



## Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 09:05 PM UTC

PDB ID : 9NKF / pdb\_00009nkf  
EMDB ID : EMD-49507  
Title : Structure of human substrate-free 26S proteasome in the presence of ATPgS and MG-132,SA-like state (composite map)  
Authors : Peddada, N.; Beutler, B.  
Deposited on : 2025-02-28  
Resolution : 2.90 Å(reported)  
Based on initial model : 6MSB

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:

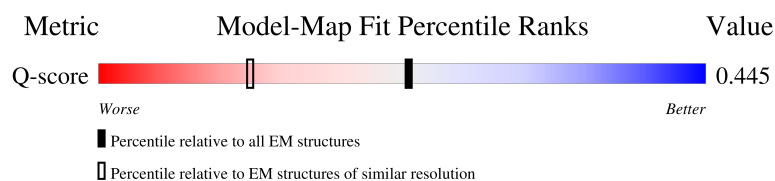
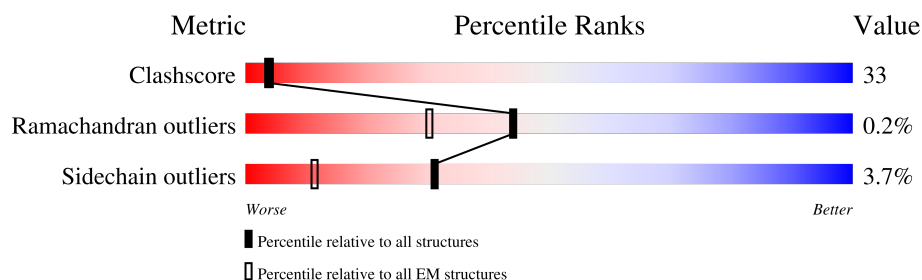
EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (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 2.90 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.



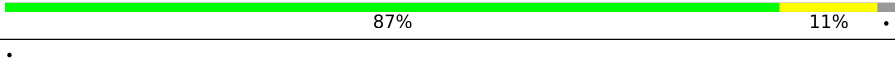
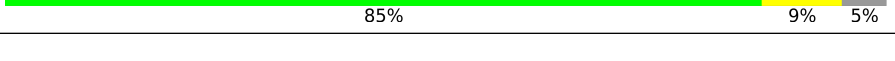
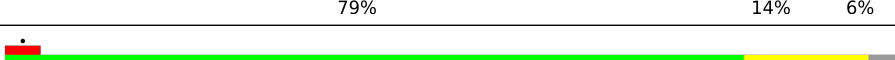
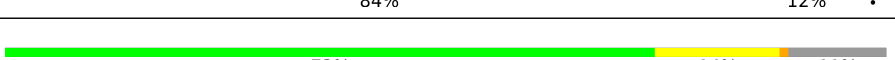
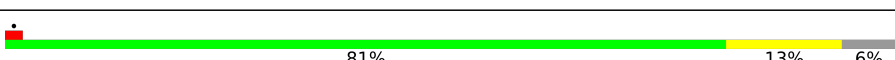
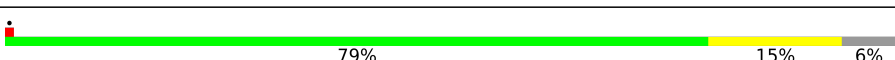
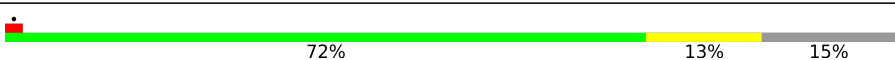
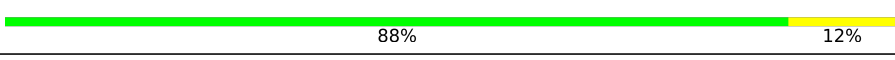
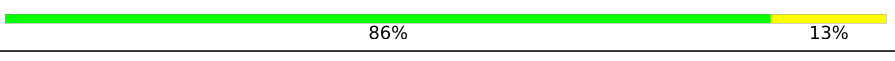
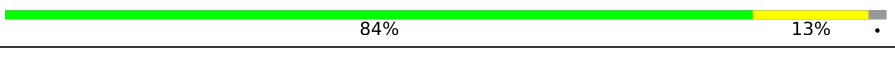
| Metric                | Whole archive<br>(#Entries) | EM structures<br>(#Entries) | Similar EM resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-----------------------------|----------------------------------------------------------|
| Clashscore            | 229148                      | 23984                       | -                                                        |
| Ramachandran outliers | 224038                      | 23583                       | -                                                        |
| Sidechain outliers    | 223484                      | 23102                       | -                                                        |
| Q-score               | -                           | 25397                       | 13054 ( 2.40 - 3.40 )                                    |

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   | A     | 433    |                  |
| 2   | B     | 440    |                  |
| 3   | C     | 406    |                  |
| 4   | D     | 418    |                  |

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| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 5   | E     | 403    |    |
| 6   | G     | 246    |    |
| 6   | g     | 246    |    |
| 7   | H     | 234    |    |
| 7   | h     | 234    |    |
| 8   | I     | 261    |    |
| 8   | i     | 261    |    |
| 9   | J     | 248    |    |
| 9   | j     | 248    |    |
| 10  | K     | 241    |    |
| 10  | k     | 241    |    |
| 11  | L     | 263    |  |
| 11  | l     | 263    |  |
| 12  | M     | 255    |  |
| 12  | m     | 255    |  |
| 13  | N     | 239    |  |
| 13  | n     | 239    |  |
| 14  | O     | 277    |  |
| 14  | o     | 277    |  |
| 15  | P     | 205    |  |
| 15  | p     | 205    |  |
| 16  | Q     | 201    |  |
| 16  | q     | 201    |  |
| 17  | R     | 263    |  |
| 17  | r     | 263    |  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 18  | S     | 241    |                  |
| 18  | s     | 241    |                  |
| 19  | T     | 264    |                  |
| 19  | t     | 264    |                  |
| 20  | V     | 534    |                  |
| 21  | W     | 456    |                  |
| 22  | X     | 422    |                  |
| 23  | Y     | 389    |                  |
| 24  | Z     | 324    |                  |
| 25  | a     | 376    |                  |
| 26  | b     | 377    |                  |
| 27  | c     | 310    |                  |
| 28  | d     | 350    |                  |
| 29  | e     | 70     |                  |
| 30  | f     | 908    |                  |
| 31  | F     | 439    |                  |
| 32  | U     | 953    |                  |

## 2 Entry composition [i](#)

There are 37 unique types of molecules in this entry. The entry contains 145524 atoms, of which 44186 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 26S proteasome regulatory subunit 7.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 1   | A     | 366      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2863  | 1805 | 503 | 537 | 18 |         |       |

- Molecule 2 is a protein called 26S proteasome regulatory subunit 4.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 2   | B     | 388      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3042  | 1915 | 519 | 593 | 15 |         |       |

- Molecule 3 is a protein called 26S protease regulatory subunit 8.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 3   | C     | 379      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2968  | 1867 | 534 | 551 | 16 |         |       |

- Molecule 4 is a protein called 26S proteasome regulatory subunit 6B.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 4   | D     | 380      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3039  | 1923 | 524 | 579 | 13 |         |       |

- Molecule 5 is a protein called 26S proteasome regulatory subunit 10B.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 5   | E     | 375      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2860  | 1796 | 512 | 536 | 16 |         |       |

- Molecule 6 is a protein called Proteasome subunit alpha type-6.

| Mol | Chain | Residues | Atoms |      |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|----|---------|-------|
| 6   | G     | 240      | Total | C    | H    | N   | O   | S  | 0       | 0     |
|     |       |          | 3402  | 1108 | 1660 | 304 | 318 | 12 |         |       |

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| Mol | Chain | Residues | Atoms |      |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|----|---------|-------|
| 6   | g     | 240      | Total | C    | H    | N   | O   | S  | 0       | 0     |
|     |       |          | 3445  | 1124 | 1687 | 306 | 316 | 12 |         |       |

- Molecule 7 is a protein called Proteasome subunit alpha type-2.

| Mol | Chain | Residues | Atoms |      |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|---|---------|-------|
| 7   | H     | 229      | Total | C    | H    | N   | O   | S | 0       | 0     |
|     |       |          | 3252  | 1080 | 1590 | 288 | 288 | 6 |         |       |
| 7   | h     | 229      | Total | C    | H    | N   | O   | S | 0       | 0     |
|     |       |          | 3252  | 1080 | 1590 | 288 | 288 | 6 |         |       |

- Molecule 8 is a protein called Proteasome subunit alpha type-4.

| Mol | Chain | Residues | Atoms |      |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|----|---------|-------|
| 8   | I     | 247      | Total | C    | H    | N   | O   | S  | 0       | 0     |
|     |       |          | 3543  | 1150 | 1741 | 322 | 320 | 10 |         |       |
| 8   | i     | 247      | Total | C    | H    | N   | O   | S  | 0       | 0     |
|     |       |          | 3503  | 1143 | 1717 | 320 | 313 | 10 |         |       |

- Molecule 9 is a protein called Proteasome subunit alpha type-7.

| Mol | Chain | Residues | Atoms |      |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|---|---------|-------|
| 9   | J     | 232      | Total | C    | H    | N   | O   | S | 0       | 0     |
|     |       |          | 3151  | 1038 | 1518 | 306 | 284 | 5 |         |       |
| 9   | j     | 232      | Total | C    | H    | N   | O   | S | 0       | 0     |
|     |       |          | 3151  | 1038 | 1518 | 306 | 284 | 5 |         |       |

- Molecule 10 is a protein called Proteasome subunit alpha type-5.

| Mol | Chain | Residues | Atoms |      |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|----|---------|-------|
| 10  | K     | 233      | Total | C    | H    | N   | O   | S  | 0       | 0     |
|     |       |          | 3255  | 1057 | 1592 | 287 | 308 | 11 |         |       |
| 10  | k     | 233      | Total | C    | H    | N   | O   | S  | 0       | 0     |
|     |       |          | 3249  | 1056 | 1589 | 287 | 306 | 11 |         |       |

- Molecule 11 is a protein called Proteasome subunit alpha type-1.

| Mol | Chain | Residues | Atoms |      |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|----|---------|-------|
| 11  | L     | 233      | Total | C    | H    | N   | O   | S  | 0       | 0     |
|     |       |          | 3359  | 1090 | 1649 | 318 | 293 | 9  |         |       |
| 11  | l     | 233      | Total | C    | H    | N   | O   | S  | 0       | 0     |
|     |       |          | 3352  | 1089 | 1645 | 315 | 293 | 10 |         |       |

- Molecule 12 is a protein called Proteasome subunit alpha type-3.

| Mol | Chain | Residues | Atoms |      |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|----|---------|-------|
| 12  | M     | 239      | Total | C    | H    | N   | O   | S  | 0       | 0     |
|     |       |          | 3440  | 1131 | 1680 | 308 | 311 | 10 |         |       |
| 12  | m     | 239      | Total | C    | H    | N   | O   | S  | 0       | 0     |
|     |       |          | 3444  | 1131 | 1683 | 308 | 312 | 10 |         |       |

- Molecule 13 is a protein called Proteasome subunit beta type-6.

| Mol | Chain | Residues | Atoms |     |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|----|---------|-------|
| 13  | N     | 202      | Total | C   | H    | N   | O   | S  | 0       | 0     |
|     |       |          | 2891  | 928 | 1422 | 257 | 272 | 12 |         |       |
| 13  | n     | 202      | Total | C   | H    | N   | O   | S  | 0       | 0     |
|     |       |          | 2881  | 926 | 1416 | 256 | 271 | 12 |         |       |

- Molecule 14 is a protein called Proteasome subunit beta type-7.

| Mol | Chain | Residues | Atoms |      |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|---|---------|-------|
| 14  | O     | 220      | Total | C    | H    | N   | O   | S | 0       | 0     |
|     |       |          | 3139  | 1005 | 1559 | 272 | 294 | 9 |         |       |
| 14  | o     | 220      | Total | C    | H    | N   | O   | S | 0       | 0     |
|     |       |          | 3131  | 1003 | 1555 | 272 | 292 | 9 |         |       |

- Molecule 15 is a protein called Proteasome subunit beta type-3.

| Mol | Chain | Residues | Atoms |     |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|----|---------|-------|
| 15  | P     | 204      | Total | C   | H    | N   | O   | S  | 0       | 0     |
|     |       |          | 3096  | 992 | 1550 | 262 | 273 | 19 |         |       |
| 15  | p     | 204      | Total | C   | H    | N   | O   | S  | 0       | 0     |
|     |       |          | 3081  | 989 | 1543 | 263 | 268 | 18 |         |       |

- Molecule 16 is a protein called Proteasome subunit beta type-2.

| Mol | Chain | Residues | Atoms |     |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|---------|-------|
| 16  | Q     | 196      | Total | C   | H    | N   | O   | S | 0       | 0     |
|     |       |          | 2986  | 974 | 1477 | 259 | 268 | 8 |         |       |
| 16  | q     | 196      | Total | C   | H    | N   | O   | S | 0       | 0     |
|     |       |          | 2981  | 973 | 1475 | 259 | 266 | 8 |         |       |

- Molecule 17 is a protein called Proteasome subunit beta type-5.

| Mol | Chain | Residues | Atoms |     |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|---------|-------|
| 17  | R     | 200      | Total | C   | H    | N   | O   | S | 0       | 0     |
|     |       |          | 2953  | 957 | 1449 | 271 | 267 | 9 |         |       |
| 17  | r     | 200      | Total | C   | H    | N   | O   | S | 0       | 0     |
|     |       |          | 2938  | 954 | 1438 | 270 | 267 | 9 |         |       |

- Molecule 18 is a protein called Proteasome subunit beta type-1.

| Mol | Chain | Residues | Atoms |      |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|----|---------|-------|
| 18  | S     | 212      | Total | C    | H    | N   | O   | S  | 0       | 0     |
|     |       |          | 3163  | 1016 | 1579 | 279 | 279 | 10 |         |       |
| 18  | s     | 212      | Total | C    | H    | N   | O   | S  | 0       | 0     |
|     |       |          | 3168  | 1017 | 1581 | 279 | 281 | 10 |         |       |

- Molecule 19 is a protein called Proteasome subunit beta type-4.

| Mol | Chain | Residues | Atoms |      |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|----|---------|-------|
| 19  | T     | 212      | Total | C    | H    | N   | O   | S  | 0       | 0     |
|     |       |          | 3102  | 1003 | 1526 | 280 | 282 | 11 |         |       |
| 19  | t     | 212      | Total | C    | H    | N   | O   | S  | 0       | 0     |
|     |       |          | 3079  | 998  | 1511 | 279 | 280 | 11 |         |       |

- Molecule 20 is a protein called 26S proteasome non-ATPase regulatory subunit 3.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 20  | V     | 472      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3754  | 2387 | 673 | 681 | 13 |         |       |

- Molecule 21 is a protein called 26S proteasome non-ATPase regulatory subunit 12.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 21  | W     | 446      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3635  | 2302 | 622 | 687 | 24 |         |       |

- Molecule 22 is a protein called 26S proteasome non-ATPase regulatory subunit 11.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 22  | X     | 334      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2664  | 1696 | 448 | 508 | 12 |         |       |

- Molecule 23 is a protein called 26S proteasome non-ATPase regulatory subunit 6.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 23  | Y     | 378      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3115  | 1987 | 533 | 578 | 17 |         |       |

- Molecule 24 is a protein called 26S proteasome non-ATPase regulatory subunit 7.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 24  | Z     | 286      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2281  | 1457 | 392 | 427 | 5 |         |       |

- Molecule 25 is a protein called 26S proteasome non-ATPase regulatory subunit 13.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 25  | a     | 373      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2995  | 1911 | 510 | 559 | 15 |         |       |

- Molecule 26 is a protein called 26S proteasome non-ATPase regulatory subunit 4.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 26  | b     | 191      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1458  | 910 | 261 | 279 | 8 |         |       |

- Molecule 27 is a protein called 26S proteasome non-ATPase regulatory subunit 14.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 27  | c     | 287      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2260  | 1430 | 389 | 422 | 19 |         |       |

- Molecule 28 is a protein called 26S proteasome non-ATPase regulatory subunit 8.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 28  | d     | 257      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2116  | 1371 | 346 | 390 | 9 |         |       |

- Molecule 29 is a protein called 26S proteasome complex subunit SEM1.

| Mol | Chain | Residues | Atoms |     |    |     | AltConf | Trace |
|-----|-------|----------|-------|-----|----|-----|---------|-------|
| 29  | e     | 50       | Total | C   | N  | O   | 0       | 0     |
|     |       |          | 425   | 260 | 65 | 100 |         |       |

- Molecule 30 is a protein called 26S proteasome non-ATPase regulatory subunit 2.

| Mol | Chain | Residues | Atoms |      |      |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
| 30  | f     | 889      | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 6866  | 4315 | 1174 | 1331 | 46 |         |       |

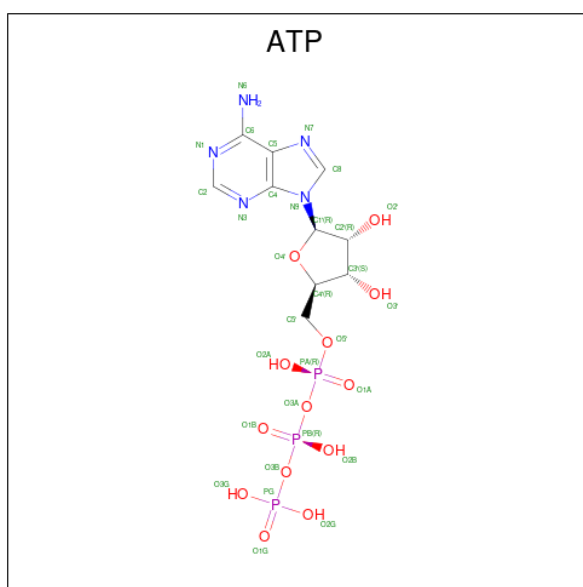
- Molecule 31 is a protein called 26S proteasome regulatory subunit 6A.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 31  | F     | 376      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2858  | 1802 | 496 | 545 | 15 |         |       |

- Molecule 32 is a protein called 26S proteasome non-ATPase regulatory subunit 1.

| Mol | Chain | Residues | Atoms |      |      |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
| 32  | U     | 808      | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 6304  | 4003 | 1074 | 1183 | 44 |         |       |

- Molecule 33 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula:  $C_{10}H_{16}N_5O_{13}P_3$ ) (labeled as "Ligand of Interest" by depositor).

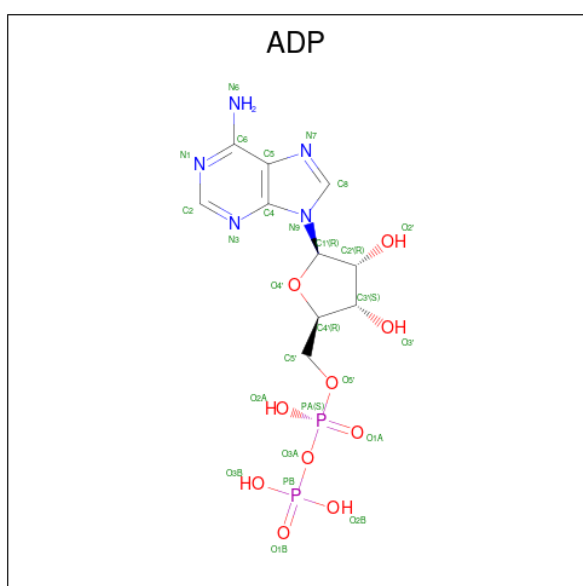


| Mol | Chain | Residues | Atoms |    |   |    |   | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|
| 33  | A     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 31    | 10 | 5 | 13 | 3 |         |
| 33  | B     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 31    | 10 | 5 | 13 | 3 |         |
| 33  | D     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 31    | 10 | 5 | 13 | 3 |         |
| 33  | E     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 31    | 10 | 5 | 13 | 3 |         |

- Molecule 34 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

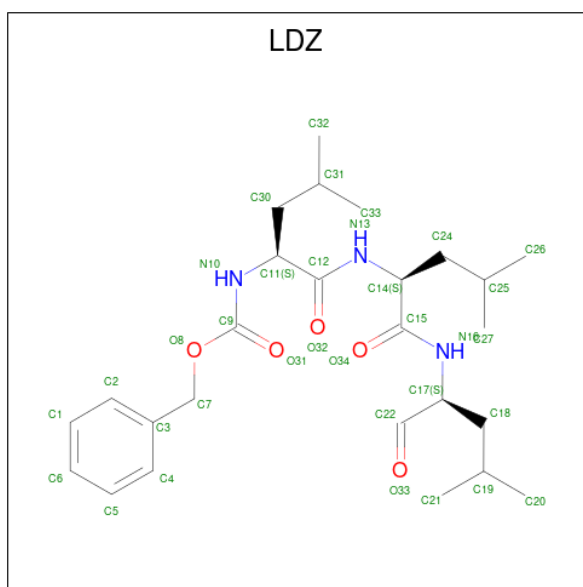
| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 34  | A     | 2        | Total | Mg | 0       |
|     |       |          | 2     | 2  |         |
| 34  | B     | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |
| 34  | E     | 2        | Total | Mg | 0       |
|     |       |          | 2     | 2  |         |

- Molecule 35 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>10</sub>P<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



| Mol | Chain | Residues | Atoms |    |   |    |   | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|
| 35  | C     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 27    | 10 | 5 | 10 | 2 |         |
| 35  | F     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 27    | 10 | 5 | 10 | 2 |         |

- Molecule 36 is N-[(benzyloxy)carbonyl]-L-leucyl-N-[(2S)-4-methyl-1-oxopentan-2-yl]-L-leucinamide (CCD ID: LDZ) (formula: C<sub>26</sub>H<sub>41</sub>N<sub>3</sub>O<sub>5</sub>) (labeled as "Ligand of Interest" by depositor).



| Mol | Chain | Residues | Atoms |    |    |   |   | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 36  | N     | 1        | Total | C  | H  | N | O | 0       |
|     |       |          | 75    | 26 | 41 | 3 | 5 |         |
| 36  | O     | 1        | Total | C  | H  | N | O | 0       |
|     |       |          | 75    | 26 | 41 | 3 | 5 |         |
| 36  | R     | 1        | Total | C  | H  | N | O | 0       |
|     |       |          | 75    | 26 | 41 | 3 | 5 |         |
| 36  | n     | 1        | Total | C  | H  | N | O | 0       |
|     |       |          | 75    | 26 | 41 | 3 | 5 |         |
| 36  | o     | 1        | Total | C  | H  | N | O | 0       |
|     |       |          | 75    | 26 | 41 | 3 | 5 |         |
| 36  | r     | 1        | Total | C  | H  | N | O | 0       |
|     |       |          | 75    | 26 | 41 | 3 | 5 |         |

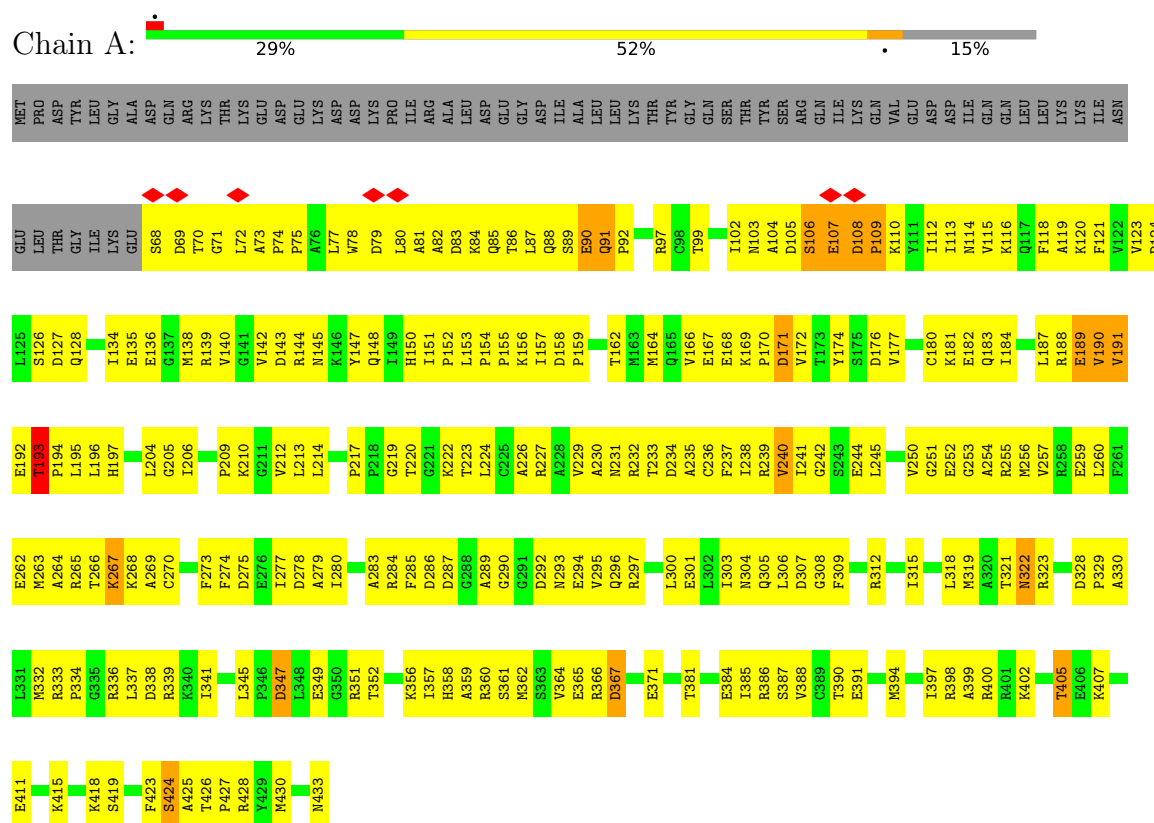
- Molecule 37 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 37  | c     | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |

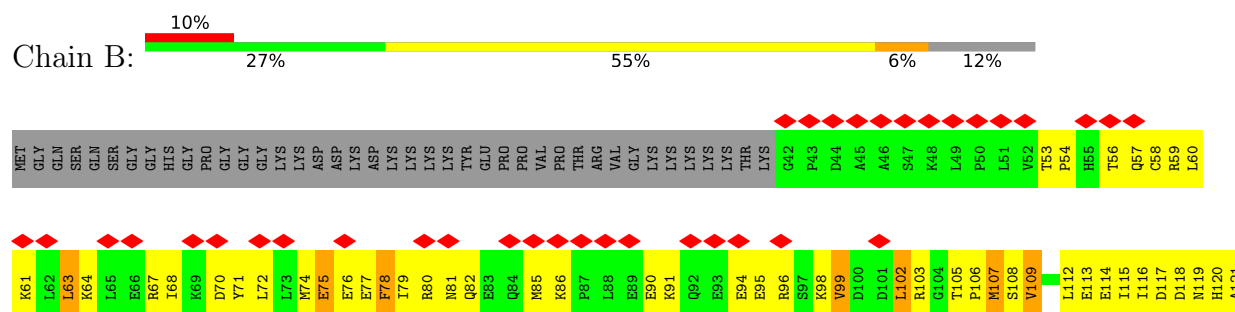
### 3 Residue-property plots [i](#)

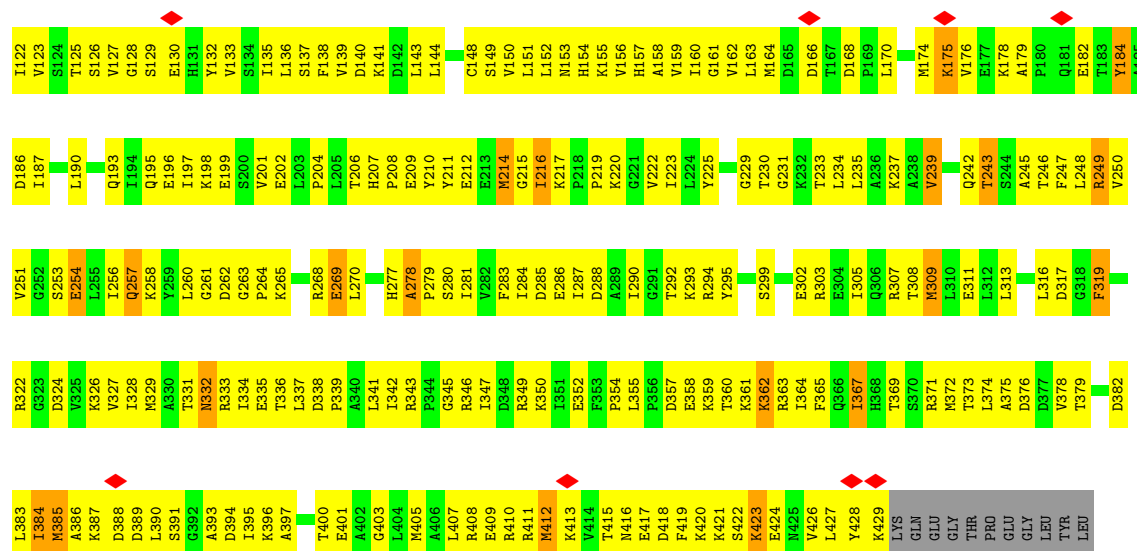
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: 26S proteasome regulatory subunit 7

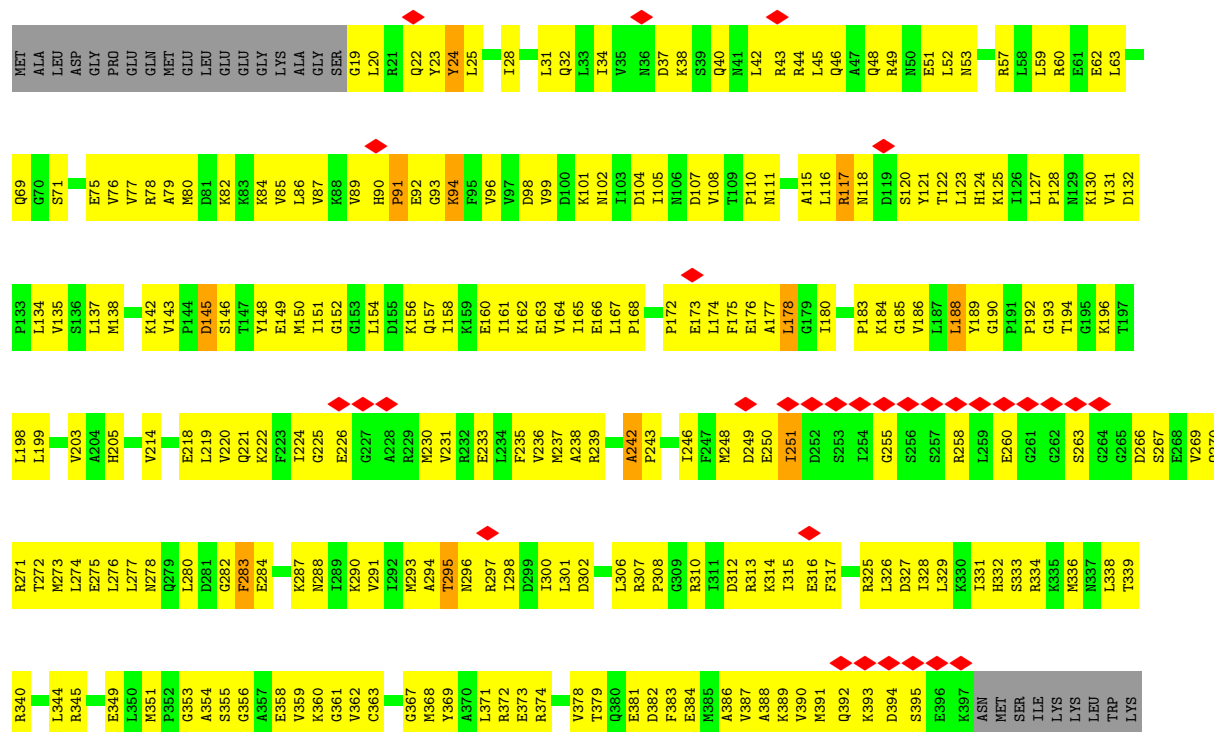


- Molecule 2: 26S proteasome regulatory subunit 4

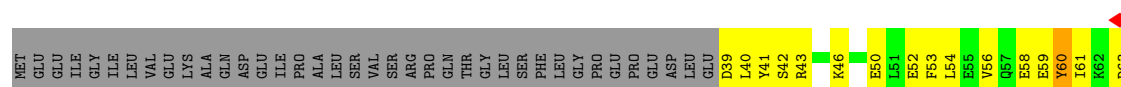


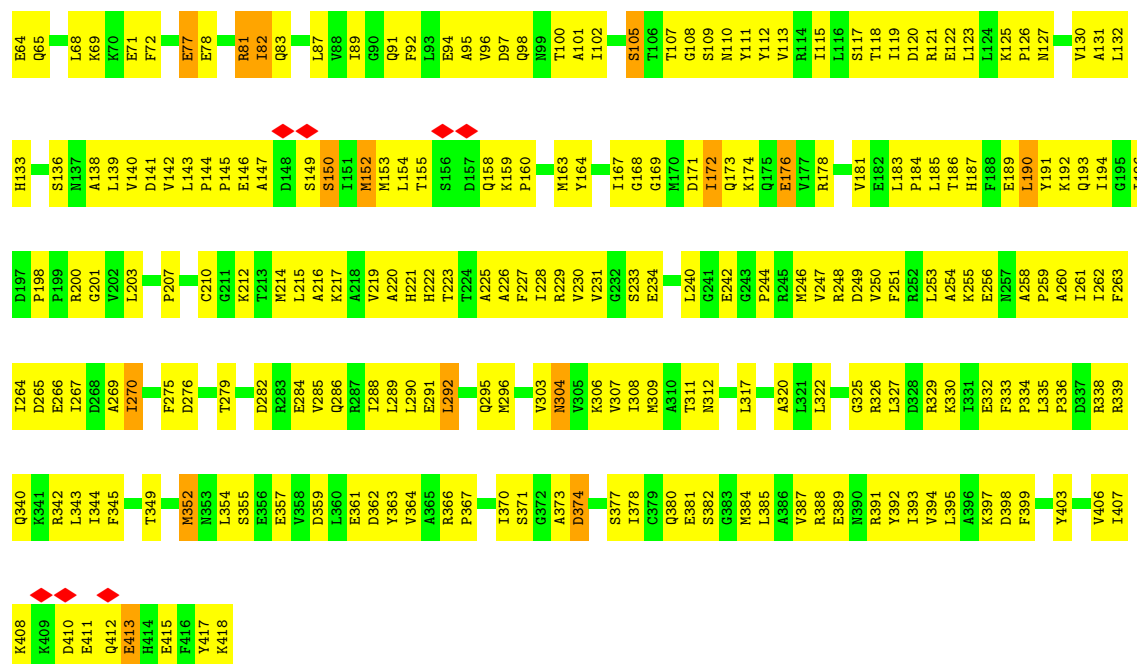


• Molecule 3: 26S protease regulatory subunit 8

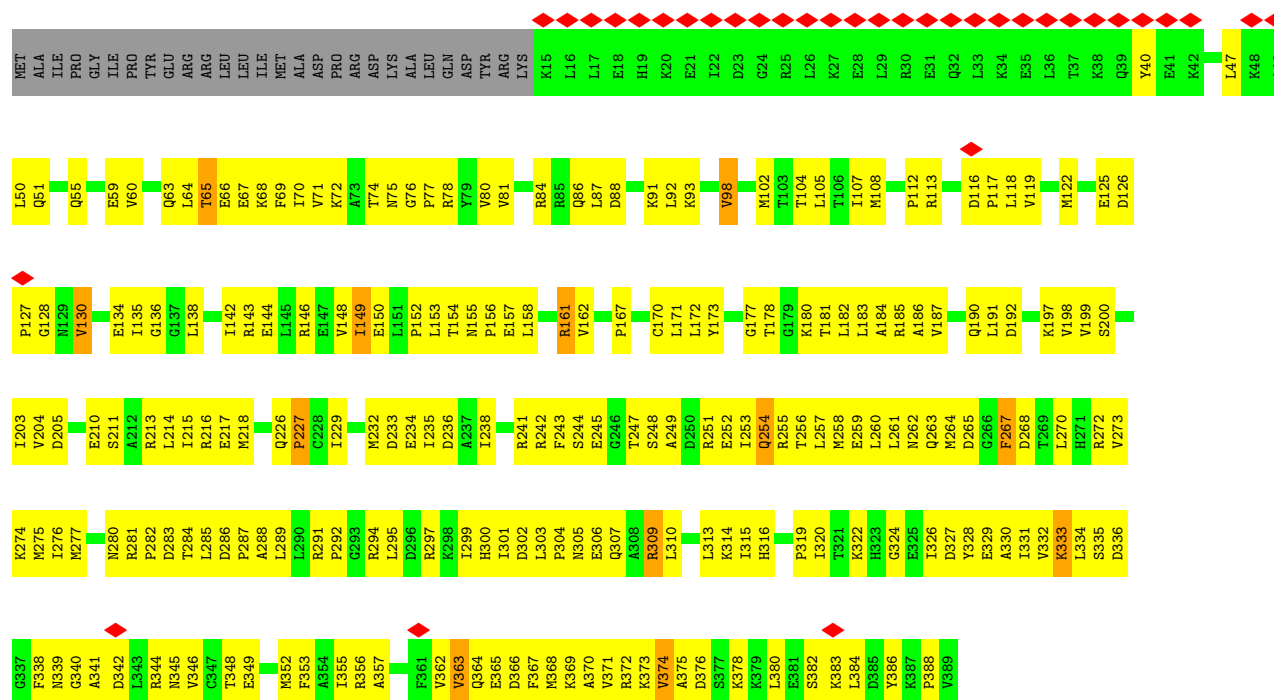


• Molecule 4: 26S proteasome regulatory subunit 6B

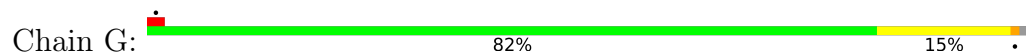


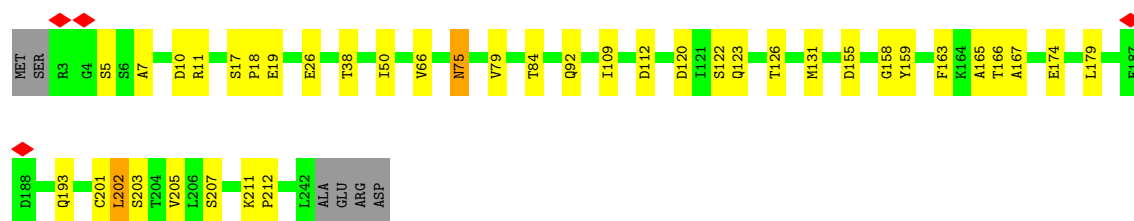


• Molecule 5: 26S proteasome regulatory subunit 10B

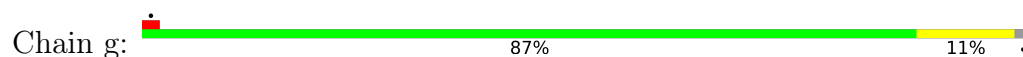


• Molecule 6: Proteasome subunit alpha type-6

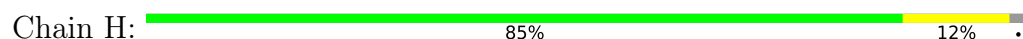




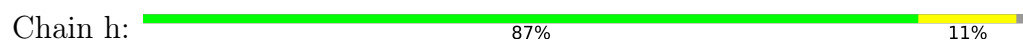
- Molecule 6: Proteasome subunit alpha type-6



- Molecule 7: Proteasome subunit alpha type-2



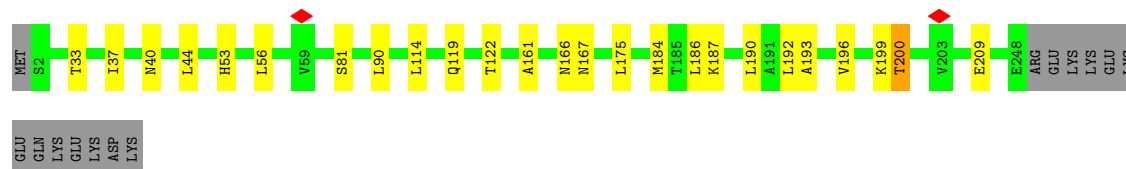
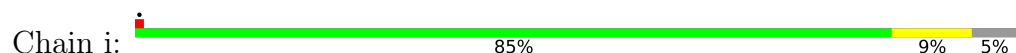
- Molecule 7: Proteasome subunit alpha type-2



- Molecule 8: Proteasome subunit alpha type-4

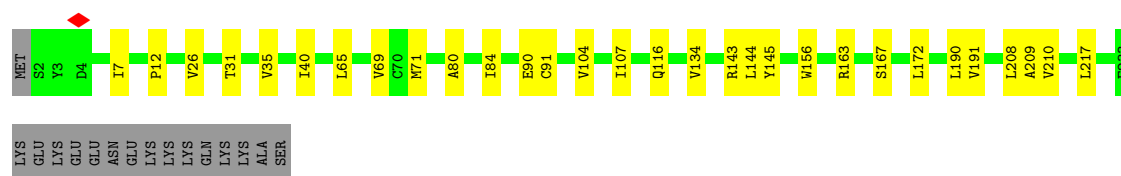


- Molecule 8: Proteasome subunit alpha type-4



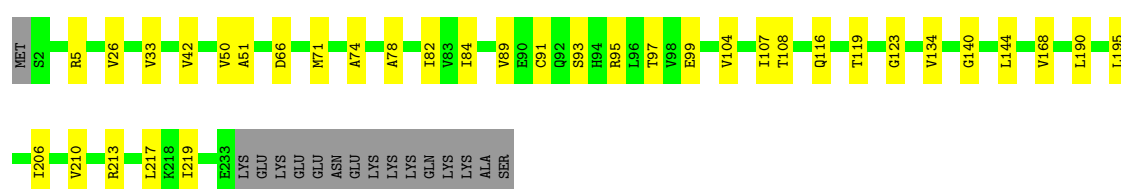
- Molecule 9: Proteasome subunit alpha type-7

Chain J:  81% 12% 6%



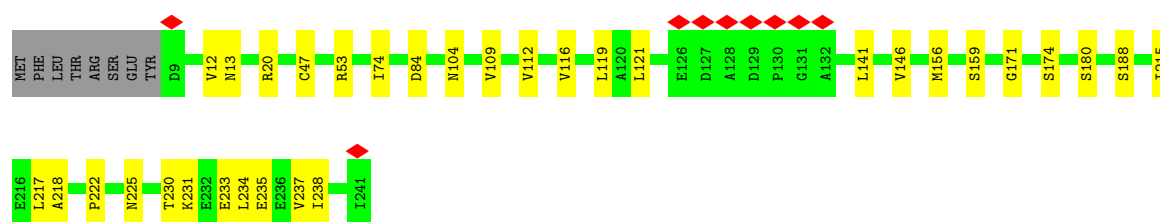
- Molecule 9: Proteasome subunit alpha type-7

Chain j:  79% 14% 6%



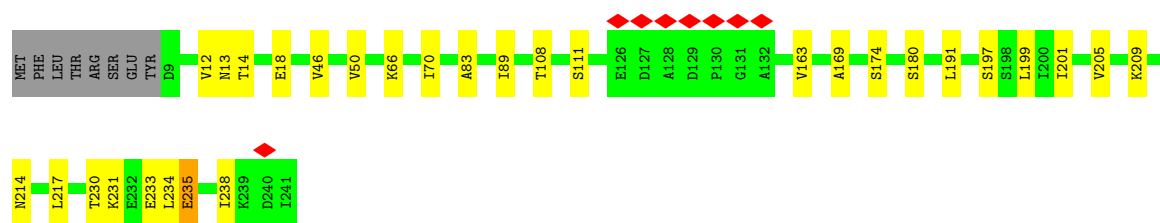
- Molecule 10: Proteasome subunit alpha type-5

Chain K:  83% 14% 3%



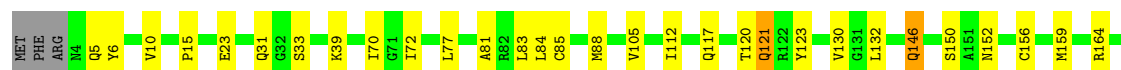
- Molecule 10: Proteasome subunit alpha type-5

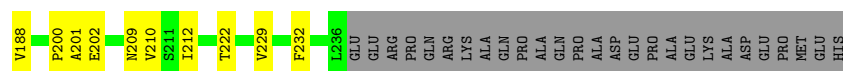
Chain k:  84% 12% 4%



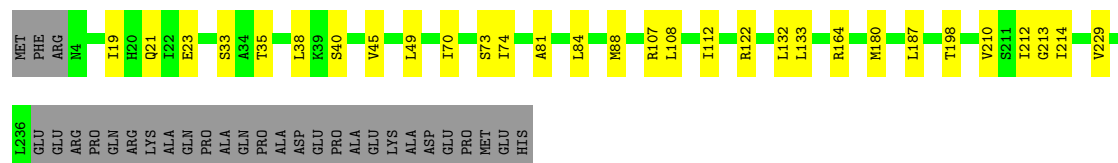
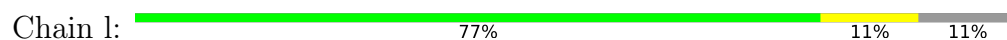
- Molecule 11: Proteasome subunit alpha type-1

Chain L:  73% 14% 11%

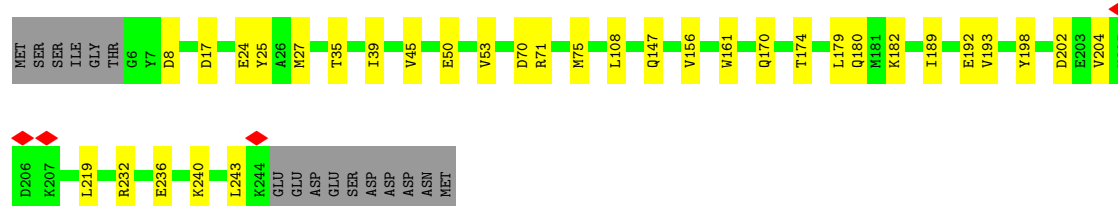
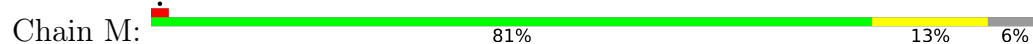




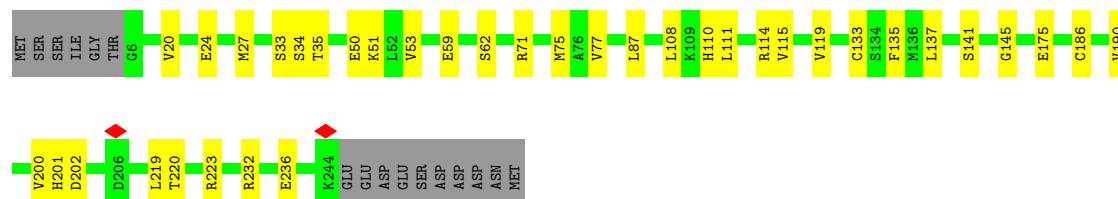
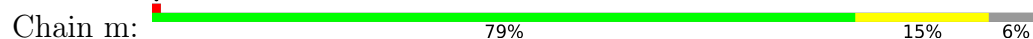
• Molecule 11: Proteasome subunit alpha type-1



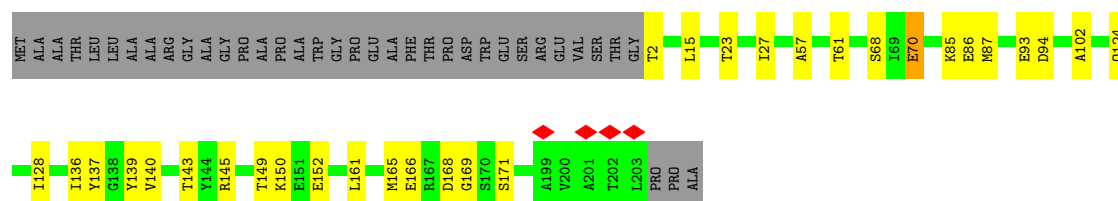
• Molecule 12: Proteasome subunit alpha type-3



• Molecule 12: Proteasome subunit alpha type-3

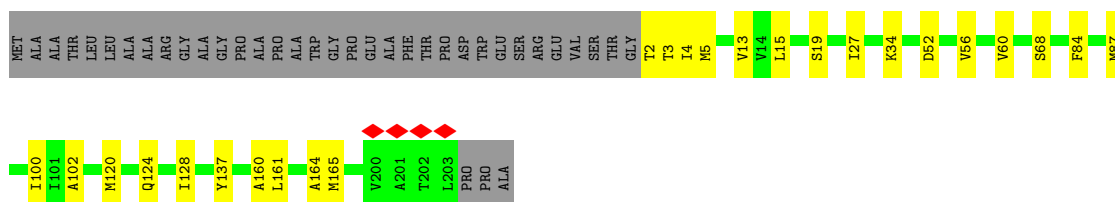


• Molecule 13: Proteasome subunit beta type-6

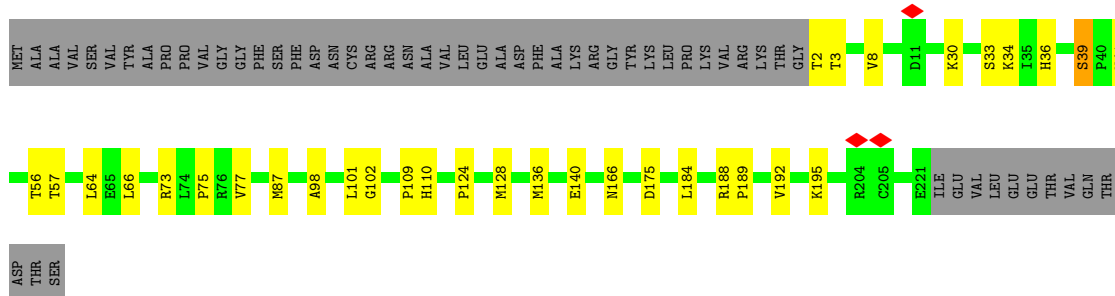


• Molecule 13: Proteasome subunit beta type-6

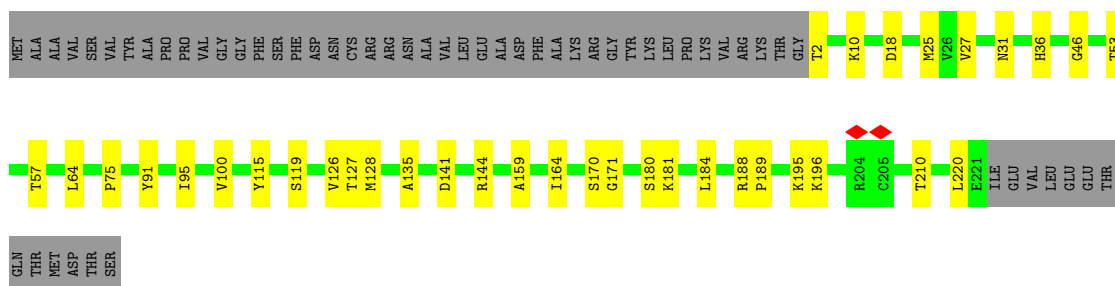




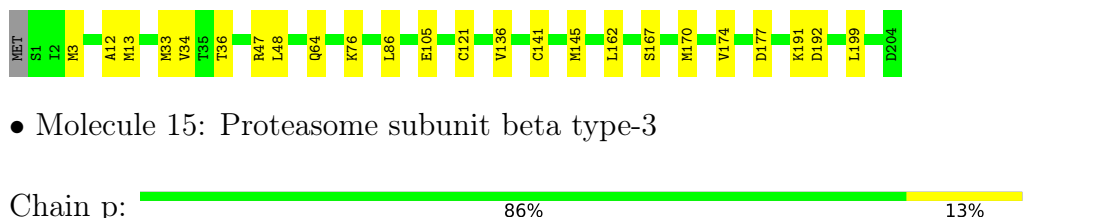
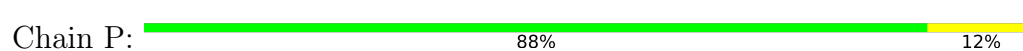
• Molecule 14: Proteasome subunit beta type-7



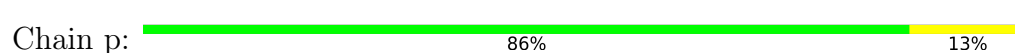
• Molecule 14: Proteasome subunit beta type-7



• Molecule 15: Proteasome subunit beta type-3



• Molecule 15: Proteasome subunit beta type-3



• Molecule 16: Proteasome subunit beta type-2

Chain Q:  84% 13%



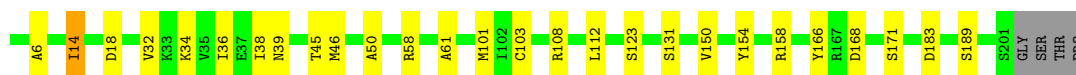
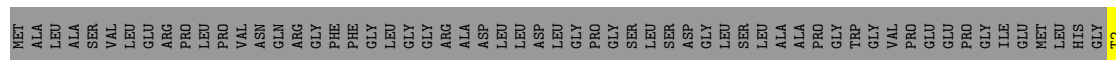
- Molecule 16: Proteasome subunit beta type-2

Chain q:  84% 13%



- Molecule 17: Proteasome subunit beta type-5

Chain R:  65% 10% 24%



- Molecule 17: Proteasome subunit beta type-5

Chain r:  65% 10% 24%



THR  
PRO

- Molecule 18: Proteasome subunit beta type-1

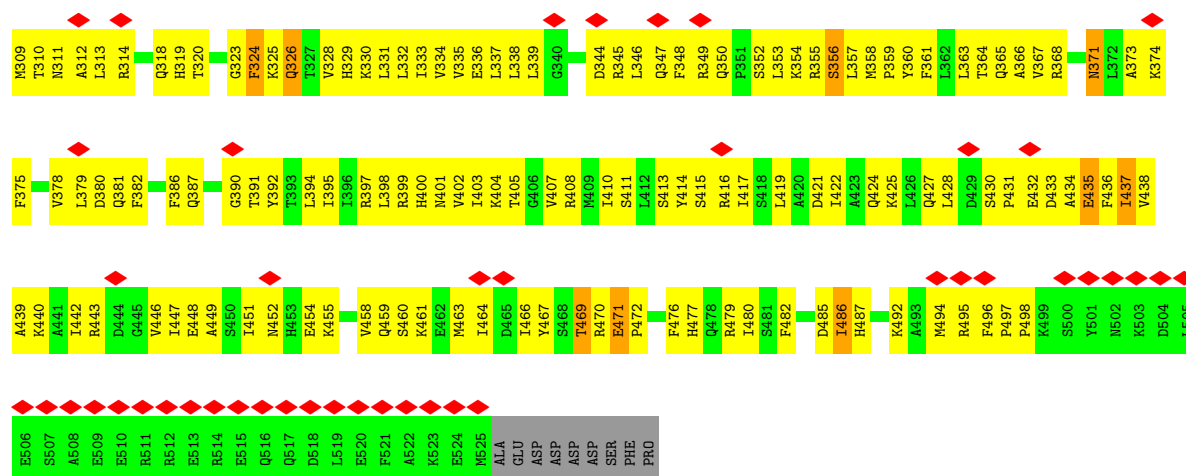
Chain S:  81% 7% 12%



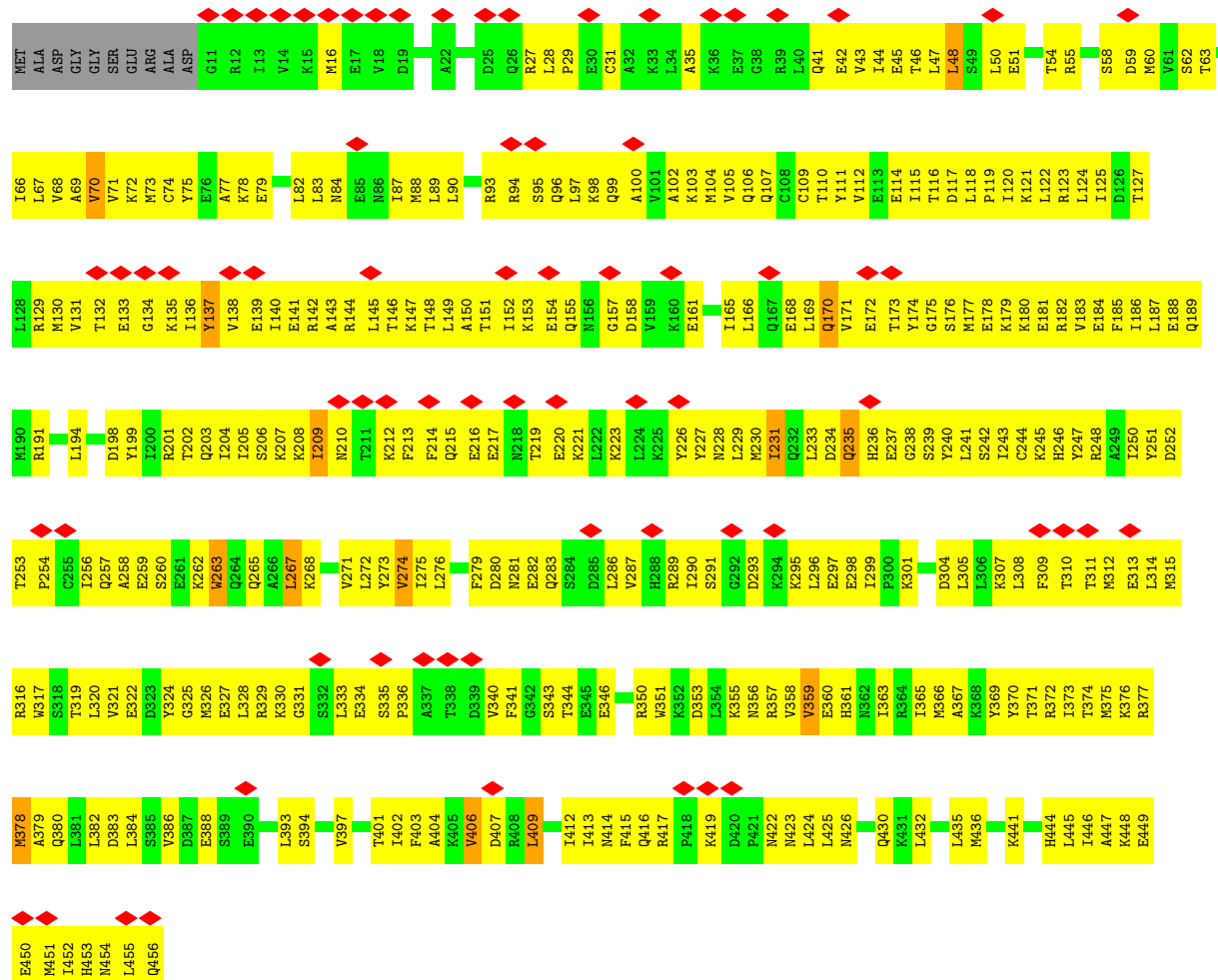
- Molecule 18: Proteasome subunit beta type-1

Chain s:  78% 10% 12%

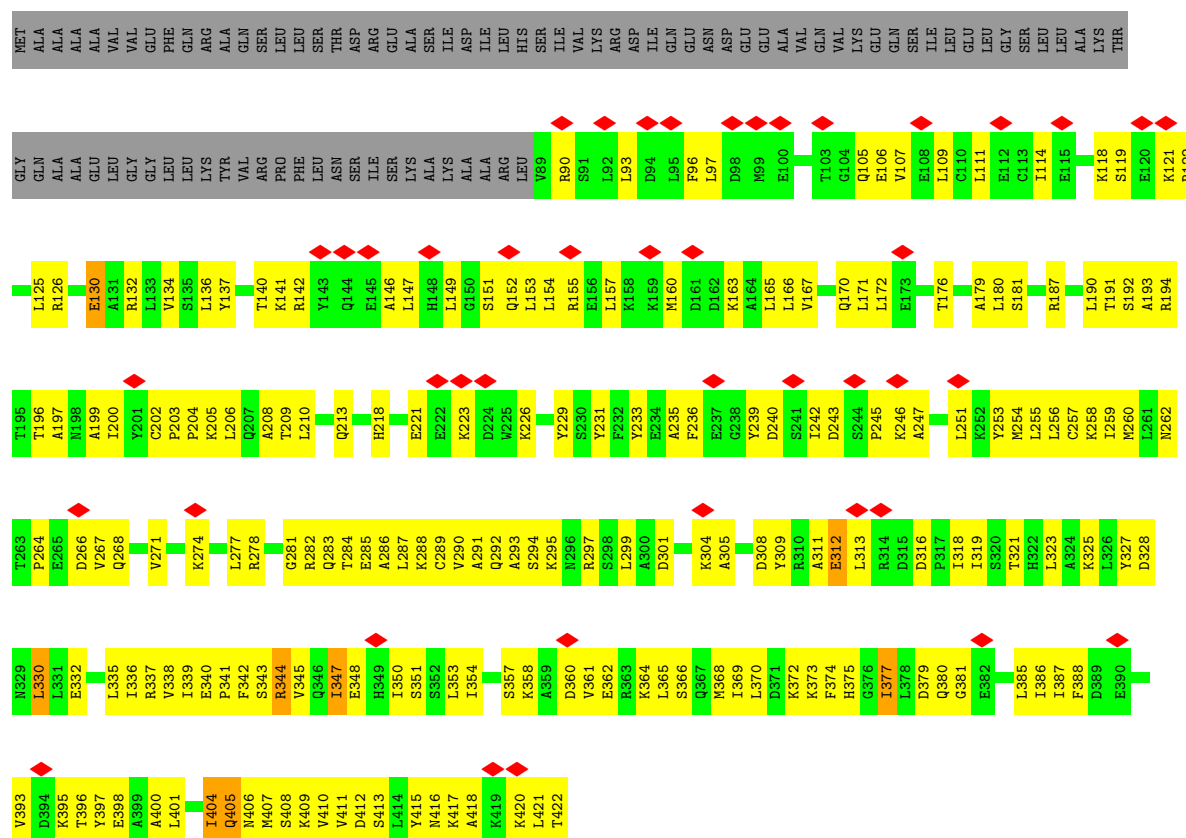




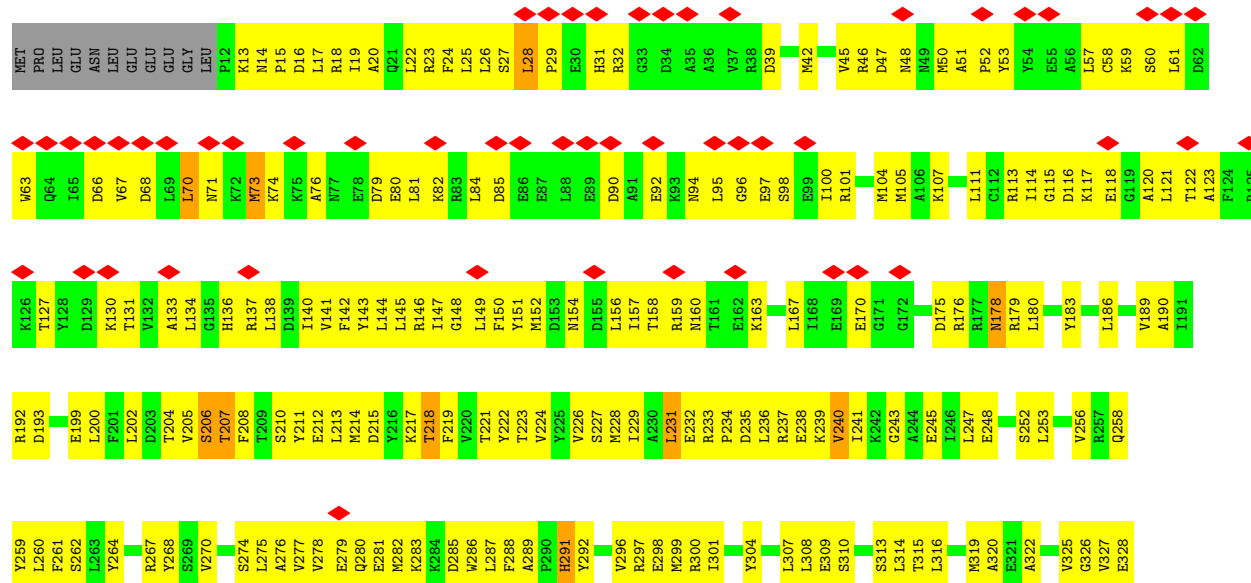
• Molecule 21: 26S proteasome non-ATPase regulatory subunit 12

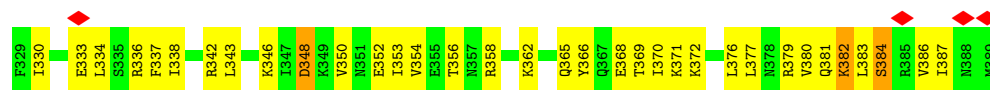


• Molecule 22: 26S proteasome non-ATPase regulatory subunit 11

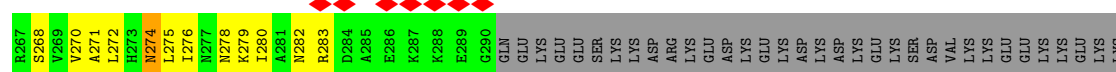
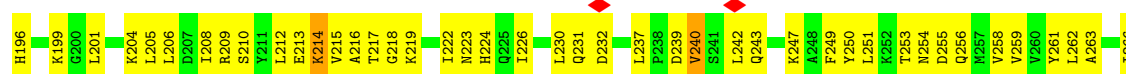
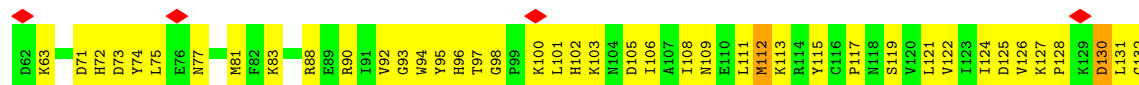
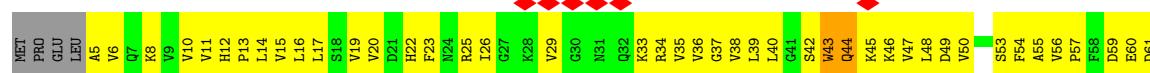


• Molecule 23: 26S proteasome non-ATPase regulatory subunit 6

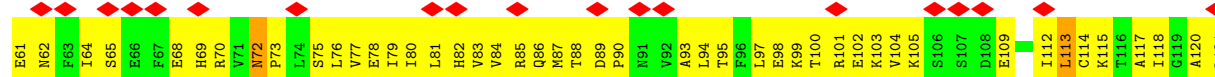
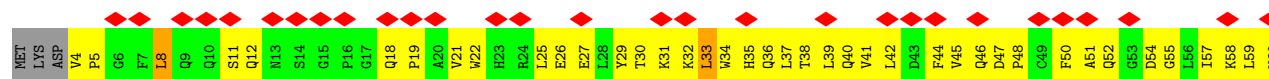




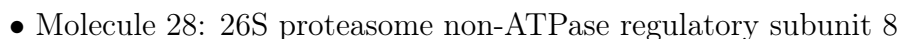
• Molecule 24: 26S proteasome non-ATPase regulatory subunit 7

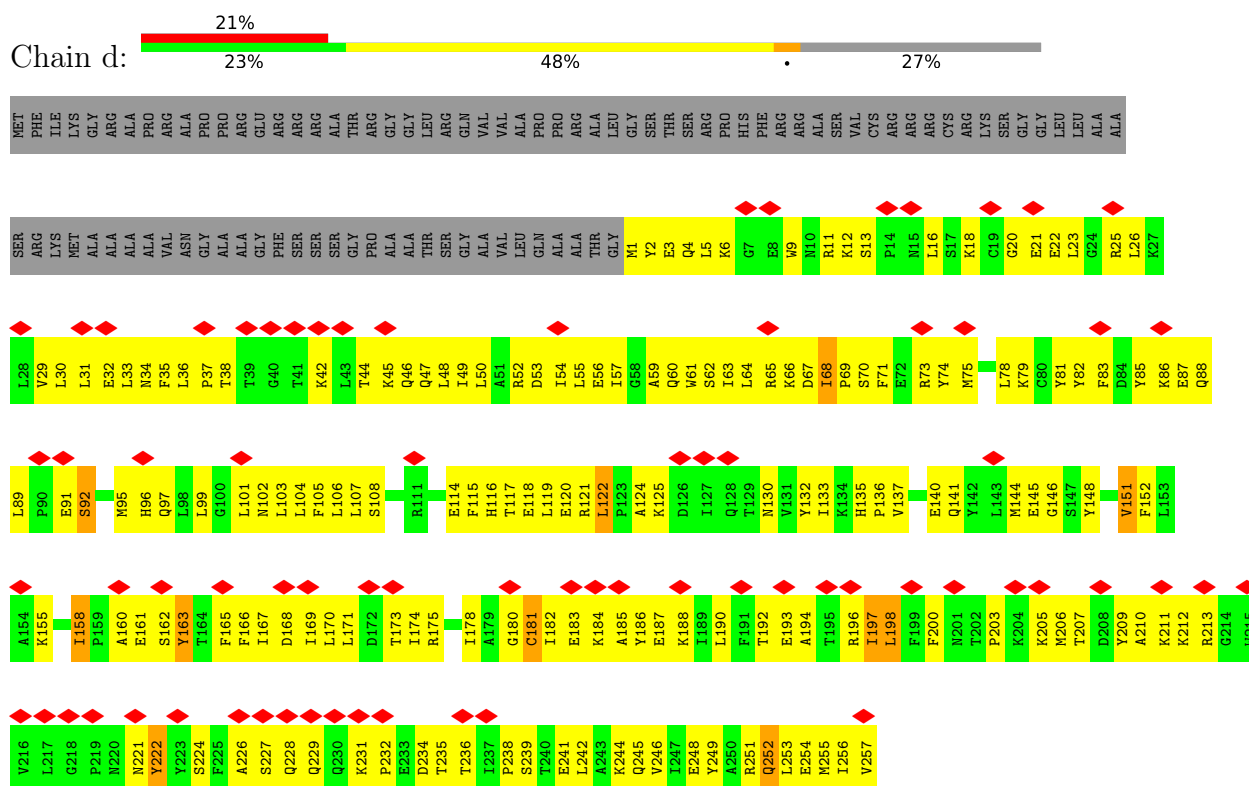


• Molecule 25: 26S proteasome non-ATPase regulatory subunit 13

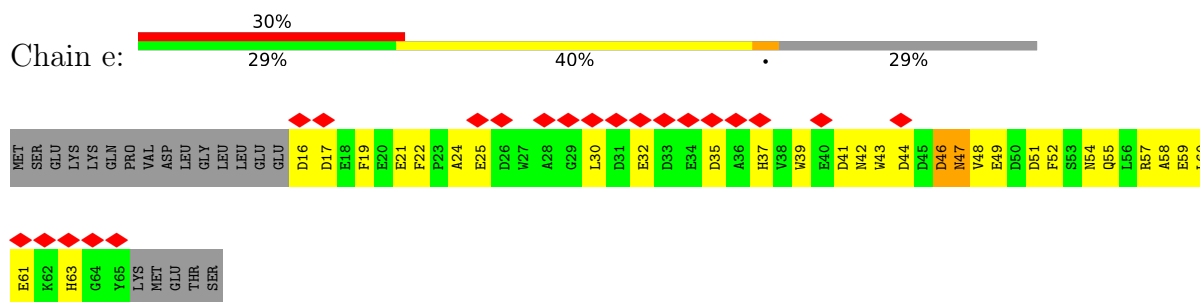


Chain b: 

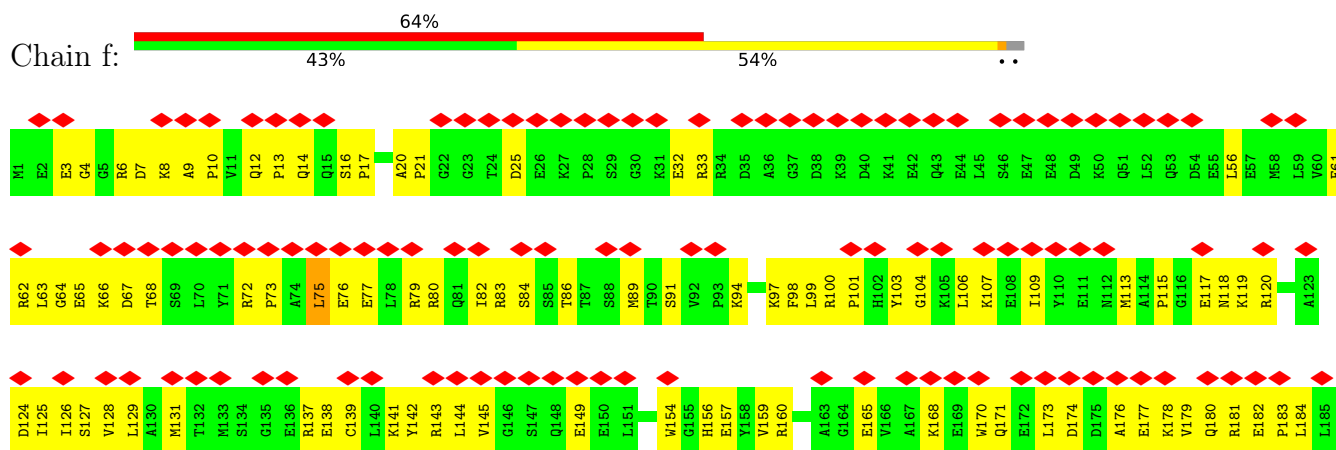


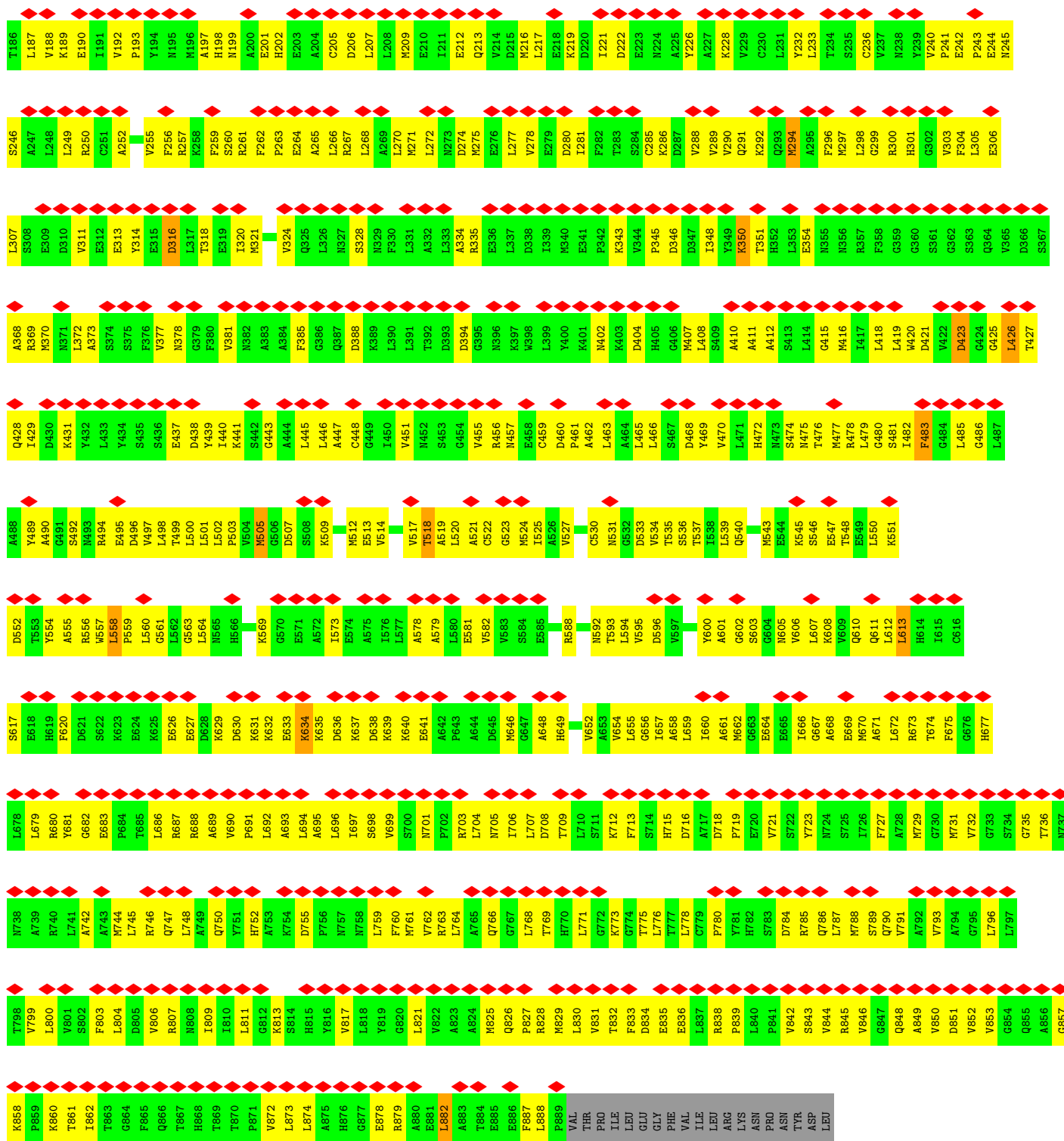


• Molecule 29: 26S proteasome complex subunit SEM1

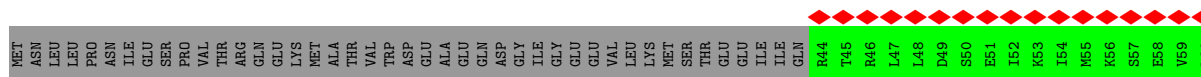


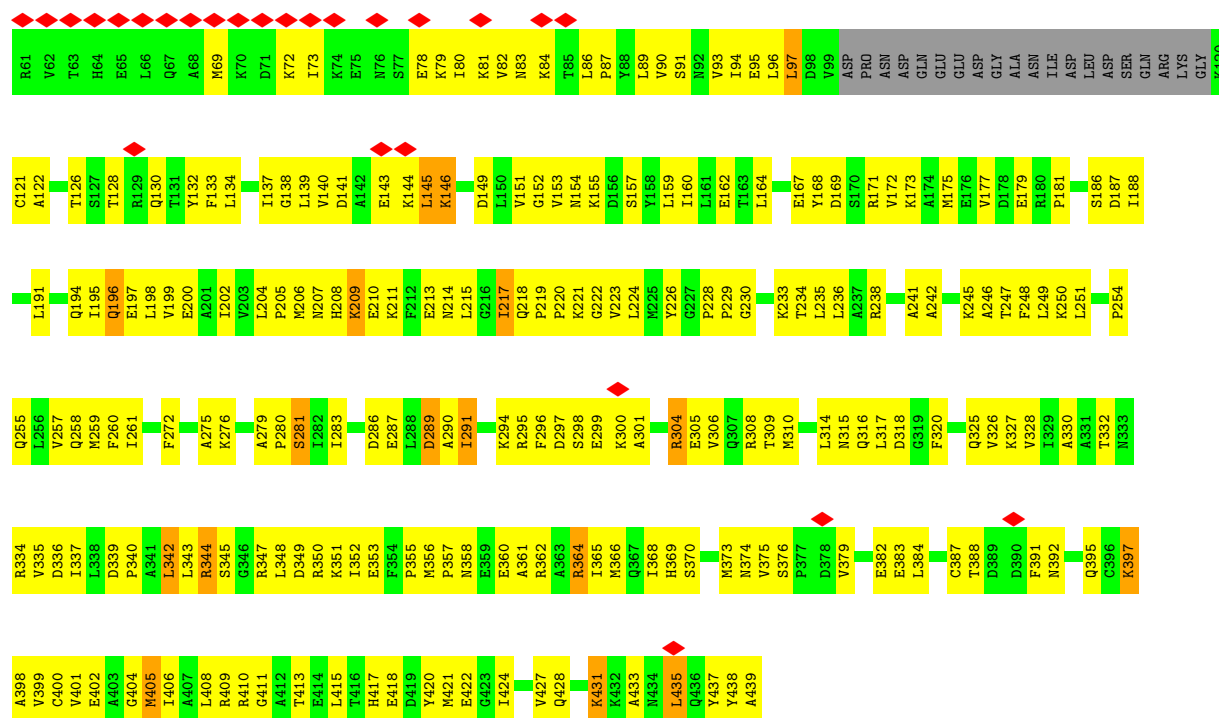
• Molecule 30: 26S proteasome non-ATPase regulatory subunit 2



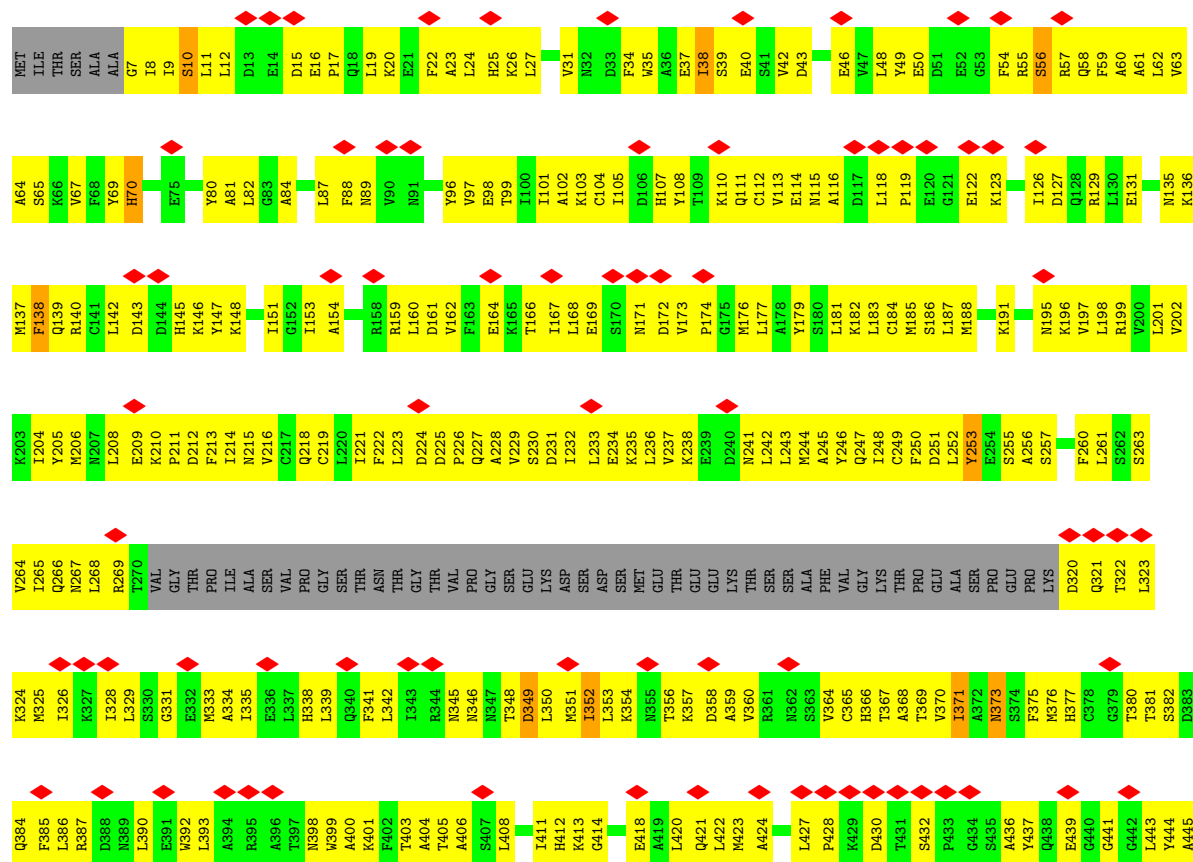


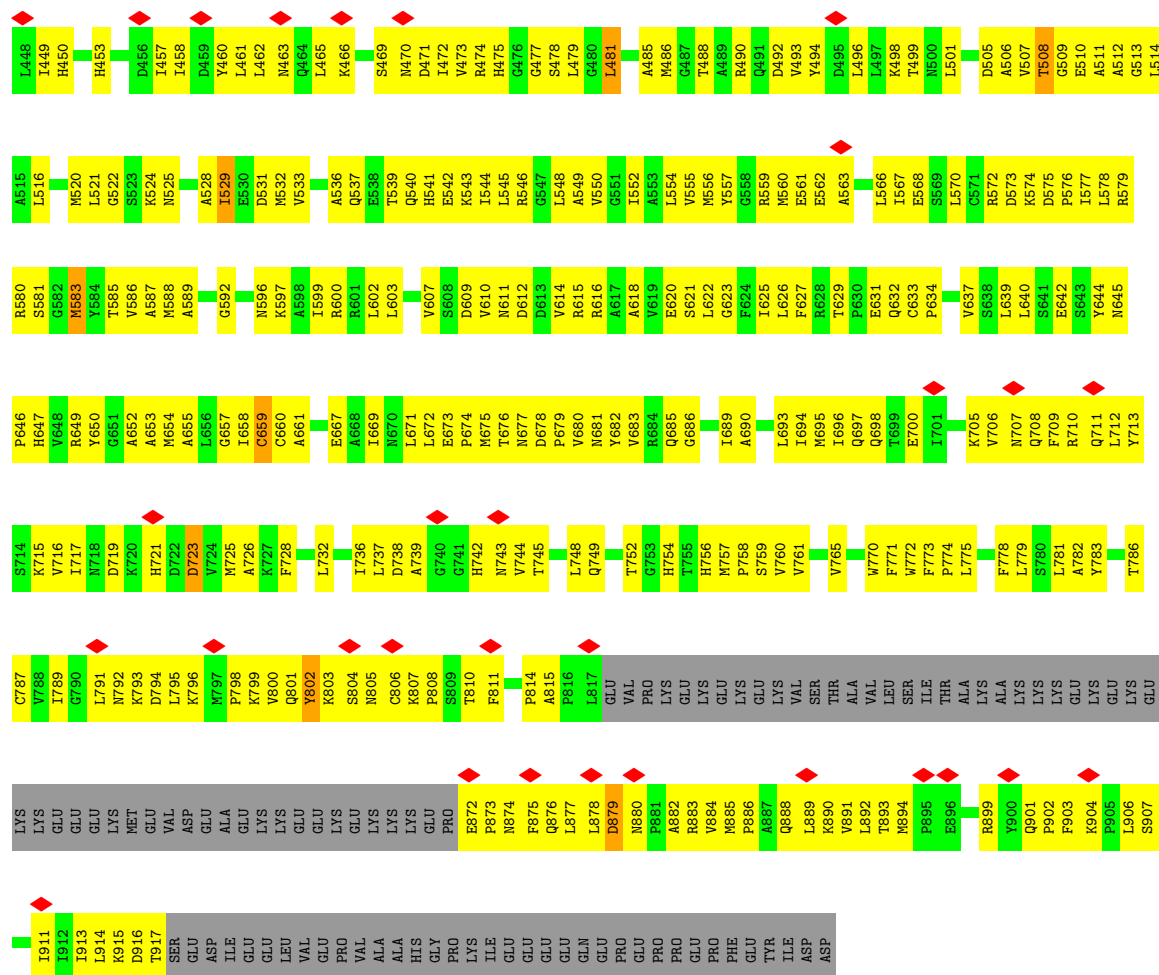
• Molecule 31: 26S proteasome regulatory subunit 6A





• Molecule 32: 26S proteasome non-ATPase regulatory subunit 1





## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|-----------------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, Not provided                     |           |
| Number of particles used             | 106182                                  | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF                       | Depositor |
| CTF correction method                | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope                           | TFS KRIOS                               | Depositor |
| Voltage (kV)                         | 300                                     | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 50                                      | Depositor |
| Minimum defocus (nm)                 | 1100                                    | Depositor |
| Maximum defocus (nm)                 | 2700                                    | Depositor |
| Magnification                        | 81000                                   | Depositor |
| Image detector                       | GATAN K3 BIOQUANTUM (6k x 4k)           | Depositor |
| Maximum map value                    | 1.990                                   | Depositor |
| Minimum map value                    | -0.002                                  | Depositor |
| Average map value                    | 0.002                                   | Depositor |
| Map value standard deviation         | 0.021                                   | Depositor |
| Recommended contour level            | 0.165                                   | Depositor |
| Map size (Å)                         | 691.656, 689.508, 691.656               | wwPDB     |
| Map dimensions                       | 644, 642, 644                           | wwPDB     |
| Map angles (°)                       | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing (Å)                    | 1.074, 1.074, 1.074                     | Depositor |

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: LDZ, MG, ZN, ATP, ADP

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   | A     | 0.19         | 0/2914      | 0.36        | 0/3937      |
| 2   | B     | 0.18         | 0/3086      | 0.37        | 0/4164      |
| 3   | C     | 0.19         | 0/3007      | 0.36        | 0/4045      |
| 4   | D     | 0.19         | 0/3089      | 0.32        | 0/4168      |
| 5   | E     | 0.19         | 0/2904      | 0.34        | 0/3924      |
| 6   | G     | 0.17         | 0/1771      | 0.30        | 0/2403      |
| 6   | g     | 0.16         | 0/1790      | 0.27        | 0/2429      |
| 7   | H     | 0.17         | 0/1701      | 0.29        | 0/2318      |
| 7   | h     | 0.17         | 0/1701      | 0.28        | 0/2318      |
| 8   | I     | 0.19         | 0/1831      | 0.31        | 0/2487      |
| 8   | i     | 0.16         | 0/1815      | 0.27        | 0/2466      |
| 9   | J     | 0.17         | 0/1657      | 0.28        | 0/2261      |
| 9   | j     | 0.16         | 0/1657      | 0.29        | 0/2261      |
| 10  | K     | 0.17         | 0/1689      | 0.28        | 0/2294      |
| 10  | k     | 0.15         | 0/1686      | 0.24        | 0/2290      |
| 11  | L     | 0.18         | 0/1744      | 0.29        | 0/2371      |
| 11  | l     | 0.16         | 0/1741      | 0.27        | 0/2367      |
| 12  | M     | 0.17         | 0/1795      | 0.28        | 0/2434      |
| 12  | m     | 0.16         | 0/1796      | 0.27        | 0/2435      |
| 13  | N     | 0.16         | 0/1495      | 0.25        | 0/2026      |
| 13  | n     | 0.16         | 0/1491      | 0.24        | 0/2021      |
| 14  | O     | 0.16         | 0/1607      | 0.28        | 0/2185      |
| 14  | o     | 0.17         | 0/1603      | 0.26        | 0/2180      |
| 15  | P     | 0.17         | 0/1575      | 0.29        | 0/2128      |
| 15  | p     | 0.18         | 0/1567      | 0.29        | 0/2118      |
| 16  | Q     | 0.16         | 0/1541      | 0.25        | 0/2092      |
| 16  | q     | 0.16         | 0/1538      | 0.28        | 0/2088      |
| 17  | R     | 0.16         | 0/1535      | 0.25        | 0/2080      |
| 17  | r     | 0.16         | 0/1531      | 0.26        | 0/2076      |
| 18  | S     | 0.16         | 0/1614      | 0.27        | 0/2178      |
| 18  | s     | 0.16         | 0/1617      | 0.27        | 0/2182      |
| 19  | T     | 0.17         | 0/1606      | 0.26        | 0/2179      |

| Mol | Chain | Bond lengths |          | Bond angles |          |
|-----|-------|--------------|----------|-------------|----------|
|     |       | RMSZ         | # Z  >5  | RMSZ        | # Z  >5  |
| 19  | t     | 0.17         | 0/1598   | 0.28        | 0/2170   |
| 20  | V     | 0.15         | 0/3824   | 0.30        | 0/5170   |
| 21  | W     | 0.15         | 0/3683   | 0.32        | 0/4952   |
| 22  | X     | 0.13         | 0/2705   | 0.29        | 0/3648   |
| 23  | Y     | 0.16         | 0/3173   | 0.28        | 0/4273   |
| 24  | Z     | 0.18         | 0/2324   | 0.29        | 0/3150   |
| 25  | a     | 0.16         | 0/3053   | 0.33        | 0/4133   |
| 26  | b     | 0.15         | 0/1478   | 0.38        | 0/2001   |
| 27  | c     | 0.19         | 0/2302   | 0.33        | 0/3110   |
| 28  | d     | 0.15         | 0/2162   | 0.31        | 0/2919   |
| 29  | e     | 0.12         | 0/437    | 0.25        | 0/595    |
| 30  | f     | 0.08         | 0/6980   | 0.25        | 0/9433   |
| 31  | F     | 0.19         | 0/2896   | 0.33        | 0/3912   |
| 32  | U     | 0.16         | 0/6417   | 0.32        | 0/8684   |
| All | All   | 0.16         | 0/102726 | 0.30        | 0/139055 |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 2863  | 0        | 2895     | 357     | 0            |
| 2   | B     | 3042  | 0        | 3100     | 418     | 0            |
| 3   | C     | 2968  | 0        | 3066     | 334     | 0            |
| 4   | D     | 3039  | 0        | 3074     | 353     | 0            |
| 5   | E     | 2860  | 0        | 2828     | 338     | 0            |
| 6   | G     | 1742  | 1660     | 1660     | 27      | 0            |
| 6   | g     | 1758  | 1687     | 1687     | 19      | 0            |
| 7   | H     | 1662  | 1590     | 1590     | 23      | 0            |
| 7   | h     | 1662  | 1590     | 1590     | 18      | 0            |
| 8   | I     | 1802  | 1741     | 1741     | 26      | 0            |
| 8   | i     | 1786  | 1717     | 1717     | 15      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 9   | J     | 1633  | 1518     | 1518     | 22      | 0            |
| 9   | j     | 1633  | 1518     | 1518     | 20      | 0            |
| 10  | K     | 1663  | 1592     | 1591     | 26      | 0            |
| 10  | k     | 1660  | 1589     | 1589     | 16      | 0            |
| 11  | L     | 1710  | 1649     | 1649     | 27      | 0            |
| 11  | l     | 1707  | 1645     | 1645     | 22      | 0            |
| 12  | M     | 1760  | 1680     | 1680     | 21      | 0            |
| 12  | m     | 1761  | 1683     | 1683     | 21      | 0            |
| 13  | N     | 1469  | 1422     | 1422     | 18      | 0            |
| 13  | n     | 1465  | 1416     | 1416     | 17      | 0            |
| 14  | O     | 1580  | 1559     | 1559     | 23      | 0            |
| 14  | o     | 1576  | 1555     | 1555     | 28      | 0            |
| 15  | P     | 1546  | 1550     | 1552     | 19      | 0            |
| 15  | p     | 1538  | 1543     | 1545     | 24      | 0            |
| 16  | Q     | 1509  | 1477     | 1477     | 17      | 0            |
| 16  | q     | 1506  | 1475     | 1475     | 17      | 0            |
| 17  | R     | 1504  | 1449     | 1449     | 23      | 0            |
| 17  | r     | 1500  | 1438     | 1438     | 18      | 0            |
| 18  | S     | 1584  | 1579     | 1579     | 11      | 0            |
| 18  | s     | 1587  | 1581     | 1581     | 14      | 0            |
| 19  | T     | 1576  | 1526     | 1528     | 20      | 0            |
| 19  | t     | 1568  | 1511     | 1513     | 14      | 0            |
| 20  | V     | 3754  | 0        | 3749     | 429     | 0            |
| 21  | W     | 3635  | 0        | 3762     | 522     | 0            |
| 22  | X     | 2664  | 0        | 2732     | 248     | 0            |
| 23  | Y     | 3115  | 0        | 3120     | 375     | 0            |
| 24  | Z     | 2281  | 0        | 2312     | 297     | 0            |
| 25  | a     | 2995  | 0        | 3012     | 397     | 0            |
| 26  | b     | 1458  | 0        | 1505     | 247     | 0            |
| 27  | c     | 2260  | 0        | 2276     | 292     | 0            |
| 28  | d     | 2116  | 0        | 2146     | 278     | 0            |
| 29  | e     | 425   | 0        | 328      | 40      | 0            |
| 30  | f     | 6866  | 0        | 6866     | 794     | 0            |
| 31  | F     | 2858  | 0        | 2853     | 288     | 0            |
| 32  | U     | 6304  | 0        | 6334     | 785     | 0            |
| 33  | A     | 31    | 0        | 12       | 4       | 0            |
| 33  | B     | 31    | 0        | 12       | 3       | 0            |
| 33  | D     | 31    | 0        | 12       | 8       | 0            |
| 33  | E     | 31    | 0        | 12       | 7       | 0            |
| 34  | A     | 2     | 0        | 0        | 0       | 0            |
| 34  | B     | 1     | 0        | 0        | 0       | 0            |
| 34  | E     | 2     | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H  | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 35  | C     | 27     | 0        | 12       | 4       | 0            |
| 35  | F     | 27     | 0        | 12       | 2       | 0            |
| 36  | N     | 34     | 41       | 41       | 1       | 0            |
| 36  | O     | 34     | 41       | 41       | 0       | 0            |
| 36  | R     | 34     | 41       | 41       | 7       | 0            |
| 36  | n     | 34     | 41       | 41       | 3       | 0            |
| 36  | o     | 34     | 41       | 41       | 1       | 0            |
| 36  | r     | 34     | 41       | 41       | 0       | 0            |
| 37  | c     | 1      | 0        | 0        | 0       | 0            |
| All | All   | 101338 | 44186    | 100223   | 6735    | 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 33.

All (6735) 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) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:217:LYS:HA    | 2:B:217:LYS:HE3   | 1.20                     | 1.17              |
| 2:B:361:LYS:HD3   | 2:B:390:LEU:HD11  | 1.25                     | 1.15              |
| 26:b:111:ALA:HB3  | 26:b:140:ILE:HA   | 1.29                     | 1.14              |
| 2:B:342:ILE:HG23  | 2:B:347:ILE:HD11  | 1.29                     | 1.13              |
| 3:C:248:MET:HE1   | 3:C:273:MET:HG3   | 1.14                     | 1.13              |
| 2:B:95:GLU:HA     | 2:B:98:LYS:HE2    | 1.31                     | 1.12              |
| 3:C:251:ILE:HG12  | 3:C:296:ASN:HD21  | 1.05                     | 1.12              |
| 2:B:278:ALA:HB1   | 2:B:279:PRO:HD2   | 1.31                     | 1.11              |
| 27:c:27:THR:HG21  | 27:c:177:THR:HA   | 1.25                     | 1.11              |
| 21:W:248:ARG:HD2  | 21:W:290:ILE:HD11 | 1.29                     | 1.10              |
| 30:f:99:LEU:HG    | 30:f:101:PRO:HD2  | 1.34                     | 1.10              |
| 30:f:681:TYR:HB3  | 30:f:761:MET:HE3  | 1.31                     | 1.09              |
| 31:F:373:MET:HE2  | 31:F:415:LEU:HD11 | 1.30                     | 1.09              |
| 20:V:428:LEU:HD21 | 20:V:437:ILE:HD11 | 1.25                     | 1.09              |
| 25:a:197:ALA:HA   | 25:a:222:LEU:HD13 | 1.27                     | 1.08              |
| 24:Z:172:VAL:HG13 | 27:c:217:LEU:HD21 | 1.31                     | 1.08              |
| 32:U:137:MET:HE2  | 32:U:137:MET:HA   | 1.27                     | 1.08              |
| 3:C:146:SER:HA    | 3:C:150:MET:HE3   | 1.35                     | 1.08              |
| 23:Y:27:SER:HA    | 23:Y:59:LYS:HE2   | 1.36                     | 1.08              |
| 30:f:370:MET:HE3  | 30:f:370:MET:HA   | 1.32                     | 1.07              |
| 28:d:231:LYS:HG3  | 28:d:232:PRO:HD3  | 1.32                     | 1.07              |
| 14:o:2:THR:N      | 14:o:170:SER:HG   | 1.51                     | 1.07              |
| 1:A:268:LYS:HG2   | 30:f:354:GLU:HG2  | 1.29                     | 1.06              |
| 30:f:545:LYS:HE2  | 30:f:547:GLU:HB3  | 1.38                     | 1.06              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 25:a:112:ILE:HD12 | 25:a:151:VAL:HG21 | 1.32                     | 1.05              |
| 30:f:729:MET:HA   | 30:f:729:MET:HE3  | 1.36                     | 1.05              |
| 32:U:894:MET:HE2  | 32:U:902:PRO:HD3  | 1.35                     | 1.05              |
| 28:d:36:LEU:HG    | 28:d:37:PRO:HD2   | 1.38                     | 1.05              |
| 30:f:385:PHE:HB3  | 30:f:388:ASP:HB2  | 1.33                     | 1.05              |
| 23:Y:96:GLY:HA2   | 23:Y:100:ILE:HG23 | 1.39                     | 1.04              |
| 26:b:22:LEU:HB3   | 26:b:23:PRO:HD3   | 1.37                     | 1.04              |
| 32:U:38:ILE:HD13  | 32:U:42:VAL:HB    | 1.36                     | 1.04              |
| 30:f:138:GLU:HA   | 30:f:141:LYS:HE3  | 1.40                     | 1.04              |
| 5:E:355:ILE:HD11  | 31:F:211:LYS:HD2  | 1.34                     | 1.03              |
| 21:W:60:MET:HE1   | 21:W:99:GLN:HB2   | 1.37                     | 1.03              |
| 20:V:333:ILE:HD11 | 20:V:360:TYR:HB3  | 1.41                     | 1.03              |
| 20:V:443:ARG:HG2  | 28:d:184:LYS:HZ1  | 1.23                     | 1.03              |
| 30:f:786:GLN:HB3  | 30:f:788:MET:HE1  | 1.39                     | 1.02              |
| 4:D:56:VAL:HG23   | 32:U:600:ARG:HE   | 1.22                     | 1.02              |
| 30:f:479:LEU:HD13 | 30:f:514:VAL:HG22 | 1.39                     | 1.02              |
| 30:f:829:MET:HE3  | 30:f:829:MET:H    | 1.18                     | 1.01              |
| 21:W:105:VAL:HG21 | 21:W:140:ILE:HD13 | 1.43                     | 1.01              |
| 1:A:85:GLN:HA     | 1:A:88:GLN:HB3    | 1.42                     | 1.01              |
| 24:Z:142:GLU:HG2  | 24:Z:153:LYS:HG3  | 1.41                     | 1.01              |
| 30:f:791:VAL:HG22 | 30:f:800:LEU:HD11 | 1.40                     | 1.01              |
| 1:A:196:LEU:HD13  | 30:f:348:ILE:HD13 | 1.39                     | 1.00              |
| 5:E:380:LEU:HD11  | 31:F:351:LYS:HE3  | 1.42                     | 1.00              |
| 24:Z:34:ARG:NH2   | 24:Z:105:ASP:OD2  | 1.95                     | 1.00              |
| 30:f:744:MET:HE1  | 30:f:745:LEU:HD23 | 1.41                     | 1.00              |
| 23:Y:232:GLU:HG2  | 23:Y:234:PRO:HD2  | 1.44                     | 1.00              |
| 4:D:64:GLU:HB3    | 32:U:607:VAL:HG21 | 1.41                     | 0.99              |
| 24:Z:19:VAL:HG21  | 24:Z:124:ILE:HD11 | 1.41                     | 0.99              |
| 5:E:330:ALA:HA    | 5:E:333:LYS:HE2   | 1.42                     | 0.99              |
| 31:F:188:ILE:HG12 | 31:F:235:LEU:HD23 | 1.44                     | 0.99              |
| 28:d:206:MET:HE3  | 28:d:206:MET:H    | 1.21                     | 0.99              |
| 3:C:249:ASP:OD1   | 3:C:250:GLU:N     | 1.94                     | 0.99              |
| 27:c:163:ILE:HD11 | 27:c:199:HIS:HA   | 1.41                     | 0.99              |
| 23:Y:18:ARG:HH11  | 23:Y:22:LEU:HD21  | 1.28                     | 0.98              |
| 3:C:196:LYS:HD2   | 3:C:294:ALA:HB1   | 1.43                     | 0.98              |
| 25:a:41:VAL:HG11  | 25:a:79:ILE:HD11  | 1.41                     | 0.98              |
| 1:A:151:ILE:HD12  | 1:A:152:PRO:HD2   | 1.45                     | 0.98              |
| 23:Y:29:PRO:HB2   | 23:Y:32:ARG:HG2   | 1.43                     | 0.98              |
| 32:U:789:ILE:HG13 | 32:U:911:ILE:HA   | 1.45                     | 0.98              |
| 1:A:196:LEU:HD11  | 30:f:345:PRO:HD2  | 1.45                     | 0.97              |
| 30:f:520:LEU:HD23 | 30:f:557:TRP:HB2  | 1.44                     | 0.97              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 25:a:200:LEU:HD22 | 25:a:222:LEU:HD12 | 1.45                     | 0.97              |
| 30:f:536:SER:HA   | 30:f:539:LEU:HD12 | 1.46                     | 0.97              |
| 20:V:452:ASN:ND2  | 28:d:187:GLU:OE2  | 1.96                     | 0.97              |
| 32:U:509:GLY:HA3  | 32:U:544:ILE:HG13 | 1.46                     | 0.97              |
| 30:f:125:ILE:HG21 | 30:f:129:LEU:HB2  | 1.42                     | 0.97              |
| 32:U:377:HIS:HB3  | 32:U:380:THR:HG22 | 1.45                     | 0.97              |
| 23:Y:237:ARG:HA   | 23:Y:241:ILE:HD12 | 1.46                     | 0.97              |
| 26:b:19:GLY:HA2   | 26:b:24:THR:HA    | 1.44                     | 0.97              |
| 1:A:99:THR:HG21   | 1:A:113:ILE:HD11  | 1.47                     | 0.97              |
| 1:A:306:LEU:HA    | 1:A:312:ARG:HD3   | 1.45                     | 0.96              |
| 30:f:559:PRO:HB2  | 30:f:594:LEU:HD23 | 1.45                     | 0.96              |
| 21:W:373:ILE:HD11 | 21:W:377:ARG:HG2  | 1.46                     | 0.96              |
| 32:U:576:PRO:HB3  | 32:U:611:ASN:HD22 | 1.30                     | 0.96              |
| 20:V:480:ILE:HD11 | 24:Z:261:TYR:HA   | 1.44                     | 0.95              |
| 23:Y:301:ILE:HD12 | 23:Y:342:ARG:HH21 | 1.28                     | 0.95              |
| 30:f:79:ARG:HB3   | 30:f:82:ILE:HG22  | 1.47                     | 0.95              |
| 32:U:525:ASN:OD1  | 32:U:528:ALA:N    | 1.99                     | 0.95              |
| 30:f:703:ARG:HA   | 30:f:706:ILE:HD12 | 1.46                     | 0.95              |
| 26:b:51:LEU:HD13  | 26:b:75:LEU:HD22  | 1.49                     | 0.95              |
| 1:A:268:LYS:HE2   | 1:A:268:LYS:N     | 1.82                     | 0.95              |
| 26:b:129:LYS:HG2  | 26:b:133:LYS:HZ1  | 1.30                     | 0.95              |
| 4:D:41:TYR:HD2    | 32:U:183:LEU:HD11 | 1.32                     | 0.95              |
| 27:c:167:MET:HE2  | 27:c:172:HIS:HB3  | 1.47                     | 0.95              |
| 26:b:52:ILE:HG13  | 26:b:60:VAL:HG23  | 1.50                     | 0.94              |
| 20:V:289:LEU:HB2  | 20:V:312:ALA:HB2  | 1.47                     | 0.94              |
| 26:b:8:VAL:HG22   | 26:b:110:ILE:HD11 | 1.47                     | 0.94              |
| 28:d:144:MET:HE2  | 28:d:144:MET:HA   | 1.49                     | 0.94              |
| 30:f:180:GLN:HG3  | 30:f:219:LYS:HZ2  | 1.31                     | 0.94              |
| 32:U:458:ILE:HD13 | 32:U:490:ARG:HH12 | 1.30                     | 0.94              |
| 25:a:149:THR:HG23 | 25:a:183:VAL:HB   | 1.50                     | 0.93              |
| 23:Y:52:PRO:HD3   | 23:Y:115:GLY:HA2  | 1.51                     | 0.93              |
| 3:C:354:ALA:HB1   | 3:C:358:GLU:HB2   | 1.50                     | 0.93              |
| 23:Y:238:GLU:OE1  | 23:Y:238:GLU:N    | 2.01                     | 0.93              |
| 2:B:212:GLU:HA    | 30:f:845:ARG:HG3  | 1.49                     | 0.93              |
| 22:X:233:TYR:HA   | 22:X:254:MET:HE1  | 1.51                     | 0.93              |
| 25:a:227:ASN:OD1  | 25:a:228:THR:N    | 2.02                     | 0.93              |
| 21:W:253:THR:O    | 21:W:257:GLN:N    | 2.01                     | 0.93              |
| 25:a:126:GLY:HA3  | 25:a:130:VAL:HG21 | 1.50                     | 0.93              |
| 25:a:278:MET:CE   | 25:a:319:LEU:HG   | 1.97                     | 0.93              |
| 32:U:188:MET:HE2  | 32:U:188:MET:HA   | 1.51                     | 0.93              |
| 24:Z:193:ASN:HB2  | 27:c:228:GLY:HA2  | 1.49                     | 0.92              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 21:W:363:ILE:HD11 | 21:W:393:LEU:HD13 | 1.49                     | 0.92              |
| 31:F:291:ILE:HD11 | 31:F:309:THR:HB   | 1.51                     | 0.92              |
| 4:D:266:GLU:HB3   | 5:E:258:MET:HE3   | 1.52                     | 0.92              |
| 32:U:757:MET:HE3  | 32:U:758:PRO:HD3  | 1.51                     | 0.92              |
| 24:Z:144:VAL:HA   | 24:Z:152:SER:HB3  | 1.51                     | 0.92              |
| 24:Z:176:LEU:HD21 | 27:c:217:LEU:HD22 | 1.52                     | 0.92              |
| 32:U:333:MET:SD   | 32:U:334:ALA:N    | 2.43                     | 0.92              |
| 24:Z:48:LEU:HD11  | 24:Z:92:VAL:HG21  | 1.50                     | 0.92              |
| 30:f:270:LEU:HB2  | 30:f:271:MET:HE3  | 1.52                     | 0.91              |
| 27:c:265:MET:HG2  | 27:c:266:THR:HG22 | 1.52                     | 0.91              |
| 32:U:82:LEU:HB3   | 32:U:129:ARG:HD3  | 1.52                     | 0.91              |
| 21:W:297:GLU:OE1  | 21:W:297:GLU:N    | 2.03                     | 0.91              |
| 25:a:97:LEU:HD13  | 25:a:118:ILE:HD13 | 1.52                     | 0.91              |
| 32:U:465:LEU:HD11 | 32:U:477:GLY:HA3  | 1.51                     | 0.91              |
| 1:A:319:MET:HE2   | 1:A:337:LEU:HD13  | 1.49                     | 0.91              |
| 5:E:215:ILE:HD13  | 5:E:260:LEU:HB2   | 1.53                     | 0.91              |
| 30:f:686:LEU:HD13 | 30:f:687:ARG:HG3  | 1.49                     | 0.91              |
| 4:D:332:GLU:HG3   | 4:D:334:PRO:HD3   | 1.51                     | 0.91              |
| 23:Y:26:LEU:HD23  | 23:Y:59:LYS:HD2   | 1.52                     | 0.91              |
| 2:B:292:THR:HG21  | 2:B:333:ARG:HH12  | 1.34                     | 0.91              |
| 30:f:334:ALA:HB1  | 30:f:335:ARG:HH21 | 1.33                     | 0.91              |
| 22:X:286:ALA:HA   | 22:X:309:TYR:HD2  | 1.33                     | 0.90              |
| 30:f:261:ARG:HA   | 30:f:267:ARG:HH12 | 1.36                     | 0.90              |
| 30:f:407:MET:HE1  | 30:f:440:ILE:HA   | 1.49                     | 0.90              |
| 1:A:371:GLU:N     | 1:A:371:GLU:OE2   | 2.04                     | 0.90              |
| 4:D:407:ILE:HD12  | 4:D:408:LYS:N     | 1.85                     | 0.90              |
| 28:d:13:SER:HB3   | 28:d:16:LEU:HB2   | 1.50                     | 0.90              |
| 23:Y:144:LEU:HA   | 23:Y:147:ILE:HD11 | 1.53                     | 0.90              |
| 23:Y:387:ILE:HG21 | 24:Z:276:ILE:HD11 | 1.52                     | 0.90              |
| 28:d:82:TYR:HD2   | 28:d:95:MET:HE1   | 1.37                     | 0.90              |
| 21:W:419:LYS:HG2  | 21:W:424:LEU:HD13 | 1.51                     | 0.90              |
| 32:U:669:ILE:HD13 | 32:U:695:MET:HE2  | 1.51                     | 0.90              |
| 13:N:145:ARG:NH2  | 13:N:152:GLU:OE2  | 2.05                     | 0.90              |
| 3:C:251:ILE:HG12  | 3:C:296:ASN:ND2   | 1.86                     | 0.89              |
| 5:E:306:GLU:N     | 5:E:306:GLU:OE2   | 2.04                     | 0.89              |
| 21:W:406:VAL:HG13 | 22:X:342:PHE:HB3  | 1.53                     | 0.89              |
| 27:c:260:GLU:N    | 27:c:260:GLU:OE2  | 2.04                     | 0.89              |
| 30:f:170:TRP:HE1  | 30:f:181:ARG:HB2  | 1.37                     | 0.89              |
| 1:A:113:ILE:HD11  | 1:A:142:VAL:HG11  | 1.52                     | 0.89              |
| 2:B:426:VAL:HG12  | 2:B:427:LEU:HD12  | 1.54                     | 0.89              |
| 1:A:143:ASP:OD1   | 1:A:145:ASN:N     | 2.03                     | 0.89              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:116:ILE:HG21  | 2:B:132:TYR:HE2   | 1.37                     | 0.89              |
| 4:D:267:ILE:HG12  | 4:D:309:MET:CE    | 2.03                     | 0.89              |
| 28:d:95:MET:HA    | 28:d:95:MET:HE3   | 1.55                     | 0.89              |
| 28:d:206:MET:HA   | 28:d:209:TYR:HB2  | 1.53                     | 0.89              |
| 21:W:155:GLN:HB2  | 21:W:161:GLU:OE1  | 1.72                     | 0.89              |
| 21:W:268:LYS:HZ1  | 21:W:301:LYS:HE3  | 1.38                     | 0.89              |
| 22:X:142:ARG:HB2  | 22:X:146:ALA:HB2  | 1.54                     | 0.89              |
| 31:F:224:LEU:HD13 | 31:F:348:LEU:HD22 | 1.53                     | 0.89              |
| 32:U:529:ILE:HD11 | 32:U:555:VAL:HG11 | 1.54                     | 0.89              |
| 3:C:218:GLU:OE1   | 3:C:218:GLU:N     | 2.06                     | 0.89              |
| 31:F:418:GLU:OE1  | 31:F:418:GLU:N    | 2.04                     | 0.89              |
| 27:c:51:MET:HA    | 27:c:82:VAL:HG13  | 1.56                     | 0.88              |
| 20:V:212:TYR:HA   | 20:V:253:LEU:HD11 | 1.55                     | 0.88              |
| 5:E:352:MET:HE2   | 5:E:352:MET:HA    | 1.55                     | 0.88              |
| 21:W:202:THR:HG22 | 21:W:233:LEU:HD22 | 1.54                     | 0.88              |
| 30:f:813:LYS:HB2  | 30:f:882:LEU:HD11 | 1.53                     | 0.88              |
| 2:B:90:GLU:H      | 2:B:94:GLU:HB3    | 1.36                     | 0.88              |
| 5:E:149:ILE:HD11  | 5:E:276:ILE:HD11  | 1.53                     | 0.88              |
| 28:d:23:LEU:HA    | 28:d:26:LEU:HD21  | 1.55                     | 0.88              |
| 20:V:482:PHE:HE2  | 23:Y:377:LEU:HD11 | 1.39                     | 0.88              |
| 32:U:554:LEU:HD11 | 32:U:761:VAL:HG23 | 1.54                     | 0.88              |
| 32:U:201:LEU:HD22 | 32:U:204:ILE:HD11 | 1.56                     | 0.88              |
| 20:V:244:ALA:HA   | 20:V:247:GLN:HE22 | 1.39                     | 0.87              |
| 21:W:445:LEU:HD22 | 24:Z:226:ILE:HG12 | 1.56                     | 0.87              |
| 25:a:278:MET:HE1  | 25:a:319:LEU:HG   | 1.52                     | 0.87              |
| 31:F:317:LEU:HD21 | 31:F:328:VAL:HG21 | 1.53                     | 0.87              |
| 1:A:323:ARG:HH22  | 1:A:433:ASN:HA    | 1.39                     | 0.87              |
| 1:A:364:VAL:HG23  | 1:A:366:ARG:H     | 1.38                     | 0.87              |
| 27:c:63:ASP:OD1   | 32:U:541:HIS:ND1  | 2.08                     | 0.87              |
| 32:U:242:LEU:O    | 32:U:246:TYR:HB2  | 1.74                     | 0.87              |
| 2:B:357:ASP:OD1   | 2:B:358:GLU:N     | 2.07                     | 0.87              |
| 20:V:443:ARG:HG2  | 28:d:184:LYS:NZ   | 1.87                     | 0.87              |
| 30:f:209:MET:HG3  | 30:f:212:GLU:HB2  | 1.54                     | 0.87              |
| 31:F:299:GLU:OE1  | 31:F:299:GLU:N    | 2.07                     | 0.87              |
| 3:C:44:ARG:NH1    | 3:C:44:ARG:O      | 2.07                     | 0.87              |
| 3:C:69:GLN:OE1    | 3:C:69:GLN:N      | 2.06                     | 0.87              |
| 30:f:813:LYS:HD2  | 30:f:882:LEU:HD21 | 1.55                     | 0.87              |
| 1:A:139:ARG:O     | 1:A:153:LEU:N     | 2.08                     | 0.86              |
| 4:D:393:ILE:HG12  | 21:W:133:GLU:HB3  | 1.57                     | 0.86              |
| 23:Y:275:LEU:HD21 | 23:Y:296:VAL:HG13 | 1.55                     | 0.86              |
| 30:f:673:ARG:HH21 | 30:f:707:LEU:HD22 | 1.38                     | 0.86              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 30:f:842:VAL:HG11 | 30:f:862:ILE:HB   | 1.56                     | 0.86              |
| 32:U:9:ILE:HD13   | 32:U:42:VAL:HG11  | 1.57                     | 0.86              |
| 32:U:801:GLN:HE21 | 32:U:877:LEU:HA   | 1.39                     | 0.86              |
| 3:C:336:MET:HE1   | 3:C:367:GLY:HA3   | 1.56                     | 0.86              |
| 32:U:422:LEU:HG   | 32:U:423:MET:CE   | 2.05                     | 0.86              |
| 4:D:269:ALA:HB1   | 5:E:255:ARG:HG2   | 1.57                     | 0.86              |
| 22:X:369:ILE:HD12 | 23:Y:310:SER:HA   | 1.55                     | 0.86              |
| 3:C:132:ASP:HB3   | 3:C:135:VAL:HG23  | 1.55                     | 0.86              |
| 30:f:159:VAL:HG13 | 30:f:160:ARG:HH11 | 1.40                     | 0.86              |
| 3:C:90:HIS:ND1    | 3:C:91:PRO:HD2    | 1.91                     | 0.86              |
| 30:f:759:LEU:HB2  | 30:f:809:ILE:HD12 | 1.57                     | 0.86              |
| 31:F:162:GLU:OE1  | 31:F:162:GLU:N    | 2.08                     | 0.86              |
| 23:Y:282:MET:HG3  | 23:Y:288:PHE:HB3  | 1.58                     | 0.85              |
| 28:d:206:MET:H    | 28:d:206:MET:CE   | 1.89                     | 0.85              |
| 30:f:62:ARG:HH22  | 30:f:66:LYS:HD3   | 1.41                     | 0.85              |
| 21:W:45:GLU:OE1   | 21:W:45:GLU:N     | 2.08                     | 0.85              |
| 32:U:642:GLU:N    | 32:U:642:GLU:OE1  | 2.09                     | 0.85              |
| 30:f:512:MET:O    | 30:f:512:MET:HE3  | 1.76                     | 0.85              |
| 1:A:264:ALA:HA    | 1:A:267:LYS:HD2   | 1.57                     | 0.85              |
| 3:C:172:PRO:O     | 3:C:173:GLU:HG3   | 1.77                     | 0.85              |
| 4:D:269:ALA:HB2   | 5:E:258:MET:HE2   | 1.58                     | 0.85              |
| 21:W:136:ILE:O    | 21:W:137:TYR:HB2  | 1.76                     | 0.85              |
| 26:b:147:GLU:CD   | 26:b:150:THR:HA   | 2.00                     | 0.85              |
| 32:U:872:GLU:OE1  | 32:U:872:GLU:N    | 2.09                     | 0.85              |
| 5:E:204:VAL:HG21  | 5:E:253:ILE:HD11  | 1.57                     | 0.85              |
| 20:V:259:LEU:HD13 | 20:V:264:TYR:HE1  | 1.42                     | 0.85              |
| 24:Z:43:TRP:HB3   | 24:Z:48:LEU:HA    | 1.59                     | 0.85              |
| 32:U:357:LYS:HE3  | 32:U:357:LYS:HA   | 1.58                     | 0.85              |
| 1:A:115:VAL:HG21  | 1:A:118:PHE:HB2   | 1.59                     | 0.85              |
| 21:W:169:LEU:HD11 | 21:W:173:THR:HG23 | 1.59                     | 0.84              |
| 30:f:271:MET:HB2  | 30:f:275:MET:HE1  | 1.59                     | 0.84              |
| 20:V:337:LEU:HD22 | 20:V:367:VAL:HG11 | 1.57                     | 0.84              |
| 27:c:241:ASN:HD21 | 27:c:295:ASN:HD21 | 1.22                     | 0.84              |
| 30:f:139:CYS:HA   | 30:f:143:ARG:HH21 | 1.43                     | 0.84              |
| 2:B:379:THR:OG1   | 2:B:382:ASP:OD2   | 1.94                     | 0.84              |
| 3:C:62:GLU:OE2    | 4:D:117:SER:OG    | 1.95                     | 0.84              |
| 28:d:44:THR:OG1   | 28:d:47:GLN:NE2   | 2.11                     | 0.84              |
| 4:D:154:LEU:N     | 4:D:158:GLN:OE1   | 2.11                     | 0.84              |
| 20:V:337:LEU:O    | 20:V:401:ASN:ND2  | 2.11                     | 0.84              |
| 24:Z:243:GLN:N    | 24:Z:243:GLN:OE1  | 2.11                     | 0.84              |
| 26:b:19:GLY:CA    | 26:b:24:THR:HA    | 2.07                     | 0.84              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 32:U:209:GLU:HB2  | 32:U:210:LYS:NZ   | 1.93                     | 0.84              |
| 20:V:410:ILE:HD13 | 20:V:422:ILE:HD13 | 1.60                     | 0.84              |
| 27:c:27:THR:CG2   | 27:c:177:THR:HA   | 2.08                     | 0.84              |
| 2:B:387:LYS:HZ1   | 2:B:427:LEU:HB2   | 1.43                     | 0.84              |
| 30:f:412:ALA:HB2  | 30:f:446:LEU:HD12 | 1.56                     | 0.84              |
| 25:a:57:ILE:HD11  | 25:a:60:TYR:CD2   | 2.13                     | 0.83              |
| 30:f:664:GLU:OE1  | 30:f:667:GLY:N    | 2.11                     | 0.83              |
| 32:U:199:ARG:O    | 32:U:202:VAL:HG22 | 1.78                     | 0.83              |
| 32:U:901:GLN:HE21 | 32:U:915:LYS:HB3  | 1.42                     | 0.83              |
| 24:Z:8:LYS:NZ     | 24:Z:161:GLU:HG2  | 1.92                     | 0.83              |
| 31:F:221:LYS:HA   | 31:F:221:LYS:HE3  | 1.59                     | 0.83              |
| 1:A:182:GLU:N     | 1:A:182:GLU:OE2   | 2.12                     | 0.83              |
| 4:D:336:PRO:HD2   | 4:D:371:SER:HA    | 1.60                     | 0.83              |
| 5:E:352:MET:HE2   | 5:E:355:ILE:HG21  | 1.59                     | 0.83              |
| 22:X:239:TYR:HE1  | 22:X:246:LYS:HB2  | 1.43                     | 0.83              |
| 23:Y:189:VAL:HG13 | 23:Y:287:LEU:HD21 | 1.60                     | 0.83              |
| 25:a:4:VAL:HB     | 25:a:5:PRO:HD3    | 1.58                     | 0.83              |
| 32:U:131:GLU:OE1  | 32:U:135:ASN:ND2  | 2.11                     | 0.83              |
| 5:E:270:LEU:HD21  | 5:E:273:VAL:HB    | 1.59                     | 0.83              |
| 26:b:51:LEU:HD23  | 26:b:62:THR:HB    | 1.60                     | 0.83              |
| 6:g:174:GLU:N     | 6:g:174:GLU:OE2   | 2.12                     | 0.83              |
| 1:A:394:MET:HE3   | 2:B:199:GLU:HG3   | 1.60                     | 0.83              |
| 32:U:609:ASP:OD1  | 32:U:610:VAL:N    | 2.10                     | 0.83              |
| 21:W:367:ALA:HA   | 21:W:415:PHE:HD2  | 1.44                     | 0.83              |
| 22:X:130:GLU:HG3  | 22:X:149:LEU:HD11 | 1.58                     | 0.83              |
| 32:U:226:PRO:HA   | 32:U:260:PHE:HE1  | 1.40                     | 0.83              |
| 32:U:457:ILE:H    | 32:U:457:ILE:HD12 | 1.44                     | 0.83              |
| 32:U:694:ILE:HG23 | 32:U:695:MET:SD   | 2.18                     | 0.83              |
| 2:B:196:GLU:N     | 2:B:196:GLU:OE1   | 2.12                     | 0.83              |
| 27:c:34:SER:OG    | 27:c:37:ALA:N     | 2.12                     | 0.83              |
| 32:U:757:MET:HE3  | 32:U:758:PRO:CD   | 2.08                     | 0.83              |
| 3:C:86:LEU:HD12   | 3:C:96:VAL:HG22   | 1.58                     | 0.82              |
| 4:D:41:TYR:CD2    | 32:U:183:LEU:HD11 | 2.13                     | 0.82              |
| 21:W:273:TYR:HA   | 21:W:276:LEU:HD23 | 1.60                     | 0.82              |
| 22:X:233:TYR:CA   | 22:X:254:MET:HE1  | 2.09                     | 0.82              |
| 30:f:786:GLN:HB3  | 30:f:788:MET:CE   | 2.09                     | 0.82              |
| 3:C:59:LEU:HD22   | 4:D:72:PHE:HE1    | 1.44                     | 0.82              |
| 22:X:256:LEU:HD13 | 22:X:319:ILE:CD1  | 2.09                     | 0.82              |
| 27:c:25:VAL:HG22  | 27:c:175:ARG:HA   | 1.60                     | 0.82              |
| 24:Z:101:LEU:HD12 | 24:Z:138:TYR:HE2  | 1.44                     | 0.82              |
| 25:a:286:ALA:HA   | 25:a:289:ARG:HE   | 1.44                     | 0.82              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 25:a:175:ASP:OD1  | 25:a:176:ALA:N    | 2.12                     | 0.82              |
| 5:E:277:MET:HE1   | 5:E:289:LEU:HD11  | 1.60                     | 0.82              |
| 28:d:256:ILE:HD12 | 28:d:256:ILE:O    | 1.79                     | 0.82              |
| 30:f:415:GLY:HA3  | 30:f:447:ALA:HB1  | 1.60                     | 0.82              |
| 32:U:167:ILE:HB   | 32:U:204:ILE:HG21 | 1.61                     | 0.82              |
| 3:C:379:THR:OG1   | 3:C:382:ASP:OD2   | 1.97                     | 0.82              |
| 21:W:131:VAL:HG13 | 21:W:144:ARG:HD2  | 1.62                     | 0.82              |
| 26:b:187:PRO:HG2  | 26:b:188:ILE:HD12 | 1.62                     | 0.82              |
| 3:C:273:MET:HE2   | 3:C:293:MET:HG3   | 1.62                     | 0.82              |
| 4:D:61:ILE:HD11   | 32:U:639:LEU:HD13 | 1.60                     | 0.82              |
| 4:D:415:GLU:OE1   | 4:D:415:GLU:N     | 2.13                     | 0.82              |
| 21:W:236:HIS:ND1  | 21:W:237:GLU:OE1  | 2.13                     | 0.82              |
| 31:F:357:PRO:HB3  | 31:F:361:ALA:HB3  | 1.62                     | 0.82              |
| 25:a:347:LYS:HD2  | 25:a:347:LYS:O    | 1.80                     | 0.82              |
| 28:d:125:LYS:HB3  | 28:d:130:ASN:HB2  | 1.60                     | 0.82              |
| 23:Y:224:VAL:HG23 | 23:Y:260:LEU:HD12 | 1.61                     | 0.81              |
| 14:o:2:THR:OG1    | 36:o:301:LDZ:O33  | 1.96                     | 0.81              |
| 31:F:384:LEU:HD11 | 31:F:420:TYR:HB3  | 1.62                     | 0.81              |
| 2:B:390:LEU:HD22  | 2:B:395:ILE:HD11  | 1.60                     | 0.81              |
| 26:b:115:SER:OG   | 26:b:116:PRO:HD2  | 1.78                     | 0.81              |
| 28:d:75:MET:SD    | 28:d:78:LEU:HD11  | 2.19                     | 0.81              |
| 1:A:177:VAL:HG12  | 1:A:224:LEU:HD23  | 1.62                     | 0.81              |
| 24:Z:22:HIS:HA    | 24:Z:25:ARG:HD2   | 1.61                     | 0.81              |
| 24:Z:199:LYS:HZ1  | 25:a:364:GLU:HG2  | 1.46                     | 0.81              |
| 26:b:100:ARG:HG3  | 26:b:101:GLN:O    | 1.80                     | 0.81              |
| 30:f:270:LEU:HB2  | 30:f:271:MET:CE   | 2.11                     | 0.81              |
| 30:f:701:ASN:OD1  | 30:f:704:LEU:N    | 2.12                     | 0.81              |
| 32:U:173:VAL:HG13 | 32:U:177:LEU:HB3  | 1.59                     | 0.81              |
| 30:f:605:ASN:HD21 | 30:f:608:LYS:HB3  | 1.43                     | 0.81              |
| 32:U:38:ILE:CD1   | 32:U:42:VAL:HB    | 2.10                     | 0.81              |
| 32:U:333:MET:HE3  | 32:U:333:MET:H    | 1.44                     | 0.81              |
| 23:Y:70:LEU:HG    | 23:Y:74:LYS:NZ    | 1.95                     | 0.81              |
| 3:C:273:MET:HE1   | 3:C:293:MET:SD    | 2.20                     | 0.81              |
| 30:f:828:ARG:HE   | 30:f:861:THR:HG21 | 1.45                     | 0.81              |
| 3:C:164:VAL:HG21  | 3:C:186:VAL:HG11  | 1.63                     | 0.81              |
| 3:C:173:GLU:HA    | 3:C:176:GLU:HG3   | 1.60                     | 0.81              |
| 5:E:199:VAL:HG13  | 31:F:315:ASN:ND2  | 1.95                     | 0.81              |
| 21:W:219:THR:HG23 | 21:W:223:LYS:H    | 1.45                     | 0.81              |
| 2:B:223:ILE:HB    | 2:B:347:ILE:HD12  | 1.63                     | 0.81              |
| 3:C:273:MET:CE    | 3:C:293:MET:HG3   | 2.11                     | 0.81              |
| 5:E:241:ARG:H     | 31:F:304:ARG:HH12 | 1.27                     | 0.81              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:84:LYS:NZ     | 1:A:84:LYS:O      | 2.13                     | 0.81              |
| 26:b:121:GLU:O    | 26:b:123:ASP:N    | 2.14                     | 0.81              |
| 26:b:156:PHE:O    | 26:b:159:THR:OG1  | 1.96                     | 0.81              |
| 28:d:30:LEU:HD12  | 28:d:31:LEU:H     | 1.45                     | 0.81              |
| 3:C:250:GLU:HG3   | 3:C:269:VAL:HG21  | 1.61                     | 0.81              |
| 23:Y:328:GLU:OE1  | 23:Y:328:GLU:N    | 2.14                     | 0.81              |
| 24:Z:239:ASP:OD2  | 24:Z:243:GLN:NE2  | 2.13                     | 0.81              |
| 1:A:102:ILE:HD11  | 1:A:114:ASN:HB3   | 1.63                     | 0.80              |
| 1:A:112:ILE:HD11  | 31:F:164:LEU:HD23 | 1.62                     | 0.80              |
| 1:A:322:ASN:ND2   | 1:A:322:ASN:O     | 2.14                     | 0.80              |
| 3:C:374:ARG:HD3   | 4:D:190:LEU:HD11  | 1.62                     | 0.80              |
| 7:H:15:SER:OG     | 7:H:17:LYS:NZ     | 2.14                     | 0.80              |
| 20:V:236:ARG:HA   | 32:U:70:HIS:NE2   | 1.96                     | 0.80              |
| 25:a:57:ILE:HD12  | 25:a:60:TYR:HB3   | 1.63                     | 0.80              |
| 25:a:363:MET:HA   | 25:a:363:MET:HE2  | 1.62                     | 0.80              |
| 26:b:36:VAL:O     | 26:b:40:LYS:N     | 2.12                     | 0.80              |
| 27:c:71:ASP:OD1   | 27:c:72:VAL:N     | 2.14                     | 0.80              |
| 11:l:45:VAL:HG22  | 11:l:214:ILE:HD12 | 1.63                     | 0.80              |
| 32:U:247:GLN:NE2  | 32:U:904:LYS:HD2  | 1.96                     | 0.80              |
| 5:E:342:ASP:HA    | 5:E:345:ASN:HB2   | 1.63                     | 0.80              |
| 20:V:492:LYS:HE2  | 20:V:492:LYS:HA   | 1.61                     | 0.80              |
| 21:W:298:GLU:OE1  | 21:W:298:GLU:N    | 2.14                     | 0.80              |
| 30:f:821:LEU:HD21 | 30:f:882:LEU:HD13 | 1.60                     | 0.80              |
| 4:D:200:ARG:HG2   | 4:D:200:ARG:HH11  | 1.45                     | 0.80              |
| 20:V:477:HIS:HD1  | 28:d:249:TYR:HH   | 1.29                     | 0.80              |
| 23:Y:278:VAL:HA   | 23:Y:281:GLU:HG3  | 1.62                     | 0.80              |
| 4:D:338:ARG:NH2   | 4:D:366:ARG:O     | 2.14                     | 0.80              |
| 20:V:294:ARG:NH2  | 20:V:390:GLY:O    | 2.13                     | 0.80              |
| 22:X:339:ILE:HD11 | 22:X:350:ILE:CD1  | 2.12                     | 0.80              |
| 26:b:135:LYS:HA   | 26:b:135:LYS:HE3  | 1.63                     | 0.80              |
| 21:W:59:ASP:HB3   | 21:W:62:SER:HB2   | 1.64                     | 0.80              |
| 21:W:169:LEU:CD1  | 21:W:172:GLU:HB2  | 2.10                     | 0.80              |
| 24:Z:11:VAL:HG21  | 24:Z:135:THR:HG21 | 1.63                     | 0.80              |
| 25:a:94:LEU:HG    | 25:a:121:LEU:HD23 | 1.63                     | 0.80              |
| 30:f:833:PHE:HE1  | 30:f:842:VAL:HG23 | 1.47                     | 0.80              |
| 32:U:667:GLU:N    | 32:U:667:GLU:OE1  | 2.14                     | 0.80              |
| 32:U:810:THR:OG1  | 32:U:888:GLN:OE1  | 1.98                     | 0.80              |
| 3:C:57:ARG:HH22   | 32:U:649:ARG:HH12 | 1.30                     | 0.80              |
| 1:A:81:ALA:HB2    | 2:B:137:SER:HB2   | 1.63                     | 0.80              |
| 21:W:170:GLN:OE1  | 21:W:174:TYR:HB2  | 1.82                     | 0.80              |
| 30:f:368:ALA:HB2  | 30:f:402:ASN:HA   | 1.63                     | 0.80              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 31:F:79:LYS:HA    | 31:F:79:LYS:HE3   | 1.64                     | 0.80              |
| 32:U:901:GLN:O    | 32:U:915:LYS:N    | 2.13                     | 0.80              |
| 4:D:389:GLU:OE1   | 4:D:389:GLU:N     | 2.15                     | 0.80              |
| 20:V:115:LYS:O    | 20:V:119:GLY:N    | 2.14                     | 0.80              |
| 30:f:266:LEU:HD23 | 30:f:270:LEU:HD11 | 1.62                     | 0.80              |
| 30:f:775:THR:O    | 30:f:778:LEU:HD22 | 1.80                     | 0.80              |
| 32:U:137:MET:HA   | 32:U:137:MET:CE   | 2.09                     | 0.80              |
| 1:A:280:ILE:HA    | 1:A:295:VAL:HG13  | 1.61                     | 0.80              |
| 27:c:49:VAL:HG12  | 27:c:50:PRO:HD3   | 1.63                     | 0.80              |
| 28:d:33:LEU:HG    | 28:d:47:GLN:HB2   | 1.64                     | 0.80              |
| 28:d:71:PHE:HE2   | 28:d:75:MET:HE2   | 1.43                     | 0.80              |
| 5:E:309:ARG:NH1   | 5:E:335:SER:O     | 2.15                     | 0.80              |
| 20:V:244:ALA:HA   | 20:V:247:GLN:NE2  | 1.96                     | 0.80              |
| 20:V:273:LYS:HE3  | 32:U:39:SER:HB2   | 1.64                     | 0.79              |
| 30:f:474:SER:HB3  | 30:f:477:MET:HG3  | 1.63                     | 0.79              |
| 26:b:7:MET:HB2    | 26:b:109:ILE:HG22 | 1.62                     | 0.79              |
| 28:d:35:PHE:HB2   | 28:d:81:TYR:OH    | 1.82                     | 0.79              |
| 5:E:300:HIS:ND1   | 5:E:300:HIS:O     | 2.15                     | 0.79              |
| 20:V:256:ARG:NH1  | 29:e:21:GLU:OE2   | 2.14                     | 0.79              |
| 32:U:167:ILE:HD12 | 32:U:204:ILE:HG22 | 1.64                     | 0.79              |
| 22:X:167:VAL:HG21 | 22:X:197:ALA:HB2  | 1.64                     | 0.79              |
| 23:Y:147:ILE:HD12 | 23:Y:148:GLY:H    | 1.46                     | 0.79              |
| 26:b:18:ASN:OD1   | 26:b:25:ARG:NE    | 2.16                     | 0.79              |
| 1:A:103:ASN:OD1   | 1:A:104:ALA:N     | 2.16                     | 0.79              |
| 1:A:113:ILE:CD1   | 1:A:142:VAL:HG11  | 2.11                     | 0.79              |
| 24:Z:8:LYS:HZ2    | 24:Z:161:GLU:HG2  | 1.47                     | 0.79              |
| 25:a:247:ARG:O    | 25:a:251:LEU:HD13 | 1.82                     | 0.79              |
| 26:b:22:LEU:CB    | 26:b:23:PRO:HD3   | 2.13                     | 0.79              |
| 30:f:683:GLU:H    | 30:f:688:ARG:HE   | 1.30                     | 0.79              |
| 32:U:233:LEU:HD22 | 32:U:268:LEU:HD21 | 1.64                     | 0.79              |
| 32:U:457:ILE:HG22 | 32:U:461:LEU:HD23 | 1.65                     | 0.79              |
| 32:U:744:VAL:HG21 | 32:U:783:TYR:HB3  | 1.65                     | 0.79              |
| 1:A:387:SER:HA    | 1:A:390:THR:HG22  | 1.65                     | 0.79              |
| 5:E:50:LEU:HD13   | 31:F:82:VAL:HG11  | 1.64                     | 0.79              |
| 32:U:902:PRO:HA   | 32:U:914:LEU:HD12 | 1.62                     | 0.79              |
| 2:B:95:GLU:HA     | 2:B:98:LYS:CE     | 2.13                     | 0.79              |
| 25:a:90:PRO:HB3   | 25:a:121:LEU:HD11 | 1.64                     | 0.79              |
| 14:O:98:ALA:HB1   | 14:O:128:MET:CE   | 2.13                     | 0.79              |
| 27:c:31:VAL:HG22  | 27:c:67:VAL:HG13  | 1.64                     | 0.79              |
| 32:U:368:ALA:O    | 32:U:371:ILE:HG22 | 1.83                     | 0.79              |
| 32:U:405:THR:HG21 | 32:U:441:GLY:HA3  | 1.64                     | 0.79              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 23:Y:383:LEU:O    | 23:Y:386:VAL:HG12 | 1.83                     | 0.78              |
| 25:a:87:MET:SD    | 25:a:88:THR:N     | 2.56                     | 0.78              |
| 32:U:602:LEU:HD11 | 32:U:621:SER:HB2  | 1.66                     | 0.78              |
| 1:A:268:LYS:HG2   | 30:f:354:GLU:CG   | 2.13                     | 0.78              |
| 21:W:220:GLU:O    | 21:W:257:GLN:NE2  | 2.15                     | 0.78              |
| 21:W:210:ASN:HA   | 21:W:213:PHE:HE1  | 1.48                     | 0.78              |
| 4:D:392:TYR:O     | 4:D:393:ILE:HD13  | 1.84                     | 0.78              |
| 21:W:182:ARG:O    | 21:W:186:ILE:HG22 | 1.82                     | 0.78              |
| 2:B:212:GLU:CA    | 30:f:845:ARG:HG3  | 2.13                     | 0.78              |
| 20:V:449:ALA:HB3  | 20:V:460:SER:HA   | 1.64                     | 0.78              |
| 22:X:325:LYS:HA   | 22:X:325:LYS:HE2  | 1.65                     | 0.78              |
| 1:A:323:ARG:HG2   | 1:A:323:ARG:HH11  | 1.49                     | 0.78              |
| 22:X:172:LEU:O    | 22:X:176:THR:HG23 | 1.82                     | 0.78              |
| 30:f:462:ALA:HB3  | 30:f:489:TYR:OH   | 1.82                     | 0.78              |
| 4:D:266:GLU:HB3   | 5:E:258:MET:CE    | 2.13                     | 0.78              |
| 20:V:72:LEU:CD2   | 20:V:112:VAL:HG22 | 2.14                     | 0.78              |
| 26:b:41:THR:HA    | 26:b:47:ASN:HD22  | 1.48                     | 0.78              |
| 1:A:151:ILE:HD12  | 1:A:152:PRO:CD    | 2.14                     | 0.78              |
| 21:W:28:LEU:HD11  | 21:W:69:ALA:HB2   | 1.66                     | 0.78              |
| 30:f:445:LEU:CD2  | 30:f:481:SER:HA   | 2.14                     | 0.78              |
| 20:V:466:ILE:HD11 | 20:V:471:GLU:HG2  | 1.66                     | 0.78              |
| 27:c:179:SER:OG   | 32:U:770:TRP:O    | 2.02                     | 0.78              |
| 32:U:450:HIS:HD1  | 32:U:457:ILE:HG12 | 1.49                     | 0.78              |
| 1:A:357:ILE:HD12  | 1:A:360:ARG:HE    | 1.48                     | 0.77              |
| 2:B:217:LYS:HE3   | 2:B:217:LYS:CA    | 2.08                     | 0.77              |
| 3:C:44:ARG:HH22   | 3:C:45:LEU:HD13   | 1.49                     | 0.77              |
| 25:a:57:ILE:HD11  | 25:a:60:TYR:HD2   | 1.48                     | 0.77              |
| 30:f:545:LYS:NZ   | 30:f:548:THR:OG1  | 2.18                     | 0.77              |
| 1:A:239:ARG:HG2   | 2:B:319:PHE:CZ    | 2.19                     | 0.77              |
| 5:E:313:LEU:HD11  | 5:E:331:ILE:HG21  | 1.66                     | 0.77              |
| 20:V:247:GLN:OE1  | 20:V:247:GLN:N    | 2.17                     | 0.77              |
| 21:W:372:ARG:CZ   | 25:a:327:VAL:HG21 | 2.15                     | 0.77              |
| 32:U:377:HIS:HB3  | 32:U:380:THR:CG2  | 2.14                     | 0.77              |
| 3:C:351:MET:HE1   | 3:C:362:VAL:HG21  | 1.67                     | 0.77              |
| 22:X:415:TYR:HE2  | 23:Y:382:LYS:HE3  | 1.47                     | 0.77              |
| 23:Y:336:ARG:NH1  | 29:e:47:ASN:OD1   | 2.18                     | 0.77              |
| 32:U:437:TYR:HE1  | 32:U:472:ILE:HB   | 1.49                     | 0.77              |
| 32:U:713:TYR:O    | 32:U:717:ILE:HG23 | 1.84                     | 0.77              |
| 3:C:77:VAL:CG2    | 3:C:86:LEU:HD23   | 2.14                     | 0.77              |
| 5:E:98:VAL:HB     | 5:E:107:ILE:HG23  | 1.65                     | 0.77              |
| 5:E:355:ILE:HD11  | 31:F:211:LYS:CD   | 2.14                     | 0.77              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 21:W:254:PRO:HA   | 21:W:257:GLN:O    | 1.84                     | 0.77              |
| 32:U:236:LEU:CB   | 32:U:245:ALA:HB2  | 2.15                     | 0.77              |
| 20:V:192:MET:HE1  | 20:V:211:TYR:HD1  | 1.49                     | 0.77              |
| 21:W:117:ASP:O    | 21:W:120:ILE:HG22 | 1.85                     | 0.77              |
| 22:X:105:GLN:OE1  | 22:X:105:GLN:N    | 2.18                     | 0.77              |
| 24:Z:19:VAL:HG21  | 24:Z:124:ILE:CD1  | 2.15                     | 0.77              |
| 28:d:78:LEU:HD12  | 28:d:79:LYS:H     | 1.47                     | 0.77              |
| 4:D:173:GLN:HE21  | 4:D:334:PRO:HD2   | 1.50                     | 0.77              |
| 4:D:248:ARG:HG3   | 4:D:295:GLN:HE22  | 1.50                     | 0.77              |
| 3:C:270:GLN:NE2   | 3:C:302:ASP:OD1   | 2.18                     | 0.77              |
| 20:V:482:PHE:CE2  | 23:Y:377:LEU:HD11 | 2.20                     | 0.77              |
| 28:d:78:LEU:HD12  | 28:d:79:LYS:N     | 2.00                     | 0.77              |
| 29:e:51:ASP:O     | 29:e:55:GLN:NE2   | 2.17                     | 0.77              |
| 30:f:673:ARG:HH21 | 30:f:707:LEU:CD2  | 1.98                     | 0.77              |
| 32:U:552:ILE:HD11 | 32:U:566:LEU:HD21 | 1.65                     | 0.77              |
| 4:D:87:LEU:HB2    | 5:E:80:VAL:CG1    | 2.15                     | 0.77              |
| 25:a:5:PRO:O      | 25:a:8:LEU:HG     | 1.85                     | 0.77              |
| 25:a:41:VAL:HG11  | 25:a:79:ILE:CD1   | 2.13                     | 0.77              |
| 26:b:90:ILE:HD12  | 26:b:90:ILE:H     | 1.49                     | 0.77              |
| 28:d:82:TYR:CD2   | 28:d:95:MET:HE1   | 2.20                     | 0.77              |
| 1:A:279:ALA:HB1   | 2:B:307:ARG:HG2   | 1.66                     | 0.77              |
| 3:C:351:MET:HE3   | 3:C:387:VAL:HG12  | 1.65                     | 0.77              |
| 4:D:159:LYS:HG3   | 4:D:160:PRO:HD2   | 1.66                     | 0.77              |
| 23:Y:70:LEU:O     | 23:Y:74:LYS:NZ    | 2.17                     | 0.77              |
| 26:b:108:ARG:HH12 | 26:b:137:ASN:HD21 | 1.33                     | 0.77              |
| 2:B:217:LYS:HA    | 2:B:217:LYS:CE    | 2.04                     | 0.76              |
| 20:V:159:LEU:HD22 | 20:V:163:VAL:HG11 | 1.67                     | 0.76              |
| 23:Y:307:LEU:HD22 | 23:Y:319:MET:HE3  | 1.67                     | 0.76              |
| 26:b:51:LEU:HD22  | 26:b:71:ILE:HG23  | 1.66                     | 0.76              |
| 30:f:177:GLU:HG2  | 30:f:835:GLU:HA   | 1.67                     | 0.76              |
| 32:U:413:LYS:HA   | 32:U:449:ILE:HA   | 1.67                     | 0.76              |
| 32:U:516:LEU:HG   | 32:U:532:MET:HE2  | 1.64                     | 0.76              |
| 1:A:334:PRO:HG2   | 31:F:395:GLN:HA   | 1.65                     | 0.76              |
| 3:C:52:LEU:HD11   | 4:D:69:LYS:HG3    | 1.66                     | 0.76              |
| 3:C:328:ILE:HG22  | 3:C:359:VAL:HG11  | 1.66                     | 0.76              |
| 30:f:825:MET:HG2  | 30:f:827:PRO:HD3  | 1.67                     | 0.76              |
| 14:o:127:THR:HG21 | 14:o:135:ALA:HB3  | 1.66                     | 0.76              |
| 2:B:56:THR:HB     | 30:f:835:GLU:OE2  | 1.83                     | 0.76              |
| 5:E:59:GLU:N      | 5:E:59:GLU:OE1    | 2.16                     | 0.76              |
| 20:V:72:LEU:HD21  | 20:V:112:VAL:HG22 | 1.67                     | 0.76              |
| 24:Z:6:VAL:HG23   | 24:Z:158:VAL:HG11 | 1.65                     | 0.76              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 25:a:80:ILE:O     | 25:a:83:VAL:HG12  | 1.85                     | 0.76              |
| 32:U:599:ILE:HD11 | 32:U:626:LEU:HD21 | 1.67                     | 0.76              |
| 1:A:415:LYS:HA    | 1:A:419:SER:HB3   | 1.65                     | 0.76              |
| 3:C:151:ILE:CD1   | 3:C:198:LEU:HD12  | 2.16                     | 0.76              |
| 20:V:463:MET:HE3  | 20:V:464:ILE:N    | 2.00                     | 0.76              |
| 1:A:73:ALA:HB1    | 1:A:74:PRO:HD2    | 1.68                     | 0.76              |
| 24:Z:96:HIS:CE1   | 24:Z:98:GLY:HA3   | 2.20                     | 0.76              |
| 24:Z:259:VAL:HG13 | 27:c:291:LEU:HD13 | 1.66                     | 0.76              |
| 25:a:76:LEU:O     | 25:a:79:ILE:HG22  | 1.85                     | 0.76              |
| 28:d:170:LEU:O    | 28:d:174:ILE:HG22 | 1.85                     | 0.76              |
| 30:f:266:LEU:HD21 | 30:f:270:LEU:HD21 | 1.68                     | 0.76              |
| 30:f:603:SER:HB2  | 30:f:639:LYS:HZ2  | 1.49                     | 0.76              |
| 4:D:56:VAL:HG23   | 32:U:600:ARG:NE   | 2.00                     | 0.76              |
| 20:V:497:PRO:HG2  | 20:V:498:PRO:HD3  | 1.66                     | 0.76              |
| 22:X:151:SER:HB3  | 22:X:155:ARG:HH21 | 1.49                     | 0.76              |
| 30:f:543:MET:HE2  | 30:f:543:MET:O    | 1.86                     | 0.76              |
| 32:U:11:LEU:HD12  | 32:U:11:LEU:O     | 1.85                     | 0.76              |
| 5:E:84:ARG:HD2    | 27:c:50:PRO:HG3   | 1.68                     | 0.76              |
| 24:Z:213:GLU:OE1  | 25:a:350:LYS:NZ   | 2.13                     | 0.76              |
| 30:f:656:GLY:HA2  | 30:f:660:ILE:HD13 | 1.68                     | 0.76              |
| 31:F:279:ALA:HB1  | 31:F:280:PRO:HD2  | 1.66                     | 0.76              |
| 32:U:708:GLN:O    | 32:U:711:GLN:HG2  | 1.85                     | 0.76              |
| 3:C:75:GLU:OE1    | 3:C:111:ASN:HA    | 1.85                     | 0.76              |
| 32:U:481:LEU:HD11 | 32:U:493:VAL:CG1  | 2.16                     | 0.76              |
| 32:U:800:VAL:HG22 | 32:U:880:ASN:ND2  | 2.00                     | 0.76              |
| 3:C:248:MET:CE    | 3:C:273:MET:HG3   | 2.07                     | 0.76              |
| 4:D:279:THR:HG1   | 5:E:248:SER:HG    | 1.29                     | 0.76              |
| 22:X:415:TYR:CE2  | 23:Y:382:LYS:HE3  | 2.21                     | 0.76              |
| 3:C:242:ALA:HB1   | 3:C:243:PRO:HD2   | 1.67                     | 0.76              |
| 4:D:122:GLU:OE1   | 4:D:122:GLU:HA    | 1.86                     | 0.76              |
| 20:V:428:LEU:CD2  | 20:V:437:ILE:HD11 | 2.12                     | 0.76              |
| 25:a:168:ASN:ND2  | 25:a:171:SER:OG   | 2.19                     | 0.76              |
| 27:c:130:GLN:HE21 | 27:c:142:ALA:HB2  | 1.51                     | 0.76              |
| 28:d:29:VAL:O     | 28:d:33:LEU:N     | 2.15                     | 0.76              |
| 32:U:481:LEU:HD11 | 32:U:493:VAL:HG11 | 1.66                     | 0.76              |
| 1:A:322:ASN:C     | 1:A:322:ASN:HD22  | 1.92                     | 0.75              |
| 21:W:102:ALA:HB2  | 21:W:139:GLU:HB3  | 1.66                     | 0.75              |
| 32:U:548:LEU:O    | 32:U:552:ILE:HG22 | 1.85                     | 0.75              |
| 5:E:341:ALA:O     | 5:E:345:ASN:N     | 2.17                     | 0.75              |
| 30:f:125:ILE:HG21 | 30:f:129:LEU:CB   | 2.16                     | 0.75              |
| 32:U:583:MET:HE2  | 32:U:602:LEU:HD12 | 1.67                     | 0.75              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:D:335:LEU:HD13  | 4:D:371:SER:HB3   | 1.66                     | 0.75              |
| 21:W:186:ILE:CD1  | 21:W:208:LYS:HG2  | 2.16                     | 0.75              |
| 23:Y:371:LYS:NZ   | 23:Y:372:LYS:HE2  | 2.01                     | 0.75              |
| 27:c:31:VAL:HG23  | 27:c:203:ILE:HG21 | 1.68                     | 0.75              |
| 28:d:188:LYS:HA   | 28:d:222:TYR:O    | 1.85                     | 0.75              |
| 32:U:627:PHE:CE2  | 32:U:749:GLN:HG3  | 2.20                     | 0.75              |
| 1:A:136:GLU:N     | 1:A:136:GLU:OE2   | 2.20                     | 0.75              |
| 2:B:119:ASN:OD1   | 2:B:120:HIS:ND1   | 2.18                     | 0.75              |
| 3:C:128:PRO:HD3   | 4:D:96:VAL:HG23   | 1.68                     | 0.75              |
| 20:V:259:LEU:HG   | 20:V:291:TYR:CD1  | 2.22                     | 0.75              |
| 20:V:323:GLY:HA2  | 29:e:24:ALA:HA    | 1.68                     | 0.75              |
| 26:b:129:LYS:HG2  | 26:b:133:LYS:NZ   | 2.00                     | 0.75              |
| 30:f:267:ARG:HA   | 30:f:271:MET:HE1  | 1.69                     | 0.75              |
| 32:U:472:ILE:HD12 | 32:U:473:VAL:HG13 | 1.68                     | 0.75              |
| 30:f:160:ARG:NH2  | 30:f:190:GLU:OE2  | 2.19                     | 0.75              |
| 23:Y:336:ARG:NH2  | 29:e:49:GLU:OE2   | 2.18                     | 0.75              |
| 30:f:182:GLU:HG3  | 30:f:183:PRO:HD3  | 1.67                     | 0.75              |
| 30:f:209:MET:CG   | 30:f:212:GLU:HB2  | 2.17                     | 0.75              |
| 30:f:638:ASP:O    | 30:f:640:LYS:HG2  | 1.87                     | 0.75              |
| 4:D:91:GLN:HE21   | 4:D:127:ASN:HB2   | 1.52                     | 0.75              |
| 20:V:371:ASN:HB2  | 20:V:427:GLN:HE21 | 1.50                     | 0.75              |
| 22:X:285:GLU:HA   | 22:X:288:LYS:HB2  | 1.67                     | 0.75              |
| 1:A:425:ALA:HB2   | 2:B:339:PRO:O     | 1.87                     | 0.75              |
| 4:D:403:TYR:CE2   | 4:D:407:ILE:HG12  | 2.22                     | 0.75              |
| 20:V:486:ILE:HD11 | 24:Z:268:SER:HB2  | 1.68                     | 0.75              |
| 25:a:93:ALA:O     | 25:a:97:LEU:N     | 2.15                     | 0.75              |
| 25:a:301:LYS:C    | 25:a:302:ILE:HD12 | 2.12                     | 0.75              |
| 26:b:9:CYS:O      | 26:b:112:PHE:HB2  | 1.85                     | 0.75              |
| 32:U:236:LEU:HB3  | 32:U:245:ALA:HB2  | 1.69                     | 0.75              |
| 2:B:223:ILE:CG2   | 2:B:350:LYS:HG2   | 2.17                     | 0.75              |
| 30:f:126:ILE:HD11 | 30:f:178:LYS:HD3  | 1.68                     | 0.75              |
| 30:f:177:GLU:HG2  | 30:f:835:GLU:HB2  | 1.68                     | 0.75              |
| 30:f:554:TYR:HB3  | 30:f:557:TRP:CH2  | 2.22                     | 0.75              |
| 3:C:19:GLY:HA3    | 32:U:146:LYS:CE   | 2.17                     | 0.74              |
| 26:b:83:LYS:HD2   | 26:b:84:ILE:H     | 1.50                     | 0.74              |
| 27:c:219:ASN:O    | 27:c:220:LEU:HD23 | 1.87                     | 0.74              |
| 32:U:352:ILE:HG21 | 32:U:376:MET:HE1  | 1.69                     | 0.74              |
| 2:B:59:ARG:HB2    | 30:f:184:LEU:HD22 | 1.69                     | 0.74              |
| 21:W:131:VAL:CG1  | 21:W:144:ARG:HD2  | 2.16                     | 0.74              |
| 21:W:201:ARG:O    | 21:W:205:ILE:HG22 | 1.86                     | 0.74              |
| 22:X:226:LYS:O    | 22:X:226:LYS:NZ   | 2.16                     | 0.74              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 23:Y:61:LEU:HG    | 23:Y:63:TRP:HD1   | 1.50                     | 0.74              |
| 2:B:365:PHE:HE2   | 2:B:395:ILE:HD12  | 1.51                     | 0.74              |
| 22:X:194:ARG:HD2  | 22:X:210:LEU:HD21 | 1.69                     | 0.74              |
| 3:C:194:THR:HG21  | 3:C:317:PHE:HB3   | 1.69                     | 0.74              |
| 21:W:177:MET:HE1  | 21:W:181:GLU:OE1  | 1.86                     | 0.74              |
| 25:a:174:LYS:HG3  | 25:a:178:ARG:HH22 | 1.50                     | 0.74              |
| 2:B:182:GLU:OE1   | 2:B:182:GLU:N     | 2.20                     | 0.74              |
| 5:E:138:LEU:HD21  | 5:E:301:ILE:HG23  | 1.69                     | 0.74              |
| 5:E:226:GLN:HB3   | 5:E:227:PRO:HD2   | 1.69                     | 0.74              |
| 21:W:130:MET:HE3  | 21:W:131:VAL:N    | 2.00                     | 0.74              |
| 25:a:148:VAL:HG13 | 25:a:149:THR:H    | 1.53                     | 0.74              |
| 25:a:163:TYR:HA   | 25:a:166:ILE:HG22 | 1.70                     | 0.74              |
| 27:c:128:ASN:HA   | 27:c:131:GLN:OE1  | 1.87                     | 0.74              |
| 30:f:744:MET:CE   | 30:f:745:LEU:HD23 | 2.16                     | 0.74              |
| 32:U:685:GLN:HB2  | 32:U:725:MET:HE1  | 1.70                     | 0.74              |
| 1:A:82:ALA:HB3    | 1:A:85:GLN:HG2    | 1.69                     | 0.74              |
| 1:A:278:ASP:OD2   | 1:A:321:THR:OG1   | 2.04                     | 0.74              |
| 22:X:281:GLY:O    | 22:X:284:THR:HG22 | 1.87                     | 0.74              |
| 24:Z:172:VAL:HG13 | 27:c:217:LEU:CD2  | 2.13                     | 0.74              |
| 1:A:143:ASP:OD1   | 1:A:144:ARG:N     | 2.21                     | 0.74              |
| 5:E:198:VAL:HG22  | 5:E:200:SER:H     | 1.52                     | 0.74              |
| 22:X:137:TYR:HD2  | 22:X:146:ALA:HA   | 1.52                     | 0.74              |
| 22:X:418:ALA:O    | 22:X:422:THR:HG22 | 1.88                     | 0.74              |
| 31:F:276:LYS:HB2  | 31:F:276:LYS:NZ   | 2.02                     | 0.74              |
| 32:U:172:ASP:C    | 32:U:174:PRO:HD3  | 2.13                     | 0.74              |
| 32:U:408:LEU:O    | 32:U:411:ILE:HG22 | 1.86                     | 0.74              |
| 32:U:627:PHE:HE2  | 32:U:749:GLN:HG3  | 1.53                     | 0.74              |
| 1:A:119:ALA:HB3   | 1:A:121:PHE:CE2   | 2.22                     | 0.74              |
| 4:D:322:LEU:HD22  | 4:D:330:LYS:HE3   | 1.68                     | 0.74              |
| 20:V:306:ARG:HD3  | 20:V:336:GLU:HG3  | 1.69                     | 0.74              |
| 21:W:178:GLU:OE1  | 21:W:178:GLU:HA   | 1.87                     | 0.74              |
| 31:F:198:LEU:HD12 | 31:F:223:VAL:HG11 | 1.70                     | 0.74              |
| 32:U:625:ILE:HG22 | 32:U:626:LEU:HD23 | 1.67                     | 0.74              |
| 2:B:407:LEU:HD11  | 3:C:174:LEU:HD22  | 1.70                     | 0.74              |
| 21:W:198:ASP:OD1  | 21:W:201:ARG:HB2  | 1.87                     | 0.74              |
| 18:s:83:MET:HE1   | 18:s:91:MET:HE2   | 1.70                     | 0.74              |
| 32:U:202:VAL:HG12 | 32:U:219:CYS:SG   | 2.27                     | 0.74              |
| 32:U:685:GLN:CB   | 32:U:725:MET:HE1  | 2.17                     | 0.74              |
| 1:A:400:ARG:CZ    | 1:A:400:ARG:HA    | 2.18                     | 0.74              |
| 2:B:209:GLU:HA    | 2:B:212:GLU:HB2   | 1.68                     | 0.74              |
| 20:V:443:ARG:CG   | 28:d:184:LYS:HZ1  | 2.00                     | 0.74              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 23:Y:245:GLU:OE1  | 23:Y:245:GLU:N    | 2.21                     | 0.74              |
| 30:f:86:THR:O     | 30:f:89:MET:HE3   | 1.88                     | 0.74              |
| 32:U:115:ASN:HD21 | 32:U:123:LYS:HD3  | 1.53                     | 0.74              |
| 32:U:808:PRO:HD3  | 32:U:873:PRO:O    | 1.88                     | 0.74              |
| 1:A:394:MET:HG3   | 2:B:199:GLU:OE1   | 1.88                     | 0.73              |
| 4:D:364:VAL:HG23  | 4:D:364:VAL:O     | 1.88                     | 0.73              |
| 21:W:75:TYR:HB2   | 21:W:111:TYR:CE2  | 2.22                     | 0.73              |
| 22:X:239:TYR:CE1  | 22:X:246:LYS:HB2  | 2.23                     | 0.73              |
| 26:b:110:ILE:HG22 | 26:b:139:ASP:HB3  | 1.70                     | 0.73              |
| 31:F:143:GLU:OE1  | 31:F:143:GLU:N    | 2.20                     | 0.73              |
| 32:U:479:LEU:HD21 | 32:U:511:ALA:HA   | 1.70                     | 0.73              |
| 3:C:273:MET:O     | 3:C:277:LEU:N     | 2.20                     | 0.73              |
| 21:W:373:ILE:CD1  | 25:a:326:GLU:HG3  | 2.18                     | 0.73              |
| 27:c:31:VAL:HG22  | 27:c:67:VAL:CG1   | 2.18                     | 0.73              |
| 14:o:195:LYS:NZ   | 14:o:196:LYS:O    | 2.21                     | 0.73              |
| 31:F:175:MET:HG3  | 31:F:249:LEU:HD22 | 1.68                     | 0.73              |
| 32:U:213:PHE:HA   | 32:U:216:VAL:HG12 | 1.69                     | 0.73              |
| 2:B:365:PHE:CE2   | 2:B:395:ILE:HD12  | 2.23                     | 0.73              |
| 7:H:64:VAL:O      | 7:H:219:ARG:NH1   | 2.21                     | 0.73              |
| 20:V:175:MET:HE1  | 20:V:183:GLU:HB2  | 1.67                     | 0.73              |
| 20:V:365:GLN:NE2  | 29:e:46:ASP:O     | 2.20                     | 0.73              |
| 20:V:404:LYS:HD2  | 20:V:446:VAL:HG21 | 1.70                     | 0.73              |
| 21:W:169:LEU:O    | 21:W:173:THR:OG1  | 2.05                     | 0.73              |
| 23:Y:214:MET:HG3  | 23:Y:214:MET:O    | 1.87                     | 0.73              |
| 28:d:103:LEU:HD12 | 28:d:133:ILE:HD11 | 1.68                     | 0.73              |
| 30:f:192:VAL:HB   | 30:f:193:PRO:HD3  | 1.70                     | 0.73              |
| 32:U:803:LYS:O    | 32:U:893:THR:N    | 2.19                     | 0.73              |
| 2:B:56:THR:OG1    | 30:f:181:ARG:NH2  | 2.22                     | 0.73              |
| 2:B:387:LYS:NZ    | 2:B:427:LEU:HB2   | 2.04                     | 0.73              |
| 20:V:449:ALA:HB2  | 20:V:461:LYS:N    | 2.03                     | 0.73              |
| 27:c:163:ILE:O    | 27:c:163:ILE:HD12 | 1.88                     | 0.73              |
| 27:c:292:MET:HE1  | 28:d:253:LEU:HD13 | 1.69                     | 0.73              |
| 2:B:278:ALA:HB1   | 2:B:279:PRO:CD    | 2.15                     | 0.73              |
| 4:D:123:LEU:HB3   | 4:D:142:VAL:HG11  | 1.71                     | 0.73              |
| 5:E:118:LEU:HD13  | 5:E:214:LEU:HD11  | 1.69                     | 0.73              |
| 20:V:477:HIS:ND1  | 28:d:249:TYR:OH   | 2.20                     | 0.73              |
| 21:W:60:MET:CE    | 21:W:99:GLN:HB2   | 2.15                     | 0.73              |
| 23:Y:180:LEU:HD12 | 23:Y:180:LEU:O    | 1.89                     | 0.73              |
| 25:a:134:THR:O    | 25:a:138:VAL:HG23 | 1.89                     | 0.73              |
| 30:f:658:ALA:HA   | 30:f:662:MET:HE1  | 1.69                     | 0.73              |
| 6:g:158:GLY:O     | 7:h:83:ARG:NH2    | 2.22                     | 0.73              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:205:GLY:C     | 1:A:206:ILE:HD12  | 2.13                     | 0.73              |
| 3:C:151:ILE:HD12  | 3:C:198:LEU:HD12  | 1.70                     | 0.73              |
| 4:D:120:ASP:HB3   | 4:D:123:LEU:CD2   | 2.18                     | 0.73              |
| 8:I:34:CYS:SG     | 8:I:75:SER:OG     | 2.46                     | 0.73              |
| 21:W:140:ILE:HG13 | 21:W:140:ILE:O    | 1.87                     | 0.73              |
| 25:a:59:LEU:HD23  | 25:a:60:TYR:H     | 1.51                     | 0.73              |
| 32:U:792:ASN:N    | 32:U:796:LYS:O    | 2.20                     | 0.73              |
| 4:D:339:ARG:HH21  | 4:D:342:ARG:HG2   | 1.52                     | 0.73              |
| 20:V:349:ARG:HA   | 20:V:354:LYS:HE2  | 1.71                     | 0.73              |
| 23:Y:85:ASP:OD1   | 23:Y:107:LYS:NZ   | 2.21                     | 0.73              |
| 29:e:48:VAL:O     | 29:e:48:VAL:HG13  | 1.88                     | 0.73              |
| 31:F:289:ASP:OD1  | 31:F:332:THR:HG23 | 1.88                     | 0.73              |
| 1:A:262:GLU:O     | 1:A:266:THR:HG23  | 1.88                     | 0.73              |
| 2:B:109:VAL:HG11  | 3:C:94:LYS:HD3    | 1.69                     | 0.73              |
| 2:B:281:ILE:HD12  | 2:B:326:LYS:HB2   | 1.71                     | 0.73              |
| 8:I:67:LYS:O      | 8:I:91:ARG:NH1    | 2.21                     | 0.73              |
| 21:W:140:ILE:HD12 | 21:W:143:ALA:HB3  | 1.69                     | 0.73              |
| 21:W:158:ASP:H    | 21:W:161:GLU:HG3  | 1.54                     | 0.73              |
| 27:c:289:ASP:O    | 27:c:293:THR:HG23 | 1.88                     | 0.73              |
| 32:U:681:ASN:OD1  | 32:U:682:TYR:N    | 2.21                     | 0.73              |
| 2:B:127:VAL:HG23  | 2:B:128:GLY:H     | 1.53                     | 0.73              |
| 20:V:361:PHE:O    | 20:V:364:THR:HG22 | 1.88                     | 0.73              |
| 22:X:289:CYS:SG   | 22:X:305:ALA:HB1  | 2.28                     | 0.73              |
| 32:U:198:LEU:HB3  | 32:U:223:LEU:HD21 | 1.69                     | 0.73              |
| 22:X:297:ARG:HH21 | 22:X:337:ARG:HG3  | 1.53                     | 0.73              |
| 23:Y:247:LEU:HD12 | 23:Y:248:GLU:N    | 2.03                     | 0.73              |
| 28:d:36:LEU:HG    | 28:d:37:PRO:CD    | 2.15                     | 0.73              |
| 30:f:826:GLN:CB   | 30:f:846:VAL:HA   | 2.19                     | 0.73              |
| 21:W:308:LEU:HD22 | 21:W:315:MET:HE1  | 1.70                     | 0.72              |
| 22:X:256:LEU:HD13 | 22:X:319:ILE:HD12 | 1.70                     | 0.72              |
| 23:Y:189:VAL:CG1  | 23:Y:287:LEU:HD21 | 2.19                     | 0.72              |
| 25:a:229:ASP:OD1  | 25:a:230:ARG:N    | 2.21                     | 0.72              |
| 30:f:457:ASN:ND2  | 30:f:459:CYS:SG   | 2.62                     | 0.72              |
| 30:f:784:ASP:HA   | 30:f:787:LEU:HD21 | 1.70                     | 0.72              |
| 30:f:825:MET:N    | 30:f:825:MET:HE3  | 2.04                     | 0.72              |
| 10:k:108:THR:OG1  | 10:k:111:SER:OG   | 2.06                     | 0.72              |
| 4:D:392:TYR:C     | 4:D:393:ILE:HD13  | 2.15                     | 0.72              |
| 20:V:227:VAL:HG22 | 20:V:231:LEU:CD2  | 2.19                     | 0.72              |
| 20:V:329:HIS:O    | 20:V:333:ILE:HG23 | 1.88                     | 0.72              |
| 21:W:217:GLU:N    | 21:W:217:GLU:OE1  | 2.21                     | 0.72              |
| 21:W:251:TYR:C    | 21:W:254:PRO:HD2  | 2.13                     | 0.72              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 27:c:50:PRO:HG2   | 27:c:51:MET:SD    | 2.30                     | 0.72              |
| 30:f:221:ILE:HG23 | 30:f:768:LEU:HD21 | 1.71                     | 0.72              |
| 22:X:253:TYR:CZ   | 22:X:318:ILE:HD11 | 2.24                     | 0.72              |
| 23:Y:147:ILE:HD12 | 23:Y:148:GLY:N    | 2.02                     | 0.72              |
| 26:b:138:VAL:HG12 | 26:b:160:LEU:CD1  | 2.19                     | 0.72              |
| 28:d:95:MET:HE3   | 28:d:95:MET:CA    | 2.19                     | 0.72              |
| 30:f:445:LEU:HD21 | 30:f:481:SER:HA   | 1.71                     | 0.72              |
| 30:f:788:MET:N    | 30:f:788:MET:SD   | 2.63                     | 0.72              |
| 3:C:333:SER:OG    | 3:C:338:LEU:HD11  | 1.89                     | 0.72              |
| 23:Y:26:LEU:CD2   | 23:Y:59:LYS:HD2   | 2.19                     | 0.72              |
| 4:D:267:ILE:HG12  | 4:D:309:MET:HE1   | 1.69                     | 0.72              |
| 5:E:63:GLN:HG3    | 5:E:69:PHE:CE2    | 2.25                     | 0.72              |
| 22:X:218:HIS:HE1  | 22:X:231:TYR:CE2  | 2.07                     | 0.72              |
| 26:b:113:VAL:HG12 | 26:b:141:ILE:O    | 1.90                     | 0.72              |
| 28:d:155:LYS:HE2  | 28:d:167:ILE:HG23 | 1.70                     | 0.72              |
| 32:U:195:ASN:OD1  | 32:U:196:LYS:N    | 2.22                     | 0.72              |
| 32:U:206:MET:HE2  | 32:U:206:MET:HA   | 1.70                     | 0.72              |
| 20:V:236:ARG:HA   | 32:U:70:HIS:CE1   | 2.22                     | 0.72              |
| 21:W:68:VAL:CG2   | 21:W:72:LYS:HE3   | 2.20                     | 0.72              |
| 30:f:79:ARG:HB3   | 30:f:82:ILE:CG2   | 2.19                     | 0.72              |
| 32:U:351:MET:HE2  | 32:U:351:MET:N    | 2.05                     | 0.72              |
| 3:C:24:TYR:CD1    | 4:D:40:LEU:HB3    | 2.24                     | 0.72              |
| 20:V:289:LEU:CB   | 20:V:312:ALA:HB2  | 2.17                     | 0.72              |
| 22:X:218:HIS:HE1  | 22:X:231:TYR:HE2  | 1.36                     | 0.72              |
| 22:X:282:ARG:HD3  | 22:X:312:GLU:OE2  | 1.89                     | 0.72              |
| 23:Y:27:SER:HA    | 23:Y:59:LYS:CE    | 2.18                     | 0.72              |
| 24:Z:40:LEU:HD11  | 24:Z:54:PHE:CD1   | 2.24                     | 0.72              |
| 25:a:37:LEU:HA    | 25:a:40:GLN:NE2   | 2.05                     | 0.72              |
| 30:f:267:ARG:HG3  | 30:f:271:MET:SD   | 2.30                     | 0.72              |
| 30:f:712:LYS:HZ3  | 30:f:750:GLN:HA   | 1.54                     | 0.72              |
| 32:U:247:GLN:CG   | 32:U:913:ILE:HD13 | 2.20                     | 0.72              |
| 22:X:338:VAL:HG13 | 22:X:339:ILE:HD13 | 1.71                     | 0.72              |
| 27:c:210:ASN:OD1  | 27:c:213:GLU:HB2  | 1.88                     | 0.72              |
| 27:c:219:ASN:C    | 27:c:220:LEU:HD23 | 2.15                     | 0.72              |
| 29:e:54:ASN:OD1   | 29:e:57:ARG:NH2   | 2.23                     | 0.72              |
| 30:f:370:MET:HA   | 30:f:370:MET:CE   | 2.14                     | 0.72              |
| 30:f:455:VAL:O    | 30:f:456:ARG:HG3  | 1.88                     | 0.72              |
| 31:F:287:GLU:HA   | 31:F:287:GLU:OE2  | 1.87                     | 0.72              |
| 1:A:285:PHE:CZ    | 1:A:287:ASP:HB3   | 2.24                     | 0.72              |
| 3:C:173:GLU:HA    | 3:C:176:GLU:CG    | 2.18                     | 0.72              |
| 4:D:52:GLU:HG3    | 32:U:596:ASN:OD1  | 1.90                     | 0.72              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 21:W:133:GLU:C    | 21:W:136:ILE:HD13 | 2.14                     | 0.72              |
| 21:W:371:THR:HG22 | 21:W:372:ARG:HG2  | 1.70                     | 0.72              |
| 30:f:477:MET:CE   | 30:f:478:ARG:HB3  | 2.20                     | 0.72              |
| 30:f:482:ILE:HB   | 30:f:518:THR:CG2  | 2.19                     | 0.72              |
| 10:k:18:GLU:OE1   | 10:k:18:GLU:N     | 2.22                     | 0.72              |
| 32:U:247:GLN:NE2  | 32:U:904:LYS:HB2  | 2.05                     | 0.72              |
| 1:A:166:VAL:CG2   | 1:A:237:PHE:HB3   | 2.20                     | 0.72              |
| 1:A:300:LEU:O     | 1:A:303:ILE:HG22  | 1.90                     | 0.72              |
| 2:B:278:ALA:CB    | 2:B:279:PRO:HD2   | 2.17                     | 0.72              |
| 5:E:384:LEU:HD12  | 5:E:386:TYR:HE1   | 1.54                     | 0.72              |
| 21:W:79:GLU:HB3   | 21:W:82:LEU:HB2   | 1.72                     | 0.72              |
| 23:Y:145:LEU:HD22 | 23:Y:160:ASN:ND2  | 2.05                     | 0.72              |
| 25:a:97:LEU:HD13  | 25:a:118:ILE:CD1  | 2.19                     | 0.72              |
| 26:b:8:VAL:HA     | 26:b:110:ILE:CD1  | 2.20                     | 0.72              |
| 27:c:33:ILE:O     | 27:c:69:VAL:HG22  | 1.89                     | 0.72              |
| 30:f:790:GLN:HA   | 30:f:796:LEU:HD22 | 1.71                     | 0.72              |
| 32:U:139:GLN:OE1  | 32:U:139:GLN:HA   | 1.89                     | 0.72              |
| 32:U:360:VAL:HA   | 32:U:365:CYS:SG   | 2.30                     | 0.72              |
| 32:U:626:LEU:HD13 | 32:U:632:GLN:HE22 | 1.55                     | 0.72              |
| 21:W:201:ARG:HD2  | 21:W:204:ILE:HD11 | 1.72                     | 0.71              |
| 30:f:729:MET:HA   | 30:f:729:MET:CE   | 2.15                     | 0.71              |
| 1:A:268:LYS:CG    | 30:f:354:GLU:HG2  | 2.17                     | 0.71              |
| 20:V:192:MET:HE1  | 20:V:211:TYR:CD1  | 2.25                     | 0.71              |
| 20:V:470:ARG:O    | 20:V:470:ARG:HG2  | 1.90                     | 0.71              |
| 24:Z:38:VAL:HG21  | 24:Z:75:LEU:HD11  | 1.71                     | 0.71              |
| 26:b:53:THR:HG22  | 26:b:55:ALA:H     | 1.54                     | 0.71              |
| 28:d:125:LYS:HB3  | 28:d:130:ASN:CB   | 2.20                     | 0.71              |
| 31:F:134:LEU:HD13 | 31:F:159:LEU:HA   | 1.71                     | 0.71              |
| 32:U:325:MET:SD   | 32:U:325:MET:N    | 2.63                     | 0.71              |
| 32:U:400:ALA:HA   | 32:U:403:THR:OG1  | 1.90                     | 0.71              |
| 32:U:458:ILE:HD13 | 32:U:490:ARG:NH1  | 2.04                     | 0.71              |
| 2:B:287:ILE:HG22  | 2:B:331:THR:HB    | 1.72                     | 0.71              |
| 3:C:392:GLN:CD    | 22:X:199:ALA:HB2  | 2.15                     | 0.71              |
| 20:V:114:TYR:HE1  | 20:V:137:GLU:HG2  | 1.56                     | 0.71              |
| 20:V:309:MET:HE1  | 20:V:331:LEU:HB3  | 1.71                     | 0.71              |
| 26:b:29:GLN:HA    | 26:b:29:GLN:HE21  | 1.55                     | 0.71              |
| 28:d:235:THR:HA   | 28:d:238:PRO:HG2  | 1.71                     | 0.71              |
| 32:U:360:VAL:HG11 | 32:U:392:TRP:HE1  | 1.55                     | 0.71              |
| 32:U:723:ASP:OD1  | 32:U:726:ALA:N    | 2.23                     | 0.71              |
| 1:A:213:LEU:HD12  | 1:A:337:LEU:HD21  | 1.71                     | 0.71              |
| 22:X:339:ILE:HD11 | 22:X:350:ILE:HD11 | 1.70                     | 0.71              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 23:Y:183:TYR:HE1  | 23:Y:213:LEU:HD21 | 1.55                     | 0.71              |
| 24:Z:249:PHE:HE1  | 27:c:302:ALA:HB1  | 1.55                     | 0.71              |
| 27:c:29:GLU:OE1   | 27:c:29:GLU:N     | 2.23                     | 0.71              |
| 32:U:16:GLU:O     | 32:U:20:LYS:HG3   | 1.89                     | 0.71              |
| 32:U:804:SER:HB3  | 32:U:876:GLN:HB2  | 1.72                     | 0.71              |
| 2:B:311:GLU:HA    | 2:B:311:GLU:OE2   | 1.90                     | 0.71              |
| 3:C:24:TYR:HD1    | 4:D:40:LEU:HB3    | 1.54                     | 0.71              |
| 20:V:231:LEU:HD12 | 20:V:250:LEU:HD22 | 1.72                     | 0.71              |
| 24:Z:164:ALA:HB2  | 27:c:221:HIS:CE1  | 2.25                     | 0.71              |
| 25:a:94:LEU:HG    | 25:a:121:LEU:CD2  | 2.21                     | 0.71              |
| 26:b:1:MET:O      | 26:b:2:VAL:HG12   | 1.89                     | 0.71              |
| 30:f:499:THR:HA   | 30:f:502:LEU:HD12 | 1.72                     | 0.71              |
| 32:U:446:LEU:HD23 | 32:U:457:ILE:HG23 | 1.70                     | 0.71              |
| 3:C:20:LEU:HD21   | 32:U:137:MET:SD   | 2.31                     | 0.71              |
| 26:b:15:TYR:HB2   | 26:b:115:SER:OG   | 1.91                     | 0.71              |
| 26:b:41:THR:HA    | 26:b:47:ASN:ND2   | 2.04                     | 0.71              |
| 30:f:103:TYR:CE1  | 30:f:106:LEU:HD23 | 2.26                     | 0.71              |
| 30:f:479:LEU:O    | 30:f:482:ILE:HG12 | 1.89                     | 0.71              |
| 30:f:498:LEU:HA   | 30:f:501:LEU:HD21 | 1.73                     | 0.71              |
| 1:A:284:ARG:HG3   | 1:A:296:GLN:NE2   | 2.05                     | 0.71              |
| 4:D:153:MET:HE1   | 5:E:267:PHE:CE2   | 2.26                     | 0.71              |
| 5:E:365:GLU:HA    | 5:E:365:GLU:OE1   | 1.89                     | 0.71              |
| 21:W:124:LEU:HD21 | 21:W:147:LYS:HD3  | 1.71                     | 0.71              |
| 21:W:367:ALA:HA   | 21:W:415:PHE:CD2  | 2.24                     | 0.71              |
| 30:f:259:PHE:HA   | 30:f:262:PHE:CZ   | 2.26                     | 0.71              |
| 1:A:196:LEU:HD11  | 30:f:345:PRO:CD   | 2.20                     | 0.71              |
| 1:A:257:VAL:HG11  | 1:A:301:GLU:HB3   | 1.73                     | 0.71              |
| 3:C:219:LEU:HD22  | 4:D:289:LEU:HD23  | 1.73                     | 0.71              |
| 4:D:115:ILE:HG22  | 4:D:139:LEU:HD12  | 1.72                     | 0.71              |
| 4:D:191:TYR:HD1   | 4:D:198:PRO:HG3   | 1.55                     | 0.71              |
| 21:W:75:TYR:HB2   | 21:W:111:TYR:HE2  | 1.56                     | 0.71              |
| 30:f:3:GLU:OE1    | 30:f:3:GLU:N      | 2.24                     | 0.71              |
| 30:f:165:GLU:HA   | 30:f:168:LYS:HE2  | 1.73                     | 0.71              |
| 2:B:56:THR:HG1    | 30:f:181:ARG:HH21 | 1.38                     | 0.71              |
| 27:c:292:MET:HE2  | 28:d:253:LEU:HD22 | 1.73                     | 0.71              |
| 28:d:231:LYS:CG   | 28:d:232:PRO:HD3  | 2.17                     | 0.71              |
| 32:U:84:ALA:HB3   | 32:U:88:PHE:HB2   | 1.72                     | 0.71              |
| 32:U:583:MET:CE   | 32:U:602:LEU:HD12 | 2.19                     | 0.71              |
| 3:C:336:MET:HE1   | 3:C:367:GLY:CA    | 2.20                     | 0.71              |
| 4:D:59:GLU:OE1    | 4:D:59:GLU:HA     | 1.88                     | 0.71              |
| 5:E:197:LYS:HD2   | 5:E:198:VAL:N     | 2.06                     | 0.71              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:G:165:ALA:HB1   | 6:G:179:LEU:HD13  | 1.71                     | 0.71              |
| 13:N:27:ILE:O     | 19:T:179:ARG:NH1  | 2.24                     | 0.71              |
| 23:Y:352:GLU:OE1  | 23:Y:352:GLU:HA   | 1.89                     | 0.71              |
| 26:b:33:VAL:HG12  | 26:b:112:PHE:HE2  | 1.56                     | 0.71              |
| 28:d:26:LEU:HD23  | 28:d:26:LEU:H     | 1.56                     | 0.71              |
| 32:U:320:ASP:HB3  | 32:U:323:LEU:HD13 | 1.72                     | 0.71              |
| 3:C:115:ALA:O     | 3:C:116:LEU:HD13  | 1.91                     | 0.70              |
| 20:V:375:PHE:O    | 20:V:378:VAL:HG12 | 1.91                     | 0.70              |
| 20:V:452:ASN:OD1  | 20:V:455:LYS:HB2  | 1.91                     | 0.70              |
| 25:a:42:LEU:O     | 25:a:45:VAL:HG22  | 1.91                     | 0.70              |
| 27:c:25:VAL:CG2   | 27:c:175:ARG:HA   | 2.20                     | 0.70              |
| 28:d:1:MET:HG3    | 28:d:2:TYR:HD1    | 1.56                     | 0.70              |
| 31:F:81:LYS:HA    | 31:F:84:LYS:HD3   | 1.71                     | 0.70              |
| 3:C:90:HIS:CG     | 3:C:91:PRO:HD2    | 2.26                     | 0.70              |
| 12:M:170:GLN:O    | 12:M:174:THR:HG23 | 1.90                     | 0.70              |
| 22:X:233:TYR:HA   | 22:X:254:MET:CE   | 2.19                     | 0.70              |
| 23:Y:233:ARG:HH12 | 23:Y:264:TYR:HA   | 1.54                     | 0.70              |
| 26:b:128:ALA:HB1  | 26:b:160:LEU:HD21 | 1.71                     | 0.70              |
| 30:f:731:MET:HE2  | 30:f:735:GLY:HA3  | 1.71                     | 0.70              |
| 32:U:351:MET:HA   | 32:U:354:LYS:HB2  | 1.72                     | 0.70              |
| 1:A:82:ALA:O      | 1:A:85:GLN:HG3    | 1.91                     | 0.70              |
| 21:W:78:LYS:HE2   | 21:W:78:LYS:HA    | 1.73                     | 0.70              |
| 24:Z:191:ILE:HG22 | 25:a:375:LEU:HD23 | 1.71                     | 0.70              |
| 30:f:660:ILE:HA   | 30:f:669:GLU:OE1  | 1.91                     | 0.70              |
| 31:F:383:GLU:OE2  | 31:F:417:HIS:NE2  | 2.24                     | 0.70              |
| 32:U:567:ILE:CD1  | 32:U:586:VAL:HG23 | 2.21                     | 0.70              |
| 5:E:65:THR:CG2    | 5:E:68:LYS:HB2    | 2.22                     | 0.70              |
| 21:W:373:ILE:HD13 | 25:a:326:GLU:HG3  | 1.73                     | 0.70              |
| 22:X:338:VAL:CG2  | 22:X:353:LEU:HD13 | 2.22                     | 0.70              |
| 19:t:38:ASN:OD1   | 19:t:186:ARG:NH2  | 2.25                     | 0.70              |
| 31:F:247:THR:OG1  | 31:F:281:SER:HB3  | 1.91                     | 0.70              |
| 5:E:277:MET:HE3   | 5:E:295:LEU:HD11  | 1.72                     | 0.70              |
| 6:G:158:GLY:O     | 7:H:83:ARG:NH2    | 2.25                     | 0.70              |
| 20:V:161:PRO:HB3  | 20:V:198:GLN:OE1  | 1.91                     | 0.70              |
| 20:V:313:LEU:HD11 | 20:V:329:HIS:CE1  | 2.26                     | 0.70              |
| 22:X:342:PHE:CE1  | 22:X:345:VAL:HG11 | 2.26                     | 0.70              |
| 22:X:397:TYR:OH   | 24:Z:258:VAL:HG21 | 1.91                     | 0.70              |
| 24:Z:101:LEU:HD12 | 24:Z:138:TYR:CE2  | 2.27                     | 0.70              |
| 24:Z:193:ASN:HB2  | 27:c:228:GLY:CA   | 2.21                     | 0.70              |
| 25:a:149:THR:HA   | 25:a:152:HIS:ND1  | 2.06                     | 0.70              |
| 28:d:184:LYS:HB2  | 28:d:186:TYR:CE1  | 2.27                     | 0.70              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 30:f:557:TRP:HA   | 30:f:560:LEU:CD1  | 2.21                     | 0.70              |
| 32:U:251:ASP:OD1  | 32:U:252:LEU:N    | 2.24                     | 0.70              |
| 1:A:189:GLU:HB2   | 31:F:405:MET:HE1  | 1.73                     | 0.70              |
| 1:A:430:MET:HE2   | 9:J:12:PRO:HB3    | 1.74                     | 0.70              |
| 3:C:28:ILE:HD11   | 4:D:43:ARG:HG2    | 1.74                     | 0.70              |
| 10:K:20:ARG:NH2   | 31:F:435:LEU:HA   | 2.07                     | 0.70              |
| 21:W:27:ARG:HG2   | 21:W:50:LEU:HD11  | 1.73                     | 0.70              |
| 21:W:158:ASP:N    | 21:W:161:GLU:HG3  | 2.06                     | 0.70              |
| 22:X:292:GLN:OE1  | 22:X:292:GLN:HA   | 1.90                     | 0.70              |
| 25:a:18:GLN:HG3   | 25:a:22:TRP:HE1   | 1.56                     | 0.70              |
| 25:a:269:LEU:O    | 25:a:273:GLN:HB2  | 1.91                     | 0.70              |
| 27:c:151:VAL:HG23 | 27:c:152:LYS:N    | 2.06                     | 0.70              |
| 27:c:152:LYS:HE2  | 27:c:152:LYS:HA   | 1.72                     | 0.70              |
| 27:c:196:LEU:HG   | 27:c:197:ASN:OD1  | 1.91                     | 0.70              |
| 27:c:282:ARG:HG2  | 27:c:282:ARG:HH11 | 1.56                     | 0.70              |
| 28:d:99:LEU:HD23  | 28:d:122:LEU:HD11 | 1.72                     | 0.70              |
| 30:f:243:PRO:O    | 30:f:246:SER:OG   | 2.09                     | 0.70              |
| 30:f:475:ASN:OD1  | 30:f:514:VAL:HG21 | 1.92                     | 0.70              |
| 30:f:680:ARG:HB2  | 30:f:715:HIS:HA   | 1.74                     | 0.70              |
| 32:U:147:TYR:CZ   | 32:U:169:GLU:HB2  | 2.25                     | 0.70              |
| 1:A:81:ALA:CB     | 2:B:137:SER:HB2   | 2.21                     | 0.70              |
| 1:A:140:VAL:HG12  | 1:A:152:PRO:HA    | 1.73                     | 0.70              |
| 5:E:341:ALA:CB    | 31:F:345:SER:HB2  | 2.21                     | 0.70              |
| 23:Y:123:ALA:O    | 23:Y:127:THR:HG23 | 1.91                     | 0.70              |
| 25:a:18:GLN:O     | 25:a:21:VAL:HG22  | 1.91                     | 0.70              |
| 25:a:79:ILE:HG23  | 25:a:80:ILE:HD12  | 1.74                     | 0.70              |
| 25:a:126:GLY:HA3  | 25:a:130:VAL:CG2  | 2.20                     | 0.70              |
| 26:b:110:ILE:HD12 | 26:b:110:ILE:O    | 1.92                     | 0.70              |
| 32:U:49:TYR:O     | 32:U:57:ARG:HG3   | 1.92                     | 0.70              |
| 2:B:103:ARG:HG2   | 2:B:160:ILE:HG21  | 1.72                     | 0.70              |
| 3:C:277:LEU:HD13  | 3:C:310:ARG:HG3   | 1.72                     | 0.70              |
| 23:Y:51:ALA:HB3   | 23:Y:115:GLY:HA3  | 1.71                     | 0.70              |
| 25:a:173:TYR:CE2  | 25:a:216:LEU:HD12 | 2.27                     | 0.70              |
| 26:b:129:LYS:O    | 26:b:133:LYS:HG2  | 1.91                     | 0.70              |
| 30:f:696:LEU:CD2  | 30:f:708:ASP:HB2  | 2.22                     | 0.70              |
| 31:F:169:ASP:OD2  | 31:F:171:ARG:NH2  | 2.19                     | 0.70              |
| 32:U:9:ILE:CG2    | 32:U:27:LEU:HD21  | 2.22                     | 0.70              |
| 4:D:152:MET:SD    | 4:D:152:MET:N     | 2.63                     | 0.70              |
| 17:R:2:THR:N      | 17:R:131:SER:HG   | 1.90                     | 0.70              |
| 28:d:212:LYS:NZ   | 28:d:213:ARG:HG2  | 2.07                     | 0.70              |
| 8:i:44:LEU:HD22   | 8:i:190:LEU:HD23  | 1.74                     | 0.70              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 32:U:137:MET:HE1  | 32:U:140:ARG:NE   | 2.07                     | 0.70              |
| 1:A:99:THR:HG22   | 1:A:140:VAL:O     | 1.91                     | 0.70              |
| 2:B:179:ALA:HB1   | 2:B:182:GLU:OE2   | 1.91                     | 0.70              |
| 5:E:150:GLU:O     | 5:E:154:THR:HG22  | 1.91                     | 0.70              |
| 20:V:71:THR:O     | 20:V:75:ILE:HD12  | 1.91                     | 0.70              |
| 21:W:326:MET:HE3  | 21:W:331:GLY:HA3  | 1.74                     | 0.70              |
| 28:d:193:GLU:O    | 28:d:197:ILE:HG23 | 1.91                     | 0.70              |
| 32:U:423:MET:HE2  | 32:U:423:MET:N    | 2.06                     | 0.70              |
| 3:C:287:LYS:C     | 3:C:288:ASN:HD22  | 1.99                     | 0.69              |
| 21:W:229:LEU:HD22 | 21:W:229:LEU:H    | 1.56                     | 0.69              |
| 21:W:447:ALA:O    | 21:W:451:MET:HG2  | 1.92                     | 0.69              |
| 23:Y:70:LEU:HG    | 23:Y:74:LYS:HZ3   | 1.54                     | 0.69              |
| 25:a:186:LYS:HD2  | 25:a:221:VAL:HG13 | 1.74                     | 0.69              |
| 26:b:23:PRO:O     | 26:b:24:THR:OG1   | 2.11                     | 0.69              |
| 26:b:51:LEU:C     | 26:b:52:ILE:HD12  | 2.17                     | 0.69              |
| 26:b:132:LYS:HB3  | 26:b:160:LEU:HD22 | 1.73                     | 0.69              |
| 27:c:143:VAL:HG22 | 27:c:159:ALA:HB2  | 1.73                     | 0.69              |
| 28:d:75:MET:HG2   | 28:d:102:ASN:HB2  | 1.74                     | 0.69              |
| 30:f:369:ARG:O    | 30:f:369:ARG:NH1  | 2.19                     | 0.69              |
| 4:D:87:LEU:HB2    | 5:E:80:VAL:HG12   | 1.71                     | 0.69              |
| 8:I:48:GLU:OE2    | 8:I:50:ARG:NH1    | 2.24                     | 0.69              |
| 20:V:355:ARG:NE   | 20:V:355:ARG:HA   | 2.06                     | 0.69              |
| 20:V:359:PRO:HA   | 20:V:382:PHE:CD2  | 2.28                     | 0.69              |
| 21:W:60:MET:HA    | 21:W:97:LEU:HD23  | 1.73                     | 0.69              |
| 27:c:88:ASP:OD1   | 27:c:90:VAL:HG12  | 1.91                     | 0.69              |
| 8:i:161:ALA:HB1   | 8:i:175:LEU:HD13  | 1.75                     | 0.69              |
| 5:E:330:ALA:CA    | 5:E:333:LYS:HE2   | 2.22                     | 0.69              |
| 20:V:410:ILE:CD1  | 20:V:422:ILE:HD13 | 2.22                     | 0.69              |
| 22:X:308:ASP:OD1  | 22:X:309:TYR:N    | 2.25                     | 0.69              |
| 24:Z:23:PHE:HD2   | 24:Z:126:VAL:HG11 | 1.57                     | 0.69              |
| 1:A:108:ASP:CB    | 1:A:109:PRO:HD3   | 2.22                     | 0.69              |
| 18:S:136:LYS:NZ   | 17:r:28:ALA:O     | 2.24                     | 0.69              |
| 20:V:255:LEU:O    | 20:V:259:LEU:HD23 | 1.92                     | 0.69              |
| 20:V:300:LEU:HD11 | 28:d:116:HIS:ND1  | 2.07                     | 0.69              |
| 21:W:257:GLN:O    | 21:W:262:LYS:NZ   | 2.22                     | 0.69              |
| 30:f:500:LEU:O    | 30:f:503:PRO:HD2  | 1.93                     | 0.69              |
| 32:U:236:LEU:HD13 | 32:U:244:MET:HG2  | 1.74                     | 0.69              |
| 1:A:139:ARG:HB2   | 1:A:153:LEU:O     | 1.92                     | 0.69              |
| 1:A:205:GLY:O     | 31:F:373:MET:HB3  | 1.93                     | 0.69              |
| 1:A:209:PRO:HG2   | 1:A:339:ARG:NH2   | 2.08                     | 0.69              |
| 4:D:374:ASP:OD1   | 4:D:374:ASP:N     | 2.24                     | 0.69              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:E:342:ASP:HB2   | 5:E:374:VAL:HG11  | 1.74                     | 0.69              |
| 20:V:332:LEU:O    | 20:V:335:VAL:HG12 | 1.93                     | 0.69              |
| 23:Y:67:VAL:O     | 23:Y:70:LEU:HD23  | 1.92                     | 0.69              |
| 23:Y:202:LEU:HB3  | 23:Y:239:LYS:HZ1  | 1.58                     | 0.69              |
| 27:c:167:MET:HE2  | 27:c:172:HIS:CB   | 2.19                     | 0.69              |
| 30:f:495:GLU:O    | 30:f:499:THR:HG22 | 1.93                     | 0.69              |
| 31:F:370:SER:OG   | 31:F:420:TYR:OH   | 2.09                     | 0.69              |
| 32:U:98:GLU:HA    | 32:U:101:ILE:CG2  | 2.23                     | 0.69              |
| 32:U:234:GLU:HA   | 32:U:237:VAL:HG12 | 1.74                     | 0.69              |
| 1:A:241:ILE:HG21  | 2:B:311:GLU:OE2   | 1.90                     | 0.69              |
| 20:V:296:LYS:HZ3  | 20:V:308:THR:HG21 | 1.58                     | 0.69              |
| 21:W:373:ILE:HA   | 25:a:326:GLU:HG2  | 1.73                     | 0.69              |
| 23:Y:175:ASP:OD2  | 23:Y:179:ARG:NH2  | 2.24                     | 0.69              |
| 24:Z:250:TYR:HA   | 24:Z:253:THR:HG22 | 1.75                     | 0.69              |
| 25:a:84:VAL:O     | 25:a:87:MET:HG3   | 1.93                     | 0.69              |
| 30:f:718:ASP:OD1  | 30:f:755:ASP:HB3  | 1.92                     | 0.69              |
| 30:f:828:ARG:NE   | 30:f:861:THR:HG21 | 2.07                     | 0.69              |
| 16:q:67:TYR:O     | 16:q:71:ASN:ND2   | 2.25                     | 0.69              |
| 32:U:324:LYS:HE2  | 32:U:325:MET:HE1  | 1.74                     | 0.69              |
| 1:A:86:THR:O      | 1:A:90:GLU:N      | 2.26                     | 0.69              |
| 1:A:322:ASN:ND2   | 1:A:322:ASN:C     | 2.48                     | 0.69              |
| 2:B:90:GLU:HB3    | 2:B:94:GLU:H      | 1.56                     | 0.69              |
| 3:C:137:LEU:HD12  | 3:C:220:VAL:HG21  | 1.75                     | 0.69              |
| 3:C:354:ALA:CB    | 3:C:358:GLU:HB2   | 2.22                     | 0.69              |
| 4:D:258:ALA:HB3   | 4:D:259:PRO:HD3   | 1.74                     | 0.69              |
| 23:Y:51:ALA:HB3   | 23:Y:115:GLY:CA   | 2.22                     | 0.69              |
| 30:f:680:ARG:HD3  | 30:f:760:PHE:CE2  | 2.27                     | 0.69              |
| 31:F:172:VAL:O    | 31:F:175:MET:HG2  | 1.93                     | 0.69              |
| 31:F:373:MET:HE2  | 31:F:415:LEU:CD1  | 2.16                     | 0.69              |
| 1:A:209:PRO:HG2   | 1:A:339:ARG:HH21  | 1.57                     | 0.69              |
| 4:D:108:GLY:O     | 4:D:109:SER:OG    | 2.10                     | 0.69              |
| 4:D:214:MET:N     | 33:D:501:ATP:O1A  | 2.26                     | 0.69              |
| 5:E:270:LEU:HD21  | 5:E:273:VAL:CB    | 2.23                     | 0.69              |
| 5:E:382:SER:OG    | 31:F:340:PRO:HG3  | 1.93                     | 0.69              |
| 20:V:195:ILE:HD12 | 20:V:196:SER:N    | 2.08                     | 0.69              |
| 20:V:492:LYS:HE2  | 20:V:492:LYS:CA   | 2.22                     | 0.69              |
| 23:Y:236:LEU:O    | 23:Y:241:ILE:HG13 | 1.93                     | 0.69              |
| 24:Z:190:ARG:HH12 | 27:c:297:VAL:HA   | 1.56                     | 0.69              |
| 27:c:41:MET:HG2   | 27:c:112:TYR:CD2  | 2.27                     | 0.69              |
| 28:d:152:PHE:HE2  | 28:d:198:LEU:HB3  | 1.56                     | 0.69              |
| 30:f:477:MET:HE3  | 30:f:478:ARG:HB3  | 1.75                     | 0.69              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 30:f:494:ARG:HG3  | 30:f:497:VAL:HG22 | 1.75                     | 0.69              |
| 30:f:559:PRO:CB   | 30:f:594:LEU:HD23 | 2.21                     | 0.69              |
| 30:f:689:ALA:O    | 30:f:693:ALA:HB3  | 1.93                     | 0.69              |
| 32:U:204:ILE:HD12 | 32:U:205:TYR:N    | 2.08                     | 0.69              |
| 1:A:262:GLU:HA    | 1:A:265:ARG:HD2   | 1.75                     | 0.69              |
| 5:E:330:ALA:HA    | 5:E:333:LYS:CE    | 2.21                     | 0.69              |
| 20:V:192:MET:HE3  | 20:V:230:PHE:CZ   | 2.27                     | 0.69              |
| 25:a:54:ASP:O     | 25:a:57:ILE:HG22  | 1.93                     | 0.69              |
| 30:f:466:LEU:HD12 | 30:f:481:SER:OG   | 1.93                     | 0.69              |
| 4:D:335:LEU:CD1   | 4:D:371:SER:HB3   | 2.23                     | 0.69              |
| 20:V:399:ARG:O    | 20:V:402:VAL:HG22 | 1.93                     | 0.69              |
| 20:V:407:VAL:HA   | 20:V:410:ILE:HG22 | 1.75                     | 0.69              |
| 20:V:416:ARG:HH12 | 23:Y:350:VAL:CG2  | 2.05                     | 0.69              |
| 27:c:26:ASP:HA    | 27:c:176:GLN:HE21 | 1.57                     | 0.69              |
| 28:d:52:ARG:HH22  | 28:d:89:LEU:HD21  | 1.58                     | 0.69              |
| 28:d:194:ALA:HA   | 28:d:197:ILE:CD1  | 2.23                     | 0.69              |
| 1:A:239:ARG:HG2   | 2:B:319:PHE:CE1   | 2.28                     | 0.68              |
| 4:D:153:MET:HE1   | 5:E:267:PHE:HE2   | 1.56                     | 0.68              |
| 5:E:356:ARG:HH11  | 5:E:356:ARG:HG3   | 1.58                     | 0.68              |
| 20:V:466:ILE:HD12 | 20:V:469:THR:OG1  | 1.92                     | 0.68              |
| 24:Z:164:ALA:HB1  | 24:Z:169:GLU:CG   | 2.22                     | 0.68              |
| 25:a:33:LEU:HD13  | 25:a:36:GLN:HG3   | 1.75                     | 0.68              |
| 25:a:273:GLN:HE21 | 25:a:302:ILE:HD11 | 1.56                     | 0.68              |
| 26:b:135:LYS:H    | 26:b:135:LYS:HD2  | 1.58                     | 0.68              |
| 27:c:49:VAL:HG21  | 27:c:148:ILE:HD11 | 1.75                     | 0.68              |
| 28:d:13:SER:HB3   | 28:d:16:LEU:CB    | 2.23                     | 0.68              |
| 32:U:58:GLN:HG2   | 32:U:87:LEU:HD22  | 1.75                     | 0.68              |
| 32:U:602:LEU:CD2  | 32:U:622:LEU:HG   | 2.23                     | 0.68              |
| 32:U:700:GLU:OE2  | 32:U:707:ASN:ND2  | 2.26                     | 0.68              |
| 1:A:213:LEU:HD21  | 1:A:321:THR:HG22  | 1.75                     | 0.68              |
| 1:A:279:ALA:CB    | 2:B:307:ARG:HG2   | 2.23                     | 0.68              |
| 2:B:74:MET:HE2    | 2:B:74:MET:C      | 2.18                     | 0.68              |
| 3:C:137:LEU:HD23  | 3:C:138:MET:HE3   | 1.75                     | 0.68              |
| 4:D:248:ARG:HG3   | 4:D:295:GLN:NE2   | 2.08                     | 0.68              |
| 5:E:342:ASP:HA    | 5:E:345:ASN:CB    | 2.23                     | 0.68              |
| 21:W:35:ALA:HB2   | 21:W:43:VAL:HG21  | 1.74                     | 0.68              |
| 22:X:218:HIS:CE1  | 22:X:231:TYR:CE2  | 2.80                     | 0.68              |
| 23:Y:186:LEU:O    | 23:Y:189:VAL:HG12 | 1.93                     | 0.68              |
| 25:a:113:LEU:HD11 | 25:a:154:ARG:HH12 | 1.56                     | 0.68              |
| 25:a:293:PHE:CD2  | 25:a:329:LYS:HG3  | 2.28                     | 0.68              |
| 28:d:52:ARG:HH22  | 28:d:89:LEU:HD11  | 1.58                     | 0.68              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 32:U:9:ILE:HG22   | 32:U:27:LEU:HD21  | 1.75                     | 0.68              |
| 32:U:583:MET:HA   | 32:U:583:MET:HE3  | 1.75                     | 0.68              |
| 32:U:696:ILE:O    | 32:U:697:GLN:HG2  | 1.93                     | 0.68              |
| 1:A:339:ARG:NH2   | 31:F:402:GLU:OE2  | 2.27                     | 0.68              |
| 2:B:67:ARG:HH21   | 30:f:226:TYR:HD1  | 1.40                     | 0.68              |
| 3:C:368:MET:HB3   | 3:C:372:ARG:HH21  | 1.59                     | 0.68              |
| 20:V:324:PHE:O    | 20:V:328:VAL:HG12 | 1.92                     | 0.68              |
| 20:V:415:SER:HA   | 23:Y:346:LYS:NZ   | 2.07                     | 0.68              |
| 20:V:437:ILE:HG22 | 28:d:146:GLY:H    | 1.58                     | 0.68              |
| 21:W:257:GLN:HB2  | 21:W:262:LYS:NZ   | 2.08                     | 0.68              |
| 24:Z:59:ASP:HB2   | 26:b:99:HIS:NE2   | 2.08                     | 0.68              |
| 27:c:111:TRP:HE1  | 27:c:130:GLN:HG2  | 1.59                     | 0.68              |
| 29:e:42:ASN:HD21  | 29:e:44:ASP:HB2   | 1.59                     | 0.68              |
| 31:F:374:ASN:ND2  | 31:F:413:THR:O    | 2.24                     | 0.68              |
| 5:E:65:THR:HG22   | 5:E:68:LYS:HB2    | 1.75                     | 0.68              |
| 20:V:432:GLU:CD   | 20:V:432:GLU:H    | 2.01                     | 0.68              |
| 22:X:365:LEU:O    | 22:X:369:ILE:HG12 | 1.93                     | 0.68              |
| 23:Y:186:LEU:HD11 | 23:Y:213:LEU:HD13 | 1.75                     | 0.68              |
| 25:a:173:TYR:HE2  | 25:a:216:LEU:HD12 | 1.58                     | 0.68              |
| 30:f:212:GLU:O    | 30:f:216:MET:HE2  | 1.93                     | 0.68              |
| 30:f:294:MET:SD   | 30:f:294:MET:N    | 2.66                     | 0.68              |
| 30:f:617:SER:HA   | 30:f:620:PHE:CE1  | 2.29                     | 0.68              |
| 30:f:826:GLN:HB3  | 30:f:846:VAL:HA   | 1.74                     | 0.68              |
| 31:F:226:TYR:HA   | 31:F:332:THR:O    | 1.93                     | 0.68              |
| 2:B:190:LEU:HD23  | 2:B:193:GLN:NE2   | 2.09                     | 0.68              |
| 2:B:223:ILE:HG21  | 2:B:350:LYS:HG2   | 1.76                     | 0.68              |
| 2:B:290:ILE:HG23  | 2:B:309:MET:HE1   | 1.74                     | 0.68              |
| 2:B:401:GLU:OE1   | 2:B:401:GLU:HA    | 1.92                     | 0.68              |
| 20:V:400:HIS:HD2  | 28:d:145:GLU:HB3  | 1.56                     | 0.68              |
| 21:W:124:LEU:HD21 | 21:W:147:LYS:CD   | 2.23                     | 0.68              |
| 30:f:373:ALA:HB1  | 30:f:747:GLN:HE22 | 1.57                     | 0.68              |
| 32:U:748:LEU:H    | 32:U:748:LEU:HD12 | 1.59                     | 0.68              |
| 32:U:884:VAL:CG1  | 32:U:889:LEU:HA   | 2.23                     | 0.68              |
| 3:C:326:LEU:HD22  | 3:C:345:ARG:HE    | 1.59                     | 0.68              |
| 5:E:309:ARG:NH1   | 5:E:336:ASP:HA    | 2.09                     | 0.68              |
| 21:W:179:LYS:HD2  | 21:W:179:LYS:O    | 1.94                     | 0.68              |
| 23:Y:100:ILE:HD12 | 23:Y:101:ARG:N    | 2.08                     | 0.68              |
| 1:A:82:ALA:O      | 1:A:85:GLN:N      | 2.27                     | 0.68              |
| 1:A:166:VAL:HG21  | 1:A:237:PHE:HB3   | 1.74                     | 0.68              |
| 4:D:153:MET:HE2   | 4:D:229:ARG:HB3   | 1.76                     | 0.68              |
| 21:W:310:THR:O    | 21:W:313:GLU:HG2  | 1.93                     | 0.68              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 31:F:152:GLY:HA3  | 31:F:162:GLU:OE2  | 1.93                     | 0.68              |
| 31:F:382:GLU:OE1  | 31:F:382:GLU:HA   | 1.94                     | 0.68              |
| 32:U:341:PHE:CZ   | 32:U:787:CYS:HB3  | 2.29                     | 0.68              |
| 32:U:357:LYS:HE2  | 32:U:360:VAL:HG21 | 1.74                     | 0.68              |
| 32:U:878:LEU:HB3  | 32:U:882:ALA:HB1  | 1.74                     | 0.68              |
| 2:B:288:ASP:OD2   | 2:B:333:ARG:HG3   | 1.93                     | 0.68              |
| 5:E:136:GLY:O     | 33:E:402:ATP:N6   | 2.26                     | 0.68              |
| 21:W:133:GLU:HA   | 21:W:136:ILE:HG21 | 1.76                     | 0.68              |
| 21:W:335:SER:OG   | 21:W:336:PRO:HD3  | 1.94                     | 0.68              |
| 23:Y:334:LEU:O    | 23:Y:338:ILE:HG12 | 1.94                     | 0.68              |
| 25:a:78:GLU:HA    | 25:a:81:LEU:CD2   | 2.24                     | 0.68              |
| 26:b:123:ASP:OD1  | 26:b:127:LEU:HD23 | 1.94                     | 0.68              |
| 27:c:193:ILE:HG22 | 27:c:194:HIS:HD2  | 1.58                     | 0.68              |
| 28:d:75:MET:CG    | 28:d:102:ASN:HB2  | 2.23                     | 0.68              |
| 32:U:58:GLN:OE1   | 32:U:58:GLN:N     | 2.27                     | 0.68              |
| 32:U:118:LEU:HD21 | 32:U:122:GLU:OE2  | 1.93                     | 0.68              |
| 32:U:227:GLN:O    | 32:U:230:SER:OG   | 2.07                     | 0.68              |
| 32:U:529:ILE:HD11 | 32:U:555:VAL:CG1  | 2.23                     | 0.68              |
| 4:D:100:THR:HG21  | 4:D:112:TYR:CZ    | 2.28                     | 0.68              |
| 4:D:338:ARG:HH22  | 4:D:367:PRO:HA    | 1.59                     | 0.68              |
| 5:E:348:THR:HA    | 31:F:217:ILE:HD12 | 1.74                     | 0.68              |
| 21:W:112:VAL:HG11 | 21:W:147:LYS:HE2  | 1.75                     | 0.68              |
| 22:X:338:VAL:HG23 | 22:X:353:LEU:HD13 | 1.76                     | 0.68              |
| 24:Z:11:VAL:HA    | 24:Z:50:VAL:HG23  | 1.76                     | 0.68              |
| 25:a:240:PHE:CE1  | 25:a:272:ILE:HB   | 2.29                     | 0.68              |
| 26:b:14:GLU:HG3   | 26:b:15:TYR:HD1   | 1.58                     | 0.68              |
| 27:c:54:MET:SD    | 27:c:87:VAL:HG12  | 2.33                     | 0.68              |
| 30:f:692:LEU:HD21 | 30:f:696:LEU:HD11 | 1.76                     | 0.68              |
| 30:f:828:ARG:HD3  | 30:f:844:VAL:H    | 1.59                     | 0.68              |
| 32:U:803:LYS:HA   | 32:U:876:GLN:O    | 1.94                     | 0.68              |
| 2:B:316:LEU:HD22  | 2:B:327:VAL:HG21  | 1.76                     | 0.68              |
| 3:C:231:VAL:HG11  | 3:C:272:THR:HG23  | 1.75                     | 0.68              |
| 20:V:476:PHE:CZ   | 24:Z:258:VAL:HG22 | 2.28                     | 0.68              |
| 23:Y:14:ASN:HB2   | 23:Y:15:PRO:HD3   | 1.73                     | 0.68              |
| 25:a:324:ILE:HD13 | 25:a:331:VAL:HG22 | 1.76                     | 0.68              |
| 13:n:4:ILE:HG13   | 13:n:100:ILE:HD12 | 1.74                     | 0.68              |
| 32:U:680:VAL:HG12 | 32:U:683:VAL:H    | 1.59                     | 0.68              |
| 3:C:49:ARG:HA     | 4:D:65:GLN:HE22   | 1.59                     | 0.67              |
| 23:Y:50:MET:SD    | 23:Y:51:ALA:N     | 2.67                     | 0.67              |
| 25:a:35:HIS:HB3   | 26:b:15:TYR:CE1   | 2.29                     | 0.67              |
| 27:c:236:GLU:HG2  | 27:c:239:LYS:HE3  | 1.75                     | 0.67              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 28:d:71:PHE:HE1   | 28:d:166:PHE:HZ   | 1.41                     | 0.67              |
| 30:f:505:MET:HE1  | 30:f:522:CYS:SG   | 2.34                     | 0.67              |
| 30:f:750:GLN:N    | 30:f:750:GLN:OE1  | 2.27                     | 0.67              |
| 31:F:80:ILE:O     | 31:F:84:LYS:N     | 2.26                     | 0.67              |
| 32:U:418:GLU:HG2  | 32:U:421:GLN:NE2  | 2.09                     | 0.67              |
| 32:U:423:MET:HG3  | 32:U:446:LEU:CD1  | 2.23                     | 0.67              |
| 32:U:496:LEU:O    | 32:U:499:THR:HG22 | 1.94                     | 0.67              |
| 32:U:529:ILE:CD1  | 32:U:555:VAL:HG11 | 2.24                     | 0.67              |
| 32:U:808:PRO:HG3  | 32:U:873:PRO:HD2  | 1.76                     | 0.67              |
| 1:A:85:GLN:O      | 1:A:89:SER:N      | 2.28                     | 0.67              |
| 2:B:388:ASP:OD1   | 2:B:389:ASP:N     | 2.27                     | 0.67              |
| 20:V:430:SER:HB2  | 20:V:432:GLU:OE1  | 1.94                     | 0.67              |
| 21:W:239:SER:OG   | 21:W:242:SER:HB3  | 1.94                     | 0.67              |
| 21:W:406:VAL:HG13 | 22:X:342:PHE:CB   | 2.25                     | 0.67              |
| 26:b:16:MET:SD    | 26:b:25:ARG:HB2   | 2.33                     | 0.67              |
| 26:b:140:ILE:O    | 26:b:170:LEU:HD12 | 1.95                     | 0.67              |
| 27:c:151:VAL:HG23 | 27:c:152:LYS:H    | 1.59                     | 0.67              |
| 30:f:160:ARG:CZ   | 30:f:160:ARG:HA   | 2.25                     | 0.67              |
| 30:f:313:GLU:HB2  | 30:f:316:ASP:OD1  | 1.93                     | 0.67              |
| 1:A:166:VAL:HG22  | 1:A:237:PHE:O     | 1.94                     | 0.67              |
| 1:A:181:LYS:O     | 1:A:181:LYS:HD3   | 1.94                     | 0.67              |
| 2:B:176:VAL:CG2   | 2:B:247:PHE:HB3   | 2.24                     | 0.67              |
| 5:E:345:ASN:HA    | 5:E:348:THR:CG2   | 2.23                     | 0.67              |
| 6:G:92:GLN:NE2    | 13:N:70:GLU:OE2   | 2.27                     | 0.67              |
| 24:Z:199:LYS:NZ   | 25:a:364:GLU:HG2  | 2.09                     | 0.67              |
| 28:d:18:LYS:NZ    | 28:d:21:GLU:OE1   | 2.26                     | 0.67              |
| 32:U:450:HIS:ND1  | 32:U:457:ILE:HG12 | 2.09                     | 0.67              |
| 32:U:888:GLN:O    | 32:U:891:VAL:HG22 | 1.94                     | 0.67              |
| 2:B:133:VAL:HG12  | 2:B:157:HIS:O     | 1.94                     | 0.67              |
| 2:B:260:LEU:CD2   | 2:B:299:SER:HB2   | 2.24                     | 0.67              |
| 4:D:64:GLU:HB3    | 32:U:607:VAL:CG2  | 2.23                     | 0.67              |
| 20:V:273:LYS:NZ   | 32:U:40:GLU:HB3   | 2.09                     | 0.67              |
| 24:Z:170:VAL:HG22 | 27:c:151:VAL:O    | 1.94                     | 0.67              |
| 1:A:139:ARG:NE    | 1:A:154:PRO:O     | 2.25                     | 0.67              |
| 1:A:259:GLU:HA    | 1:A:259:GLU:OE1   | 1.93                     | 0.67              |
| 3:C:23:TYR:CE2    | 32:U:105:ILE:HB   | 2.29                     | 0.67              |
| 3:C:189:TYR:HE2   | 3:C:316:GLU:HG2   | 1.59                     | 0.67              |
| 4:D:181:VAL:O     | 4:D:185:LEU:HD13  | 1.94                     | 0.67              |
| 22:X:283:GLN:OE1  | 22:X:283:GLN:HA   | 1.93                     | 0.67              |
| 25:a:246:GLU:O    | 25:a:250:THR:HG23 | 1.94                     | 0.67              |
| 26:b:48:ASN:HD21  | 26:b:64:LEU:HB3   | 1.56                     | 0.67              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 30:f:466:LEU:HB3  | 30:f:485:LEU:HD21 | 1.76                     | 0.67              |
| 4:D:50:GLU:OE1    | 4:D:50:GLU:HA     | 1.93                     | 0.67              |
| 21:W:207:LYS:HA   | 21:W:210:ASN:OD1  | 1.95                     | 0.67              |
| 22:X:364:LYS:HD2  | 22:X:364:LYS:O    | 1.95                     | 0.67              |
| 23:Y:192:ARG:CZ   | 23:Y:291:HIS:HB3  | 2.24                     | 0.67              |
| 32:U:765:VAL:HG11 | 32:U:778:PHE:CD2  | 2.30                     | 0.67              |
| 1:A:116:LYS:HG2   | 2:B:130:GLU:OE1   | 1.95                     | 0.67              |
| 2:B:70:ASP:O      | 30:f:606:VAL:HG11 | 1.94                     | 0.67              |
| 3:C:146:SER:CA    | 3:C:150:MET:HE3   | 2.18                     | 0.67              |
| 21:W:268:LYS:HB2  | 21:W:336:PRO:HG2  | 1.77                     | 0.67              |
| 30:f:415:GLY:HA3  | 30:f:447:ALA:CB   | 2.23                     | 0.67              |
| 30:f:638:ASP:O    | 30:f:639:LYS:HG3  | 1.94                     | 0.67              |
| 30:f:707:LEU:HD11 | 30:f:785:ARG:HD2  | 1.75                     | 0.67              |
| 32:U:226:PRO:HA   | 32:U:260:PHE:CE1  | 2.27                     | 0.67              |
| 32:U:437:TYR:CE1  | 32:U:472:ILE:HB   | 2.30                     | 0.67              |
| 1:A:239:ARG:O     | 1:A:240:VAL:HG23  | 1.95                     | 0.67              |
| 2:B:116:ILE:HG22  | 2:B:121:ALA:HA    | 1.77                     | 0.67              |
| 21:W:131:VAL:HG21 | 21:W:140:ILE:HG13 | 1.76                     | 0.67              |
| 21:W:186:ILE:HD11 | 21:W:208:LYS:HG2  | 1.77                     | 0.67              |
| 21:W:210:ASN:HA   | 21:W:213:PHE:CE1  | 2.30                     | 0.67              |
| 25:a:185:ILE:HD12 | 25:a:185:ILE:O    | 1.94                     | 0.67              |
| 30:f:789:SER:HA   | 30:f:793:VAL:HB   | 1.77                     | 0.67              |
| 32:U:577:ILE:O    | 32:U:580:ARG:HG2  | 1.95                     | 0.67              |
| 20:V:259:LEU:HG   | 20:V:291:TYR:HD1  | 1.58                     | 0.67              |
| 21:W:267:LEU:HD12 | 21:W:296:LEU:HD21 | 1.76                     | 0.67              |
| 21:W:289:ARG:HH11 | 21:W:289:ARG:HG3  | 1.58                     | 0.67              |
| 26:b:1:MET:HA     | 26:b:44:ASN:HB2   | 1.74                     | 0.67              |
| 32:U:366:HIS:O    | 32:U:369:THR:HG22 | 1.95                     | 0.67              |
| 32:U:657:GLY:O    | 32:U:661:ALA:HB2  | 1.95                     | 0.67              |
| 1:A:262:GLU:O     | 1:A:265:ARG:HG2   | 1.95                     | 0.67              |
| 4:D:336:PRO:HG2   | 4:D:371:SER:O     | 1.95                     | 0.67              |
| 24:Z:11:VAL:HA    | 24:Z:50:VAL:CG2   | 2.25                     | 0.67              |
| 24:Z:81:MET:HE1   | 27:c:94:LYS:HD3   | 1.76                     | 0.67              |
| 24:Z:181:ASP:O    | 24:Z:184:VAL:HG22 | 1.95                     | 0.67              |
| 25:a:233:LEU:O    | 25:a:236:THR:HG22 | 1.95                     | 0.67              |
| 31:F:348:LEU:HD12 | 31:F:348:LEU:O    | 1.95                     | 0.67              |
| 32:U:98:GLU:HA    | 32:U:101:ILE:HG22 | 1.77                     | 0.67              |
| 32:U:164:GLU:O    | 32:U:167:ILE:HG12 | 1.95                     | 0.67              |
| 3:C:381:GLU:CG    | 22:X:191:THR:HG23 | 2.25                     | 0.66              |
| 21:W:31:CYS:HB3   | 21:W:43:VAL:HG13  | 1.77                     | 0.66              |
| 21:W:68:VAL:HG22  | 21:W:72:LYS:HE3   | 1.77                     | 0.66              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 21:W:257:GLN:HB2  | 21:W:262:LYS:HZ1  | 1.59                     | 0.66              |
| 21:W:451:MET:HE3  | 24:Z:100:LYS:O    | 1.94                     | 0.66              |
| 23:Y:16:ASP:OD1   | 23:Y:18:ARG:N     | 2.29                     | 0.66              |
| 23:Y:138:LEU:HA   | 23:Y:141:VAL:HG12 | 1.76                     | 0.66              |
| 23:Y:190:ALA:O    | 23:Y:291:HIS:NE2  | 2.28                     | 0.66              |
| 28:d:229:GLN:C    | 28:d:232:PRO:HD2  | 2.20                     | 0.66              |
| 30:f:91:SER:HA    | 30:f:94:LYS:HE2   | 1.78                     | 0.66              |
| 30:f:143:ARG:HH12 | 30:f:189:LYS:HA   | 1.60                     | 0.66              |
| 30:f:557:TRP:HA   | 30:f:560:LEU:HG   | 1.76                     | 0.66              |
| 30:f:637:LYS:HG2  | 30:f:677:HIS:CD2  | 2.30                     | 0.66              |
| 32:U:266:GLN:N    | 32:U:266:GLN:OE1  | 2.28                     | 0.66              |
| 1:A:169:LYS:NZ    | 1:A:231:ASN:O     | 2.17                     | 0.66              |
| 9:J:104:VAL:HG21  | 9:J:143:ARG:HB2   | 1.77                     | 0.66              |
| 21:W:136:ILE:HA   | 21:W:140:ILE:HG23 | 1.78                     | 0.66              |
| 21:W:214:PHE:HA   | 21:W:216:GLU:OE2  | 1.95                     | 0.66              |
| 24:Z:249:PHE:O    | 24:Z:253:THR:HG22 | 1.95                     | 0.66              |
| 25:a:48:PRO:HB2   | 25:a:51:ALA:HA    | 1.78                     | 0.66              |
| 25:a:87:MET:HE1   | 25:a:89:ASP:OD1   | 1.95                     | 0.66              |
| 25:a:252:LYS:HB2  | 25:a:255:TRP:CZ3  | 2.31                     | 0.66              |
| 26:b:85:THR:HG23  | 26:b:85:THR:O     | 1.95                     | 0.66              |
| 27:c:55:GLY:C     | 27:c:56:LEU:HD23  | 2.20                     | 0.66              |
| 28:d:144:MET:HE2  | 28:d:144:MET:CA   | 2.23                     | 0.66              |
| 30:f:216:MET:HA   | 30:f:219:LYS:CE   | 2.25                     | 0.66              |
| 30:f:301:HIS:NE2  | 30:f:305:LEU:HD23 | 2.10                     | 0.66              |
| 30:f:369:ARG:NH2  | 30:f:744:MET:HB3  | 2.10                     | 0.66              |
| 32:U:377:HIS:O    | 32:U:411:ILE:HA   | 1.94                     | 0.66              |
| 1:A:82:ALA:HB3    | 1:A:85:GLN:CG     | 2.24                     | 0.66              |
| 2:B:337:LEU:HD21  | 2:B:342:ILE:HD11  | 1.76                     | 0.66              |
| 3:C:161:ILE:HG21  | 3:C:199:LEU:HD11  | 1.77                     | 0.66              |
| 3:C:360:LYS:HA    | 3:C:363:CYS:SG    | 2.35                     | 0.66              |
| 21:W:401:THR:HG22 | 21:W:402:ILE:HD13 | 1.75                     | 0.66              |
| 22:X:122:ARG:HG3  | 22:X:125:LEU:HB3  | 1.77                     | 0.66              |
| 25:a:57:ILE:CD1   | 25:a:60:TYR:HB3   | 2.24                     | 0.66              |
| 25:a:311:VAL:HG21 | 25:a:324:ILE:HD11 | 1.77                     | 0.66              |
| 28:d:53:ASP:HA    | 28:d:56:GLU:OE2   | 1.95                     | 0.66              |
| 30:f:690:VAL:O    | 30:f:694:LEU:HD22 | 1.95                     | 0.66              |
| 32:U:234:GLU:O    | 32:U:237:VAL:HG12 | 1.95                     | 0.66              |
| 32:U:609:ASP:OD2  | 32:U:614:VAL:HG11 | 1.94                     | 0.66              |
| 20:V:442:ILE:HB   | 28:d:184:LYS:HE3  | 1.75                     | 0.66              |
| 21:W:169:LEU:O    | 21:W:169:LEU:HD12 | 1.96                     | 0.66              |
| 21:W:330:LYS:HG2  | 21:W:331:GLY:H    | 1.60                     | 0.66              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 25:a:219:HIS:CE1  | 25:a:221:VAL:HB   | 2.31                     | 0.66              |
| 30:f:274:ASP:HB3  | 30:f:275:MET:CE   | 2.25                     | 0.66              |
| 32:U:60:ALA:O     | 32:U:64:ALA:N     | 2.24                     | 0.66              |
| 32:U:516:LEU:CG   | 32:U:532:MET:HE2  | 2.25                     | 0.66              |
| 32:U:541:HIS:HB2  | 32:U:544:ILE:HD13 | 1.78                     | 0.66              |
| 4:D:91:GLN:NE2    | 4:D:127:ASN:HB2   | 2.10                     | 0.66              |
| 8:I:165:GLY:O     | 8:I:168:SER:OG    | 2.14                     | 0.66              |
| 26:b:51:LEU:CD2   | 26:b:62:THR:HB    | 2.24                     | 0.66              |
| 26:b:181:ASP:OD1  | 26:b:183:LEU:N    | 2.29                     | 0.66              |
| 28:d:103:LEU:CD1  | 28:d:133:ILE:HD11 | 2.25                     | 0.66              |
| 31:F:209:LYS:O    | 31:F:213:GLU:HG3  | 1.95                     | 0.66              |
| 3:C:332:HIS:CD2   | 3:C:360:LYS:HB2   | 2.31                     | 0.66              |
| 22:X:167:VAL:CG1  | 22:X:206:LEU:HD13 | 2.25                     | 0.66              |
| 22:X:351:SER:HA   | 22:X:354:ILE:HG22 | 1.78                     | 0.66              |
| 28:d:50:LEU:H     | 28:d:50:LEU:HD22  | 1.60                     | 0.66              |
| 30:f:65:GLU:HB3   | 30:f:97:LYS:HE2   | 1.77                     | 0.66              |
| 32:U:490:ARG:HD3  | 32:U:492:ASP:HB3  | 1.77                     | 0.66              |
| 32:U:536:ALA:HB2  | 32:U:548:LEU:HD12 | 1.77                     | 0.66              |
| 2:B:389:ASP:OD1   | 2:B:389:ASP:O     | 2.14                     | 0.66              |
| 5:E:210:GLU:HG2   | 5:E:213:ARG:HH21  | 1.61                     | 0.66              |
| 12:M:39:ILE:HD12  | 12:M:193:VAL:HG22 | 1.77                     | 0.66              |
| 31:F:384:LEU:HD11 | 31:F:420:TYR:CB   | 2.25                     | 0.66              |
| 32:U:349:ASP:HB2  | 32:U:352:ILE:HB   | 1.78                     | 0.66              |
| 2:B:361:LYS:CD    | 2:B:390:LEU:HD11  | 2.15                     | 0.66              |
| 3:C:388:ALA:HA    | 3:C:392:GLN:HB3   | 1.77                     | 0.66              |
| 5:E:242:ARG:HA    | 5:E:254:GLN:NE2   | 2.11                     | 0.66              |
| 20:V:168:GLN:HB2  | 20:V:191:LEU:HD23 | 1.77                     | 0.66              |
| 20:V:247:GLN:NE2  | 20:V:277:PRO:HG3  | 2.11                     | 0.66              |
| 21:W:169:LEU:HD13 | 21:W:172:GLU:HB2  | 1.77                     | 0.66              |
| 21:W:216:GLU:HA   | 21:W:219:THR:OG1  | 1.95                     | 0.66              |
| 27:c:30:GLN:HA    | 27:c:204:THR:HG23 | 1.78                     | 0.66              |
| 28:d:36:LEU:HD23  | 28:d:38:THR:N     | 2.11                     | 0.66              |
| 30:f:679:LEU:HD21 | 30:f:681:TYR:CE2  | 2.31                     | 0.66              |
| 4:D:138:ALA:O     | 4:D:140:VAL:HG23  | 1.96                     | 0.66              |
| 24:Z:249:PHE:CE1  | 27:c:302:ALA:HB1  | 2.31                     | 0.66              |
| 26:b:128:ALA:HB1  | 26:b:160:LEU:CD2  | 2.26                     | 0.66              |
| 27:c:167:MET:O    | 27:c:171:GLY:N    | 2.29                     | 0.66              |
| 27:c:258:ALA:HA   | 27:c:261:GLU:OE2  | 1.95                     | 0.66              |
| 30:f:420:TRP:H    | 30:f:451:VAL:HG23 | 1.61                     | 0.66              |
| 31:F:272:PHE:CD2  | 31:F:316:GLN:HG2  | 2.31                     | 0.66              |
| 31:F:392:ASN:OD1  | 31:F:395:GLN:NE2  | 2.26                     | 0.66              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 32:U:177:LEU:HD11 | 32:U:204:ILE:HD13 | 1.78                     | 0.66              |
| 32:U:198:LEU:HD23 | 32:U:223:LEU:CD2  | 2.26                     | 0.66              |
| 32:U:249:CYS:SG   | 32:U:329:LEU:HD13 | 2.35                     | 0.66              |
| 1:A:250:VAL:HG13  | 1:A:294:GLU:OE1   | 1.96                     | 0.66              |
| 20:V:234:ARG:HB3  | 20:V:250:LEU:HD11 | 1.78                     | 0.66              |
| 22:X:372:LYS:O    | 22:X:372:LYS:HG2  | 1.94                     | 0.66              |
| 22:X:395:LYS:O    | 22:X:396:THR:HG22 | 1.95                     | 0.66              |
| 24:Z:135:THR:HG22 | 24:Z:160:SER:OG   | 1.96                     | 0.66              |
| 24:Z:199:LYS:HE2  | 24:Z:199:LYS:HA   | 1.77                     | 0.66              |
| 25:a:186:LYS:HG2  | 25:a:193:GLN:NE2  | 2.09                     | 0.66              |
| 25:a:278:MET:SD   | 25:a:319:LEU:HG   | 2.36                     | 0.66              |
| 27:c:60:GLU:N     | 27:c:60:GLU:OE2   | 2.28                     | 0.66              |
| 28:d:181:CYS:O    | 28:d:184:LYS:HG3  | 1.96                     | 0.66              |
| 32:U:261:LEU:O    | 32:U:264:VAL:HG12 | 1.95                     | 0.66              |
| 32:U:353:LEU:HD12 | 32:U:385:PHE:CD2  | 2.30                     | 0.66              |
| 32:U:719:ASP:OD1  | 32:U:721:HIS:N    | 2.29                     | 0.66              |
| 4:D:249:ASP:OD1   | 4:D:250:VAL:N     | 2.29                     | 0.65              |
| 23:Y:239:LYS:HZ3  | 23:Y:239:LYS:HB3  | 1.61                     | 0.65              |
| 10:k:231:LYS:NZ   | 10:k:235:GLU:OE2  | 2.29                     | 0.65              |
| 31:F:169:ASP:O    | 31:F:172:VAL:HG12 | 1.95                     | 0.65              |
| 32:U:247:GLN:CB   | 32:U:913:ILE:HD13 | 2.26                     | 0.65              |
| 2:B:378:VAL:HA    | 2:B:416:ASN:OD1   | 1.96                     | 0.65              |
| 3:C:40:GLN:HA     | 3:C:43:ARG:NH2    | 2.11                     | 0.65              |
| 25:a:36:GLN:O     | 25:a:40:GLN:NE2   | 2.29                     | 0.65              |
| 28:d:70:SER:HA    | 28:d:73:ARG:HH21  | 1.59                     | 0.65              |
| 30:f:106:LEU:O    | 30:f:109:ILE:HG22 | 1.96                     | 0.65              |
| 32:U:568:GLU:OE1  | 32:U:572:ARG:NH2  | 2.21                     | 0.65              |
| 32:U:798:PRO:HG2  | 32:U:880:ASN:HD21 | 1.60                     | 0.65              |
| 1:A:361:SER:CB    | 30:f:849:ALA:HB3  | 2.26                     | 0.65              |
| 2:B:59:ARG:O      | 2:B:63:LEU:HD22   | 1.96                     | 0.65              |
| 3:C:24:TYR:HE2    | 32:U:153:ILE:HD11 | 1.62                     | 0.65              |
| 21:W:455:LEU:O    | 21:W:456:GLN:HG2  | 1.96                     | 0.65              |
| 23:Y:61:LEU:HG    | 23:Y:63:TRP:CD1   | 2.30                     | 0.65              |
| 24:Z:190:ARG:HH22 | 27:c:297:VAL:HA   | 1.60                     | 0.65              |
| 24:Z:250:TYR:HA   | 24:Z:253:THR:CG2  | 2.26                     | 0.65              |
| 30:f:462:ALA:HB3  | 30:f:489:TYR:CZ   | 2.32                     | 0.65              |
| 32:U:801:GLN:NE2  | 32:U:877:LEU:HA   | 2.11                     | 0.65              |
| 32:U:901:GLN:N    | 32:U:915:LYS:O    | 2.21                     | 0.65              |
| 2:B:58:CYS:HA     | 30:f:184:LEU:HD11 | 1.79                     | 0.65              |
| 4:D:91:GLN:HE22   | 4:D:248:ARG:CD    | 2.09                     | 0.65              |
| 4:D:285:VAL:HG21  | 5:E:255:ARG:NH2   | 2.10                     | 0.65              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:D:391:ARG:NH2   | 4:D:398:ASP:OD2   | 2.29                     | 0.65              |
| 5:E:226:GLN:CB    | 5:E:227:PRO:HD2   | 2.26                     | 0.65              |
| 11:L:212:ILE:HD12 | 11:L:229:VAL:HG13 | 1.76                     | 0.65              |
| 20:V:428:LEU:HD21 | 20:V:434:ALA:HA   | 1.77                     | 0.65              |
| 23:Y:183:TYR:CE1  | 23:Y:213:LEU:HD21 | 2.31                     | 0.65              |
| 25:a:347:LYS:HD2  | 25:a:347:LYS:C    | 2.20                     | 0.65              |
| 27:c:161:ARG:HD2  | 27:c:201:TYR:OH   | 1.96                     | 0.65              |
| 30:f:548:THR:O    | 30:f:552:ASP:HB2  | 1.97                     | 0.65              |
| 30:f:761:MET:HA   | 30:f:761:MET:HE2  | 1.78                     | 0.65              |
| 32:U:58:GLN:HG2   | 32:U:87:LEU:CD2   | 2.27                     | 0.65              |
| 4:D:201:GLY:HA2   | 4:D:307:VAL:O     | 1.97                     | 0.65              |
| 20:V:428:LEU:HD23 | 20:V:434:ALA:HB2  | 1.79                     | 0.65              |
| 22:X:297:ARG:NH2  | 22:X:337:ARG:HG3  | 2.10                     | 0.65              |
| 24:Z:40:LEU:HD11  | 24:Z:54:PHE:CE1   | 2.30                     | 0.65              |
| 26:b:51:LEU:HD13  | 26:b:75:LEU:CD2   | 2.25                     | 0.65              |
| 28:d:105:PHE:O    | 28:d:108:SER:OG   | 2.14                     | 0.65              |
| 30:f:729:MET:HE1  | 30:f:732:VAL:HB   | 1.78                     | 0.65              |
| 31:F:89:LEU:HD21  | 31:F:126:THR:HB   | 1.78                     | 0.65              |
| 31:F:224:LEU:HD13 | 31:F:348:LEU:CD2  | 2.25                     | 0.65              |
| 32:U:567:ILE:HD12 | 32:U:586:VAL:HG23 | 1.78                     | 0.65              |
| 2:B:103:ARG:HG2   | 2:B:160:ILE:CG2   | 2.25                     | 0.65              |
| 5:E:349:GLU:HG3   | 5:E:373:LYS:HE3   | 1.78                     | 0.65              |
| 17:R:32:VAL:HG11  | 36:R:301:LDZ:H19  | 1.78                     | 0.65              |
| 25:a:112:ILE:HG21 | 25:a:140:GLU:OE2  | 1.96                     | 0.65              |
| 25:a:163:TYR:HA   | 25:a:166:ILE:CG2  | 2.27                     | 0.65              |
| 28:d:148:TYR:HD1  | 28:d:178:ILE:HD11 | 1.61                     | 0.65              |
| 1:A:217:PRO:O     | 1:A:220:THR:OG1   | 2.10                     | 0.65              |
| 2:B:127:VAL:HG23  | 2:B:128:GLY:N     | 2.12                     | 0.65              |
| 5:E:310:LEU:HD12  | 5:E:310:LEU:O     | 1.97                     | 0.65              |
| 20:V:130:PHE:HD2  | 20:V:134:PHE:HE2  | 1.43                     | 0.65              |
| 20:V:471:GLU:HG3  | 20:V:472:PRO:HD3  | 1.77                     | 0.65              |
| 23:Y:101:ARG:NH2  | 23:Y:105:MET:HE2  | 2.12                     | 0.65              |
| 23:Y:243:GLY:O    | 23:Y:247:LEU:HG   | 1.97                     | 0.65              |
| 24:Z:37:GLY:HA3   | 24:Z:95:TYR:CE1   | 2.32                     | 0.65              |
| 24:Z:212:LEU:O    | 24:Z:215:VAL:HG13 | 1.96                     | 0.65              |
| 25:a:321:LYS:HG3  | 25:a:335:TRP:HE3  | 1.61                     | 0.65              |
| 30:f:531:ASN:O    | 30:f:535:THR:HG22 | 1.97                     | 0.65              |
| 30:f:828:ARG:CZ   | 30:f:843:SER:HA   | 2.26                     | 0.65              |
| 31:F:175:MET:HG3  | 31:F:249:LEU:CD2  | 2.26                     | 0.65              |
| 31:F:226:TYR:CD2  | 31:F:335:VAL:HG21 | 2.32                     | 0.65              |
| 32:U:885:MET:N    | 32:U:885:MET:SD   | 2.69                     | 0.65              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:323:ARG:NH2   | 1:A:433:ASN:HA    | 2.10                     | 0.65              |
| 2:B:68:ILE:H      | 2:B:68:ILE:HD12   | 1.62                     | 0.65              |
| 5:E:313:LEU:HD11  | 5:E:331:ILE:CG2   | 2.27                     | 0.65              |
| 21:W:89:LEU:O     | 21:W:93:ARG:HG3   | 1.96                     | 0.65              |
| 30:f:177:GLU:HG2  | 30:f:835:GLU:CB   | 2.25                     | 0.65              |
| 30:f:744:MET:O    | 30:f:748:LEU:HD12 | 1.97                     | 0.65              |
| 4:D:230:VAL:HG22  | 4:D:263:PHE:O     | 1.97                     | 0.65              |
| 21:W:312:MET:HE2  | 21:W:312:MET:HA   | 1.79                     | 0.65              |
| 21:W:409:LEU:O    | 21:W:409:LEU:HD13 | 1.97                     | 0.65              |
| 22:X:93:LEU:O     | 22:X:97:LEU:HD23  | 1.97                     | 0.65              |
| 22:X:344:ARG:HB2  | 22:X:386:ILE:HD13 | 1.78                     | 0.65              |
| 22:X:407:MET:HE2  | 24:Z:266:ILE:HD12 | 1.77                     | 0.65              |
| 23:Y:387:ILE:HG21 | 24:Z:276:ILE:CD1  | 2.27                     | 0.65              |
| 25:a:278:MET:HE2  | 25:a:320:VAL:CG1  | 2.27                     | 0.65              |
| 4:D:322:LEU:HD22  | 4:D:330:LYS:CE    | 2.26                     | 0.65              |
| 20:V:108:LEU:HD22 | 20:V:170:LEU:HD12 | 1.77                     | 0.65              |
| 21:W:452:ILE:HG22 | 21:W:453:HIS:ND1  | 2.12                     | 0.65              |
| 22:X:122:ARG:CG   | 22:X:125:LEU:HB3  | 2.27                     | 0.65              |
| 22:X:243:ASP:OD1  | 22:X:245:PRO:HD2  | 1.97                     | 0.65              |
| 23:Y:239:LYS:HE2  | 23:Y:239:LYS:HA   | 1.79                     | 0.65              |
| 23:Y:366:TYR:HA   | 23:Y:369:THR:HG22 | 1.79                     | 0.65              |
| 25:a:217:LEU:HD21 | 25:a:238:TYR:CD1  | 2.32                     | 0.65              |
| 26:b:40:LYS:HE2   | 26:b:40:LYS:HA    | 1.77                     | 0.65              |
| 27:c:152:LYS:HA   | 27:c:152:LYS:CE   | 2.25                     | 0.65              |
| 30:f:373:ALA:CB   | 30:f:747:GLN:HE22 | 2.10                     | 0.65              |
| 30:f:771:LEU:HD22 | 30:f:807:ARG:HH21 | 1.62                     | 0.65              |
| 27:c:266:THR:HG23 | 27:c:269:GLN:HB3  | 1.77                     | 0.64              |
| 28:d:42:LYS:HA    | 28:d:86:LYS:HZ3   | 1.62                     | 0.64              |
| 30:f:474:SER:HB3  | 30:f:477:MET:CG   | 2.27                     | 0.64              |
| 30:f:746:ARG:HG3  | 30:f:750:GLN:NE2  | 2.11                     | 0.64              |
| 32:U:209:GLU:HB2  | 32:U:210:LYS:HZ3  | 1.62                     | 0.64              |
| 32:U:506:ALA:HA   | 32:U:544:ILE:HD11 | 1.77                     | 0.64              |
| 1:A:349:GLU:O     | 1:A:352:THR:HG22  | 1.97                     | 0.64              |
| 2:B:424:GLU:O     | 2:B:428:TYR:HB3   | 1.97                     | 0.64              |
| 5:E:72:LYS:HB2    | 5:E:78:ARG:HD3    | 1.79                     | 0.64              |
| 5:E:74:THR:O      | 5:E:74:THR:HG23   | 1.96                     | 0.64              |
| 5:E:198:VAL:CG1   | 5:E:232:MET:HA    | 2.26                     | 0.64              |
| 20:V:82:LEU:O     | 20:V:86:VAL:HG22  | 1.97                     | 0.64              |
| 21:W:112:VAL:HG23 | 21:W:120:ILE:HD11 | 1.79                     | 0.64              |
| 21:W:240:TYR:O    | 21:W:243:ILE:HG12 | 1.97                     | 0.64              |
| 21:W:312:MET:HB3  | 21:W:365:ILE:HD11 | 1.79                     | 0.64              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 25:a:297:ALA:HB1  | 25:a:302:ILE:O    | 1.97                     | 0.64              |
| 28:d:95:MET:HA    | 28:d:95:MET:CE    | 2.25                     | 0.64              |
| 31:F:195:ILE:O    | 31:F:199:VAL:HG22 | 1.97                     | 0.64              |
| 32:U:757:MET:HE3  | 32:U:758:PRO:N    | 2.11                     | 0.64              |
| 32:U:807:LYS:H    | 32:U:807:LYS:CD   | 2.10                     | 0.64              |
| 2:B:202:GLU:O     | 2:B:206:THR:HG23  | 1.98                     | 0.64              |
| 2:B:417:GLU:O     | 2:B:421:LYS:HG2   | 1.98                     | 0.64              |
| 3:C:332:HIS:HD2   | 3:C:360:LYS:HB2   | 1.62                     | 0.64              |
| 5:E:182:LEU:HD22  | 33:E:402:ATP:H2'  | 1.79                     | 0.64              |
| 21:W:102:ALA:O    | 21:W:106:GLN:HG2  | 1.97                     | 0.64              |
| 26:b:127:LEU:O    | 26:b:131:LEU:HG   | 1.97                     | 0.64              |
| 26:b:147:GLU:OE2  | 26:b:150:THR:HA   | 1.97                     | 0.64              |
| 28:d:161:GLU:CD   | 28:d:163:TYR:H    | 2.04                     | 0.64              |
| 30:f:445:LEU:HA   | 30:f:448:CYS:SG   | 2.37                     | 0.64              |
| 8:i:119:GLN:HG3   | 9:j:78:ALA:HB1    | 1.78                     | 0.64              |
| 1:A:213:LEU:HD12  | 1:A:337:LEU:CD2   | 2.27                     | 0.64              |
| 2:B:428:TYR:CD1   | 2:B:429:LYS:HB2   | 2.31                     | 0.64              |
| 4:D:83:GLN:HA     | 4:D:140:VAL:HG11  | 1.79                     | 0.64              |
| 5:E:242:ARG:HD3   | 5:E:254:GLN:HG3   | 1.78                     | 0.64              |
| 20:V:185:GLN:HB2  | 20:V:221:LEU:HD11 | 1.80                     | 0.64              |
| 21:W:287:VAL:HB   | 21:W:309:PHE:CZ   | 2.33                     | 0.64              |
| 23:Y:279:GLU:CD   | 23:Y:296:VAL:HG21 | 2.23                     | 0.64              |
| 23:Y:366:TYR:HA   | 23:Y:369:THR:CG2  | 2.28                     | 0.64              |
| 32:U:901:GLN:HG3  | 32:U:915:LYS:HB3  | 1.80                     | 0.64              |
| 1:A:361:SER:O     | 2:B:215:GLY:HA3   | 1.98                     | 0.64              |
| 2:B:223:ILE:HD12  | 2:B:329:MET:O     | 1.97                     | 0.64              |
| 4:D:219:VAL:O     | 4:D:223:THR:HB    | 1.97                     | 0.64              |
| 5:E:197:LYS:HG2   | 31:F:320:PHE:CD2  | 2.32                     | 0.64              |
| 5:E:352:MET:CE    | 5:E:355:ILE:HG21  | 2.26                     | 0.64              |
| 24:Z:130:ASP:N    | 24:Z:130:ASP:OD1  | 2.31                     | 0.64              |
| 25:a:247:ARG:HH21 | 25:a:251:LEU:HD11 | 1.62                     | 0.64              |
| 26:b:8:VAL:HA     | 26:b:110:ILE:HD12 | 1.80                     | 0.64              |
| 27:c:75:MET:HE1   | 27:c:88:ASP:H     | 1.62                     | 0.64              |
| 31:F:187:ASP:O    | 31:F:368:ILE:HD13 | 1.97                     | 0.64              |
| 32:U:405:THR:CG2  | 32:U:441:GLY:HA3  | 2.28                     | 0.64              |
| 2:B:197:ILE:HD13  | 2:B:222:VAL:HG21  | 1.80                     | 0.64              |
| 3:C:242:ALA:HB1   | 3:C:243:PRO:CD    | 2.27                     | 0.64              |
| 3:C:381:GLU:HG2   | 22:X:191:THR:HG23 | 1.78                     | 0.64              |
| 4:D:42:SER:O      | 4:D:46:LYS:HB2    | 1.97                     | 0.64              |
| 5:E:93:LYS:HB2    | 5:E:93:LYS:NZ     | 2.13                     | 0.64              |
| 15:P:47:ARG:NH1   | 15:P:191:LYS:O    | 2.31                     | 0.64              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 20:V:281:ASN:ND2  | 20:V:284:GLU:OE2  | 2.31                     | 0.64              |
| 22:X:126:ARG:HH11 | 22:X:126:ARG:HG3  | 1.61                     | 0.64              |
| 25:a:35:HIS:CD2   | 26:b:15:TYR:HA    | 2.33                     | 0.64              |
| 30:f:240:VAL:CG1  | 30:f:241:PRO:HD3  | 2.28                     | 0.64              |
| 32:U:807:LYS:HD2  | 32:U:807:LYS:N    | 2.13                     | 0.64              |
| 1:A:264:ALA:HB1   | 1:A:315:ILE:HD12  | 1.80                     | 0.64              |
| 2:B:295:TYR:CZ    | 3:C:271:ARG:HD3   | 2.32                     | 0.64              |
| 4:D:340:GLN:O     | 4:D:344:ILE:HG13  | 1.98                     | 0.64              |
| 25:a:149:THR:CG2  | 25:a:183:VAL:HB   | 2.26                     | 0.64              |
| 28:d:30:LEU:HD12  | 28:d:31:LEU:N     | 2.12                     | 0.64              |
| 28:d:158:ILE:O    | 28:d:158:ILE:HD12 | 1.98                     | 0.64              |
| 30:f:694:LEU:HD23 | 30:f:695:ALA:H    | 1.63                     | 0.64              |
| 6:g:192:GLU:OE1   | 6:g:192:GLU:N     | 2.29                     | 0.64              |
| 31:F:361:ALA:O    | 31:F:365:ILE:HB   | 1.98                     | 0.64              |
| 1:A:264:ALA:HA    | 1:A:267:LYS:CD    | 2.27                     | 0.64              |
| 1:A:387:SER:HA    | 1:A:390:THR:CG2   | 2.27                     | 0.64              |
| 5:E:157:GLU:OE2   | 5:E:158:LEU:HG    | 1.98                     | 0.64              |
| 20:V:150:ARG:NH1  | 20:V:157:THR:O    | 2.30                     | 0.64              |
| 20:V:449:ALA:HB2  | 20:V:461:LYS:H    | 1.62                     | 0.64              |
| 22:X:408:SER:O    | 22:X:411:VAL:HG12 | 1.98                     | 0.64              |
| 25:a:226:ARG:HH12 | 25:a:230:ARG:HG2  | 1.62                     | 0.64              |
| 28:d:205:LYS:HG2  | 28:d:209:TYR:CD2  | 2.31                     | 0.64              |
| 30:f:686:LEU:CD1  | 30:f:687:ARG:HG3  | 2.27                     | 0.64              |
| 1:A:356:LYS:O     | 1:A:360:ARG:HG3   | 1.98                     | 0.64              |
| 10:K:20:ARG:HE    | 31:F:435:LEU:HD23 | 1.61                     | 0.64              |
| 20:V:175:MET:HE1  | 20:V:180:ARG:HB3  | 1.80                     | 0.64              |
| 30:f:828:ARG:NH2  | 30:f:842:VAL:O    | 2.31                     | 0.64              |
| 17:r:161:ILE:O    | 17:r:165:THR:HG23 | 1.98                     | 0.64              |
| 32:U:16:GLU:HG3   | 32:U:19:LEU:HB3   | 1.79                     | 0.64              |
| 32:U:352:ILE:CG2  | 32:U:376:MET:HE1  | 2.28                     | 0.64              |
| 2:B:373:THR:OG1   | 2:B:412:MET:O     | 2.16                     | 0.64              |
| 13:N:2:THR:N      | 13:N:171:SER:HG   | 1.96                     | 0.64              |
| 21:W:75:TYR:OH    | 21:W:114:GLU:OE2  | 2.15                     | 0.64              |
| 21:W:251:TYR:O    | 21:W:254:PRO:HD2  | 1.98                     | 0.64              |
| 21:W:268:LYS:HE3  | 21:W:301:LYS:NZ   | 2.12                     | 0.64              |
| 22:X:258:LYS:HD3  | 22:X:266:ASP:HB2  | 1.79                     | 0.64              |
| 24:Z:38:VAL:HG21  | 24:Z:75:LEU:CD1   | 2.27                     | 0.64              |
| 25:a:291:LEU:H    | 25:a:291:LEU:HD12 | 1.61                     | 0.64              |
| 26:b:93:ALA:O     | 26:b:97:LEU:HD13  | 1.98                     | 0.64              |
| 30:f:8:LYS:HD3    | 30:f:9:ALA:H      | 1.62                     | 0.64              |
| 30:f:266:LEU:O    | 30:f:270:LEU:HG   | 1.97                     | 0.64              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 30:f:281:ILE:HD12 | 30:f:286:LYS:HD3  | 1.79                     | 0.64              |
| 30:f:729:MET:CE   | 30:f:732:VAL:HB   | 2.28                     | 0.64              |
| 30:f:766:GLN:HG3  | 30:f:768:LEU:HD12 | 1.80                     | 0.64              |
| 30:f:813:LYS:HD2  | 30:f:821:LEU:HD11 | 1.79                     | 0.64              |
| 32:U:904:LYS:HE3  | 32:U:908:ILE:HD12 | 1.79                     | 0.64              |
| 1:A:187:LEU:O     | 1:A:191:VAL:HG22  | 1.96                     | 0.63              |
| 1:A:227:ARG:HD3   | 2:B:319:PHE:O     | 1.99                     | 0.63              |
| 4:D:61:ILE:HD13   | 4:D:64:GLU:OE2    | 1.98                     | 0.63              |
| 5:E:86:GLN:OE1    | 5:E:86:GLN:N      | 2.20                     | 0.63              |
| 15:P:48:LEU:HD21  | 15:P:86:LEU:HD22  | 1.79                     | 0.63              |
| 20:V:114:TYR:CE1  | 20:V:137:GLU:HG2  | 2.33                     | 0.63              |
| 20:V:311:ASN:HA   | 20:V:314:ARG:HH11 | 1.63                     | 0.63              |
| 21:W:355:LYS:O    | 21:W:358:VAL:HG12 | 1.98                     | 0.63              |
| 24:Z:247:LYS:NZ   | 24:Z:247:LYS:HB3  | 2.13                     | 0.63              |
| 25:a:324:ILE:HG22 | 25:a:326:GLU:OE2  | 1.98                     | 0.63              |
| 30:f:593:THR:OG1  | 30:f:631:LYS:NZ   | 2.31                     | 0.63              |
| 11:l:74:ILE:HG21  | 11:l:81:ALA:HB1   | 1.80                     | 0.63              |
| 1:A:85:GLN:CA     | 1:A:88:GLN:HB3    | 2.23                     | 0.63              |
| 1:A:263:MET:HG2   | 1:A:267:LYS:NZ    | 2.12                     | 0.63              |
| 1:A:280:ILE:O     | 1:A:280:ILE:HD12  | 1.98                     | 0.63              |
| 4:D:153:MET:HE2   | 4:D:229:ARG:CB    | 2.28                     | 0.63              |
| 17:R:168:ASP:OD2  | 17:R:171:SER:OG   | 2.16                     | 0.63              |
| 20:V:183:GLU:O    | 20:V:187:ILE:HG22 | 1.97                     | 0.63              |
| 20:V:310:THR:O    | 20:V:314:ARG:HG2  | 1.98                     | 0.63              |
| 22:X:286:ALA:CB   | 22:X:312:GLU:HG3  | 2.28                     | 0.63              |
| 23:Y:275:LEU:CD2  | 23:Y:296:VAL:HG13 | 2.26                     | 0.63              |
| 23:Y:275:LEU:HA   | 23:Y:278:VAL:HG12 | 1.80                     | 0.63              |
| 25:a:191:SER:HA   | 25:a:194:GLN:NE2  | 2.13                     | 0.63              |
| 25:a:213:PHE:HE1  | 25:a:240:PHE:HD2  | 1.46                     | 0.63              |
| 26:b:7:MET:CE     | 26:b:52:ILE:HD11  | 2.28                     | 0.63              |
| 26:b:88:THR:HA    | 26:b:91:ARG:HD2   | 1.79                     | 0.63              |
| 27:c:27:THR:HA    | 27:c:175:ARG:HH21 | 1.61                     | 0.63              |
| 30:f:61:GLU:OE2   | 30:f:97:LYS:HB2   | 1.98                     | 0.63              |
| 30:f:291:GLN:HG2  | 30:f:879:ARG:HD3  | 1.81                     | 0.63              |
| 30:f:416:MET:HE1  | 30:f:447:ALA:HA   | 1.80                     | 0.63              |
| 30:f:530:CYS:SG   | 30:f:533:ASP:HB2  | 2.38                     | 0.63              |
| 6:g:83:MET:O      | 6:g:87:SER:OG     | 2.16                     | 0.63              |
| 32:U:422:LEU:C    | 32:U:423:MET:HE2  | 2.23                     | 0.63              |
| 32:U:889:LEU:O    | 32:U:892:LEU:HD22 | 1.98                     | 0.63              |
| 1:A:345:LEU:HD11  | 1:A:426:THR:HG21  | 1.80                     | 0.63              |
| 5:E:149:ILE:CD1   | 5:E:276:ILE:HD11  | 2.27                     | 0.63              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:E:345:ASN:HA    | 5:E:348:THR:HG22  | 1.80                     | 0.63              |
| 5:E:352:MET:O     | 5:E:355:ILE:HG22  | 1.98                     | 0.63              |
| 20:V:466:ILE:O    | 20:V:469:THR:OG1  | 2.15                     | 0.63              |
| 21:W:116:THR:O    | 21:W:117:ASP:HB3  | 1.98                     | 0.63              |
| 21:W:307:LYS:HG2  | 21:W:315:MET:HE2  | 1.80                     | 0.63              |
| 24:Z:42:SER:HA    | 24:Z:90:ARG:CZ    | 2.29                     | 0.63              |
| 25:a:223:GLU:HB3  | 25:a:234:ILE:HD11 | 1.80                     | 0.63              |
| 25:a:360:VAL:HG23 | 27:c:308:VAL:HG13 | 1.79                     | 0.63              |
| 28:d:61:TRP:CZ3   | 28:d:65:ARG:HD2   | 2.33                     | 0.63              |
| 30:f:141:LYS:HZ2  | 30:f:142:TYR:HB2  | 1.63                     | 0.63              |
| 30:f:180:GLN:HG3  | 30:f:219:LYS:NZ   | 2.11                     | 0.63              |
| 30:f:240:VAL:HG13 | 30:f:241:PRO:HD3  | 1.80                     | 0.63              |
| 30:f:787:LEU:HD22 | 30:f:791:VAL:HB   | 1.80                     | 0.63              |
| 32:U:475:HIS:ND1  | 32:U:507:VAL:O    | 2.31                     | 0.63              |
| 32:U:700:GLU:OE1  | 32:U:700:GLU:N    | 2.31                     | 0.63              |
| 32:U:715:LYS:HB2  | 32:U:715:LYS:NZ   | 2.14                     | 0.63              |
| 2:B:60:LEU:HA     | 2:B:63:LEU:HD23   | 1.80                     | 0.63              |
| 5:E:368:MET:O     | 5:E:372:ARG:NE    | 2.32                     | 0.63              |
| 11:L:146:GLN:NE2  | 11:L:159:MET:SD   | 2.71                     | 0.63              |
| 13:N:15:LEU:HD11  | 13:N:102:ALA:HB3  | 1.79                     | 0.63              |
| 21:W:131:VAL:CG2  | 21:W:140:ILE:HG13 | 2.29                     | 0.63              |
| 21:W:186:ILE:HD12 | 21:W:208:LYS:HG2  | 1.80                     | 0.63              |
| 22:X:205:LYS:HZ1  | 22:X:206:LEU:HD23 | 1.63                     | 0.63              |
| 22:X:286:ALA:HB2  | 22:X:312:GLU:HG3  | 1.81                     | 0.63              |
| 23:Y:278:VAL:HG23 | 23:Y:281:GLU:OE2  | 1.98                     | 0.63              |
| 28:d:144:MET:HA   | 28:d:144:MET:CE   | 2.26                     | 0.63              |
| 28:d:188:LYS:HB2  | 28:d:221:ASN:ND2  | 2.12                     | 0.63              |
| 30:f:560:LEU:HD23 | 30:f:594:LEU:CD2  | 2.28                     | 0.63              |
| 2:B:74:MET:HB2    | 30:f:610:GLN:CD   | 2.23                     | 0.63              |
| 2:B:292:THR:HG23  | 2:B:333:ARG:HH22  | 1.64                     | 0.63              |
| 5:E:242:ARG:HA    | 5:E:254:GLN:CD    | 2.23                     | 0.63              |
| 5:E:324:GLY:O     | 5:E:326:ILE:HD12  | 1.99                     | 0.63              |
| 22:X:119:SER:O    | 22:X:121:LYS:NZ   | 2.31                     | 0.63              |
| 22:X:122:ARG:CZ   | 22:X:122:ARG:HB2  | 2.28                     | 0.63              |
| 23:Y:104:MET:HE3  | 23:Y:127:THR:HA   | 1.81                     | 0.63              |
| 23:Y:377:LEU:O    | 23:Y:380:VAL:HG12 | 1.99                     | 0.63              |
| 25:a:161:LYS:NZ   | 25:a:164:GLN:OE1  | 2.31                     | 0.63              |
| 28:d:52:ARG:HG3   | 28:d:81:TYR:CD2   | 2.34                     | 0.63              |
| 30:f:303:VAL:O    | 30:f:306:GLU:HG3  | 1.97                     | 0.63              |
| 30:f:592:ASN:O    | 30:f:595:VAL:HG12 | 1.99                     | 0.63              |
| 32:U:544:ILE:HD12 | 32:U:544:ILE:H    | 1.64                     | 0.63              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:115:VAL:CG2   | 1:A:118:PHE:HB2   | 2.28                     | 0.63              |
| 2:B:207:HIS:HB3   | 2:B:210:TYR:CE1   | 2.33                     | 0.63              |
| 4:D:160:PRO:HG2   | 4:D:220:ALA:HB3   | 1.80                     | 0.63              |
| 4:D:266:GLU:HA    | 4:D:266:GLU:OE2   | 1.98                     | 0.63              |
| 20:V:193:GLN:HA   | 20:V:193:GLN:OE1  | 1.98                     | 0.63              |
| 20:V:496:PHE:N    | 20:V:497:PRO:HD2  | 2.14                     | 0.63              |
| 21:W:93:ARG:HB2   | 21:W:96:GLN:HE22  | 1.63                     | 0.63              |
| 21:W:209:ILE:HD13 | 21:W:227:TYR:HE2  | 1.64                     | 0.63              |
| 21:W:401:THR:O    | 21:W:402:ILE:HD12 | 1.99                     | 0.63              |
| 24:Z:165:GLU:HG3  | 24:Z:166:GLU:N    | 2.12                     | 0.63              |
| 26:b:86:PHE:CE2   | 26:b:90:ILE:HD11  | 2.33                     | 0.63              |
| 26:b:138:VAL:HG12 | 26:b:160:LEU:HD12 | 1.79                     | 0.63              |
| 27:c:38:LEU:HD11  | 27:c:155:VAL:HG11 | 1.80                     | 0.63              |
| 30:f:271:MET:HE3  | 30:f:271:MET:N    | 2.13                     | 0.63              |
| 30:f:608:LYS:HE2  | 30:f:639:LYS:CE   | 2.29                     | 0.63              |
| 30:f:829:MET:HE3  | 30:f:829:MET:N    | 2.02                     | 0.63              |
| 31:F:276:LYS:HB2  | 31:F:276:LYS:HZ3  | 1.63                     | 0.63              |
| 31:F:344:ARG:HH21 | 31:F:347:ARG:CZ   | 2.11                     | 0.63              |
| 32:U:599:ILE:HG23 | 32:U:603:LEU:HD23 | 1.80                     | 0.63              |
| 32:U:878:LEU:HB3  | 32:U:882:ALA:CB   | 2.28                     | 0.63              |
| 3:C:86:LEU:HD12   | 3:C:96:VAL:CG2    | 2.28                     | 0.63              |
| 3:C:162:LYS:HD2   | 23:Y:95:LEU:HD11  | 1.81                     | 0.63              |
| 20:V:480:ILE:HD11 | 24:Z:261:TYR:CA   | 2.24                     | 0.63              |
| 21:W:201:ARG:CZ   | 21:W:201:ARG:HB3  | 2.29                     | 0.63              |
| 22:X:213:GLN:OE1  | 22:X:213:GLN:HA   | 1.98                     | 0.63              |
| 25:a:136:GLU:OE1  | 25:a:136:GLU:HA   | 1.98                     | 0.63              |
| 25:a:244:ASN:HB3  | 25:a:247:ARG:HB2  | 1.81                     | 0.63              |
| 28:d:74:TYR:O     | 28:d:78:LEU:HG    | 1.98                     | 0.63              |
| 14:o:210:THR:HG21 | 15:p:167:SER:HB2  | 1.81                     | 0.63              |
| 2:B:77:GLU:O      | 2:B:81:ASN:HB2    | 1.98                     | 0.63              |
| 2:B:166:ASP:CG    | 3:C:78:ARG:HH12   | 2.05                     | 0.63              |
| 2:B:396:LYS:O     | 2:B:400:THR:HG22  | 1.98                     | 0.63              |
| 5:E:309:ARG:HB3   | 5:E:332:VAL:HG13  | 1.80                     | 0.63              |
| 5:E:352:MET:HE2   | 5:E:355:ILE:CG2   | 2.28                     | 0.63              |
| 20:V:245:ASP:OD1  | 20:V:245:ASP:O    | 2.17                     | 0.63              |
| 20:V:259:LEU:HD13 | 20:V:264:TYR:CE1  | 2.31                     | 0.63              |
| 20:V:280:ALA:HB3  | 20:V:285:TRP:HE3  | 1.64                     | 0.63              |
| 22:X:132:ARG:HD3  | 22:X:136:LEU:HD23 | 1.80                     | 0.63              |
| 25:a:61:GLU:HA    | 25:a:64:ILE:CG1   | 2.28                     | 0.63              |
| 30:f:461:PRO:HB2  | 30:f:465:LEU:HD11 | 1.81                     | 0.63              |
| 30:f:744:MET:HB2  | 30:f:748:LEU:CD1  | 2.29                     | 0.63              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 32:U:161:ASP:OD1  | 32:U:162:VAL:N    | 2.32                     | 0.63              |
| 32:U:463:ASN:HA   | 32:U:466:LYS:HZ3  | 1.64                     | 0.63              |
| 32:U:552:ILE:CD1  | 32:U:570:LEU:HD11 | 2.29                     | 0.63              |
| 32:U:680:VAL:O    | 32:U:683:VAL:HG12 | 1.98                     | 0.63              |
| 1:A:319:MET:HE2   | 1:A:337:LEU:CD1   | 2.28                     | 0.63              |
| 5:E:138:LEU:HD21  | 5:E:301:ILE:CG2   | 2.29                     | 0.63              |
| 24:Z:176:LEU:HD21 | 27:c:217:LEU:CD2  | 2.28                     | 0.63              |
| 26:b:52:ILE:HD12  | 26:b:52:ILE:N     | 2.14                     | 0.63              |
| 27:c:56:LEU:HB2   | 27:c:73:PHE:CE1   | 2.34                     | 0.63              |
| 28:d:252:GLN:HG3  | 28:d:252:GLN:O    | 1.99                     | 0.63              |
| 30:f:180:GLN:N    | 30:f:180:GLN:OE1  | 2.32                     | 0.63              |
| 30:f:482:ILE:HB   | 30:f:518:THR:HG22 | 1.80                     | 0.63              |
| 31:F:230:GLY:O    | 31:F:392:ASN:HB2  | 1.98                     | 0.63              |
| 32:U:213:PHE:HA   | 32:U:216:VAL:CG1  | 2.29                     | 0.63              |
| 32:U:423:MET:HG3  | 32:U:446:LEU:HD12 | 1.81                     | 0.63              |
| 1:A:78:TRP:O      | 1:A:81:ALA:HB3    | 1.99                     | 0.62              |
| 1:A:240:VAL:HG11  | 1:A:274:PHE:CD1   | 2.33                     | 0.62              |
| 2:B:211:TYR:HA    | 2:B:216:ILE:CD1   | 2.29                     | 0.62              |
| 4:D:374:ASP:O     | 4:D:378:ILE:HG13  | 1.99                     | 0.62              |
| 17:R:2:THR:OG1    | 17:R:34:LYS:NZ    | 2.31                     | 0.62              |
| 21:W:216:GLU:HA   | 21:W:219:THR:CB   | 2.28                     | 0.62              |
| 21:W:356:ASN:O    | 21:W:359:VAL:HG12 | 1.99                     | 0.62              |
| 26:b:97:LEU:HD23  | 26:b:107:MET:HB2  | 1.79                     | 0.62              |
| 27:c:33:ILE:HD12  | 27:c:205:ILE:HD11 | 1.81                     | 0.62              |
| 13:n:60:VAL:HG23  | 13:n:87:MET:CE    | 2.28                     | 0.62              |
| 31:F:406:ILE:HD13 | 31:F:422:GLU:OE1  | 1.98                     | 0.62              |
| 32:U:884:VAL:HG11 | 32:U:889:LEU:HA   | 1.81                     | 0.62              |
| 1:A:273:PHE:HA    | 1:A:318:LEU:O     | 1.99                     | 0.62              |
| 2:B:70:ASP:C      | 30:f:606:VAL:HG11 | 2.23                     | 0.62              |
| 2:B:374:LEU:HD23  | 2:B:378:VAL:CG1   | 2.29                     | 0.62              |
| 3:C:134:LEU:HD23  | 3:C:237:MET:SD    | 2.39                     | 0.62              |
| 4:D:217:LYS:HA    | 5:E:267:PHE:CE1   | 2.34                     | 0.62              |
| 20:V:227:VAL:HG22 | 20:V:231:LEU:HD21 | 1.80                     | 0.62              |
| 22:X:206:LEU:HA   | 22:X:209:THR:HG22 | 1.81                     | 0.62              |
| 25:a:341:LEU:HB3  | 25:a:345:GLN:HB2  | 1.81                     | 0.62              |
| 27:c:54:MET:HG2   | 27:c:55:GLY:N     | 2.14                     | 0.62              |
| 32:U:148:LYS:HE2  | 32:U:148:LYS:HA   | 1.80                     | 0.62              |
| 32:U:353:LEU:O    | 32:U:356:THR:OG1  | 2.12                     | 0.62              |
| 32:U:792:ASN:HB3  | 32:U:796:LYS:HB3  | 1.81                     | 0.62              |
| 32:U:892:LEU:HD11 | 32:U:906:LEU:HD11 | 1.81                     | 0.62              |
| 1:A:174:TYR:HD2   | 1:A:188:ARG:HH11  | 1.47                     | 0.62              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:74:MET:SD     | 2:B:75:GLU:N      | 2.73                     | 0.62              |
| 8:I:35:LEU:HD11   | 8:I:175:LEU:HD11  | 1.81                     | 0.62              |
| 9:J:104:VAL:HG21  | 9:J:143:ARG:CB    | 2.29                     | 0.62              |
| 20:V:251:LEU:HD11 | 20:V:270:LEU:HD21 | 1.80                     | 0.62              |
| 21:W:307:LYS:HD2  | 21:W:315:MET:HE2  | 1.80                     | 0.62              |
| 22:X:253:TYR:CE2  | 22:X:318:ILE:HD11 | 2.34                     | 0.62              |
| 22:X:347:ILE:O    | 22:X:350:ILE:HG22 | 1.99                     | 0.62              |
| 24:Z:173:GLU:OE1  | 27:c:152:LYS:NZ   | 2.22                     | 0.62              |
| 25:a:33:LEU:HD11  | 25:a:36:GLN:HB2   | 1.80                     | 0.62              |
| 30:f:189:LYS:HD3  | 30:f:190:GLU:HG3  | 1.81                     | 0.62              |
| 30:f:346:ASP:OD2  | 30:f:378:ASN:ND2  | 2.32                     | 0.62              |
| 30:f:637:LYS:HD2  | 30:f:637:LYS:C    | 2.24                     | 0.62              |
| 1:A:222:LYS:HB2   | 33:A:501:ATP:O2B  | 2.00                     | 0.62              |
| 3:C:150:MET:HA    | 3:C:331:ILE:HG21  | 1.80                     | 0.62              |
| 4:D:53:PHE:O      | 4:D:56:VAL:HG12   | 1.98                     | 0.62              |
| 5:E:60:VAL:HG23   | 5:E:98:VAL:HG21   | 1.82                     | 0.62              |
| 5:E:275:MET:O     | 5:E:276:ILE:HD13  | 1.97                     | 0.62              |
| 5:E:281:ARG:HB3   | 5:E:281:ARG:HH11  | 1.64                     | 0.62              |
| 5:E:281:ARG:HB3   | 5:E:281:ARG:NH1   | 2.14                     | 0.62              |
| 5:E:331:ILE:HG12  | 5:E:371:VAL:HG21  | 1.81                     | 0.62              |
| 9:J:80:ALA:O      | 9:J:84:ILE:HD13   | 2.00                     | 0.62              |
| 20:V:337:LEU:HD22 | 20:V:367:VAL:CG1  | 2.27                     | 0.62              |
| 20:V:449:ALA:CB   | 20:V:460:SER:HA   | 2.27                     | 0.62              |
| 23:Y:186:LEU:HD22 | 23:Y:287:LEU:HD13 | 1.81                     | 0.62              |
| 24:Z:39:LEU:HD23  | 24:Z:53:SER:HB3   | 1.80                     | 0.62              |
| 26:b:188:ILE:HD12 | 26:b:188:ILE:H    | 1.64                     | 0.62              |
| 30:f:744:MET:HB2  | 30:f:748:LEU:HD12 | 1.80                     | 0.62              |
| 31:F:246:ALA:HB1  | 31:F:280:PRO:O    | 1.98                     | 0.62              |
| 31:F:384:LEU:HD22 | 31:F:424:ILE:HD11 | 1.80                     | 0.62              |
| 1:A:102:ILE:N     | 1:A:102:ILE:HD12  | 2.15                     | 0.62              |
| 2:B:223:ILE:HD13  | 2:B:329:MET:HB2   | 1.81                     | 0.62              |
| 3:C:192:PRO:HG3   | 3:C:296:ASN:OD1   | 1.99                     | 0.62              |
| 4:D:335:LEU:HD13  | 4:D:371:SER:CB    | 2.30                     | 0.62              |
| 5:E:81:VAL:HB     | 5:E:105:LEU:O     | 2.00                     | 0.62              |
| 20:V:187:ILE:HA   | 20:V:190:ASP:OD2  | 1.98                     | 0.62              |
| 21:W:372:ARG:HD2  | 21:W:414:ASN:HB3  | 1.81                     | 0.62              |
| 21:W:412:ILE:O    | 21:W:412:ILE:HG13 | 1.98                     | 0.62              |
| 23:Y:104:MET:HE1  | 23:Y:130:LYS:HG3  | 1.82                     | 0.62              |
| 24:Z:164:ALA:HB1  | 24:Z:169:GLU:HG3  | 1.81                     | 0.62              |
| 25:a:302:ILE:HG22 | 25:a:303:THR:O    | 2.00                     | 0.62              |
| 25:a:311:VAL:HG21 | 25:a:324:ILE:CD1  | 2.30                     | 0.62              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 26:b:29:GLN:HA    | 26:b:29:GLN:NE2   | 2.14                     | 0.62              |
| 28:d:42:LYS:HE2   | 28:d:87:GLU:HG2   | 1.82                     | 0.62              |
| 16:q:180:VAL:HG21 | 16:q:194:ILE:HD13 | 1.82                     | 0.62              |
| 32:U:599:ILE:CD1  | 32:U:626:LEU:HD21 | 2.29                     | 0.62              |
| 32:U:609:ASP:O    | 32:U:615:ARG:NH1  | 2.32                     | 0.62              |
| 32:U:736:ILE:HD11 | 32:U:779:LEU:HD23 | 1.79                     | 0.62              |
| 32:U:759:SER:HA   | 32:U:782:ALA:HA   | 1.79                     | 0.62              |
| 2:B:390:LEU:HD12  | 2:B:390:LEU:O     | 1.99                     | 0.62              |
| 3:C:166:GLU:OE1   | 3:C:167:LEU:HD23  | 2.00                     | 0.62              |
| 5:E:226:GLN:HB3   | 5:E:227:PRO:CD    | 2.29                     | 0.62              |
| 10:K:104:ASN:OD1  | 17:R:58:ARG:NH2   | 2.32                     | 0.62              |
| 20:V:463:MET:HE3  | 20:V:463:MET:C    | 2.25                     | 0.62              |
| 20:V:471:GLU:HG3  | 20:V:472:PRO:CD   | 2.30                     | 0.62              |
| 23:Y:24:PHE:CZ    | 23:Y:28:LEU:HD22  | 2.34                     | 0.62              |
| 23:Y:167:LEU:O    | 23:Y:170:GLU:HG2  | 1.98                     | 0.62              |
| 23:Y:233:ARG:NH1  | 23:Y:264:TYR:HA   | 2.14                     | 0.62              |
| 26:b:77:THR:HA    | 26:b:79:GLN:NE2   | 2.14                     | 0.62              |
| 26:b:129:LYS:O    | 26:b:133:LYS:NZ   | 2.23                     | 0.62              |
| 30:f:263:PRO:HB2  | 30:f:266:LEU:CD2  | 2.29                     | 0.62              |
| 30:f:346:ASP:HB2  | 30:f:350:LYS:HZ1  | 1.64                     | 0.62              |
| 30:f:698:SER:O    | 30:f:705:ASN:ND2  | 2.31                     | 0.62              |
| 30:f:716:ASP:HB2  | 30:f:719:PRO:HG3  | 1.80                     | 0.62              |
| 32:U:209:GLU:HB2  | 32:U:210:LYS:HZ2  | 1.63                     | 0.62              |
| 32:U:772:TRP:CD1  | 32:U:774:PRO:HG2  | 2.34                     | 0.62              |
| 1:A:319:MET:CE    | 1:A:337:LEU:HD22  | 2.30                     | 0.62              |
| 4:D:203:LEU:HD12  | 4:D:309:MET:O     | 2.00                     | 0.62              |
| 5:E:272:ARG:HG3   | 5:E:272:ARG:HH11  | 1.65                     | 0.62              |
| 20:V:415:SER:HB3  | 23:Y:348:ASP:OD1  | 1.99                     | 0.62              |
| 20:V:424:GLN:OE1  | 20:V:424:GLN:HA   | 1.99                     | 0.62              |
| 21:W:333:LEU:HD23 | 21:W:334:GLU:H    | 1.63                     | 0.62              |
| 25:a:22:TRP:O     | 25:a:26:GLU:HG2   | 2.00                     | 0.62              |
| 28:d:75:MET:HA    | 28:d:78:LEU:HD11  | 1.82                     | 0.62              |
| 30:f:474:SER:O    | 30:f:477:MET:HE3  | 2.00                     | 0.62              |
| 30:f:705:ASN:HA   | 30:f:708:ASP:OD2  | 1.99                     | 0.62              |
| 31:F:78:GLU:OE1   | 31:F:81:LYS:HD3   | 2.00                     | 0.62              |
| 32:U:222:PHE:HE1  | 32:U:754:HIS:HD1  | 1.47                     | 0.62              |
| 1:A:268:LYS:HE3   | 30:f:354:GLU:CB   | 2.29                     | 0.62              |
| 2:B:342:ILE:HG23  | 2:B:347:ILE:CD1   | 2.18                     | 0.62              |
| 2:B:428:TYR:CE1   | 2:B:429:LYS:HB2   | 2.33                     | 0.62              |
| 3:C:151:ILE:HG12  | 3:C:158:ILE:HD11  | 1.82                     | 0.62              |
| 21:W:435:LEU:CD1  | 24:Z:237:LEU:HD23 | 2.30                     | 0.62              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 21:W:445:LEU:HD22 | 24:Z:226:ILE:CG1  | 2.30                     | 0.62              |
| 22:X:348:GLU:HA   | 22:X:348:GLU:OE2  | 2.00                     | 0.62              |
| 23:Y:133:ALA:O    | 23:Y:137:ARG:HG3  | 1.98                     | 0.62              |
| 24:Z:22:HIS:O     | 24:Z:26:ILE:HG22  | 1.99                     | 0.62              |
| 24:Z:259:VAL:HG11 | 27:c:291:LEU:HD22 | 1.82                     | 0.62              |
| 30:f:736:THR:O    | 30:f:746:ARG:NH2  | 2.33                     | 0.62              |
| 30:f:787:LEU:CD2  | 30:f:791:VAL:HB   | 2.30                     | 0.62              |
| 32:U:206:MET:HE2  | 32:U:206:MET:CA   | 2.30                     | 0.62              |
| 3:C:193:GLY:HA2   | 35:C:501:ADP:O3A  | 1.99                     | 0.62              |
| 21:W:201:ARG:O    | 21:W:204:ILE:HG13 | 1.99                     | 0.62              |
| 22:X:235:ALA:O    | 22:X:239:TYR:HB2  | 2.00                     | 0.62              |
| 24:Z:209:ARG:HG2  | 24:Z:209:ARG:HH11 | 1.65                     | 0.62              |
| 24:Z:270:VAL:HG23 | 27:c:281:LYS:HE3  | 1.82                     | 0.62              |
| 26:b:91:ARG:HB3   | 26:b:91:ARG:NH1   | 2.15                     | 0.62              |
| 30:f:228:LYS:HE3  | 30:f:233:LEU:HD12 | 1.82                     | 0.62              |
| 30:f:320:ILE:HG23 | 30:f:324:VAL:HG11 | 1.81                     | 0.62              |
| 30:f:705:ASN:O    | 30:f:709:THR:HG22 | 2.00                     | 0.62              |
| 32:U:380:THR:HG23 | 32:U:382:SER:H    | 1.63                     | 0.62              |
| 32:U:713:TYR:O    | 32:U:716:VAL:HG22 | 1.99                     | 0.62              |
| 32:U:902:PRO:CA   | 32:U:914:LEU:HD12 | 2.29                     | 0.62              |
| 1:A:230:ALA:HA    | 1:A:233:THR:HG22  | 1.80                     | 0.62              |
| 2:B:106:PRO:HB3   | 3:C:121:TYR:CD1   | 2.35                     | 0.62              |
| 2:B:279:PRO:HB3   | 2:B:324:ASP:OD2   | 1.99                     | 0.62              |
| 4:D:59:GLU:O      | 4:D:63:ASP:HB2    | 1.99                     | 0.62              |
| 4:D:61:ILE:HD11   | 32:U:639:LEU:CD1  | 2.29                     | 0.62              |
| 21:W:149:LEU:HB2  | 21:W:185:PHE:HE2  | 1.65                     | 0.62              |
| 24:Z:223:ASN:O    | 24:Z:224:HIS:HB2  | 2.00                     | 0.62              |
| 30:f:126:ILE:HD13 | 30:f:173:LEU:HD22 | 1.80                     | 0.62              |
| 30:f:796:LEU:O    | 30:f:796:LEU:HD23 | 2.00                     | 0.62              |
| 32:U:148:LYS:O    | 32:U:151:ILE:HG22 | 2.00                     | 0.62              |
| 32:U:250:PHE:CD2  | 32:U:911:ILE:HG21 | 2.35                     | 0.62              |
| 32:U:424:ALA:HA   | 32:U:427:LEU:HD13 | 1.82                     | 0.62              |
| 32:U:892:LEU:HD11 | 32:U:906:LEU:CD1  | 2.28                     | 0.62              |
| 2:B:159:VAL:C     | 2:B:160:ILE:HD12  | 2.24                     | 0.61              |
| 2:B:264:PRO:HB3   | 2:B:311:GLU:CB    | 2.30                     | 0.61              |
| 20:V:296:LYS:NZ   | 20:V:308:THR:HG21 | 2.14                     | 0.61              |
| 21:W:268:LYS:HE3  | 21:W:301:LYS:HZ2  | 1.65                     | 0.61              |
| 21:W:316:ARG:NH1  | 21:W:380:GLN:O    | 2.33                     | 0.61              |
| 21:W:394:SER:HA   | 21:W:397:VAL:HG12 | 1.82                     | 0.61              |
| 25:a:252:LYS:HA   | 25:a:255:TRP:CD2  | 2.35                     | 0.61              |
| 28:d:52:ARG:NH2   | 28:d:89:LEU:HD21  | 2.14                     | 0.61              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 32:U:98:GLU:OE1   | 32:U:98:GLU:N     | 2.33                     | 0.61              |
| 32:U:268:LEU:HD23 | 32:U:325:MET:HB2  | 1.82                     | 0.61              |
| 32:U:510:GLU:HG3  | 32:U:543:LYS:HG2  | 1.81                     | 0.61              |
| 32:U:546:ARG:HD3  | 32:U:771:PHE:CG   | 2.34                     | 0.61              |
| 1:A:364:VAL:HG23  | 1:A:366:ARG:N     | 2.14                     | 0.61              |
| 22:X:202:CYS:O    | 22:X:204:PRO:HD3  | 1.99                     | 0.61              |
| 26:b:142:ASN:HB3  | 26:b:172:THR:HA   | 1.80                     | 0.61              |
| 30:f:346:ASP:HB2  | 30:f:350:LYS:NZ   | 2.14                     | 0.61              |
| 30:f:416:MET:HE1  | 30:f:447:ALA:CB   | 2.30                     | 0.61              |
| 32:U:186:SER:O    | 32:U:187:LEU:HD23 | 1.99                     | 0.61              |
| 32:U:445:ALA:O    | 32:U:449:ILE:HG22 | 2.00                     | 0.61              |
| 32:U:792:ASN:OD1  | 32:U:795:LEU:N    | 2.32                     | 0.61              |
| 1:A:106:SER:O     | 1:A:107:GLU:HB2   | 1.99                     | 0.61              |
| 3:C:82:LYS:HB3    | 3:C:82:LYS:HZ3    | 1.63                     | 0.61              |
| 3:C:194:THR:CG2   | 3:C:317:PHE:HB3   | 2.30                     | 0.61              |
| 5:E:161:ARG:NH2   | 21:W:173:THR:O    | 2.33                     | 0.61              |
| 20:V:127:THR:HB   | 20:V:131:LEU:HD12 | 1.82                     | 0.61              |
| 24:Z:230:LEU:CD2  | 25:a:349:MET:HE3  | 2.30                     | 0.61              |
| 25:a:8:LEU:HA     | 25:a:11:SER:OG    | 2.00                     | 0.61              |
| 25:a:112:ILE:HD12 | 25:a:151:VAL:CG2  | 2.20                     | 0.61              |
| 26:b:48:ASN:HD22  | 26:b:64:LEU:HG    | 1.65                     | 0.61              |
| 28:d:33:LEU:HD22  | 28:d:34:ASN:H     | 1.64                     | 0.61              |
| 28:d:203:PRO:C    | 28:d:206:MET:HE1  | 2.25                     | 0.61              |
| 30:f:141:LYS:NZ   | 30:f:142:TYR:HB2  | 2.15                     | 0.61              |
| 30:f:177:GLU:CG   | 30:f:835:GLU:HB2  | 2.29                     | 0.61              |
| 32:U:24:LEU:O     | 32:U:24:LEU:HD23  | 1.99                     | 0.61              |
| 32:U:177:LEU:HD11 | 32:U:204:ILE:CD1  | 2.30                     | 0.61              |
| 2:B:53:THR:OG1    | 2:B:54:PRO:HD3    | 1.99                     | 0.61              |
| 4:D:284:GLU:O     | 4:D:288:ILE:HG12  | 2.00                     | 0.61              |
| 4:D:374:ASP:HA    | 4:D:377:SER:HB3   | 1.81                     | 0.61              |
| 5:E:367:PHE:O     | 5:E:371:VAL:HG23  | 1.99                     | 0.61              |
| 20:V:106:ARG:HE   | 20:V:106:ARG:H    | 1.46                     | 0.61              |
| 20:V:436:PHE:O    | 20:V:440:LYS:N    | 2.26                     | 0.61              |
| 20:V:492:LYS:HA   | 20:V:492:LYS:CE   | 2.26                     | 0.61              |
| 23:Y:224:VAL:CG2  | 23:Y:260:LEU:HD12 | 2.29                     | 0.61              |
| 25:a:124:ASN:O    | 25:a:125:ILE:HG23 | 2.01                     | 0.61              |
| 29:e:46:ASP:OD1   | 29:e:46:ASP:N     | 2.32                     | 0.61              |
| 31:F:332:THR:HG22 | 31:F:334:ARG:H    | 1.65                     | 0.61              |
| 32:U:350:LEU:HD22 | 32:U:385:PHE:CZ   | 2.34                     | 0.61              |
| 32:U:892:LEU:HD11 | 32:U:906:LEU:CG   | 2.31                     | 0.61              |
| 2:B:56:THR:HG23   | 2:B:58:CYS:H      | 1.65                     | 0.61              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:C:138:MET:N     | 3:C:138:MET:HE2   | 2.16                     | 0.61              |
| 4:D:109:SER:C     | 4:D:110:ASN:HD22  | 2.08                     | 0.61              |
| 5:E:185:ARG:HD3   | 31:F:320:PHE:HA   | 1.83                     | 0.61              |
| 5:E:270:LEU:HD11  | 5:E:273:VAL:HG11  | 1.80                     | 0.61              |
| 21:W:142:ARG:O    | 21:W:142:ARG:HD3  | 2.00                     | 0.61              |
| 21:W:166:LEU:HD13 | 21:W:166:LEU:O    | 2.00                     | 0.61              |
| 21:W:371:THR:HG22 | 21:W:372:ARG:CG   | 2.29                     | 0.61              |
| 21:W:435:LEU:HD11 | 24:Z:237:LEU:HD23 | 1.82                     | 0.61              |
| 22:X:240:ASP:O    | 22:X:242:ILE:HG23 | 2.00                     | 0.61              |
| 25:a:78:GLU:HA    | 25:a:81:LEU:HD23  | 1.83                     | 0.61              |
| 28:d:59:ALA:HA    | 28:d:62:SER:OG    | 2.01                     | 0.61              |
| 30:f:126:ILE:HG23 | 30:f:127:SER:H    | 1.65                     | 0.61              |
| 15:p:137:VAL:HG11 | 15:p:145:MET:HB3  | 1.81                     | 0.61              |
| 32:U:108:TYR:HE2  | 32:U:126:ILE:HG21 | 1.65                     | 0.61              |
| 32:U:375:PHE:HE2  | 32:U:732:LEU:HD21 | 1.66                     | 0.61              |
| 1:A:190:VAL:HG23  | 1:A:209:PRO:O     | 2.00                     | 0.61              |
| 3:C:250:GLU:OE1   | 3:C:295:THR:HB    | 2.00                     | 0.61              |
| 20:V:288:TYR:HD1  | 20:V:289:LEU:HD23 | 1.66                     | 0.61              |
| 23:Y:179:ARG:HD3  | 23:Y:210:SER:OG   | 1.99                     | 0.61              |
| 24:Z:247:LYS:HB3  | 24:Z:247:LYS:HZ1  | 1.66                     | 0.61              |
| 26:b:41:THR:HG22  | 26:b:42:ARG:H     | 1.63                     | 0.61              |
| 30:f:266:LEU:HD23 | 30:f:266:LEU:H    | 1.66                     | 0.61              |
| 30:f:462:ALA:O    | 30:f:466:LEU:HB2  | 2.01                     | 0.61              |
| 15:p:202:ARG:NH2  | 15:p:204:ASP:OD2  | 2.33                     | 0.61              |
| 32:U:353:LEU:HD11 | 32:U:373:ASN:HB2  | 1.81                     | 0.61              |
| 32:U:576:PRO:CB   | 32:U:611:ASN:HD22 | 2.10                     | 0.61              |
| 32:U:892:LEU:HD11 | 32:U:906:LEU:HG   | 1.81                     | 0.61              |
| 2:B:176:VAL:HG23  | 2:B:247:PHE:HB3   | 1.82                     | 0.61              |
| 3:C:48:GLN:O      | 3:C:51:GLU:HG3    | 1.99                     | 0.61              |
| 5:E:380:LEU:HD11  | 31:F:351:LYS:CE   | 2.24                     | 0.61              |
| 20:V:480:ILE:CD1  | 24:Z:261:TYR:HA   | 2.24                     | 0.61              |
| 21:W:133:GLU:O    | 21:W:136:ILE:HD13 | 2.00                     | 0.61              |
| 21:W:145:LEU:HD23 | 21:W:177:MET:HE3  | 1.83                     | 0.61              |
| 23:Y:101:ARG:HH21 | 23:Y:140:ILE:HD11 | 1.66                     | 0.61              |
| 32:U:188:MET:HE2  | 32:U:188:MET:CA   | 2.27                     | 0.61              |
| 32:U:250:PHE:HD2  | 32:U:911:ILE:HG21 | 1.65                     | 0.61              |
| 32:U:485:ALA:O    | 32:U:488:THR:HG23 | 1.99                     | 0.61              |
| 32:U:904:LYS:HE3  | 32:U:908:ILE:CD1  | 2.30                     | 0.61              |
| 5:E:86:GLN:H      | 5:E:86:GLN:CD     | 2.08                     | 0.61              |
| 25:a:226:ARG:NH2  | 25:a:233:LEU:HB3  | 2.16                     | 0.61              |
| 26:b:63:THR:O     | 26:b:65:THR:HG22  | 1.99                     | 0.61              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 28:d:200:PHE:HB2  | 28:d:203:PRO:HG3  | 1.83                     | 0.61              |
| 30:f:655:LEU:HA   | 30:f:659:LEU:CD1  | 2.31                     | 0.61              |
| 32:U:188:MET:HA   | 32:U:188:MET:CE   | 2.26                     | 0.61              |
| 32:U:465:LEU:HD11 | 32:U:477:GLY:CA   | 2.29                     | 0.61              |
| 1:A:387:SER:O     | 1:A:391:GLU:HB2   | 2.01                     | 0.61              |
| 10:K:20:ARG:CZ    | 31:F:435:LEU:HA   | 2.31                     | 0.61              |
| 12:M:53:VAL:O     | 12:M:53:VAL:HG23  | 1.99                     | 0.61              |
| 20:V:306:ARG:HD2  | 20:V:336:GLU:OE2  | 2.01                     | 0.61              |
| 21:W:247:TYR:O    | 21:W:250:ILE:HG12 | 2.01                     | 0.61              |
| 23:Y:379:ARG:HG2  | 23:Y:379:ARG:HH11 | 1.66                     | 0.61              |
| 24:Z:42:SER:HA    | 24:Z:90:ARG:NH1   | 2.13                     | 0.61              |
| 25:a:202:LEU:HG   | 25:a:261:LEU:HD13 | 1.83                     | 0.61              |
| 28:d:36:LEU:HD23  | 28:d:38:THR:H     | 1.65                     | 0.61              |
| 28:d:235:THR:C    | 28:d:238:PRO:HD2  | 2.26                     | 0.61              |
| 12:m:108:LEU:HD11 | 12:m:137:LEU:HB3  | 1.83                     | 0.61              |
| 32:U:214:ILE:HG13 | 32:U:215:ASN:N    | 2.15                     | 0.61              |
| 32:U:218:GLN:NE2  | 32:U:752:THR:HB   | 2.15                     | 0.61              |
| 32:U:654:MET:HE1  | 32:U:686:GLY:HA2  | 1.81                     | 0.61              |
| 1:A:156:LYS:HA    | 1:A:156:LYS:HE3   | 1.81                     | 0.61              |
| 1:A:254:ALA:HB1   | 1:A:301:GLU:HG3   | 1.83                     | 0.61              |
| 2:B:378:VAL:HG23  | 2:B:416:ASN:OD1   | 2.00                     | 0.61              |
| 5:E:197:LYS:HG2   | 31:F:320:PHE:CE2  | 2.36                     | 0.61              |
| 20:V:466:ILE:HD11 | 20:V:471:GLU:CG   | 2.30                     | 0.61              |
| 21:W:307:LYS:O    | 21:W:313:GLU:HG3  | 2.00                     | 0.61              |
| 22:X:140:THR:OG1  | 22:X:142:ARG:HD3  | 2.00                     | 0.61              |
| 23:Y:275:LEU:HA   | 23:Y:278:VAL:CG1  | 2.31                     | 0.61              |
| 26:b:132:LYS:HE2  | 26:b:133:LYS:HZ1  | 1.65                     | 0.61              |
| 26:b:135:LYS:HD2  | 26:b:135:LYS:N    | 2.16                     | 0.61              |
| 27:c:232:GLN:OE1  | 27:c:232:GLN:O    | 2.19                     | 0.61              |
| 2:B:260:LEU:HD21  | 2:B:299:SER:HB2   | 1.83                     | 0.60              |
| 20:V:212:TYR:HA   | 20:V:253:LEU:CD1  | 2.29                     | 0.60              |
| 21:W:183:VAL:HA   | 21:W:186:ILE:CG2  | 2.31                     | 0.60              |
| 21:W:307:LYS:CD   | 21:W:315:MET:HE2  | 2.31                     | 0.60              |
| 21:W:413:ILE:O    | 21:W:413:ILE:HG13 | 2.00                     | 0.60              |
| 21:W:448:LYS:HD2  | 24:Z:154:THR:HG21 | 1.82                     | 0.60              |
| 25:a:280:MET:O    | 25:a:284:ARG:HG2  | 2.00                     | 0.60              |
| 28:d:5:LEU:HD11   | 28:d:6:LYS:NZ     | 2.14                     | 0.60              |
| 30:f:301:HIS:CE1  | 30:f:318:THR:HG21 | 2.35                     | 0.60              |
| 30:f:545:LYS:NZ   | 30:f:547:GLU:OE1  | 2.32                     | 0.60              |
| 14:o:46:GLY:HA3   | 14:o:53:THR:HG21  | 1.82                     | 0.60              |
| 31:F:250:LYS:O    | 31:F:250:LYS:HG2  | 2.00                     | 0.60              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 32:U:235:LYS:HA   | 32:U:235:LYS:HE2  | 1.82                     | 0.60              |
| 32:U:346:ASN:OD1  | 32:U:348:THR:HG23 | 2.01                     | 0.60              |
| 32:U:803:LYS:HD2  | 32:U:875:PHE:CB   | 2.31                     | 0.60              |
| 1:A:251:GLY:O     | 1:A:253:GLY:N     | 2.29                     | 0.60              |
| 1:A:423:PHE:HE1   | 2:B:334:ILE:HG21  | 1.66                     | 0.60              |
| 2:B:71:TYR:CE1    | 2:B:75:GLU:HG3    | 2.36                     | 0.60              |
| 4:D:89:ILE:HD12   | 5:E:70:ILE:HG23   | 1.81                     | 0.60              |
| 21:W:244:CYS:HG   | 21:W:273:TYR:HD1  | 1.49                     | 0.60              |
| 21:W:312:MET:HE2  | 21:W:312:MET:CA   | 2.31                     | 0.60              |
| 23:Y:50:MET:HE1   | 23:Y:51:ALA:HB2   | 1.82                     | 0.60              |
| 24:Z:81:MET:HE3   | 27:c:94:LYS:HB3   | 1.83                     | 0.60              |
| 24:Z:270:VAL:CG2  | 27:c:281:LYS:HE3  | 2.31                     | 0.60              |
| 25:a:120:ALA:HA   | 25:a:123:LEU:HG   | 1.82                     | 0.60              |
| 25:a:184:ASP:O    | 25:a:185:ILE:HG13 | 2.01                     | 0.60              |
| 26:b:40:LYS:O     | 26:b:40:LYS:HD3   | 2.00                     | 0.60              |
| 26:b:128:ALA:HB2  | 26:b:156:PHE:CE1  | 2.36                     | 0.60              |
| 27:c:27:THR:HG21  | 27:c:177:THR:CA   | 2.16                     | 0.60              |
| 28:d:117:THR:HA   | 28:d:120:GLU:OE2  | 2.01                     | 0.60              |
| 30:f:99:LEU:HD12  | 30:f:100:ARG:H    | 1.65                     | 0.60              |
| 30:f:124:ASP:OD1  | 30:f:125:ILE:N    | 2.34                     | 0.60              |
| 30:f:198:HIS:HA   | 30:f:201:GLU:CD   | 2.26                     | 0.60              |
| 30:f:260:SER:O    | 30:f:270:LEU:HD13 | 2.01                     | 0.60              |
| 30:f:766:GLN:HE21 | 30:f:769:THR:HB   | 1.65                     | 0.60              |
| 31:F:122:ALA:HB2  | 31:F:137:ILE:CD1  | 2.30                     | 0.60              |
| 32:U:325:MET:O    | 32:U:328:ILE:HG12 | 2.00                     | 0.60              |
| 32:U:811:PHE:HZ   | 32:U:884:VAL:HA   | 1.66                     | 0.60              |
| 1:A:273:PHE:CD1   | 1:A:318:LEU:HD22  | 2.36                     | 0.60              |
| 2:B:166:ASP:OD1   | 3:C:78:ARG:NH1    | 2.32                     | 0.60              |
| 3:C:189:TYR:CE2   | 3:C:316:GLU:HG2   | 2.37                     | 0.60              |
| 4:D:107:THR:HG22  | 5:E:77:PRO:CG     | 2.31                     | 0.60              |
| 4:D:389:GLU:HB2   | 4:D:391:ARG:HD3   | 1.83                     | 0.60              |
| 21:W:220:GLU:HG3  | 21:W:221:LYS:CE   | 2.31                     | 0.60              |
| 23:Y:20:ALA:HB2   | 23:Y:150:PHE:CE1  | 2.36                     | 0.60              |
| 23:Y:39:ASP:OD1   | 23:Y:39:ASP:N     | 2.34                     | 0.60              |
| 24:Z:36:VAL:HG22  | 24:Z:96:HIS:HB3   | 1.82                     | 0.60              |
| 24:Z:122:VAL:HG12 | 24:Z:137:ALA:HB2  | 1.84                     | 0.60              |
| 25:a:59:LEU:HD23  | 25:a:60:TYR:N     | 2.16                     | 0.60              |
| 25:a:361:LYS:HD2  | 25:a:365:MET:HE1  | 1.82                     | 0.60              |
| 26:b:83:LYS:CD    | 26:b:84:ILE:H     | 2.14                     | 0.60              |
| 28:d:18:LYS:O     | 28:d:21:GLU:HG2   | 2.01                     | 0.60              |
| 30:f:75:LEU:HD12  | 30:f:77:GLU:H     | 1.66                     | 0.60              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 30:f:257:ARG:HB2  | 30:f:289:VAL:HG11 | 1.83                     | 0.60              |
| 30:f:687:ARG:O    | 30:f:691:PRO:HG2  | 2.00                     | 0.60              |
| 31:F:362:ARG:NE   | 31:F:388:THR:O    | 2.35                     | 0.60              |
| 32:U:82:LEU:HB3   | 32:U:129:ARG:CD   | 2.30                     | 0.60              |
| 32:U:443:LEU:HD22 | 32:U:443:LEU:H    | 1.66                     | 0.60              |
| 32:U:573:ASP:OD1  | 32:U:578:LEU:HB2  | 2.01                     | 0.60              |
| 1:A:254:ALA:O     | 1:A:257:VAL:HG12  | 2.01                     | 0.60              |
| 1:A:394:MET:HE1   | 2:B:211:TYR:CE1   | 2.36                     | 0.60              |
| 3:C:137:LEU:C     | 3:C:138:MET:HE2   | 2.26                     | 0.60              |
| 3:C:329:LEU:HD22  | 3:C:344:LEU:HD22  | 1.83                     | 0.60              |
| 4:D:122:GLU:OE2   | 27:c:278:GLN:HA   | 2.01                     | 0.60              |
| 21:W:157:GLY:HA2  | 21:W:161:GLU:HG3  | 1.83                     | 0.60              |
| 21:W:293:ASP:OD2  | 21:W:296:LEU:N    | 2.33                     | 0.60              |
| 22:X:277:LEU:HD12 | 22:X:278:ARG:N    | 2.17                     | 0.60              |
| 23:Y:192:ARG:HB2  | 23:Y:291:HIS:HD2  | 1.66                     | 0.60              |
| 23:Y:215:ASP:O    | 23:Y:218:THR:HG22 | 2.01                     | 0.60              |
| 23:Y:301:ILE:HD12 | 23:Y:342:ARG:NH2  | 2.09                     | 0.60              |
| 24:Z:126:VAL:O    | 27:c:212:LEU:HD11 | 2.01                     | 0.60              |
| 25:a:186:LYS:O    | 25:a:188:LEU:HD22 | 2.02                     | 0.60              |
| 1:A:153:LEU:HD22  | 1:A:154:PRO:HD2   | 1.82                     | 0.60              |
| 1:A:284:ARG:HG3   | 1:A:296:GLN:HE21  | 1.66                     | 0.60              |
| 3:C:154:LEU:HD22  | 3:C:157:GLN:OE1   | 2.02                     | 0.60              |
| 3:C:351:MET:HB3   | 3:C:391:MET:HE3   | 1.84                     | 0.60              |
| 5:E:173:TYR:HB2   | 5:E:282:PRO:HG3   | 1.83                     | 0.60              |
| 20:V:65:ARG:HA    | 20:V:68:ASP:OD1   | 2.01                     | 0.60              |
| 20:V:309:MET:CE   | 20:V:331:LEU:HB3  | 2.32                     | 0.60              |
| 20:V:497:PRO:CG   | 20:V:498:PRO:HD3  | 2.30                     | 0.60              |
| 21:W:79:GLU:CD    | 21:W:82:LEU:HD12  | 2.27                     | 0.60              |
| 22:X:388:PHE:CD2  | 23:Y:358:ARG:HD2  | 2.37                     | 0.60              |
| 23:Y:113:ARG:O    | 23:Y:113:ARG:HD3  | 2.02                     | 0.60              |
| 23:Y:154:ASN:O    | 23:Y:158:THR:OG1  | 2.17                     | 0.60              |
| 25:a:370:GLN:HE22 | 28:d:244:LYS:HB3  | 1.66                     | 0.60              |
| 30:f:637:LYS:HG2  | 30:f:677:HIS:HD2  | 1.66                     | 0.60              |
| 30:f:744:MET:C    | 30:f:744:MET:HE2  | 2.26                     | 0.60              |
| 7:h:35:VAL:HG11   | 7:h:193:THR:HG21  | 1.84                     | 0.60              |
| 14:o:36:HIS:HB2   | 14:o:57:THR:HG21  | 1.84                     | 0.60              |
| 31:F:188:ILE:HG12 | 31:F:235:LEU:CD2  | 2.26                     | 0.60              |
| 32:U:357:LYS:HA   | 32:U:357:LYS:CE   | 2.25                     | 0.60              |
| 1:A:219:GLY:O     | 1:A:381:THR:HB    | 2.02                     | 0.60              |
| 2:B:235:LEU:HD13  | 2:B:235:LEU:O     | 2.01                     | 0.60              |
| 4:D:173:GLN:NE2   | 4:D:334:PRO:HD2   | 2.15                     | 0.60              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:D:254:ALA:CB    | 4:D:262:ILE:HD11  | 2.32                     | 0.60              |
| 11:L:84:LEU:HD23  | 11:L:132:LEU:HD11 | 1.83                     | 0.60              |
| 20:V:417:ILE:HD11 | 20:V:421:ASP:HB3  | 1.84                     | 0.60              |
| 26:b:126:LYS:HA   | 26:b:129:LYS:HE3  | 1.82                     | 0.60              |
| 26:b:132:LYS:HE2  | 26:b:133:LYS:NZ   | 2.15                     | 0.60              |
| 30:f:106:LEU:HG   | 30:f:109:ILE:HG21 | 1.83                     | 0.60              |
| 30:f:445:LEU:HD22 | 30:f:480:GLY:C    | 2.27                     | 0.60              |
| 30:f:673:ARG:HH22 | 30:f:785:ARG:N    | 1.99                     | 0.60              |
| 31:F:95:GLU:HG3   | 31:F:97:LEU:HD13  | 1.84                     | 0.60              |
| 31:F:373:MET:CE   | 31:F:415:LEU:HD11 | 2.21                     | 0.60              |
| 32:U:554:LEU:HD12 | 32:U:588:MET:CE   | 2.32                     | 0.60              |
| 1:A:284:ARG:NH1   | 31:F:289:ASP:OD2  | 2.34                     | 0.60              |
| 3:C:334:ARG:HG2   | 23:Y:175:ASP:HB3  | 1.84                     | 0.60              |
| 4:D:43:ARG:NH1    | 4:D:43:ARG:HB2    | 2.15                     | 0.60              |
| 12:M:161:TRP:CG   | 12:M:182:LYS:HZ1  | 2.19                     | 0.60              |
| 21:W:148:THR:O    | 21:W:152:ILE:HG12 | 2.02                     | 0.60              |
| 21:W:308:LEU:CD2  | 21:W:315:MET:HE1  | 2.30                     | 0.60              |
| 23:Y:47:ASP:CG    | 23:Y:113:ARG:HE   | 2.09                     | 0.60              |
| 23:Y:53:TYR:CE2   | 23:Y:70:LEU:HD13  | 2.36                     | 0.60              |
| 23:Y:241:ILE:HG23 | 23:Y:261:PHE:HE1  | 1.67                     | 0.60              |
| 24:Z:38:VAL:HG22  | 24:Z:112:MET:SD   | 2.42                     | 0.60              |
| 24:Z:88:ARG:O     | 24:Z:88:ARG:HD2   | 2.01                     | 0.60              |
| 25:a:273:GLN:NE2  | 25:a:302:ILE:HD11 | 2.17                     | 0.60              |
| 30:f:62:ARG:O     | 30:f:65:GLU:HG2   | 2.02                     | 0.60              |
| 30:f:126:ILE:HD11 | 30:f:178:LYS:CD   | 2.31                     | 0.60              |
| 32:U:611:ASN:OD1  | 32:U:612:ASP:N    | 2.34                     | 0.60              |
| 1:A:223:THR:HG23  | 2:B:319:PHE:HB3   | 1.82                     | 0.60              |
| 3:C:250:GLU:C     | 3:C:251:ILE:HG13  | 2.27                     | 0.60              |
| 15:P:13:MET:HB3   | 15:P:162:LEU:HD11 | 1.82                     | 0.60              |
| 15:P:64:GLN:OE1   | 16:Q:86:ARG:NH2   | 2.35                     | 0.60              |
| 16:Q:137:PHE:HB3  | 17:r:134:VAL:HG21 | 1.84                     | 0.60              |
| 20:V:437:ILE:HG22 | 28:d:146:GLY:N    | 2.17                     | 0.60              |
| 21:W:219:THR:CG2  | 21:W:223:LYS:H    | 2.14                     | 0.60              |
| 22:X:377:ILE:HG23 | 23:Y:358:ARG:HH12 | 1.66                     | 0.60              |
| 24:Z:11:VAL:HG12  | 24:Z:15:VAL:CG1   | 2.32                     | 0.60              |
| 25:a:39:LEU:HD23  | 25:a:40:GLN:OE1   | 2.00                     | 0.60              |
| 25:a:363:MET:HE2  | 25:a:363:MET:CA   | 2.29                     | 0.60              |
| 27:c:63:ASP:OD1   | 32:U:506:ALA:HB2  | 2.02                     | 0.60              |
| 27:c:167:MET:HG3  | 27:c:172:HIS:O    | 2.01                     | 0.60              |
| 30:f:65:GLU:CD    | 30:f:97:LYS:HE2   | 2.26                     | 0.60              |
| 32:U:803:LYS:HG2  | 32:U:893:THR:HB   | 1.84                     | 0.60              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:323:ARG:HH12  | 1:A:433:ASN:CA    | 2.15                     | 0.60              |
| 2:B:102:LEU:O     | 2:B:102:LEU:HD13  | 2.02                     | 0.60              |
| 21:W:124:LEU:O    | 21:W:127:THR:HG22 | 2.02                     | 0.60              |
| 21:W:228:ASN:O    | 21:W:231:ILE:HG22 | 2.02                     | 0.60              |
| 21:W:330:LYS:HG2  | 21:W:331:GLY:N    | 2.16                     | 0.60              |
| 24:Z:15:VAL:HG23  | 24:Z:53:SER:OG    | 2.02                     | 0.60              |
| 28:d:148:TYR:CD1  | 28:d:178:ILE:HD11 | 2.36                     | 0.60              |
| 30:f:63:LEU:O     | 30:f:67:ASP:HB2   | 2.01                     | 0.60              |
| 7:h:188:HIS:O     | 7:h:192:LEU:HD12  | 2.02                     | 0.60              |
| 14:o:64:LEU:HD22  | 14:o:75:PRO:HB3   | 1.84                     | 0.60              |
| 31:F:410:ARG:O    | 31:F:410:ARG:HG3  | 2.00                     | 0.60              |
| 32:U:803:LYS:HD2  | 32:U:875:PHE:HA   | 1.84                     | 0.60              |
| 1:A:262:GLU:HA    | 1:A:265:ARG:CD    | 2.32                     | 0.60              |
| 4:D:115:ILE:HD12  | 4:D:121:ARG:CZ    | 2.32                     | 0.60              |
| 22:X:332:GLU:OE2  | 22:X:364:LYS:HE3  | 2.02                     | 0.60              |
| 23:Y:117:LYS:HE2  | 23:Y:151:TYR:CD1  | 2.36                     | 0.60              |
| 30:f:157:GLU:O    | 30:f:160:ARG:HG2  | 2.01                     | 0.60              |
| 30:f:833:PHE:HA   | 30:f:836:GLU:OE2  | 2.01                     | 0.60              |
| 32:U:552:ILE:HD13 | 32:U:570:LEU:HD11 | 1.82                     | 0.60              |
| 32:U:602:LEU:HD23 | 32:U:622:LEU:HG   | 1.84                     | 0.60              |
| 1:A:171:ASP:OD1   | 1:A:171:ASP:N     | 2.34                     | 0.59              |
| 1:A:204:LEU:HB3   | 1:A:206:ILE:HD13  | 1.82                     | 0.59              |
| 2:B:363:ARG:O     | 2:B:367:ILE:HG22  | 2.02                     | 0.59              |
| 5:E:84:ARG:HD2    | 27:c:50:PRO:CG    | 2.31                     | 0.59              |
| 21:W:105:VAL:CG2  | 21:W:140:ILE:HD13 | 2.27                     | 0.59              |
| 21:W:254:PRO:N    | 21:W:262:LYS:HZ3  | 2.00                     | 0.59              |
| 21:W:265:GLN:HG2  | 21:W:336:PRO:HD3  | 1.83                     | 0.59              |
| 23:Y:48:ASN:HD22  | 23:Y:73:MET:HE2   | 1.67                     | 0.59              |
| 24:Z:19:VAL:HG22  | 24:Z:95:TYR:CE2   | 2.36                     | 0.59              |
| 26:b:6:THR:HA     | 26:b:108:ARG:O    | 2.02                     | 0.59              |
| 27:c:139:ARG:HG3  | 27:c:139:ARG:HH11 | 1.67                     | 0.59              |
| 27:c:180:ASN:ND2  | 32:U:725:MET:HG3  | 2.16                     | 0.59              |
| 28:d:71:PHE:CE2   | 28:d:75:MET:HE2   | 2.30                     | 0.59              |
| 30:f:3:GLU:HG2    | 30:f:7:ASP:CG     | 2.27                     | 0.59              |
| 30:f:4:GLY:O      | 30:f:6:ARG:NE     | 2.35                     | 0.59              |
| 31:F:296:PHE:CE1  | 31:F:298:SER:HB3  | 2.37                     | 0.59              |
| 1:A:77:LEU:HD12   | 30:f:694:LEU:HD12 | 1.83                     | 0.59              |
| 2:B:79:ILE:HA     | 2:B:82:GLN:HE21   | 1.67                     | 0.59              |
| 20:V:323:GLY:CA   | 29:e:24:ALA:HA    | 2.31                     | 0.59              |
| 23:Y:229:ILE:HD11 | 23:Y:298:GLU:HG2  | 1.84                     | 0.59              |
| 27:c:303:MET:SD   | 27:c:303:MET:N    | 2.75                     | 0.59              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 30:f:182:GLU:HG3  | 30:f:183:PRO:CD   | 2.33                     | 0.59              |
| 30:f:445:LEU:HD22 | 30:f:481:SER:HA   | 1.83                     | 0.59              |
| 30:f:821:LEU:HD21 | 30:f:882:LEU:HD22 | 1.83                     | 0.59              |
| 31:F:224:LEU:HD12 | 31:F:330:ALA:HB3  | 1.83                     | 0.59              |
| 1:A:181:LYS:HD3   | 1:A:181:LYS:C     | 2.27                     | 0.59              |
| 21:W:312:MET:CG   | 21:W:365:ILE:HD11 | 2.32                     | 0.59              |
| 25:a:174:LYS:HG3  | 25:a:178:ARG:NH2  | 2.17                     | 0.59              |
| 30:f:275:MET:N    | 30:f:275:MET:HE3  | 2.16                     | 0.59              |
| 30:f:690:VAL:HB   | 30:f:691:PRO:HD3  | 1.84                     | 0.59              |
| 32:U:22:PHE:C     | 32:U:26:LYS:HZ2   | 2.10                     | 0.59              |
| 32:U:268:LEU:HD23 | 32:U:325:MET:CB   | 2.32                     | 0.59              |
| 32:U:626:LEU:HD13 | 32:U:632:GLN:NE2  | 2.16                     | 0.59              |
| 2:B:54:PRO:HA     | 30:f:834:ASP:OD2  | 2.03                     | 0.59              |
| 2:B:333:ARG:HB2   | 2:B:336:THR:HG22  | 1.84                     | 0.59              |
| 3:C:76:VAL:O      | 3:C:76:VAL:HG13   | 2.02                     | 0.59              |
| 4:D:200:ARG:HG2   | 4:D:200:ARG:NH1   | 2.15                     | 0.59              |
| 20:V:192:MET:HE3  | 20:V:230:PHE:CE2  | 2.37                     | 0.59              |
| 24:Z:251:LEU:O    | 24:Z:251:LEU:HD23 | 2.02                     | 0.59              |
| 25:a:179:PHE:HE1  | 25:a:196:ARG:NE   | 1.99                     | 0.59              |
| 28:d:25:ARG:HE    | 28:d:54:ILE:HD11  | 1.68                     | 0.59              |
| 28:d:120:GLU:OE1  | 28:d:120:GLU:N    | 2.32                     | 0.59              |
| 30:f:125:ILE:HD11 | 30:f:128:VAL:CG2  | 2.33                     | 0.59              |
| 30:f:465:LEU:O    | 30:f:466:LEU:HD22 | 2.02                     | 0.59              |
| 32:U:11:LEU:O     | 32:U:12:LEU:HD12  | 2.02                     | 0.59              |
| 32:U:509:GLY:HA3  | 32:U:544:ILE:CG1  | 2.26                     | 0.59              |
| 32:U:623:GLY:HA3  | 32:U:658:ILE:HD11 | 1.84                     | 0.59              |
| 2:B:223:ILE:CB    | 2:B:347:ILE:HD12  | 2.31                     | 0.59              |
| 2:B:251:VAL:HB    | 2:B:254:GLU:OE2   | 2.03                     | 0.59              |
| 3:C:271:ARG:O     | 3:C:275:GLU:HG2   | 2.02                     | 0.59              |
| 3:C:374:ARG:NE    | 3:C:374:ARG:HA    | 2.17                     | 0.59              |
| 20:V:201:ARG:NE   | 20:V:201:ARG:HA   | 2.18                     | 0.59              |
| 20:V:344:ASP:OD1  | 20:V:345:ARG:N    | 2.36                     | 0.59              |
| 21:W:202:THR:CG2  | 21:W:233:LEU:HD22 | 2.28                     | 0.59              |
| 23:Y:186:LEU:HD22 | 23:Y:287:LEU:CD1  | 2.32                     | 0.59              |
| 23:Y:229:ILE:HB   | 23:Y:299:MET:CE   | 2.32                     | 0.59              |
| 27:c:163:ILE:HG23 | 27:c:201:TYR:HD1  | 1.66                     | 0.59              |
| 27:c:181:LEU:O    | 27:c:181:LEU:HD23 | 2.02                     | 0.59              |
| 28:d:89:LEU:HD12  | 28:d:89:LEU:O     | 2.03                     | 0.59              |
| 30:f:833:PHE:CE1  | 30:f:842:VAL:HG23 | 2.34                     | 0.59              |
| 16:q:184:ASP:N    | 16:q:184:ASP:OD1  | 2.34                     | 0.59              |
| 31:F:167:GLU:OE1  | 31:F:167:GLU:N    | 2.32                     | 0.59              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:97:ARG:HB3    | 1:A:97:ARG:CZ     | 2.32                     | 0.59              |
| 1:A:345:LEU:HD11  | 1:A:426:THR:CG2   | 2.32                     | 0.59              |
| 1:A:361:SER:HB3   | 30:f:849:ALA:HB3  | 1.84                     | 0.59              |
| 3:C:168:PRO:HG3   | 3:C:175:PHE:CE2   | 2.37                     | 0.59              |
| 3:C:280:LEU:HD23  | 3:C:284:GLU:HG2   | 1.83                     | 0.59              |
| 12:M:39:ILE:HG21  | 12:M:189:ILE:HD12 | 1.85                     | 0.59              |
| 22:X:239:TYR:HD1  | 22:X:247:ALA:HA   | 1.68                     | 0.59              |
| 23:Y:50:MET:CE    | 23:Y:51:ALA:HB2   | 2.32                     | 0.59              |
| 28:d:22:GLU:O     | 28:d:26:LEU:HD23  | 2.03                     | 0.59              |
| 28:d:71:PHE:HE1   | 28:d:166:PHE:CZ   | 2.20                     | 0.59              |
| 28:d:120:GLU:H    | 28:d:120:GLU:CD   | 2.11                     | 0.59              |
| 30:f:216:MET:HA   | 30:f:219:LYS:NZ   | 2.17                     | 0.59              |
| 30:f:278:VAL:HG11 | 30:f:281:ILE:HG23 | 1.85                     | 0.59              |
| 30:f:800:LEU:HA   | 30:f:803:PHE:CE2  | 2.36                     | 0.59              |
| 32:U:885:MET:SD   | 32:U:888:GLN:HB2  | 2.43                     | 0.59              |
| 1:A:227:ARG:HB2   | 2:B:319:PHE:HB2   | 1.83                     | 0.59              |
| 3:C:258:ARG:NH1   | 3:C:260:GLU:O     | 2.36                     | 0.59              |
| 4:D:109:SER:HB2   | 4:D:111:TYR:HE1   | 1.68                     | 0.59              |
| 5:E:248:SER:HA    | 5:E:251:ARG:NH2   | 2.18                     | 0.59              |
| 14:O:64:LEU:HD22  | 14:O:75:PRO:HB3   | 1.85                     | 0.59              |
| 20:V:230:PHE:O    | 20:V:234:ARG:HG2  | 2.03                     | 0.59              |
| 22:X:294:SER:HA   | 22:X:330:LEU:HD11 | 1.85                     | 0.59              |
| 23:Y:314:LEU:HD23 | 23:Y:354:VAL:HG13 | 1.84                     | 0.59              |
| 24:Z:188:SER:O    | 24:Z:192:THR:N    | 2.31                     | 0.59              |
| 25:a:48:PRO:HB2   | 25:a:51:ALA:H     | 1.65                     | 0.59              |
| 25:a:366:LEU:C    | 25:a:366:LEU:HD13 | 2.28                     | 0.59              |
| 28:d:46:GLN:O     | 28:d:49:ILE:HG22  | 2.03                     | 0.59              |
| 28:d:235:THR:HA   | 28:d:238:PRO:CG   | 2.32                     | 0.59              |
| 30:f:125:ILE:HD11 | 30:f:128:VAL:HG22 | 1.85                     | 0.59              |
| 30:f:266:LEU:CD2  | 30:f:270:LEU:HD21 | 2.33                     | 0.59              |
| 30:f:686:LEU:HD12 | 30:f:687:ARG:HE   | 1.66                     | 0.59              |
| 32:U:97:VAL:O     | 32:U:101:ILE:HG22 | 2.03                     | 0.59              |
| 4:D:194:ILE:HG22  | 4:D:196:ILE:HG23  | 1.84                     | 0.59              |
| 4:D:234:GLU:HA    | 5:E:216:ARG:HH12  | 1.68                     | 0.59              |
| 5:E:117:PRO:HG3   | 31:F:94:ILE:HD13  | 1.85                     | 0.59              |
| 5:E:125:GLU:O     | 5:E:127:PRO:HD3   | 2.03                     | 0.59              |
| 20:V:431:PRO:HD2  | 20:V:432:GLU:OE2  | 2.03                     | 0.59              |
| 23:Y:275:LEU:HD11 | 23:Y:299:MET:HB3  | 1.85                     | 0.59              |
| 26:b:125:VAL:O    | 26:b:129:LYS:HB2  | 2.03                     | 0.59              |
| 28:d:148:TYR:O    | 28:d:151:VAL:HG12 | 2.03                     | 0.59              |
| 28:d:255:MET:C    | 28:d:255:MET:HE2  | 2.28                     | 0.59              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 30:f:418:LEU:HB3  | 30:f:421:ASP:OD2  | 2.01                     | 0.59              |
| 30:f:829:MET:H    | 30:f:829:MET:CE   | 2.04                     | 0.59              |
| 7:h:110:VAL:HG22  | 7:h:135:ILE:HD13  | 1.85                     | 0.59              |
| 32:U:138:PHE:CE2  | 32:U:162:VAL:HG21 | 2.38                     | 0.59              |
| 4:D:96:VAL:HG13   | 4:D:97:ASP:OD1    | 2.03                     | 0.59              |
| 10:K:233:GLU:O    | 10:K:237:VAL:HG23 | 2.03                     | 0.59              |
| 23:Y:79:ASP:O     | 23:Y:82:LYS:HG2   | 2.03                     | 0.59              |
| 25:a:205:LEU:HD12 | 25:a:268:LEU:HD11 | 1.85                     | 0.59              |
| 27:c:154:LYS:HE2  | 27:c:154:LYS:HA   | 1.85                     | 0.59              |
| 30:f:266:LEU:CD2  | 30:f:270:LEU:HD11 | 2.32                     | 0.59              |
| 30:f:524:MET:HE2  | 30:f:524:MET:O    | 2.02                     | 0.59              |
| 14:o:2:THR:N      | 14:o:170:SER:OG   | 2.30                     | 0.59              |
| 32:U:229:VAL:HG21 | 32:U:252:LEU:CD2  | 2.33                     | 0.59              |
| 32:U:458:ILE:O    | 32:U:462:LEU:HG   | 2.03                     | 0.59              |
| 32:U:580:ARG:HH22 | 32:U:771:PHE:HE2  | 1.49                     | 0.59              |
| 2:B:136:LEU:O     | 2:B:139:VAL:HG22  | 2.02                     | 0.59              |
| 2:B:222:VAL:HG22  | 2:B:328:ILE:HG12  | 1.85                     | 0.59              |
| 4:D:168:GLY:CA    | 33:D:501:ATP:HN62 | 2.16                     | 0.59              |
| 4:D:256:GLU:OE1   | 4:D:256:GLU:HA    | 2.03                     | 0.59              |
| 4:D:392:TYR:CE1   | 21:W:136:ILE:HD12 | 2.38                     | 0.59              |
| 17:R:46:MET:CE    | 36:R:301:LDZ:H17  | 2.32                     | 0.59              |
| 20:V:256:ARG:O    | 20:V:256:ARG:HD2  | 2.03                     | 0.59              |
| 21:W:55:ARG:HD3   | 21:W:96:GLN:OE1   | 2.03                     | 0.59              |
| 23:Y:232:GLU:CG   | 23:Y:234:PRO:HD2  | 2.26                     | 0.59              |
| 26:b:138:VAL:HG22 | 26:b:140:ILE:HD12 | 1.84                     | 0.59              |
| 28:d:2:TYR:HB2    | 28:d:32:GLU:OE2   | 2.02                     | 0.59              |
| 30:f:177:GLU:HG2  | 30:f:835:GLU:CA   | 2.32                     | 0.59              |
| 30:f:285:CYS:O    | 30:f:288:VAL:HG12 | 2.02                     | 0.59              |
| 15:p:58:ASP:OD1   | 16:q:93:ARG:NH2   | 2.35                     | 0.59              |
| 32:U:142:LEU:HD13 | 32:U:147:TYR:HE1  | 1.68                     | 0.59              |
| 20:V:486:ILE:HD11 | 24:Z:268:SER:CB   | 2.33                     | 0.58              |
| 22:X:153:LEU:HG   | 22:X:157:LEU:HD23 | 1.85                     | 0.58              |
| 22:X:286:ALA:HA   | 22:X:309:TYR:CD2  | 2.25                     | 0.58              |
| 23:Y:231:LEU:CD1  | 23:Y:236:LEU:HG   | 2.33                     | 0.58              |
| 23:Y:371:LYS:HZ3  | 23:Y:372:LYS:HE2  | 1.65                     | 0.58              |
| 28:d:170:LEU:O    | 28:d:173:THR:HG22 | 2.03                     | 0.58              |
| 13:n:5:MET:HE1    | 13:n:160:ALA:HB3  | 1.85                     | 0.58              |
| 31:F:366:MET:HE2  | 31:F:399:VAL:HG11 | 1.85                     | 0.58              |
| 32:U:807:LYS:H    | 32:U:807:LYS:HD2  | 1.67                     | 0.58              |
| 2:B:155:LYS:HZ3   | 2:B:155:LYS:HB2   | 1.66                     | 0.58              |
| 4:D:164:TYR:H     | 4:D:222:HIS:CE1   | 2.21                     | 0.58              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:E:143:ARG:HH11  | 5:E:143:ARG:HG3   | 1.68                     | 0.58              |
| 5:E:198:VAL:HG11  | 5:E:232:MET:HG2   | 1.85                     | 0.58              |
| 20:V:387:GLN:OE1  | 20:V:387:GLN:HA   | 2.02                     | 0.58              |
| 22:X:293:ALA:HA   | 22:X:301:ASP:OD1  | 2.03                     | 0.58              |
| 22:X:299:LEU:O    | 22:X:299:LEU:HD13 | 2.03                     | 0.58              |
| 22:X:325:LYS:HE2  | 22:X:325:LYS:CA   | 2.31                     | 0.58              |
| 24:Z:190:ARG:CZ   | 27:c:300:LEU:HD22 | 2.32                     | 0.58              |
| 25:a:230:ARG:HG2  | 25:a:230:ARG:O    | 2.02                     | 0.58              |
| 26:b:71:ILE:H     | 26:b:71:ILE:HD12  | 1.68                     | 0.58              |
| 26:b:142:ASN:N    | 26:b:171:VAL:O    | 2.37                     | 0.58              |
| 27:c:160:PHE:CE1  | 27:c:202:SER:HB2  | 2.38                     | 0.58              |
| 27:c:292:MET:CE   | 28:d:253:LEU:HD22 | 2.32                     | 0.58              |
| 30:f:198:HIS:HA   | 30:f:201:GLU:OE2  | 2.02                     | 0.58              |
| 30:f:372:LEU:HD13 | 30:f:410:ALA:HB2  | 1.84                     | 0.58              |
| 30:f:719:PRO:HG2  | 30:f:721:VAL:HG12 | 1.85                     | 0.58              |
| 30:f:784:ASP:HA   | 30:f:787:LEU:CD2  | 2.33                     | 0.58              |
| 3:C:31:LEU:HA     | 3:C:34:ILE:HG22   | 1.83                     | 0.58              |
| 5:E:59:GLU:OE2    | 5:E:72:LYS:HD3    | 2.03                     | 0.58              |
| 9:J:65:LEU:HD11   | 9:J:71:MET:HE3    | 1.84                     | 0.58              |
| 14:O:101:LEU:HD23 | 14:O:102:GLY:N    | 2.18                     | 0.58              |
| 19:T:108:ASN:HB3  | 19:T:110:MET:HE2  | 1.86                     | 0.58              |
| 20:V:175:MET:CE   | 20:V:183:GLU:HB2  | 2.32                     | 0.58              |
| 20:V:419:LEU:HD13 | 20:V:458:VAL:HG23 | 1.86                     | 0.58              |
| 21:W:147:LYS:HB2  | 21:W:147:LYS:NZ   | 2.18                     | 0.58              |
| 21:W:215:GLN:HG2  | 21:W:223:LYS:CE   | 2.33                     | 0.58              |
| 22:X:205:LYS:NZ   | 22:X:206:LEU:HD23 | 2.18                     | 0.58              |
| 22:X:362:GLU:OE2  | 22:X:380:GLN:NE2  | 2.29                     | 0.58              |
| 23:Y:117:LYS:O    | 23:Y:120:ALA:N    | 2.35                     | 0.58              |
| 23:Y:300:ARG:HH11 | 23:Y:300:ARG:HG3  | 1.67                     | 0.58              |
| 24:Z:205:LEU:HD12 | 25:a:353:LEU:HD22 | 1.84                     | 0.58              |
| 24:Z:240:VAL:HG23 | 24:Z:243:GLN:HE22 | 1.69                     | 0.58              |
| 25:a:186:LYS:CD   | 25:a:221:VAL:HG22 | 2.34                     | 0.58              |
| 28:d:99:LEU:CD2   | 28:d:122:LEU:HD11 | 2.33                     | 0.58              |
| 30:f:268:LEU:HA   | 30:f:272:LEU:HD12 | 1.84                     | 0.58              |
| 13:n:161:LEU:O    | 13:n:165:MET:HG3  | 2.03                     | 0.58              |
| 31:F:146:LYS:N    | 31:F:149:ASP:OD2  | 2.36                     | 0.58              |
| 32:U:210:LYS:H    | 32:U:210:LYS:HE2  | 1.69                     | 0.58              |
| 1:A:115:VAL:HG22  | 1:A:119:ALA:O     | 2.02                     | 0.58              |
| 3:C:351:MET:HE2   | 3:C:391:MET:HE3   | 1.85                     | 0.58              |
| 4:D:384:MET:O     | 4:D:387:VAL:HG12  | 2.04                     | 0.58              |
| 14:O:98:ALA:HB1   | 14:O:128:MET:HE1  | 1.86                     | 0.58              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 18:S:68:ILE:HD11  | 18:S:92:LEU:HD13  | 1.85                     | 0.58              |
| 21:W:138:VAL:HG12 | 21:W:176:SER:OG   | 2.04                     | 0.58              |
| 21:W:142:ARG:NH1  | 21:W:146:THR:HB   | 2.18                     | 0.58              |
| 21:W:150:ALA:HA   | 21:W:153:LYS:NZ   | 2.18                     | 0.58              |
| 21:W:251:TYR:CZ   | 21:W:267:LEU:HD21 | 2.38                     | 0.58              |
| 21:W:307:LYS:CG   | 21:W:315:MET:HE2  | 2.33                     | 0.58              |
| 22:X:385:LEU:HG   | 22:X:387:ILE:CD1  | 2.33                     | 0.58              |
| 23:Y:176:ARG:HH11 | 23:Y:179:ARG:HH22 | 1.52                     | 0.58              |
| 23:Y:276:ALA:O    | 23:Y:279:GLU:HB3  | 2.02                     | 0.58              |
| 24:Z:94:TRP:O     | 24:Z:121:LEU:HA   | 2.02                     | 0.58              |
| 26:b:111:ALA:N    | 26:b:139:ASP:O    | 2.25                     | 0.58              |
| 27:c:33:ILE:HG22  | 27:c:34:SER:N     | 2.18                     | 0.58              |
| 27:c:120:CYS:SG   | 27:c:156:VAL:HG12 | 2.42                     | 0.58              |
| 30:f:228:LYS:H    | 30:f:228:LYS:HE2  | 1.67                     | 0.58              |
| 31:F:357:PRO:HB3  | 31:F:361:ALA:CB   | 2.33                     | 0.58              |
| 32:U:449:ILE:HG12 | 32:U:450:HIS:HD2  | 1.68                     | 0.58              |
| 32:U:498:LYS:HD3  | 32:U:531:ASP:OD2  | 2.04                     | 0.58              |
| 32:U:634:PRO:HG2  | 32:U:667:GLU:OE2  | 2.03                     | 0.58              |
| 1:A:230:ALA:HA    | 1:A:233:THR:CG2   | 2.32                     | 0.58              |
| 1:A:365:GLU:O     | 1:A:367:ASP:N     | 2.35                     | 0.58              |
| 2:B:64:LYS:O      | 30:f:646:MET:HE1  | 2.04                     | 0.58              |
| 3:C:287:LYS:H     | 3:C:287:LYS:CD    | 2.16                     | 0.58              |
| 20:V:218:TYR:HA   | 20:V:221:LEU:HB2  | 1.85                     | 0.58              |
| 21:W:267:LEU:HD12 | 21:W:296:LEU:CD2  | 2.34                     | 0.58              |
| 21:W:373:ILE:HA   | 25:a:326:GLU:CG   | 2.32                     | 0.58              |
| 23:Y:53:TYR:OH    | 23:Y:66:ASP:HB2   | 2.04                     | 0.58              |
| 24:Z:23:PHE:HD2   | 24:Z:126:VAL:CG1  | 2.16                     | 0.58              |
| 30:f:778:LEU:HD23 | 30:f:778:LEU:H    | 1.68                     | 0.58              |
| 31:F:279:ALA:HB1  | 31:F:280:PRO:CD   | 2.32                     | 0.58              |
| 32:U:138:PHE:CE2  | 32:U:162:VAL:HG11 | 2.39                     | 0.58              |
| 32:U:449:ILE:HG23 | 32:U:450:HIS:CD2  | 2.39                     | 0.58              |
| 1:A:177:VAL:HG12  | 1:A:224:LEU:CD2   | 2.34                     | 0.58              |
| 2:B:361:LYS:C     | 2:B:384:ILE:HD11  | 2.28                     | 0.58              |
| 3:C:71:SER:HB2    | 4:D:112:TYR:HB3   | 1.84                     | 0.58              |
| 3:C:161:ILE:CG1   | 3:C:203:VAL:HG21  | 2.33                     | 0.58              |
| 3:C:374:ARG:HD3   | 4:D:190:LEU:CD1   | 2.32                     | 0.58              |
| 4:D:52:GLU:HA     | 4:D:52:GLU:OE1    | 2.03                     | 0.58              |
| 20:V:223:LYS:O    | 20:V:225:ASP:N    | 2.35                     | 0.58              |
| 21:W:120:ILE:O    | 21:W:124:LEU:HB2  | 2.03                     | 0.58              |
| 22:X:398:GLU:OE1  | 23:Y:365:GLN:NE2  | 2.36                     | 0.58              |
| 23:Y:221:THR:HA   | 23:Y:224:VAL:HG12 | 1.85                     | 0.58              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 30:f:180:GLN:CG   | 30:f:219:LYS:HD3  | 2.34                     | 0.58              |
| 30:f:545:LYS:CE   | 30:f:547:GLU:HB3  | 2.25                     | 0.58              |
| 30:f:557:TRP:HA   | 30:f:560:LEU:CG   | 2.34                     | 0.58              |
| 6:g:112:ASP:OD2   | 6:g:113:MET:HE3   | 2.02                     | 0.58              |
| 14:o:36:HIS:CB    | 14:o:57:THR:HG21  | 2.34                     | 0.58              |
| 31:F:343:LEU:HD23 | 31:F:348:LEU:HD11 | 1.86                     | 0.58              |
| 32:U:597:LYS:HE2  | 32:U:597:LYS:HA   | 1.85                     | 0.58              |
| 2:B:152:LEU:HA    | 2:B:158:ALA:O     | 2.03                     | 0.58              |
| 2:B:378:VAL:HG21  | 2:B:419:PHE:CD2   | 2.39                     | 0.58              |
| 3:C:132:ASP:HB3   | 3:C:135:VAL:CG2   | 2.31                     | 0.58              |
| 21:W:328:LEU:CD2  | 21:W:341:PHE:HB3  | 2.34                     | 0.58              |
| 22:X:336:ILE:HG12 | 22:X:374:PHE:HE1  | 1.68                     | 0.58              |
| 23:Y:278:VAL:HA   | 23:Y:281:GLU:CG   | 2.32                     | 0.58              |
| 25:a:61:GLU:O     | 25:a:65:SER:N     | 2.21                     | 0.58              |
| 25:a:141:MET:HE2  | 25:a:152:HIS:NE2  | 2.18                     | 0.58              |
| 25:a:321:LYS:HG3  | 25:a:335:TRP:CE3  | 2.39                     | 0.58              |
| 26:b:30:GLN:O     | 26:b:33:VAL:HG22  | 2.04                     | 0.58              |
| 28:d:30:LEU:CD1   | 28:d:31:LEU:HD13  | 2.34                     | 0.58              |
| 28:d:155:LYS:CE   | 28:d:167:ILE:HG23 | 2.32                     | 0.58              |
| 30:f:440:ILE:HG13 | 30:f:441:LYS:HD2  | 1.85                     | 0.58              |
| 31:F:79:LYS:HE3   | 31:F:79:LYS:CA    | 2.31                     | 0.58              |
| 32:U:471:ASP:OD2  | 32:U:508:THR:HB   | 2.04                     | 0.58              |
| 32:U:646:PRO:HB3  | 32:U:680:VAL:HG21 | 1.85                     | 0.58              |
| 32:U:791:LEU:HD11 | 32:U:795:LEU:O    | 2.03                     | 0.58              |
| 1:A:297:ARG:HG2   | 31:F:290:ALA:HB1  | 1.86                     | 0.58              |
| 2:B:292:THR:HG21  | 2:B:333:ARG:NH1   | 2.14                     | 0.58              |
| 5:E:309:ARG:HH12  | 5:E:336:ASP:HA    | 1.69                     | 0.58              |
| 5:E:341:ALA:HB3   | 31:F:345:SER:HB2  | 1.84                     | 0.58              |
| 13:N:15:LEU:HD11  | 13:N:102:ALA:CB   | 2.33                     | 0.58              |
| 21:W:312:MET:HE2  | 21:W:312:MET:N    | 2.19                     | 0.58              |
| 23:Y:200:LEU:O    | 23:Y:204:THR:HG23 | 2.03                     | 0.58              |
| 26:b:86:PHE:O     | 26:b:90:ILE:HD12  | 2.04                     | 0.58              |
| 27:c:163:ILE:HD11 | 27:c:199:HIS:CA   | 2.25                     | 0.58              |
| 30:f:830:LEU:HD12 | 30:f:861:THR:HB   | 1.86                     | 0.58              |
| 31:F:305:GLU:HA   | 31:F:308:ARG:NH1  | 2.19                     | 0.58              |
| 32:U:247:GLN:HE22 | 32:U:904:LYS:HD2  | 1.69                     | 0.58              |
| 32:U:658:ILE:C    | 32:U:658:ILE:HD12 | 2.27                     | 0.58              |
| 1:A:239:ARG:HG2   | 2:B:319:PHE:HZ    | 1.66                     | 0.58              |
| 2:B:116:ILE:HD13  | 2:B:132:TYR:CE2   | 2.39                     | 0.58              |
| 3:C:189:TYR:CE2   | 3:C:316:GLU:HA    | 2.38                     | 0.58              |
| 10:K:171:GLY:O    | 10:K:174:SER:OG   | 2.14                     | 0.58              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 20:V:249:THR:O    | 20:V:253:LEU:HG   | 2.04                     | 0.58              |
| 20:V:313:LEU:HD21 | 20:V:329:HIS:CE1  | 2.39                     | 0.58              |
| 20:V:414:TYR:OH   | 20:V:425:LYS:NZ   | 2.37                     | 0.58              |
| 21:W:216:GLU:HA   | 21:W:219:THR:HB   | 1.85                     | 0.58              |
| 22:X:180:LEU:O    | 22:X:181:SER:OG   | 2.18                     | 0.58              |
| 23:Y:67:VAL:HA    | 23:Y:70:LEU:CD2   | 2.34                     | 0.58              |
| 23:Y:138:LEU:HD21 | 23:Y:167:LEU:HB3  | 1.85                     | 0.58              |
| 30:f:255:VAL:HB   | 30:f:259:PHE:CZ   | 2.38                     | 0.58              |
| 30:f:556:ARG:NH2  | 30:f:627:GLU:OE1  | 2.36                     | 0.58              |
| 30:f:612:LEU:C    | 30:f:632:LYS:HD3  | 2.29                     | 0.58              |
| 30:f:771:LEU:HD22 | 30:f:807:ARG:NH2  | 2.19                     | 0.58              |
| 32:U:186:SER:C    | 32:U:187:LEU:HD23 | 2.29                     | 0.58              |
| 32:U:446:LEU:HD23 | 32:U:457:ILE:CG2  | 2.33                     | 0.58              |
| 32:U:802:TYR:OH   | 32:U:880:ASN:O    | 2.20                     | 0.58              |
| 3:C:334:ARG:HG2   | 23:Y:175:ASP:CB   | 2.34                     | 0.58              |
| 4:D:370:ILE:HG21  | 4:D:407:ILE:HG22  | 1.85                     | 0.58              |
| 5:E:170:CYS:SG    | 5:E:299:ILE:HD13  | 2.43                     | 0.58              |
| 20:V:401:ASN:O    | 20:V:405:THR:HG23 | 2.03                     | 0.58              |
| 21:W:120:ILE:O    | 21:W:124:LEU:N    | 2.36                     | 0.58              |
| 25:a:180:LEU:CD1  | 25:a:222:LEU:HG   | 2.33                     | 0.58              |
| 25:a:291:LEU:HD13 | 25:a:333:MET:HG2  | 1.86                     | 0.58              |
| 26:b:188:ILE:HD12 | 26:b:188:ILE:N    | 2.18                     | 0.58              |
| 2:B:118:ASP:OD1   | 2:B:119:ASN:N     | 2.37                     | 0.57              |
| 2:B:135:ILE:HA    | 2:B:159:VAL:HB    | 1.85                     | 0.57              |
| 3:C:164:VAL:O     | 3:C:165:ILE:HD13  | 2.03                     | 0.57              |
| 16:Q:119:ASP:OD1  | 16:Q:119:ASP:N    | 2.37                     | 0.57              |
| 20:V:120:PHE:HB3  | 20:V:159:LEU:HD11 | 1.86                     | 0.57              |
| 21:W:151:THR:HA   | 21:W:154:GLU:CG   | 2.33                     | 0.57              |
| 21:W:253:THR:O    | 21:W:256:ILE:N    | 2.35                     | 0.57              |
| 23:Y:15:PRO:HD3   | 23:Y:143:TYR:HE1  | 1.68                     | 0.57              |
| 23:Y:371:LYS:HD3  | 23:Y:372:LYS:N    | 2.19                     | 0.57              |
| 25:a:186:LYS:HG2  | 25:a:193:GLN:HE22 | 1.68                     | 0.57              |
| 27:c:58:LEU:O     | 27:c:70:ILE:HG22  | 2.03                     | 0.57              |
| 32:U:198:LEU:O    | 32:U:201:LEU:N    | 2.36                     | 0.57              |
| 32:U:422:LEU:HD12 | 32:U:422:LEU:O    | 2.03                     | 0.57              |
| 1:A:196:LEU:CD1   | 30:f:345:PRO:HD2  | 2.29                     | 0.57              |
| 1:A:323:ARG:HG2   | 1:A:323:ARG:NH1   | 2.13                     | 0.57              |
| 2:B:81:ASN:O      | 2:B:85:MET:HE1    | 2.04                     | 0.57              |
| 2:B:357:ASP:HB3   | 2:B:360:THR:HG23  | 1.86                     | 0.57              |
| 5:E:75:ASN:ND2    | 31:F:130:GLN:OE1  | 2.36                     | 0.57              |
| 20:V:265:ASP:N    | 20:V:265:ASP:OD1  | 2.34                     | 0.57              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 23:Y:376:LEU:HD23 | 23:Y:376:LEU:O    | 2.03                     | 0.57              |
| 24:Z:17:LEU:HD22  | 27:c:39:LEU:HD12  | 1.86                     | 0.57              |
| 25:a:79:ILE:HG23  | 25:a:80:ILE:CD1   | 2.34                     | 0.57              |
| 26:b:138:VAL:HG12 | 26:b:160:LEU:HD11 | 1.86                     | 0.57              |
| 30:f:296:PHE:HD2  | 30:f:300:ARG:HH12 | 1.53                     | 0.57              |
| 30:f:369:ARG:NH2  | 30:f:370:MET:HE1  | 2.18                     | 0.57              |
| 30:f:416:MET:HE3  | 30:f:416:MET:N    | 2.19                     | 0.57              |
| 30:f:461:PRO:O    | 30:f:465:LEU:HG   | 2.04                     | 0.57              |
| 9:j:99:GLU:OE1    | 9:j:99:GLU:N      | 2.36                     | 0.57              |
| 32:U:798:PRO:HG2  | 32:U:880:ASN:ND2  | 2.19                     | 0.57              |
| 1:A:262:GLU:CD    | 1:A:265:ARG:HD2   | 2.28                     | 0.57              |
| 4:D:130:VAL:CG2   | 4:D:139:LEU:HD21  | 2.34                     | 0.57              |
| 5:E:238:ILE:HD11  | 5:E:256:THR:HG21  | 1.87                     | 0.57              |
| 5:E:334:LEU:HD12  | 5:E:334:LEU:O     | 2.04                     | 0.57              |
| 20:V:102:PRO:O    | 20:V:106:ARG:NH2  | 2.28                     | 0.57              |
| 20:V:482:PHE:O    | 20:V:485:ASP:HB3  | 2.04                     | 0.57              |
| 21:W:320:LEU:HD22 | 21:W:324:TYR:HD2  | 1.69                     | 0.57              |
| 21:W:343:SER:OG   | 21:W:344:THR:N    | 2.36                     | 0.57              |
| 23:Y:138:LEU:HD12 | 23:Y:142:PHE:HE2  | 1.68                     | 0.57              |
| 26:b:125:VAL:O    | 26:b:129:LYS:N    | 2.36                     | 0.57              |
| 27:c:219:ASN:O    | 27:c:223:LYS:HD2  | 2.04                     | 0.57              |
| 30:f:791:VAL:CG2  | 30:f:800:LEU:HD11 | 2.25                     | 0.57              |
| 10:k:169:ALA:O    | 10:k:174:SER:OG   | 2.19                     | 0.57              |
| 32:U:116:ALA:O    | 32:U:119:PRO:HD3  | 2.03                     | 0.57              |
| 1:A:99:THR:HG21   | 1:A:113:ILE:CD1   | 2.30                     | 0.57              |
| 1:A:226:ALA:O     | 1:A:229:VAL:HG12  | 2.03                     | 0.57              |
| 1:A:236:CYS:SG    | 1:A:267:LYS:HD3   | 2.44                     | 0.57              |
| 1:A:397:ILE:HG13  | 2:B:210:TYR:HB3   | 1.85                     | 0.57              |
| 2:B:229:GLY:O     | 2:B:391:SER:HB2   | 2.04                     | 0.57              |
| 2:B:333:ARG:HB2   | 2:B:336:THR:CG2   | 2.35                     | 0.57              |
| 3:C:137:LEU:HD12  | 3:C:220:VAL:CG2   | 2.34                     | 0.57              |
| 21:W:68:VAL:HG21  | 21:W:72:LYS:HE3   | 1.87                     | 0.57              |
| 21:W:289:ARG:HG3  | 21:W:289:ARG:NH1  | 2.19                     | 0.57              |
| 22:X:325:LYS:O    | 22:X:325:LYS:HD3  | 2.04                     | 0.57              |
| 24:Z:81:MET:HE1   | 27:c:94:LYS:CD    | 2.33                     | 0.57              |
| 25:a:101:ARG:HB2  | 25:a:114:CYS:SG   | 2.44                     | 0.57              |
| 27:c:122:LEU:HB2  | 27:c:200:TYR:CE2  | 2.39                     | 0.57              |
| 28:d:52:ARG:NH2   | 28:d:89:LEU:HD11  | 2.19                     | 0.57              |
| 30:f:107:LYS:HA   | 30:f:137:ARG:HH22 | 1.70                     | 0.57              |
| 30:f:285:CYS:O    | 30:f:289:VAL:HG23 | 2.04                     | 0.57              |
| 30:f:696:LEU:HD22 | 30:f:708:ASP:HB2  | 1.86                     | 0.57              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 32:U:48:LEU:O     | 32:U:48:LEU:HD13  | 2.04                     | 0.57              |
| 32:U:101:ILE:O    | 32:U:105:ILE:HG13 | 2.04                     | 0.57              |
| 32:U:806:CYS:O    | 32:U:876:GLN:NE2  | 2.33                     | 0.57              |
| 2:B:287:ILE:HG12  | 2:B:329:MET:CE    | 2.35                     | 0.57              |
| 3:C:198:LEU:O     | 3:C:198:LEU:HD13  | 2.04                     | 0.57              |
| 3:C:354:ALA:HA    | 3:C:358:GLU:OE2   | 2.04                     | 0.57              |
| 5:E:161:ARG:HE    | 21:W:173:THR:HA   | 1.69                     | 0.57              |
| 5:E:384:LEU:HB3   | 5:E:386:TYR:CE1   | 2.39                     | 0.57              |
| 20:V:72:LEU:HA    | 20:V:75:ILE:HD12  | 1.85                     | 0.57              |
| 21:W:158:ASP:H    | 21:W:161:GLU:CG   | 2.17                     | 0.57              |
| 23:Y:24:PHE:CE2   | 23:Y:28:LEU:HD22  | 2.40                     | 0.57              |
| 23:Y:316:LEU:HD21 | 23:Y:352:GLU:OE1  | 2.04                     | 0.57              |
| 25:a:226:ARG:HH12 | 25:a:230:ARG:CG   | 2.16                     | 0.57              |
| 28:d:49:ILE:HG23  | 28:d:50:LEU:HD22  | 1.85                     | 0.57              |
| 28:d:133:ILE:C    | 28:d:136:PRO:HD2  | 2.29                     | 0.57              |
| 29:e:30:LEU:HD12  | 29:e:32:GLU:OE2   | 2.04                     | 0.57              |
| 30:f:145:VAL:O    | 30:f:149:GLU:HG3  | 2.04                     | 0.57              |
| 30:f:217:LEU:HD13 | 30:f:259:PHE:HZ   | 1.70                     | 0.57              |
| 30:f:240:VAL:O    | 30:f:243:PRO:HD2  | 2.04                     | 0.57              |
| 30:f:373:ALA:HB1  | 30:f:748:LEU:HD21 | 1.87                     | 0.57              |
| 30:f:826:GLN:HB2  | 30:f:846:VAL:HA   | 1.84                     | 0.57              |
| 6:g:120:ASP:OD1   | 7:h:83:ARG:NH1    | 2.38                     | 0.57              |
| 31:F:82:VAL:HG23  | 31:F:83:ASN:OD1   | 2.04                     | 0.57              |
| 32:U:472:ILE:HD12 | 32:U:473:VAL:CG1  | 2.33                     | 0.57              |
| 32:U:623:GLY:HA2  | 32:U:659:CYS:HB2  | 1.86                     | 0.57              |
| 2:B:371:ARG:HG2   | 2:B:371:ARG:HH11  | 1.68                     | 0.57              |
| 21:W:97:LEU:HB2   | 21:W:100:ALA:HB2  | 1.84                     | 0.57              |
| 21:W:280:ASP:OD2  | 21:W:283:GLN:N    | 2.35                     | 0.57              |
| 21:W:452:ILE:HD11 | 24:Z:101:LEU:HD22 | 1.86                     | 0.57              |
| 23:Y:100:ILE:HD12 | 23:Y:100:ILE:C    | 2.30                     | 0.57              |
| 25:a:189:PRO:HG2  | 25:a:192:GLU:OE1  | 2.05                     | 0.57              |
| 26:b:8:VAL:CG2    | 26:b:110:ILE:HD11 | 2.30                     | 0.57              |
| 26:b:22:LEU:HB3   | 26:b:23:PRO:CD    | 2.23                     | 0.57              |
| 27:c:29:GLU:O     | 27:c:66:THR:HA    | 2.04                     | 0.57              |
| 30:f:179:VAL:HG11 | 30:f:216:MET:HE1  | 1.86                     | 0.57              |
| 30:f:419:LEU:HD23 | 30:f:420:TRP:N    | 2.19                     | 0.57              |
| 30:f:438:ASP:HA   | 30:f:441:LYS:HG2  | 1.85                     | 0.57              |
| 30:f:672:LEU:HD13 | 30:f:707:LEU:HD12 | 1.87                     | 0.57              |
| 36:n:301:LDZ:H40  | 14:o:115:TYR:CD2  | 2.39                     | 0.57              |
| 32:U:11:LEU:HD11  | 32:U:23:ALA:HB2   | 1.87                     | 0.57              |
| 32:U:147:TYR:OH   | 32:U:169:GLU:HB2  | 2.05                     | 0.57              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:263:MET:HG2   | 1:A:267:LYS:HZ1   | 1.69                     | 0.57              |
| 5:E:384:LEU:HB3   | 5:E:386:TYR:CD1   | 2.40                     | 0.57              |
| 20:V:205:LEU:HG   | 20:V:245:ASP:OD2  | 2.05                     | 0.57              |
| 20:V:273:LYS:HZ2  | 32:U:40:GLU:HB3   | 1.67                     | 0.57              |
| 20:V:304:GLU:HG3  | 20:V:307:ARG:HE   | 1.70                     | 0.57              |
| 23:Y:46:ARG:HB2   | 23:Y:46:ARG:CZ    | 2.34                     | 0.57              |
| 24:Z:48:LEU:HD21  | 24:Z:92:VAL:CG2   | 2.34                     | 0.57              |
| 25:a:186:LYS:CG   | 25:a:221:VAL:HG13 | 2.34                     | 0.57              |
| 25:a:191:SER:O    | 25:a:194:GLN:HG2  | 2.05                     | 0.57              |
| 28:d:171:LEU:O    | 28:d:175:ARG:HG2  | 2.05                     | 0.57              |
| 30:f:502:LEU:O    | 30:f:505:MET:HG2  | 2.03                     | 0.57              |
| 30:f:780:PRO:HB3  | 30:f:803:PHE:CE2  | 2.39                     | 0.57              |
| 30:f:800:LEU:HA   | 30:f:803:PHE:CZ   | 2.40                     | 0.57              |
| 1:A:158:ASP:OD1   | 1:A:159:PRO:HD2   | 2.05                     | 0.57              |
| 1:A:257:VAL:CG1   | 1:A:301:GLU:HB3   | 2.33                     | 0.57              |
| 2:B:294:ARG:HB2   | 2:B:294:ARG:HH11  | 1.68                     | 0.57              |
| 3:C:138:MET:HE2   | 3:C:138:MET:HA    | 1.87                     | 0.57              |
| 5:E:264:MET:HE3   | 5:E:294:ARG:HB3   | 1.87                     | 0.57              |
| 20:V:334:VAL:CG2  | 20:V:395:ILE:HD11 | 2.35                     | 0.57              |
| 20:V:454:GLU:OE1  | 20:V:455:LYS:N    | 2.37                     | 0.57              |
| 21:W:155:GLN:OE1  | 21:W:155:GLN:N    | 2.37                     | 0.57              |
| 22:X:369:ILE:HD12 | 23:Y:310:SER:CA   | 2.32                     | 0.57              |
| 23:Y:138:LEU:HA   | 23:Y:141:VAL:CG1  | 2.35                     | 0.57              |
| 23:Y:146:ARG:CZ   | 23:Y:146:ARG:HB2  | 2.34                     | 0.57              |
| 24:Z:172:VAL:CG1  | 27:c:217:LEU:HD21 | 2.21                     | 0.57              |
| 24:Z:276:ILE:O    | 24:Z:280:ILE:HG22 | 2.04                     | 0.57              |
| 25:a:188:LEU:HB3  | 25:a:189:PRO:HD2  | 1.85                     | 0.57              |
| 25:a:302:ILE:HG21 | 25:a:306:GLU:HG2  | 1.85                     | 0.57              |
| 26:b:91:ARG:HB3   | 26:b:91:ARG:CZ    | 2.35                     | 0.57              |
| 27:c:55:GLY:HA3   | 27:c:112:TYR:CE1  | 2.40                     | 0.57              |
| 27:c:130:GLN:NE2  | 27:c:142:ALA:HB2  | 2.18                     | 0.57              |
| 28:d:61:TRP:HZ3   | 28:d:65:ARG:HD2   | 1.68                     | 0.57              |
| 30:f:274:ASP:HB3  | 30:f:275:MET:HE3  | 1.87                     | 0.57              |
| 32:U:9:ILE:HG22   | 32:U:27:LEU:HD11  | 1.87                     | 0.57              |
| 1:A:164:MET:HE2   | 1:A:244:GLU:OE1   | 2.05                     | 0.57              |
| 3:C:164:VAL:HG21  | 3:C:186:VAL:CG1   | 2.32                     | 0.57              |
| 5:E:344:ARG:O     | 5:E:348:THR:HG22  | 2.04                     | 0.57              |
| 21:W:94:ARG:O     | 21:W:95:SER:HB2   | 2.05                     | 0.57              |
| 21:W:137:TYR:O    | 21:W:141:GLU:N    | 2.37                     | 0.57              |
| 22:X:301:ASP:O    | 22:X:304:LYS:HG3  | 2.05                     | 0.57              |
| 22:X:415:TYR:OH   | 23:Y:382:LYS:HG2  | 2.04                     | 0.57              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 23:Y:186:LEU:CD1  | 23:Y:213:LEU:HD13 | 2.34                     | 0.57              |
| 24:Z:131:LEU:HD23 | 24:Z:131:LEU:H    | 1.69                     | 0.57              |
| 24:Z:172:VAL:O    | 24:Z:176:LEU:HG   | 2.04                     | 0.57              |
| 30:f:821:LEU:HD21 | 30:f:882:LEU:CD1  | 2.34                     | 0.57              |
| 11:l:35:THR:HG22  | 11:l:133:LEU:HD12 | 1.86                     | 0.57              |
| 32:U:173:VAL:HG11 | 32:U:177:LEU:HD22 | 1.87                     | 0.57              |
| 32:U:191:LYS:HD3  | 32:U:191:LYS:N    | 2.20                     | 0.57              |
| 1:A:264:ALA:CA    | 1:A:267:LYS:HD2   | 2.33                     | 0.57              |
| 2:B:415:THR:N     | 2:B:418:ASP:OD2   | 2.29                     | 0.57              |
| 4:D:91:GLN:HE22   | 4:D:248:ARG:NE    | 2.03                     | 0.57              |
| 4:D:229:ARG:NH1   | 5:E:268:ASP:OD1   | 2.36                     | 0.57              |
| 5:E:182:LEU:CD2   | 33:E:402:ATP:H2'  | 2.34                     | 0.57              |
| 20:V:326:GLN:OE1  | 29:e:25:GLU:HB3   | 2.04                     | 0.57              |
| 21:W:237:GLU:HG2  | 21:W:238:GLY:H    | 1.69                     | 0.57              |
| 21:W:432:LEU:HD22 | 27:c:309:PHE:CD2  | 2.40                     | 0.57              |
| 24:Z:48:LEU:CD1   | 24:Z:92:VAL:HG21  | 2.32                     | 0.57              |
| 25:a:77:VAL:HG13  | 25:a:113:LEU:HD13 | 1.85                     | 0.57              |
| 27:c:77:GLN:OE1   | 27:c:77:GLN:HA    | 2.04                     | 0.57              |
| 32:U:62:LEU:HA    | 32:U:88:PHE:CE2   | 2.39                     | 0.57              |
| 2:B:116:ILE:HG12  | 2:B:117:ASP:H     | 1.70                     | 0.56              |
| 3:C:46:GLN:OE1    | 32:U:639:LEU:HD11 | 2.05                     | 0.56              |
| 5:E:342:ASP:OD2   | 5:E:342:ASP:N     | 2.38                     | 0.56              |
| 20:V:477:HIS:CE1  | 28:d:245:GLN:HE21 | 2.23                     | 0.56              |
| 21:W:436:MET:CE   | 27:c:226:MET:HB3  | 2.35                     | 0.56              |
| 23:Y:240:VAL:CG2  | 23:Y:260:LEU:HD11 | 2.35                     | 0.56              |
| 27:c:123:SER:OG   | 27:c:124:GLY:N    | 2.38                     | 0.56              |
| 30:f:103:TYR:HA   | 30:f:106:LEU:HB2  | 1.87                     | 0.56              |
| 32:U:742:HIS:HE2  | 32:U:814:PRO:HG3  | 1.70                     | 0.56              |
| 32:U:748:LEU:HD12 | 32:U:748:LEU:N    | 2.20                     | 0.56              |
| 2:B:209:GLU:CA    | 2:B:212:GLU:HB2   | 2.35                     | 0.56              |
| 2:B:212:GLU:HG2   | 30:f:845:ARG:HG3  | 1.87                     | 0.56              |
| 2:B:369:THR:HG22  | 2:B:372:MET:HE1   | 1.88                     | 0.56              |
| 2:B:426:VAL:CG1   | 2:B:427:LEU:HD12  | 2.29                     | 0.56              |
| 5:E:299:ILE:HG22  | 5:E:301:ILE:HD12  | 1.86                     | 0.56              |
| 20:V:408:ARG:HB2  | 20:V:408:ARG:HH11 | 1.70                     | 0.56              |
| 22:X:218:HIS:CE1  | 22:X:231:TYR:HE2  | 2.16                     | 0.56              |
| 22:X:239:TYR:HE1  | 22:X:246:LYS:CB   | 2.17                     | 0.56              |
| 24:Z:25:ARG:HH21  | 27:c:104:ARG:NH1  | 2.02                     | 0.56              |
| 28:d:235:THR:O    | 28:d:239:SER:N    | 2.38                     | 0.56              |
| 32:U:213:PHE:HD1  | 32:U:216:VAL:HG11 | 1.70                     | 0.56              |
| 1:A:193:THR:H     | 1:A:194:PRO:HD2   | 1.71                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:283:ALA:HA    | 1:A:328:ASP:OD2   | 2.06                     | 0.56              |
| 1:A:303:ILE:HD11  | 1:A:330:ALA:C     | 2.29                     | 0.56              |
| 2:B:223:ILE:CD1   | 2:B:329:MET:HB2   | 2.35                     | 0.56              |
| 3:C:40:GLN:HA     | 3:C:40:GLN:OE1    | 2.04                     | 0.56              |
| 3:C:77:VAL:HG23   | 3:C:86:LEU:HD23   | 1.88                     | 0.56              |
| 3:C:340:ARG:HG3   | 23:Y:206:SER:O    | 2.05                     | 0.56              |
| 3:C:351:MET:HE2   | 3:C:391:MET:CE    | 2.35                     | 0.56              |
| 5:E:148:VAL:HG21  | 5:E:167:PRO:HB2   | 1.87                     | 0.56              |
| 33:E:402:ATP:H5'1 | 31:F:344:ARG:HH12 | 1.71                     | 0.56              |
| 19:T:6:VAL:HG11   | 13:n:120:MET:HE1  | 1.87                     | 0.56              |
| 20:V:108:LEU:CD2  | 20:V:170:LEU:HD12 | 2.36                     | 0.56              |
| 20:V:134:PHE:HB2  | 20:V:135:LEU:HD22 | 1.87                     | 0.56              |
| 20:V:166:TYR:HE1  | 20:V:170:LEU:HD21 | 1.71                     | 0.56              |
| 20:V:359:PRO:HA   | 20:V:382:PHE:HD2  | 1.67                     | 0.56              |
| 23:Y:210:SER:HB3  | 23:Y:212:GLU:OE2  | 2.06                     | 0.56              |
| 23:Y:381:GLN:O    | 23:Y:384:SER:OG   | 2.22                     | 0.56              |
| 24:Z:8:LYS:HZ1    | 24:Z:161:GLU:HG2  | 1.70                     | 0.56              |
| 24:Z:190:ARG:HE   | 24:Z:194:GLN:HG3  | 1.71                     | 0.56              |
| 25:a:231:GLN:OE1  | 25:a:231:GLN:HA   | 2.05                     | 0.56              |
| 29:e:47:ASN:O     | 29:e:48:VAL:HG12  | 2.05                     | 0.56              |
| 30:f:104:GLY:O    | 30:f:107:LYS:NZ   | 2.34                     | 0.56              |
| 30:f:106:LEU:HG   | 30:f:109:ILE:CG2  | 2.35                     | 0.56              |
| 30:f:156:HIS:O    | 30:f:159:VAL:HG12 | 2.05                     | 0.56              |
| 30:f:274:ASP:HB3  | 30:f:275:MET:HE1  | 1.87                     | 0.56              |
| 30:f:290:VAL:O    | 30:f:294:MET:HE1  | 2.05                     | 0.56              |
| 30:f:490:ALA:HA   | 30:f:524:MET:HE1  | 1.87                     | 0.56              |
| 30:f:723:TYR:CG   | 30:f:723:TYR:O    | 2.57                     | 0.56              |
| 30:f:742:ALA:HA   | 30:f:745:LEU:CD1  | 2.35                     | 0.56              |
| 30:f:766:GLN:HG3  | 30:f:768:LEU:CD1  | 2.34                     | 0.56              |
| 30:f:821:LEU:HD11 | 30:f:882:LEU:CD2  | 2.35                     | 0.56              |
| 31:F:134:LEU:CD1  | 31:F:159:LEU:HA   | 2.34                     | 0.56              |
| 31:F:196:GLN:HA   | 31:F:199:VAL:CG2  | 2.35                     | 0.56              |
| 32:U:249:CYS:SG   | 32:U:328:ILE:HG13 | 2.44                     | 0.56              |
| 32:U:672:LEU:HD23 | 32:U:675:MET:SD   | 2.44                     | 0.56              |
| 1:A:126:SER:HB3   | 1:A:150:HIS:CE1   | 2.40                     | 0.56              |
| 2:B:95:GLU:CA     | 2:B:98:LYS:HE2    | 2.21                     | 0.56              |
| 2:B:112:LEU:HD11  | 2:B:114:GLU:O     | 2.05                     | 0.56              |
| 2:B:153:ASN:OD1   | 2:B:154:HIS:N     | 2.39                     | 0.56              |
| 2:B:363:ARG:O     | 2:B:363:ARG:NH1   | 2.39                     | 0.56              |
| 3:C:328:ILE:HG12  | 35:C:501:ADP:C6   | 2.41                     | 0.56              |
| 4:D:217:LYS:HA    | 5:E:267:PHE:HE1   | 1.70                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 21:W:191:ARG:HG3  | 21:W:191:ARG:HH11 | 1.70                     | 0.56              |
| 21:W:363:ILE:CD1  | 21:W:393:LEU:HD13 | 2.30                     | 0.56              |
| 23:Y:144:LEU:HB2  | 23:Y:160:ASN:HD22 | 1.70                     | 0.56              |
| 24:Z:38:VAL:HG21  | 24:Z:75:LEU:HD21  | 1.87                     | 0.56              |
| 24:Z:71:ASP:HB3   | 24:Z:74:TYR:HB3   | 1.88                     | 0.56              |
| 25:a:35:HIS:HB3   | 26:b:15:TYR:CD1   | 2.40                     | 0.56              |
| 26:b:187:PRO:HG2  | 26:b:188:ILE:CD1  | 2.34                     | 0.56              |
| 28:d:47:GLN:HG2   | 28:d:48:LEU:N     | 2.19                     | 0.56              |
| 30:f:180:GLN:HG3  | 30:f:219:LYS:HD3  | 1.88                     | 0.56              |
| 10:k:230:THR:OG1  | 10:k:233:GLU:OE2  | 2.22                     | 0.56              |
| 31:F:81:LYS:O     | 31:F:84:LYS:HG2   | 2.04                     | 0.56              |
| 32:U:173:VAL:CG1  | 32:U:177:LEU:HB3  | 2.32                     | 0.56              |
| 32:U:201:LEU:HD13 | 32:U:201:LEU:O    | 2.05                     | 0.56              |
| 32:U:218:GLN:HE22 | 32:U:752:THR:HB   | 1.70                     | 0.56              |
| 2:B:397:ALA:HA    | 2:B:400:THR:HG22  | 1.88                     | 0.56              |
| 4:D:43:ARG:HB2    | 4:D:43:ARG:HH11   | 1.71                     | 0.56              |
| 4:D:363:TYR:HA    | 4:D:366:ARG:NH1   | 2.20                     | 0.56              |
| 7:H:230:ALA:HB1   | 22:X:90:ARG:HH12  | 1.71                     | 0.56              |
| 20:V:160:LEU:HD22 | 20:V:200:ARG:NH1  | 2.20                     | 0.56              |
| 20:V:175:MET:CE   | 20:V:180:ARG:HB3  | 2.36                     | 0.56              |
| 21:W:312:MET:HE2  | 21:W:312:MET:H    | 1.71                     | 0.56              |
| 23:Y:138:LEU:HD21 | 23:Y:167:LEU:CB   | 2.36                     | 0.56              |
| 23:Y:307:LEU:HD21 | 23:Y:314:LEU:CD1  | 2.36                     | 0.56              |
| 27:c:51:MET:CA    | 27:c:82:VAL:HG13  | 2.33                     | 0.56              |
| 30:f:199:ASN:HA   | 30:f:202:HIS:CE1  | 2.40                     | 0.56              |
| 30:f:423:ASP:O    | 30:f:427:THR:HG23 | 2.06                     | 0.56              |
| 30:f:513:GLU:O    | 30:f:517:VAL:HG22 | 2.05                     | 0.56              |
| 30:f:537:THR:HA   | 30:f:540:GLN:OE1  | 2.05                     | 0.56              |
| 30:f:608:LYS:HE2  | 30:f:639:LYS:NZ   | 2.21                     | 0.56              |
| 30:f:692:LEU:HG   | 30:f:696:LEU:HD21 | 1.86                     | 0.56              |
| 2:B:403:GLY:HA3   | 3:C:180:ILE:HG13  | 1.88                     | 0.56              |
| 3:C:104:ASP:OD1   | 3:C:107:ASP:HB2   | 2.06                     | 0.56              |
| 3:C:267:SER:OG    | 3:C:270:GLN:HB2   | 2.05                     | 0.56              |
| 20:V:394:LEU:O    | 20:V:397:ARG:HG2  | 2.06                     | 0.56              |
| 20:V:433:ASP:OD1  | 20:V:433:ASP:N    | 2.36                     | 0.56              |
| 21:W:132:THR:HG23 | 21:W:134:GLY:H    | 1.70                     | 0.56              |
| 21:W:265:GLN:OE1  | 21:W:336:PRO:HG3  | 2.05                     | 0.56              |
| 21:W:346:GLU:O    | 21:W:350:ARG:NH1  | 2.39                     | 0.56              |
| 21:W:374:THR:HG22 | 21:W:377:ARG:HB3  | 1.88                     | 0.56              |
| 23:Y:117:LYS:HB2  | 23:Y:121:LEU:CD1  | 2.35                     | 0.56              |
| 23:Y:160:ASN:HA   | 23:Y:163:LYS:HG2  | 1.87                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 24:Z:48:LEU:HD21  | 24:Z:92:VAL:HG22  | 1.87                     | 0.56              |
| 26:b:33:VAL:HA    | 26:b:36:VAL:CG1   | 2.35                     | 0.56              |
| 30:f:216:MET:HA   | 30:f:219:LYS:HE2  | 1.86                     | 0.56              |
| 30:f:672:LEU:HA   | 30:f:675:PHE:CE1  | 2.41                     | 0.56              |
| 30:f:764:LEU:O    | 30:f:858:LYS:NZ   | 2.39                     | 0.56              |
| 30:f:786:GLN:HB3  | 30:f:788:MET:SD   | 2.46                     | 0.56              |
| 30:f:828:ARG:HH12 | 30:f:831:VAL:HG22 | 1.71                     | 0.56              |
| 32:U:37:GLU:HG3   | 32:U:38:ILE:N     | 2.20                     | 0.56              |
| 32:U:236:LEU:HB2  | 32:U:245:ALA:HB2  | 1.85                     | 0.56              |
| 32:U:803:LYS:HD2  | 32:U:875:PHE:CA   | 2.36                     | 0.56              |
| 2:B:60:LEU:HG     | 2:B:64:LYS:NZ     | 2.21                     | 0.56              |
| 2:B:193:GLN:HE22  | 2:B:354:PRO:HD3   | 1.71                     | 0.56              |
| 3:C:57:ARG:HH12   | 32:U:649:ARG:NH1  | 2.04                     | 0.56              |
| 5:E:173:TYR:C     | 5:E:180:LYS:HE3   | 2.31                     | 0.56              |
| 6:G:11:ARG:HH11   | 6:G:11:ARG:HG3    | 1.70                     | 0.56              |
| 21:W:151:THR:HA   | 21:W:154:GLU:CD   | 2.31                     | 0.56              |
| 21:W:371:THR:C    | 21:W:372:ARG:HG2  | 2.30                     | 0.56              |
| 24:Z:224:HIS:HE1  | 25:a:340:VAL:HG11 | 1.71                     | 0.56              |
| 25:a:252:LYS:HA   | 25:a:255:TRP:CE2  | 2.40                     | 0.56              |
| 26:b:101:GLN:OE1  | 26:b:101:GLN:HA   | 2.06                     | 0.56              |
| 27:c:29:GLU:HA    | 27:c:65:TYR:O     | 2.06                     | 0.56              |
| 28:d:96:HIS:HB2   | 28:d:132:TYR:CD2  | 2.40                     | 0.56              |
| 30:f:117:GLU:OE1  | 30:f:120:ARG:NE   | 2.35                     | 0.56              |
| 30:f:137:ARG:HG3  | 30:f:138:GLU:N    | 2.19                     | 0.56              |
| 30:f:498:LEU:HA   | 30:f:501:LEU:CD2  | 2.36                     | 0.56              |
| 30:f:524:MET:O    | 30:f:773:LYS:NZ   | 2.35                     | 0.56              |
| 11:l:164:ARG:NH1  | 11:l:198:THR:O    | 2.39                     | 0.56              |
| 32:U:913:ILE:HD12 | 32:U:913:ILE:N    | 2.21                     | 0.56              |
| 2:B:225:TYR:OH    | 2:B:352:GLU:HB2   | 2.06                     | 0.56              |
| 21:W:98:LYS:HG3   | 21:W:139:GLU:HG2  | 1.87                     | 0.56              |
| 22:X:132:ARG:HD3  | 22:X:132:ARG:O    | 2.05                     | 0.56              |
| 23:Y:14:ASN:OD1   | 23:Y:143:TYR:OH   | 2.20                     | 0.56              |
| 23:Y:183:TYR:OH   | 23:Y:212:GLU:OE2  | 2.24                     | 0.56              |
| 25:a:319:LEU:HD12 | 25:a:337:GLN:HB2  | 1.87                     | 0.56              |
| 26:b:142:ASN:OD1  | 26:b:150:THR:OG1  | 2.23                     | 0.56              |
| 27:c:122:LEU:HD12 | 27:c:126:ASP:HB3  | 1.88                     | 0.56              |
| 27:c:181:LEU:HD23 | 27:c:181:LEU:C    | 2.31                     | 0.56              |
| 27:c:303:MET:HG2  | 28:d:242:LEU:HB3  | 1.88                     | 0.56              |
| 28:d:188:LYS:HB2  | 28:d:221:ASN:HD21 | 1.68                     | 0.56              |
| 31:F:140:VAL:HG21 | 31:F:160:ILE:HG21 | 1.88                     | 0.56              |
| 32:U:23:ALA:HA    | 32:U:26:LYS:HD2   | 1.88                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 32:U:69:TYR:CZ    | 32:U:99:THR:HG21  | 2.41                     | 0.56              |
| 32:U:469:SER:OG   | 32:U:470:ASN:N    | 2.39                     | 0.56              |
| 32:U:556:MET:SD   | 32:U:563:ALA:HA   | 2.46                     | 0.56              |
| 2:B:197:ILE:CD1   | 2:B:222:VAL:HG21  | 2.35                     | 0.56              |
| 20:V:280:ALA:HB3  | 20:V:285:TRP:CE3  | 2.41                     | 0.56              |
| 21:W:140:ILE:O    | 21:W:140:ILE:CG1  | 2.54                     | 0.56              |
| 21:W:179:LYS:CE   | 21:W:212:LYS:HD2  | 2.34                     | 0.56              |
| 21:W:187:LEU:HD21 | 21:W:226:TYR:HD2  | 1.70                     | 0.56              |
| 23:Y:217:LYS:HG3  | 23:Y:253:LEU:HD11 | 1.87                     | 0.56              |
| 23:Y:387:ILE:HD13 | 24:Z:276:ILE:HD11 | 1.88                     | 0.56              |
| 26:b:32:ALA:O     | 26:b:35:ILE:HG12  | 2.05                     | 0.56              |
| 27:c:241:ASN:ND2  | 27:c:295:ASN:HD21 | 2.00                     | 0.56              |
| 28:d:67:ASP:O     | 28:d:71:PHE:HB2   | 2.05                     | 0.56              |
| 31:F:80:ILE:O     | 31:F:84:LYS:HB3   | 2.05                     | 0.56              |
| 32:U:381:THR:HG22 | 32:U:412:HIS:HA   | 1.88                     | 0.56              |
| 2:B:115:ILE:O     | 2:B:115:ILE:HG22  | 2.06                     | 0.56              |
| 4:D:269:ALA:CB    | 5:E:258:MET:HE2   | 2.34                     | 0.56              |
| 4:D:361:GLU:OE1   | 4:D:361:GLU:HA    | 2.05                     | 0.56              |
| 5:E:148:VAL:O     | 5:E:149:ILE:HD12  | 2.06                     | 0.56              |
| 5:E:198:VAL:HG13  | 5:E:232:MET:HA    | 1.86                     | 0.56              |
| 5:E:314:LYS:HE3   | 5:E:328:TYR:HD2   | 1.69                     | 0.56              |
| 5:E:322:LYS:HB3   | 5:E:326:ILE:CD1   | 2.36                     | 0.56              |
| 20:V:302:TYR:CZ   | 20:V:338:LEU:HD13 | 2.41                     | 0.56              |
| 21:W:111:TYR:O    | 21:W:115:ILE:HG22 | 2.06                     | 0.56              |
| 21:W:326:MET:HE2  | 21:W:330:LYS:O    | 2.06                     | 0.56              |
| 23:Y:113:ARG:O    | 23:Y:113:ARG:NH1  | 2.38                     | 0.56              |
| 24:Z:23:PHE:CD2   | 24:Z:126:VAL:HG11 | 2.39                     | 0.56              |
| 25:a:18:GLN:HB3   | 25:a:19:PRO:HD3   | 1.88                     | 0.56              |
| 25:a:72:ASN:HA    | 26:b:17:ARG:HH12  | 1.71                     | 0.56              |
| 30:f:744:MET:HA   | 30:f:747:GLN:HG3  | 1.88                     | 0.56              |
| 7:h:110:VAL:HG22  | 7:h:135:ILE:CD1   | 2.36                     | 0.56              |
| 31:F:422:GLU:OE1  | 31:F:422:GLU:C    | 2.49                     | 0.56              |
| 32:U:139:GLN:NE2  | 32:U:143:ASP:OD1  | 2.39                     | 0.56              |
| 1:A:102:ILE:HD11  | 1:A:114:ASN:CB    | 2.32                     | 0.55              |
| 2:B:94:GLU:HG3    | 2:B:98:LYS:NZ     | 2.21                     | 0.55              |
| 2:B:316:LEU:CD2   | 2:B:327:VAL:HG21  | 2.36                     | 0.55              |
| 3:C:328:ILE:HG12  | 35:C:501:ADP:N1   | 2.20                     | 0.55              |
| 4:D:200:ARG:HG3   | 4:D:200:ARG:O     | 2.06                     | 0.55              |
| 5:E:297:ARG:HG2   | 5:E:299:ILE:CD1   | 2.36                     | 0.55              |
| 7:H:74:VAL:HG22   | 7:H:75:TYR:H      | 1.70                     | 0.55              |
| 17:R:2:THR:N      | 17:R:131:SER:OG   | 2.38                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 17:R:36:ILE:HD11  | 17:R:46:MET:SD    | 2.46                     | 0.55              |
| 20:V:127:THR:O    | 20:V:131:LEU:HB2  | 2.06                     | 0.55              |
| 20:V:302:TYR:CE2  | 20:V:338:LEU:HB3  | 2.42                     | 0.55              |
| 23:Y:365:GLN:O    | 23:Y:369:THR:HG22 | 2.06                     | 0.55              |
| 24:Z:209:ARG:HG2  | 24:Z:209:ARG:NH1  | 2.19                     | 0.55              |
| 25:a:213:PHE:CE1  | 25:a:240:PHE:HD2  | 2.24                     | 0.55              |
| 26:b:140:ILE:HG22 | 26:b:170:LEU:HD11 | 1.88                     | 0.55              |
| 30:f:213:GLN:OE1  | 30:f:249:LEU:HD11 | 2.06                     | 0.55              |
| 31:F:197:GLU:OE2  | 31:F:350:ARG:HB3  | 2.06                     | 0.55              |
| 31:F:376:SER:OG   | 31:F:379:VAL:HG23 | 2.06                     | 0.55              |
| 32:U:331:GLY:HA2  | 32:U:333:MET:HE1  | 1.88                     | 0.55              |
| 32:U:625:ILE:HG22 | 32:U:626:LEU:CD2  | 2.36                     | 0.55              |
| 32:U:803:LYS:CG   | 32:U:893:THR:HB   | 2.36                     | 0.55              |
| 1:A:193:THR:H     | 1:A:194:PRO:CD    | 2.19                     | 0.55              |
| 2:B:293:LYS:HB3   | 3:C:266:ASP:OD2   | 2.05                     | 0.55              |
| 3:C:161:ILE:HG13  | 3:C:203:VAL:HG21  | 1.87                     | 0.55              |
| 3:C:273:MET:CE    | 3:C:293:MET:CG    | 2.84                     | 0.55              |
| 11:L:150:SER:O    | 11:L:152:ASN:N    | 2.37                     | 0.55              |
| 20:V:114:TYR:O    | 20:V:117:VAL:HG12 | 2.07                     | 0.55              |
| 20:V:320:THR:OG1  | 29:e:16:ASP:OD1   | 2.22                     | 0.55              |
| 20:V:416:ARG:HH12 | 23:Y:350:VAL:HG21 | 1.68                     | 0.55              |
| 22:X:401:LEU:HD21 | 23:Y:368:GLU:OE1  | 2.05                     | 0.55              |
| 23:Y:160:ASN:OD1  | 23:Y:160:ASN:N    | 2.39                     | 0.55              |
| 24:Z:187:LEU:HA   | 25:a:374:ILE:CG2  | 2.37                     | 0.55              |
| 24:Z:213:GLU:HB3  | 24:Z:219:LYS:HZ2  | 1.72                     | 0.55              |
| 25:a:18:GLN:O     | 25:a:22:TRP:HD1   | 1.90                     | 0.55              |
| 26:b:110:ILE:HA   | 26:b:139:ASP:HB3  | 1.88                     | 0.55              |
| 27:c:149:GLN:O    | 27:c:151:VAL:HG13 | 2.07                     | 0.55              |
| 30:f:372:LEU:CD1  | 30:f:410:ALA:HB2  | 2.35                     | 0.55              |
| 30:f:385:PHE:CB   | 30:f:388:ASP:HB2  | 2.22                     | 0.55              |
| 30:f:600:TYR:HB3  | 30:f:603:SER:OG   | 2.06                     | 0.55              |
| 32:U:669:ILE:HD11 | 32:U:709:PHE:CE1  | 2.41                     | 0.55              |
| 2:B:135:ILE:HG22  | 2:B:141:LYS:HE2   | 1.88                     | 0.55              |
| 21:W:184:GLU:OE2  | 21:W:188:GLU:HB2  | 2.05                     | 0.55              |
| 22:X:407:MET:HG3  | 24:Z:266:ILE:HD12 | 1.88                     | 0.55              |
| 24:Z:43:TRP:H     | 24:Z:90:ARG:HH22  | 1.55                     | 0.55              |
| 24:Z:214:LYS:HG2  | 24:Z:218:GLY:HA2  | 1.88                     | 0.55              |
| 25:a:8:LEU:HD22   | 25:a:26:GLU:OE2   | 2.06                     | 0.55              |
| 30:f:472:HIS:CE1  | 30:f:474:SER:HB2  | 2.40                     | 0.55              |
| 31:F:408:LEU:HD12 | 31:F:408:LEU:O    | 2.07                     | 0.55              |
| 2:B:284:ILE:HG21  | 2:B:287:ILE:HD13  | 1.88                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:C:274:LEU:O     | 3:C:278:ASN:ND2   | 2.38                     | 0.55              |
| 20:V:181:TYR:CE2  | 20:V:220:PHE:HB3  | 2.42                     | 0.55              |
| 20:V:486:ILE:CD1  | 24:Z:268:SER:HB2  | 2.37                     | 0.55              |
| 21:W:179:LYS:HD2  | 21:W:179:LYS:C    | 2.31                     | 0.55              |
| 22:X:199:ALA:C    | 22:X:200:ILE:HD12 | 2.32                     | 0.55              |
| 25:a:35:HIS:NE2   | 26:b:17:ARG:HD3   | 2.21                     | 0.55              |
| 25:a:48:PRO:HB2   | 25:a:51:ALA:CA    | 2.37                     | 0.55              |
| 26:b:48:ASN:ND2   | 26:b:64:LEU:HG    | 2.21                     | 0.55              |
| 27:c:57:MET:HA    | 27:c:72:VAL:HG22  | 1.88                     | 0.55              |
| 30:f:468:ASP:OD1  | 30:f:468:ASP:N    | 2.40                     | 0.55              |
| 13:n:13:VAL:HG21  | 13:n:102:ALA:HB1  | 1.88                     | 0.55              |
| 32:U:472:ILE:HD12 | 32:U:472:ILE:C    | 2.31                     | 0.55              |
| 32:U:506:ALA:HA   | 32:U:544:ILE:CD1  | 2.36                     | 0.55              |
| 32:U:552:ILE:O    | 32:U:555:VAL:HG12 | 2.06                     | 0.55              |
| 1:A:292:ASP:OD1   | 1:A:292:ASP:O     | 2.23                     | 0.55              |
| 4:D:167:ILE:HD11  | 4:D:214:MET:CG    | 2.37                     | 0.55              |
| 4:D:403:TYR:O     | 4:D:407:ILE:HG13  | 2.07                     | 0.55              |
| 5:E:341:ALA:HB1   | 31:F:345:SER:HB2  | 1.88                     | 0.55              |
| 11:L:117:GLN:O    | 11:L:120:THR:OG1  | 2.20                     | 0.55              |
| 20:V:256:ARG:HD3  | 20:V:291:TYR:OH   | 2.06                     | 0.55              |
| 20:V:371:ASN:HB2  | 20:V:427:GLN:NE2  | 2.21                     | 0.55              |
| 20:V:404:LYS:CD   | 20:V:446:VAL:HG21 | 2.37                     | 0.55              |
| 23:Y:252:SER:OG   | 23:Y:253:LEU:HD12 | 2.06                     | 0.55              |
| 23:Y:286:TRP:O    | 23:Y:287:LEU:HB3  | 2.05                     | 0.55              |
| 24:Z:191:ILE:CG2  | 25:a:375:LEU:HD23 | 2.36                     | 0.55              |
| 24:Z:199:LYS:HE3  | 25:a:364:GLU:CD   | 2.31                     | 0.55              |
| 25:a:35:HIS:HA    | 25:a:38:THR:OG1   | 2.06                     | 0.55              |
| 25:a:135:ILE:HD11 | 25:a:159:SER:HB3  | 1.87                     | 0.55              |
| 25:a:278:MET:HE1  | 25:a:319:LEU:CG   | 2.31                     | 0.55              |
| 30:f:857:GLY:O    | 30:f:860:LYS:NZ   | 2.36                     | 0.55              |
| 32:U:265:ILE:HG23 | 32:U:326:ILE:CD1  | 2.36                     | 0.55              |
| 32:U:798:PRO:C    | 32:U:799:LYS:HD3  | 2.31                     | 0.55              |
| 1:A:423:PHE:CE2   | 2:B:350:LYS:HD2   | 2.42                     | 0.55              |
| 2:B:193:GLN:HE22  | 2:B:354:PRO:CD    | 2.19                     | 0.55              |
| 3:C:138:MET:HE2   | 3:C:138:MET:CA    | 2.36                     | 0.55              |
| 3:C:188:LEU:O     | 3:C:294:ALA:HA    | 2.06                     | 0.55              |
| 5:E:364:GLN:C     | 5:E:364:GLN:OE1   | 2.50                     | 0.55              |
| 20:V:254:LEU:O    | 20:V:254:LEU:HD13 | 2.06                     | 0.55              |
| 21:W:198:ASP:CG   | 21:W:201:ARG:HB2  | 2.32                     | 0.55              |
| 24:Z:39:LEU:CD2   | 24:Z:53:SER:HB3   | 2.36                     | 0.55              |
| 30:f:115:PRO:HG2  | 30:f:118:ASN:CG   | 2.31                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 30:f:407:MET:HE1  | 30:f:440:ILE:CA   | 2.30                     | 0.55              |
| 32:U:43:ASP:C     | 32:U:43:ASP:OD1   | 2.49                     | 0.55              |
| 32:U:331:GLY:O    | 32:U:335:ILE:HG12 | 2.06                     | 0.55              |
| 1:A:197:HIS:NE2   | 30:f:343:LYS:HG3  | 2.21                     | 0.55              |
| 1:A:384:GLU:O     | 1:A:388:VAL:HG23  | 2.07                     | 0.55              |
| 2:B:412:MET:O     | 2:B:412:MET:HE2   | 2.07                     | 0.55              |
| 3:C:273:MET:HE1   | 3:C:293:MET:CG    | 2.36                     | 0.55              |
| 4:D:163:MET:HE2   | 4:D:221:HIS:CE1   | 2.42                     | 0.55              |
| 4:D:201:GLY:C     | 4:D:327:LEU:HB2   | 2.32                     | 0.55              |
| 5:E:65:THR:OG1    | 5:E:66:GLU:N      | 2.40                     | 0.55              |
| 23:Y:25:LEU:O     | 23:Y:29:PRO:HG2   | 2.07                     | 0.55              |
| 24:Z:254:ASN:OD1  | 24:Z:255:ASP:N    | 2.40                     | 0.55              |
| 27:c:49:VAL:HG12  | 27:c:50:PRO:CD    | 2.36                     | 0.55              |
| 30:f:662:MET:N    | 30:f:662:MET:HE3  | 2.22                     | 0.55              |
| 7:h:64:VAL:O      | 7:h:219:ARG:NH1   | 2.38                     | 0.55              |
| 8:i:192:LEU:O     | 8:i:196:VAL:HG23  | 2.06                     | 0.55              |
| 32:U:16:GLU:HG3   | 32:U:19:LEU:CB    | 2.37                     | 0.55              |
| 32:U:350:LEU:HD13 | 32:U:385:PHE:CE2  | 2.42                     | 0.55              |
| 32:U:542:GLU:OE1  | 32:U:542:GLU:C    | 2.50                     | 0.55              |
| 32:U:883:ARG:HG3  | 32:U:883:ARG:O    | 2.06                     | 0.55              |
| 1:A:91:GLN:HB3    | 1:A:92:PRO:HD3    | 1.87                     | 0.55              |
| 1:A:143:ASP:HB3   | 1:A:148:GLN:H     | 1.72                     | 0.55              |
| 2:B:114:GLU:HG2   | 2:B:115:ILE:N     | 2.21                     | 0.55              |
| 2:B:140:ASP:CG    | 2:B:143:LEU:HG    | 2.32                     | 0.55              |
| 2:B:347:ILE:O     | 2:B:347:ILE:HG13  | 2.07                     | 0.55              |
| 4:D:231:VAL:HG11  | 5:E:259:GLU:OE1   | 2.07                     | 0.55              |
| 4:D:291:GLU:OE1   | 4:D:291:GLU:HA    | 2.07                     | 0.55              |
| 5:E:249:ALA:HB1   | 31:F:261:ILE:HG12 | 1.87                     | 0.55              |
| 16:Q:108:ASP:OD1  | 16:Q:109:GLU:N    | 2.40                     | 0.55              |
| 20:V:254:LEU:HD13 | 20:V:254:LEU:C    | 2.31                     | 0.55              |
| 23:Y:42:MET:HE3   | 23:Y:42:MET:HA    | 1.89                     | 0.55              |
| 23:Y:338:ILE:CD1  | 23:Y:343:LEU:HD22 | 2.37                     | 0.55              |
| 24:Z:164:ALA:HB2  | 27:c:221:HIS:HE1  | 1.68                     | 0.55              |
| 25:a:180:LEU:HD11 | 25:a:222:LEU:HD21 | 1.89                     | 0.55              |
| 26:b:100:ARG:HD2  | 26:b:103:LYS:HA   | 1.88                     | 0.55              |
| 27:c:152:LYS:HE2  | 27:c:152:LYS:CA   | 2.32                     | 0.55              |
| 28:d:122:LEU:HD22 | 28:d:122:LEU:N    | 2.22                     | 0.55              |
| 30:f:334:ALA:HB1  | 30:f:335:ARG:NH2  | 2.12                     | 0.55              |
| 30:f:613:LEU:HD22 | 30:f:613:LEU:H    | 1.71                     | 0.55              |
| 30:f:680:ARG:CB   | 30:f:715:HIS:HA   | 2.37                     | 0.55              |
| 30:f:784:ASP:OD1  | 30:f:791:VAL:HG21 | 2.07                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 30:f:811:LEU:HB2  | 30:f:878:GLU:OE1  | 2.07                     | 0.55              |
| 31:F:91:SER:CB    | 31:F:126:THR:HA   | 2.36                     | 0.55              |
| 32:U:890:LYS:NZ   | 32:U:891:VAL:HG12 | 2.22                     | 0.55              |
| 32:U:894:MET:CE   | 32:U:902:PRO:HD3  | 2.23                     | 0.55              |
| 1:A:277:ILE:HD12  | 1:A:280:ILE:HG13  | 1.88                     | 0.55              |
| 2:B:237:LYS:HB3   | 3:C:283:PHE:CE1   | 2.42                     | 0.55              |
| 2:B:343:ARG:HE    | 2:B:346:ARG:NH1   | 2.04                     | 0.55              |
| 3:C:156:LYS:O     | 3:C:160:GLU:HG3   | 2.05                     | 0.55              |
| 4:D:217:LYS:HG2   | 5:E:267:PHE:CE1   | 2.41                     | 0.55              |
| 5:E:252:GLU:OE1   | 5:E:252:GLU:C     | 2.49                     | 0.55              |
| 6:G:66:VAL:HG13   | 6:G:66:VAL:O      | 2.05                     | 0.55              |
| 20:V:127:THR:HA   | 20:V:130:PHE:CE1  | 2.42                     | 0.55              |
| 20:V:494:MET:HE2  | 24:Z:275:LEU:HA   | 1.89                     | 0.55              |
| 21:W:144:ARG:O    | 21:W:148:THR:HG22 | 2.06                     | 0.55              |
| 21:W:273:TYR:HB2  | 21:W:276:LEU:HB2  | 1.88                     | 0.55              |
| 22:X:377:ILE:HD12 | 22:X:377:ILE:O    | 2.07                     | 0.55              |
| 25:a:60:TYR:O     | 25:a:64:ILE:HG12  | 2.06                     | 0.55              |
| 25:a:148:VAL:HG13 | 25:a:149:THR:N    | 2.20                     | 0.55              |
| 26:b:53:THR:HG22  | 26:b:55:ALA:N     | 2.22                     | 0.55              |
| 27:c:26:ASP:HA    | 27:c:176:GLN:NE2  | 2.22                     | 0.55              |
| 27:c:208:ARG:HD2  | 27:c:209:LYS:N    | 2.21                     | 0.55              |
| 30:f:232:TYR:CE2  | 30:f:233:LEU:HG   | 2.41                     | 0.55              |
| 30:f:259:PHE:HA   | 30:f:262:PHE:CE1  | 2.41                     | 0.55              |
| 32:U:472:ILE:CD1  | 32:U:473:VAL:HG13 | 2.37                     | 0.55              |
| 32:U:803:LYS:HZ3  | 32:U:875:PHE:HB3  | 1.71                     | 0.55              |
| 1:A:84:LYS:O      | 1:A:88:GLN:N      | 2.34                     | 0.55              |
| 2:B:76:GLU:O      | 2:B:80:ARG:HG2    | 2.07                     | 0.55              |
| 2:B:223:ILE:CG2   | 2:B:347:ILE:HD12  | 2.38                     | 0.55              |
| 4:D:130:VAL:HG21  | 4:D:139:LEU:HD21  | 1.88                     | 0.55              |
| 20:V:431:PRO:HD2  | 20:V:432:GLU:CD   | 2.31                     | 0.55              |
| 21:W:67:LEU:HD12  | 21:W:90:LEU:HD13  | 1.89                     | 0.55              |
| 21:W:67:LEU:CD1   | 21:W:90:LEU:HD13  | 2.37                     | 0.55              |
| 21:W:114:GLU:C    | 21:W:114:GLU:OE1  | 2.50                     | 0.55              |
| 21:W:220:GLU:HG3  | 21:W:221:LYS:HE2  | 1.89                     | 0.55              |
| 21:W:244:CYS:SG   | 21:W:274:VAL:HG23 | 2.47                     | 0.55              |
| 22:X:421:LEU:O    | 24:Z:283:ARG:NH2  | 2.40                     | 0.55              |
| 23:Y:46:ARG:HB2   | 23:Y:46:ARG:NH1   | 2.22                     | 0.55              |
| 24:Z:61:ASP:C     | 24:Z:61:ASP:OD1   | 2.50                     | 0.55              |
| 24:Z:275:LEU:O    | 24:Z:275:LEU:HD22 | 2.06                     | 0.55              |
| 25:a:180:LEU:HD22 | 25:a:221:VAL:HG11 | 1.89                     | 0.55              |
| 27:c:123:SER:O    | 27:c:127:ILE:HG13 | 2.06                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 28:d:1:MET:CE     | 28:d:32:GLU:HG2   | 2.37                     | 0.55              |
| 28:d:42:LYS:HG3   | 28:d:86:LYS:HG3   | 1.87                     | 0.55              |
| 30:f:709:THR:O    | 30:f:712:LYS:HE3  | 2.07                     | 0.55              |
| 30:f:828:ARG:NH1  | 30:f:831:VAL:HG13 | 2.22                     | 0.55              |
| 32:U:48:LEU:HD13  | 32:U:48:LEU:C     | 2.32                     | 0.55              |
| 1:A:159:PRO:HA    | 1:A:162:THR:HG22  | 1.89                     | 0.54              |
| 4:D:150:SER:OG    | 4:D:250:VAL:HG22  | 2.08                     | 0.54              |
| 4:D:393:ILE:HG12  | 21:W:133:GLU:CB   | 2.35                     | 0.54              |
| 5:E:235:ILE:HD12  | 5:E:238:ILE:HG22  | 1.87                     | 0.54              |
| 10:K:188:SER:O    | 10:K:188:SER:OG   | 2.24                     | 0.54              |
| 20:V:85:ALA:HB2   | 20:V:93:PHE:HB2   | 1.88                     | 0.54              |
| 20:V:330:LYS:HD3  | 20:V:360:TYR:CE1  | 2.42                     | 0.54              |
| 20:V:408:ARG:HB2  | 20:V:408:ARG:NH1  | 2.21                     | 0.54              |
| 21:W:219:THR:HG22 | 21:W:219:THR:O    | 2.07                     | 0.54              |
| 24:Z:143:GLU:OE1  | 24:Z:143:GLU:N    | 2.40                     | 0.54              |
| 28:d:104:LEU:O    | 28:d:104:LEU:HD23 | 2.06                     | 0.54              |
| 30:f:498:LEU:O    | 30:f:501:LEU:HG   | 2.07                     | 0.54              |
| 31:F:286:ASP:OD1  | 31:F:287:GLU:N    | 2.39                     | 0.54              |
| 32:U:331:GLY:CA   | 32:U:333:MET:HE1  | 2.37                     | 0.54              |
| 32:U:775:LEU:HD23 | 32:U:775:LEU:O    | 2.08                     | 0.54              |
| 1:A:168:GLU:OE1   | 30:f:723:TYR:HB2  | 2.07                     | 0.54              |
| 2:B:53:THR:HG21   | 30:f:832:THR:OG1  | 2.07                     | 0.54              |
| 3:C:340:ARG:HG2   | 23:Y:208:PHE:H    | 1.71                     | 0.54              |
| 4:D:388:ARG:HB3   | 4:D:389:GLU:OE1   | 2.07                     | 0.54              |
| 12:M:219:LEU:HD23 | 12:M:219:LEU:H    | 1.72                     | 0.54              |
| 20:V:410:ILE:HD13 | 20:V:422:ILE:CD1  | 2.35                     | 0.54              |
| 21:W:48:LEU:HD22  | 21:W:48:LEU:H     | 1.71                     | 0.54              |
| 21:W:55:ARG:HH22  | 21:W:93:ARG:HH21  | 1.56                     | 0.54              |
| 21:W:187:LEU:HD21 | 21:W:226:TYR:CD2  | 2.42                     | 0.54              |
| 21:W:317:TRP:CD1  | 21:W:358:VAL:HG11 | 2.42                     | 0.54              |
| 25:a:35:HIS:O     | 25:a:38:THR:N     | 2.32                     | 0.54              |
| 26:b:57:ASP:OD1   | 26:b:57:ASP:N     | 2.38                     | 0.54              |
| 30:f:14:GLN:C     | 30:f:17:PRO:HD2   | 2.32                     | 0.54              |
| 30:f:126:ILE:HG23 | 30:f:127:SER:N    | 2.21                     | 0.54              |
| 31:F:86:LEU:C     | 31:F:86:LEU:HD13  | 2.32                     | 0.54              |
| 32:U:50:GLU:OE1   | 32:U:50:GLU:HA    | 2.08                     | 0.54              |
| 2:B:264:PRO:HB3   | 2:B:311:GLU:HB3   | 1.89                     | 0.54              |
| 4:D:159:LYS:HG3   | 4:D:160:PRO:CD    | 2.35                     | 0.54              |
| 17:R:158:ARG:NH1  | 17:R:189:SER:OG   | 2.41                     | 0.54              |
| 20:V:411:SER:HB3  | 20:V:447:ILE:HG21 | 1.87                     | 0.54              |
| 21:W:44:ILE:O     | 21:W:48:LEU:HD22  | 2.06                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 21:W:84:ASN:O     | 21:W:87:ILE:HG22  | 2.07                     | 0.54              |
| 21:W:201:ARG:HA   | 21:W:204:ILE:HD11 | 1.88                     | 0.54              |
| 23:Y:307:LEU:CD2  | 23:Y:308:LEU:HD22 | 2.38                     | 0.54              |
| 23:Y:371:LYS:HZ2  | 23:Y:372:LYS:HE2  | 1.70                     | 0.54              |
| 23:Y:377:LEU:O    | 23:Y:377:LEU:HD12 | 2.07                     | 0.54              |
| 24:Z:199:LYS:CE   | 25:a:364:GLU:HG2  | 2.37                     | 0.54              |
| 25:a:99:LYS:O     | 25:a:102:GLU:HG2  | 2.07                     | 0.54              |
| 25:a:193:GLN:HA   | 25:a:193:GLN:OE1  | 2.06                     | 0.54              |
| 30:f:183:PRO:O    | 30:f:187:LEU:HG   | 2.07                     | 0.54              |
| 30:f:274:ASP:OD1  | 30:f:277:LEU:HD12 | 2.07                     | 0.54              |
| 30:f:827:PRO:HB3  | 30:f:860:LYS:NZ   | 2.22                     | 0.54              |
| 31:F:86:LEU:N     | 31:F:87:PRO:HD2   | 2.23                     | 0.54              |
| 31:F:194:GLN:HE22 | 31:F:355:PRO:HD3  | 1.71                     | 0.54              |
| 32:U:210:LYS:HE2  | 32:U:210:LYS:N    | 2.22                     | 0.54              |
| 1:A:209:PRO:HB3   | 1:A:338:ASP:OD2   | 2.08                     | 0.54              |
| 1:A:270:CYS:HB3   | 1:A:315:ILE:HD12  | 1.89                     | 0.54              |
| 2:B:57:GLN:HG2    | 30:f:181:ARG:HH22 | 1.72                     | 0.54              |
| 2:B:405:MET:SD    | 2:B:421:LYS:HD3   | 2.47                     | 0.54              |
| 3:C:184:LYS:N     | 3:C:312:ASP:OD2   | 2.40                     | 0.54              |
| 4:D:391:ARG:NH2   | 4:D:395:LEU:HG    | 2.22                     | 0.54              |
| 4:D:393:ILE:CG1   | 21:W:133:GLU:HB3  | 2.31                     | 0.54              |
| 5:E:116:ASP:HB3   | 5:E:119:VAL:HG23  | 1.89                     | 0.54              |
| 5:E:148:VAL:HG13  | 5:E:149:ILE:HD13  | 1.89                     | 0.54              |
| 7:H:47:THR:CG2    | 7:H:74:VAL:HG21   | 2.37                     | 0.54              |
| 9:J:144:LEU:HD12  | 9:J:156:TRP:HB2   | 1.90                     | 0.54              |
| 20:V:338:LEU:HD21 | 20:V:397:ARG:HG3  | 1.89                     | 0.54              |
| 20:V:403:ILE:O    | 20:V:407:VAL:HG23 | 2.07                     | 0.54              |
| 23:Y:214:MET:HE1  | 23:Y:222:TYR:CD2  | 2.42                     | 0.54              |
| 24:Z:191:ILE:HG21 | 25:a:375:LEU:HA   | 1.90                     | 0.54              |
| 24:Z:199:LYS:HE3  | 25:a:364:GLU:HG2  | 1.90                     | 0.54              |
| 25:a:198:PHE:HE1  | 25:a:202:LEU:HD22 | 1.72                     | 0.54              |
| 27:c:206:ASN:C    | 27:c:206:ASN:OD1  | 2.51                     | 0.54              |
| 28:d:236:THR:O    | 28:d:239:SER:HB3  | 2.07                     | 0.54              |
| 30:f:266:LEU:O    | 30:f:266:LEU:HG   | 2.07                     | 0.54              |
| 30:f:377:VAL:O    | 30:f:381:VAL:HG23 | 2.06                     | 0.54              |
| 6:g:7:ALA:N       | 6:g:10:ASP:OD2    | 2.35                     | 0.54              |
| 12:m:220:THR:HG22 | 12:m:220:THR:O    | 2.08                     | 0.54              |
| 14:o:220:LEU:HD13 | 15:p:47:ARG:HH11  | 1.73                     | 0.54              |
| 18:s:70:ALA:O     | 18:s:74:MET:HG3   | 2.08                     | 0.54              |
| 32:U:204:ILE:HD12 | 32:U:205:TYR:H    | 1.71                     | 0.54              |
| 32:U:587:ALA:HB2  | 32:U:621:SER:HB3  | 1.90                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:386:ARG:O     | 1:A:390:THR:HG22  | 2.07                     | 0.54              |
| 3:C:23:TYR:CD2    | 32:U:105:ILE:HD12 | 2.43                     | 0.54              |
| 3:C:168:PRO:HG3   | 3:C:175:PHE:HE2   | 1.72                     | 0.54              |
| 3:C:371:LEU:HD22  | 4:D:191:TYR:HE2   | 1.73                     | 0.54              |
| 4:D:92:PHE:O      | 4:D:127:ASN:HA    | 2.07                     | 0.54              |
| 21:W:234:ASP:O    | 21:W:239:SER:HB3  | 2.08                     | 0.54              |
| 23:Y:48:ASN:HA    | 23:Y:73:MET:CE    | 2.38                     | 0.54              |
| 23:Y:281:GLU:OE1  | 23:Y:281:GLU:C    | 2.50                     | 0.54              |
| 23:Y:309:GLU:C    | 23:Y:309:GLU:OE1  | 2.51                     | 0.54              |
| 25:a:25:LEU:HD21  | 25:a:37:LEU:HD11  | 1.90                     | 0.54              |
| 27:c:151:VAL:O    | 27:c:152:LYS:HD2  | 2.08                     | 0.54              |
| 27:c:216:MET:HG2  | 27:c:220:LEU:HD11 | 1.89                     | 0.54              |
| 28:d:114:GLU:HA   | 28:d:117:THR:HG22 | 1.88                     | 0.54              |
| 30:f:157:GLU:OE1  | 30:f:157:GLU:N    | 2.38                     | 0.54              |
| 30:f:670:MET:SD   | 30:f:785:ARG:HD3  | 2.48                     | 0.54              |
| 31:F:219:PRO:O    | 31:F:221:LYS:HD2  | 2.08                     | 0.54              |
| 31:F:342:LEU:O    | 31:F:348:LEU:HD11 | 2.07                     | 0.54              |
| 32:U:583:MET:CE   | 32:U:583:MET:HA   | 2.33                     | 0.54              |
| 1:A:273:PHE:HD1   | 1:A:318:LEU:HD22  | 1.72                     | 0.54              |
| 4:D:163:MET:HA    | 4:D:222:HIS:HE2   | 1.72                     | 0.54              |
| 4:D:359:ASP:OD2   | 4:D:362:ASP:HB2   | 2.07                     | 0.54              |
| 17:R:46:MET:HE2   | 36:R:301:LDZ:H17  | 1.89                     | 0.54              |
| 20:V:98:LEU:O     | 20:V:101:LEU:HB3  | 2.08                     | 0.54              |
| 20:V:348:PHE:HD1  | 20:V:361:PHE:HB2  | 1.73                     | 0.54              |
| 23:Y:138:LEU:HD12 | 23:Y:142:PHE:CE2  | 2.42                     | 0.54              |
| 23:Y:314:LEU:CD2  | 23:Y:354:VAL:HG13 | 2.37                     | 0.54              |
| 24:Z:37:GLY:HA2   | 24:Z:56:VAL:HG22  | 1.88                     | 0.54              |
| 24:Z:96:HIS:ND1   | 24:Z:98:GLY:HA3   | 2.22                     | 0.54              |
| 24:Z:187:LEU:O    | 24:Z:191:ILE:HG23 | 2.07                     | 0.54              |
| 24:Z:189:GLN:OE1  | 27:c:297:VAL:HG11 | 2.08                     | 0.54              |
| 26:b:13:SER:O     | 26:b:16:MET:HB3   | 2.08                     | 0.54              |
| 27:c:27:THR:HA    | 27:c:175:ARG:NH2  | 2.23                     | 0.54              |
| 27:c:31:VAL:HG23  | 27:c:203:ILE:CG2  | 2.35                     | 0.54              |
| 27:c:49:VAL:N     | 27:c:50:PRO:HD2   | 2.22                     | 0.54              |
| 32:U:725:MET:HE3  | 32:U:725:MET:C    | 2.32                     | 0.54              |
| 1:A:267:LYS:C     | 1:A:268:LYS:HE2   | 2.32                     | 0.54              |
| 1:A:284:ARG:HA    | 1:A:296:GLN:NE2   | 2.21                     | 0.54              |
| 4:D:60:TYR:OH     | 32:U:640:LEU:HG   | 2.08                     | 0.54              |
| 4:D:251:PHE:HE2   | 4:D:292:LEU:HD23  | 1.72                     | 0.54              |
| 4:D:255:LYS:HB2   | 4:D:255:LYS:NZ    | 2.21                     | 0.54              |
| 5:E:244:SER:O     | 5:E:245:GLU:HB3   | 2.07                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 16:Q:158:GLU:HA   | 16:Q:158:GLU:OE1  | 2.07                     | 0.54              |
| 19:T:54:SER:OG    | 19:T:55:GLY:N     | 2.41                     | 0.54              |
| 20:V:194:LYS:NZ   | 20:V:194:LYS:HB3  | 2.23                     | 0.54              |
| 21:W:293:ASP:OD2  | 21:W:293:ASP:C    | 2.51                     | 0.54              |
| 22:X:274:LYS:HA   | 22:X:277:LEU:HG   | 1.89                     | 0.54              |
| 23:Y:160:ASN:HA   | 23:Y:163:LYS:CG   | 2.38                     | 0.54              |
| 26:b:130:ARG:HA   | 26:b:133:LYS:HG3  | 1.88                     | 0.54              |
| 30:f:80:ARG:HD3   | 30:f:80:ARG:H     | 1.71                     | 0.54              |
| 30:f:260:SER:O    | 30:f:263:PRO:HD2  | 2.08                     | 0.54              |
| 30:f:535:THR:O    | 30:f:539:LEU:HG   | 2.08                     | 0.54              |
| 30:f:556:ARG:O    | 30:f:559:PRO:HD2  | 2.08                     | 0.54              |
| 30:f:664:GLU:N    | 30:f:668:ALA:HB3  | 2.22                     | 0.54              |
| 30:f:712:LYS:NZ   | 30:f:713:PHE:HB2  | 2.23                     | 0.54              |
| 15:p:145:MET:HE2  | 15:p:170:MET:HE1  | 1.88                     | 0.54              |
| 32:U:213:PHE:O    | 32:U:216:VAL:HG12 | 2.07                     | 0.54              |
| 5:E:338:PHE:HA    | 5:E:342:ASP:OD1   | 2.07                     | 0.54              |
| 22:X:194:ARG:HG3  | 22:X:194:ARG:HH11 | 1.71                     | 0.54              |
| 23:Y:387:ILE:CD1  | 24:Z:276:ILE:HD11 | 2.37                     | 0.54              |
| 25:a:27:GLU:O     | 25:a:30:THR:OG1   | 2.24                     | 0.54              |
| 27:c:33:ILE:O     | 27:c:34:SER:HB3   | 2.07                     | 0.54              |
| 27:c:143:VAL:HG22 | 27:c:159:ALA:CB   | 2.36                     | 0.54              |
| 29:e:35:ASP:HB3   | 29:e:37:HIS:CD2   | 2.43                     | 0.54              |
| 30:f:463:LEU:HG   | 30:f:489:TYR:CE2  | 2.43                     | 0.54              |
| 30:f:523:GLY:HA3  | 30:f:561:GLY:HA3  | 1.89                     | 0.54              |
| 15:p:35:THR:HG22  | 15:p:37:ASP:H     | 1.72                     | 0.54              |
| 32:U:457:ILE:CG2  | 32:U:461:LEU:HD23 | 2.37                     | 0.54              |
| 32:U:557:TYR:HD1  | 32:U:588:MET:HE3  | 1.73                     | 0.54              |
| 32:U:807:LYS:CD   | 32:U:807:LYS:N    | 2.70                     | 0.54              |
| 2:B:264:PRO:HG3   | 2:B:308:THR:HA    | 1.89                     | 0.54              |
| 4:D:100:THR:HG21  | 4:D:112:TYR:OH    | 2.08                     | 0.54              |
| 11:L:5:GLN:OE1    | 11:L:5:GLN:N      | 2.41                     | 0.54              |
| 13:N:168:ASP:OD1  | 13:N:169:GLY:N    | 2.41                     | 0.54              |
| 20:V:191:LEU:C    | 20:V:191:LEU:HD13 | 2.32                     | 0.54              |
| 20:V:471:GLU:N    | 20:V:472:PRO:HD2  | 2.23                     | 0.54              |
| 23:Y:27:SER:HB2   | 23:Y:59:LYS:HG3   | 1.89                     | 0.54              |
| 25:a:100:THR:O    | 25:a:103:LYS:HG2  | 2.07                     | 0.54              |
| 25:a:148:VAL:O    | 25:a:149:THR:HG22 | 2.06                     | 0.54              |
| 25:a:278:MET:HE2  | 25:a:320:VAL:HG13 | 1.89                     | 0.54              |
| 26:b:86:PHE:CD2   | 26:b:90:ILE:HD11  | 2.43                     | 0.54              |
| 28:d:71:PHE:HE2   | 28:d:75:MET:CE    | 2.18                     | 0.54              |
| 30:f:463:LEU:HG   | 30:f:489:TYR:HE2  | 1.73                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 30:f:716:ASP:N    | 30:f:716:ASP:OD2  | 2.37                     | 0.54              |
| 32:U:127:ASP:OD1  | 32:U:129:ARG:HG2  | 2.08                     | 0.54              |
| 32:U:599:ILE:HD11 | 32:U:626:LEU:CD2  | 2.37                     | 0.54              |
| 32:U:669:ILE:CD1  | 32:U:695:MET:HE2  | 2.32                     | 0.54              |
| 1:A:338:ASP:C     | 1:A:338:ASP:OD1   | 2.51                     | 0.54              |
| 3:C:297:ARG:HB2   | 3:C:300:ILE:HG13  | 1.90                     | 0.54              |
| 4:D:144:PRO:HD2   | 5:E:64:LEU:HD21   | 1.90                     | 0.54              |
| 4:D:378:ILE:HG13  | 4:D:406:VAL:HG11  | 1.90                     | 0.54              |
| 11:L:81:ALA:HB2   | 11:L:130:VAL:HG21 | 1.89                     | 0.54              |
| 19:T:1:THR:N      | 19:T:105:PRO:O    | 2.41                     | 0.54              |
| 20:V:440:LYS:HD3  | 28:d:146:GLY:N    | 2.23                     | 0.54              |
| 21:W:78:LYS:HA    | 21:W:78:LYS:CE    | 2.37                     | 0.54              |
| 21:W:317:TRP:CE2  | 21:W:355:LYS:HG3  | 2.43                     | 0.54              |
| 21:W:448:LYS:HD2  | 24:Z:154:THR:CG2  | 2.38                     | 0.54              |
| 24:Z:191:ILE:HA   | 24:Z:195:VAL:HG12 | 1.90                     | 0.54              |
| 25:a:143:ASN:O    | 25:a:145:LEU:HD23 | 2.08                     | 0.54              |
| 25:a:217:LEU:HD11 | 25:a:238:TYR:CD1  | 2.43                     | 0.54              |
| 26:b:126:LYS:HG2  | 26:b:129:LYS:NZ   | 2.23                     | 0.54              |
| 27:c:163:ILE:HG13 | 27:c:199:HIS:C    | 2.33                     | 0.54              |
| 28:d:212:LYS:HZ2  | 28:d:213:ARG:HG2  | 1.73                     | 0.54              |
| 30:f:520:LEU:HD23 | 30:f:557:TRP:CB   | 2.28                     | 0.54              |
| 30:f:551:LYS:HA   | 30:f:551:LYS:HE3  | 1.90                     | 0.54              |
| 30:f:686:LEU:O    | 30:f:686:LEU:HD22 | 2.08                     | 0.54              |
| 30:f:768:LEU:HD12 | 30:f:769:THR:N    | 2.23                     | 0.54              |
| 11:l:213:GLY:C    | 11:l:214:ILE:HD13 | 2.33                     | 0.54              |
| 4:D:145:PRO:HG2   | 4:D:256:GLU:CD    | 2.33                     | 0.53              |
| 4:D:327:LEU:O     | 4:D:327:LEU:HD23  | 2.07                     | 0.53              |
| 4:D:339:ARG:HH22  | 4:D:343:LEU:HG    | 1.72                     | 0.53              |
| 5:E:199:VAL:O     | 5:E:200:SER:HB3   | 2.08                     | 0.53              |
| 5:E:307:GLN:OE1   | 5:E:307:GLN:HA    | 2.08                     | 0.53              |
| 12:M:192:GLU:HA   | 12:M:192:GLU:OE2  | 2.07                     | 0.53              |
| 14:O:39:SER:OG    | 14:O:41:ASN:OD1   | 2.26                     | 0.53              |
| 20:V:368:ARG:HH12 | 29:e:43:TRP:HB3   | 1.73                     | 0.53              |
| 21:W:117:ASP:CG   | 21:W:119:PRO:HD2  | 2.33                     | 0.53              |
| 21:W:123:ARG:HH12 | 21:W:124:LEU:HA   | 1.73                     | 0.53              |
| 21:W:286:LEU:HD13 | 21:W:290:ILE:HD13 | 1.89                     | 0.53              |
| 22:X:163:LYS:HB3  | 22:X:196:THR:HG23 | 1.90                     | 0.53              |
| 23:Y:17:LEU:HD12  | 23:Y:286:TRP:CH2  | 2.42                     | 0.53              |
| 25:a:25:LEU:HD23  | 25:a:25:LEU:O     | 2.08                     | 0.53              |
| 25:a:277:LEU:HD12 | 25:a:296:ILE:HD13 | 1.90                     | 0.53              |
| 28:d:3:GLU:OE1    | 28:d:3:GLU:HA     | 2.08                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 30:f:268:LEU:O    | 30:f:272:LEU:HD12 | 2.08                     | 0.53              |
| 30:f:627:GLU:HG3  | 30:f:627:GLU:O    | 2.08                     | 0.53              |
| 30:f:679:LEU:HD22 | 30:f:688:ARG:HH12 | 1.73                     | 0.53              |
| 30:f:745:LEU:HB2  | 30:f:746:ARG:HD3  | 1.89                     | 0.53              |
| 10:k:14:THR:HG23  | 11:l:21:GLN:HE22  | 1.73                     | 0.53              |
| 32:U:58:GLN:O     | 32:U:87:LEU:HD23  | 2.08                     | 0.53              |
| 32:U:436:ALA:O    | 32:U:439:GLU:HG2  | 2.08                     | 0.53              |
| 32:U:540:GLN:OE1  | 32:U:540:GLN:HA   | 2.07                     | 0.53              |
| 1:A:297:ARG:CZ    | 31:F:306:VAL:HG21 | 2.38                     | 0.53              |
| 2:B:105:THR:HB    | 2:B:106:PRO:HD3   | 1.90                     | 0.53              |
| 22:X:154:LEU:HD22 | 22:X:166:LEU:HD11 | 1.90                     | 0.53              |
| 22:X:208:ALA:HB1  | 22:X:239:TYR:HD2  | 1.73                     | 0.53              |
| 23:Y:20:ALA:HB2   | 23:Y:150:PHE:CD1  | 2.43                     | 0.53              |
| 23:Y:59:LYS:HD3   | 23:Y:60:SER:N     | 2.24                     | 0.53              |
| 24:Z:48:LEU:HD12  | 24:Z:49:ASP:H     | 1.72                     | 0.53              |
| 25:a:68:GLU:O     | 25:a:70:ARG:HD2   | 2.08                     | 0.53              |
| 25:a:73:PRO:HA    | 25:a:76:LEU:HB3   | 1.90                     | 0.53              |
| 9:j:66:ASP:OD2    | 9:j:95:ARG:NH2    | 2.41                     | 0.53              |
| 31:F:195:ILE:HG12 | 31:F:236:LEU:CD1  | 2.38                     | 0.53              |
| 32:U:195:ASN:HB2  | 32:U:223:LEU:HD11 | 1.90                     | 0.53              |
| 32:U:357:LYS:HE3  | 32:U:357:LYS:CA   | 2.25                     | 0.53              |
| 32:U:516:LEU:HB3  | 32:U:532:MET:HE2  | 1.90                     | 0.53              |
| 32:U:615:ARG:HH21 | 32:U:645:ASN:HD22 | 1.57                     | 0.53              |
| 2:B:288:ASP:O     | 2:B:292:THR:HB    | 2.08                     | 0.53              |
| 4:D:203:LEU:HD13  | 4:D:327:LEU:HD11  | 1.90                     | 0.53              |
| 4:D:207:PRO:HG2   | 4:D:335:LEU:HD23  | 1.90                     | 0.53              |
| 6:G:38:THR:HG23   | 6:G:202:LEU:HD21  | 1.91                     | 0.53              |
| 36:R:301:LDZ:H39  | 36:R:301:LDZ:C9   | 2.38                     | 0.53              |
| 20:V:176:MET:HE1  | 20:V:217:VAL:HG23 | 1.89                     | 0.53              |
| 24:Z:83:LYS:HB3   | 24:Z:83:LYS:HZ2   | 1.74                     | 0.53              |
| 24:Z:259:VAL:HG21 | 27:c:241:ASN:ND2  | 2.24                     | 0.53              |
| 25:a:130:VAL:HG12 | 25:a:131:THR:HG23 | 1.91                     | 0.53              |
| 26:b:30:GLN:OE1   | 26:b:76:HIS:ND1   | 2.39                     | 0.53              |
| 27:c:136:LEU:HD22 | 27:c:136:LEU:H    | 1.73                     | 0.53              |
| 30:f:61:GLU:CD    | 30:f:97:LYS:HB2   | 2.34                     | 0.53              |
| 30:f:154:TRP:HA   | 30:f:157:GLU:OE2  | 2.08                     | 0.53              |
| 30:f:744:MET:HB3  | 30:f:747:GLN:HE21 | 1.72                     | 0.53              |
| 32:U:221:ILE:HA   | 32:U:260:PHE:HE2  | 1.73                     | 0.53              |
| 32:U:479:LEU:CD2  | 32:U:511:ALA:HA   | 2.36                     | 0.53              |
| 32:U:610:VAL:HG23 | 32:U:611:ASN:N    | 2.23                     | 0.53              |
| 32:U:811:PHE:CD2  | 32:U:885:MET:HE1  | 2.43                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:289:ALA:HA    | 31:F:296:PHE:CE1  | 2.43                     | 0.53              |
| 2:B:116:ILE:HG21  | 2:B:132:TYR:CE2   | 2.30                     | 0.53              |
| 5:E:122:MET:SD    | 5:E:198:VAL:HB    | 2.48                     | 0.53              |
| 5:E:253:ILE:HG13  | 31:F:308:ARG:NH2  | 2.24                     | 0.53              |
| 5:E:342:ASP:HB2   | 5:E:374:VAL:CG1   | 2.38                     | 0.53              |
| 20:V:80:LYS:HG2   | 20:V:84:LYS:HE3   | 1.90                     | 0.53              |
| 20:V:301:GLU:OE1  | 20:V:301:GLU:HA   | 2.07                     | 0.53              |
| 21:W:208:LYS:O    | 21:W:208:LYS:HG3  | 2.06                     | 0.53              |
| 21:W:419:LYS:NZ   | 21:W:423:ASN:HB3  | 2.22                     | 0.53              |
| 22:X:407:MET:HE2  | 24:Z:266:ILE:HG23 | 1.90                     | 0.53              |
| 23:Y:268:TYR:HB2  | 23:Y:322:ALA:O    | 2.08                     | 0.53              |
| 23:Y:308:LEU:HD12 | 23:Y:356:THR:HG22 | 1.89                     | 0.53              |
| 26:b:8:VAL:HA     | 26:b:110:ILE:HD11 | 1.90                     | 0.53              |
| 28:d:23:LEU:HA    | 28:d:26:LEU:CD2   | 2.33                     | 0.53              |
| 28:d:206:MET:HE3  | 28:d:206:MET:N    | 2.06                     | 0.53              |
| 30:f:126:ILE:CD1  | 30:f:173:LEU:HD22 | 2.38                     | 0.53              |
| 30:f:217:LEU:HD13 | 30:f:259:PHE:CZ   | 2.43                     | 0.53              |
| 14:o:141:ASP:OD2  | 19:t:149:LEU:HD13 | 2.08                     | 0.53              |
| 19:t:9:THR:OG1    | 19:t:25:ASP:OD2   | 2.27                     | 0.53              |
| 31:F:233:LYS:HE3  | 31:F:332:THR:O    | 2.08                     | 0.53              |
| 32:U:481:LEU:O    | 32:U:481:LEU:HD22 | 2.09                     | 0.53              |
| 32:U:789:ILE:CG1  | 32:U:911:ILE:HA   | 2.28                     | 0.53              |
| 1:A:284:ARG:O     | 31:F:334:ARG:NH1  | 2.41                     | 0.53              |
| 1:A:365:GLU:OE2   | 1:A:366:ARG:NH2   | 2.42                     | 0.53              |
| 2:B:420:LYS:O     | 2:B:423:LYS:HG3   | 2.09                     | 0.53              |
| 3:C:40:GLN:OE1    | 3:C:43:ARG:NH1    | 2.41                     | 0.53              |
| 3:C:118:ASN:N     | 3:C:118:ASN:OD1   | 2.40                     | 0.53              |
| 4:D:217:LYS:HG2   | 5:E:267:PHE:CD1   | 2.43                     | 0.53              |
| 5:E:314:LYS:HE3   | 5:E:328:TYR:CD2   | 2.43                     | 0.53              |
| 20:V:65:ARG:O     | 20:V:69:THR:HG22  | 2.09                     | 0.53              |
| 21:W:241:LEU:O    | 21:W:241:LEU:HD13 | 2.08                     | 0.53              |
| 21:W:287:VAL:HB   | 21:W:309:PHE:HZ   | 1.73                     | 0.53              |
| 22:X:208:ALA:HB1  | 22:X:239:TYR:CD2  | 2.43                     | 0.53              |
| 22:X:297:ARG:HH21 | 22:X:337:ARG:CG   | 2.19                     | 0.53              |
| 22:X:400:ALA:HA   | 24:Z:262:LEU:CD1  | 2.39                     | 0.53              |
| 23:Y:24:PHE:CD2   | 23:Y:28:LEU:HD13  | 2.44                     | 0.53              |
| 24:Z:12:HIS:O     | 24:Z:15:VAL:HG12  | 2.09                     | 0.53              |
| 24:Z:75:LEU:HD23  | 24:Z:115:TYR:HE2  | 1.72                     | 0.53              |
| 25:a:34:TRP:HZ3   | 26:b:19:GLY:H     | 1.56                     | 0.53              |
| 26:b:9:CYS:SG     | 26:b:54:LEU:HD21  | 2.48                     | 0.53              |
| 26:b:11:ASP:C     | 26:b:11:ASP:OD1   | 2.52                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 30:f:292:LYS:HE2  | 30:f:807:ARG:NH1  | 2.23                     | 0.53              |
| 30:f:489:TYR:HB3  | 30:f:492:SER:HB3  | 1.90                     | 0.53              |
| 30:f:555:ALA:HA   | 30:f:558:LEU:HD23 | 1.91                     | 0.53              |
| 30:f:603:SER:CB   | 30:f:639:LYS:HZ2  | 2.21                     | 0.53              |
| 31:F:364:ARG:O    | 31:F:368:ILE:HG13 | 2.08                     | 0.53              |
| 32:U:377:HIS:HB2  | 32:U:411:ILE:HG13 | 1.91                     | 0.53              |
| 4:D:407:ILE:HD12  | 4:D:407:ILE:C     | 2.33                     | 0.53              |
| 5:E:352:MET:HA    | 5:E:355:ILE:HG22  | 1.91                     | 0.53              |
| 10:K:112:VAL:O    | 10:K:116:VAL:HG23 | 2.08                     | 0.53              |
| 11:L:6:TYR:CD2    | 11:L:15:PRO:HD3   | 2.44                     | 0.53              |
| 21:W:151:THR:O    | 21:W:154:GLU:HB2  | 2.08                     | 0.53              |
| 21:W:254:PRO:O    | 21:W:258:ALA:HB2  | 2.08                     | 0.53              |
| 21:W:268:LYS:O    | 21:W:272:LEU:HB2  | 2.09                     | 0.53              |
| 21:W:271:VAL:CG2  | 21:W:305:LEU:HB2  | 2.38                     | 0.53              |
| 21:W:325:GLY:O    | 21:W:329:ARG:NH1  | 2.42                     | 0.53              |
| 22:X:385:LEU:HG   | 22:X:387:ILE:HD11 | 1.90                     | 0.53              |
| 22:X:388:PHE:CE2  | 23:Y:358:ARG:HD2  | 2.43                     | 0.53              |
| 23:Y:214:MET:O    | 23:Y:214:MET:CG   | 2.53                     | 0.53              |
| 25:a:87:MET:CE    | 25:a:89:ASP:OD1   | 2.56                     | 0.53              |
| 25:a:102:GLU:HA   | 25:a:105:LYS:NZ   | 2.24                     | 0.53              |
| 25:a:185:ILE:HD12 | 25:a:185:ILE:C    | 2.34                     | 0.53              |
| 25:a:186:LYS:CD   | 25:a:221:VAL:HG13 | 2.37                     | 0.53              |
| 26:b:3:LEU:O      | 26:b:106:LYS:N    | 2.36                     | 0.53              |
| 26:b:91:ARG:HH22  | 26:b:130:ARG:HH12 | 1.57                     | 0.53              |
| 26:b:109:ILE:HG13 | 26:b:138:VAL:HG23 | 1.89                     | 0.53              |
| 26:b:129:LYS:HG2  | 26:b:133:LYS:CE   | 2.39                     | 0.53              |
| 27:c:104:ARG:H    | 27:c:104:ARG:HD3  | 1.73                     | 0.53              |
| 29:e:59:GLU:OE1   | 29:e:59:GLU:HA    | 2.09                     | 0.53              |
| 30:f:288:VAL:HG13 | 30:f:873:LEU:HD13 | 1.90                     | 0.53              |
| 30:f:346:ASP:O    | 30:f:350:LYS:HG2  | 2.08                     | 0.53              |
| 30:f:461:PRO:HB2  | 30:f:465:LEU:CD1  | 2.38                     | 0.53              |
| 30:f:486:GLY:HA3  | 30:f:521:ALA:HB1  | 1.90                     | 0.53              |
| 30:f:713:PHE:CE2  | 30:f:752:HIS:HB3  | 2.43                     | 0.53              |
| 17:r:36:ILE:HD11  | 17:r:46:MET:SD    | 2.49                     | 0.53              |
| 32:U:177:LEU:HD11 | 32:U:204:ILE:CG1  | 2.39                     | 0.53              |
| 32:U:213:PHE:CA   | 32:U:216:VAL:HG12 | 2.38                     | 0.53              |
| 32:U:227:GLN:HG2  | 32:U:228:ALA:N    | 2.24                     | 0.53              |
| 32:U:899:ARG:HG2  | 32:U:916:ASP:OD1  | 2.09                     | 0.53              |
| 2:B:342:ILE:HA    | 2:B:347:ILE:HG12  | 1.90                     | 0.53              |
| 4:D:163:MET:SD    | 4:D:222:HIS:NE2   | 2.82                     | 0.53              |
| 10:K:53:ARG:HH11  | 10:K:53:ARG:HG3   | 1.74                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 10:K:215:ILE:HD12 | 10:K:215:ILE:O    | 2.08                     | 0.53              |
| 11:L:31:GLN:CB    | 31:F:435:LEU:HD13 | 2.39                     | 0.53              |
| 19:T:9:THR:HG22   | 19:T:10:SER:H     | 1.74                     | 0.53              |
| 21:W:55:ARG:HH22  | 21:W:93:ARG:HE    | 1.57                     | 0.53              |
| 22:X:170:GLN:CD   | 22:X:192:SER:HG   | 2.12                     | 0.53              |
| 27:c:49:VAL:O     | 27:c:116:PRO:HG3  | 2.09                     | 0.53              |
| 27:c:163:ILE:HG23 | 27:c:201:TYR:CD1  | 2.43                     | 0.53              |
| 28:d:42:LYS:HA    | 28:d:86:LYS:NZ    | 2.23                     | 0.53              |
| 30:f:179:VAL:CG1  | 30:f:216:MET:HE1  | 2.38                     | 0.53              |
| 12:m:202:ASP:C    | 12:m:202:ASP:OD1  | 2.52                     | 0.53              |
| 32:U:463:ASN:HA   | 32:U:466:LYS:NZ   | 2.23                     | 0.53              |
| 32:U:554:LEU:HD12 | 32:U:588:MET:HE1  | 1.89                     | 0.53              |
| 1:A:143:ASP:OD1   | 1:A:143:ASP:C     | 2.52                     | 0.53              |
| 2:B:154:HIS:ND1   | 2:B:154:HIS:O     | 2.42                     | 0.53              |
| 2:B:361:LYS:HD3   | 2:B:390:LEU:CD1   | 2.18                     | 0.53              |
| 2:B:390:LEU:HD22  | 2:B:395:ILE:CD1   | 2.33                     | 0.53              |
| 13:N:128:ILE:HD11 | 13:N:137:TYR:CE1  | 2.44                     | 0.53              |
| 20:V:162:GLU:HA   | 20:V:162:GLU:OE2  | 2.08                     | 0.53              |
| 21:W:73:MET:HE1   | 21:W:77:ALA:HB2   | 1.89                     | 0.53              |
| 21:W:175:GLY:O    | 21:W:182:ARG:NH1  | 2.41                     | 0.53              |
| 21:W:214:PHE:HA   | 21:W:216:GLU:CD   | 2.34                     | 0.53              |
| 22:X:282:ARG:HA   | 22:X:285:GLU:OE1  | 2.09                     | 0.53              |
| 24:Z:190:ARG:NE   | 27:c:300:LEU:HD22 | 2.24                     | 0.53              |
| 27:c:284:LEU:O    | 27:c:288:VAL:HG23 | 2.09                     | 0.53              |
| 30:f:423:ASP:HA   | 30:f:426:LEU:HD23 | 1.90                     | 0.53              |
| 32:U:164:GLU:HA   | 32:U:167:ILE:HG23 | 1.91                     | 0.53              |
| 32:U:256:ALA:HB3  | 32:U:261:LEU:HD21 | 1.89                     | 0.53              |
| 32:U:370:VAL:HG11 | 32:U:404:ALA:HA   | 1.91                     | 0.53              |
| 32:U:765:VAL:HG13 | 32:U:775:LEU:CD2  | 2.39                     | 0.53              |
| 1:A:159:PRO:O     | 1:A:162:THR:HG22  | 2.09                     | 0.53              |
| 2:B:417:GLU:OE1   | 2:B:417:GLU:HA    | 2.07                     | 0.53              |
| 3:C:42:LEU:HD13   | 4:D:54:LEU:HD13   | 1.89                     | 0.53              |
| 4:D:233:SER:OG    | 5:E:259:GLU:OE1   | 2.21                     | 0.53              |
| 5:E:205:ASP:C     | 5:E:205:ASP:OD1   | 2.51                     | 0.53              |
| 5:E:356:ARG:HG3   | 5:E:356:ARG:NH1   | 2.24                     | 0.53              |
| 6:G:122:SER:O     | 6:G:126:THR:HG23  | 2.09                     | 0.53              |
| 15:P:48:LEU:CD2   | 15:P:86:LEU:HD22  | 2.39                     | 0.53              |
| 18:S:26:ASP:C     | 18:S:26:ASP:OD1   | 2.52                     | 0.53              |
| 20:V:254:LEU:CD1  | 20:V:270:LEU:HD13 | 2.39                     | 0.53              |
| 23:Y:247:LEU:HD12 | 23:Y:248:GLU:H    | 1.72                     | 0.53              |
| 24:Z:5:ALA:O      | 24:Z:46:LYS:HD2   | 2.09                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 24:Z:213:GLU:HB3  | 24:Z:219:LYS:NZ   | 2.24                     | 0.53              |
| 25:a:52:GLN:HA    | 25:a:86:GLN:HG2   | 1.90                     | 0.53              |
| 27:c:30:GLN:OE1   | 27:c:181:LEU:HD21 | 2.09                     | 0.53              |
| 27:c:150:SER:HB3  | 27:c:155:VAL:O    | 2.09                     | 0.53              |
| 30:f:271:MET:CE   | 30:f:271:MET:H    | 2.21                     | 0.53              |
| 30:f:479:LEU:CD1  | 30:f:514:VAL:HG22 | 2.26                     | 0.53              |
| 30:f:507:ASP:OD2  | 30:f:509:LYS:HG2  | 2.09                     | 0.53              |
| 32:U:159:ARG:HB2  | 32:U:159:ARG:HH11 | 1.74                     | 0.53              |
| 32:U:384:GLN:C    | 32:U:384:GLN:OE1  | 2.51                     | 0.53              |
| 32:U:475:HIS:HE1  | 32:U:510:GLU:HB2  | 1.73                     | 0.53              |
| 32:U:585:THR:O    | 32:U:589:ALA:N    | 2.34                     | 0.53              |
| 2:B:197:ILE:CG2   | 2:B:239:VAL:HG21  | 2.39                     | 0.53              |
| 2:B:207:HIS:HB3   | 2:B:210:TYR:HE1   | 1.71                     | 0.53              |
| 3:C:351:MET:CE    | 3:C:362:VAL:HG21  | 2.37                     | 0.53              |
| 8:I:174:MET:HE1   | 8:I:199:LYS:HB3   | 1.90                     | 0.53              |
| 9:J:134:VAL:HG12  | 9:J:144:LEU:CD2   | 2.39                     | 0.53              |
| 20:V:466:ILE:HD11 | 20:V:471:GLU:OE2  | 2.09                     | 0.53              |
| 22:X:361:VAL:O    | 22:X:365:LEU:HD23 | 2.09                     | 0.53              |
| 23:Y:48:ASN:HA    | 23:Y:73:MET:HE2   | 1.90                     | 0.53              |
| 25:a:48:PRO:CB    | 25:a:51:ALA:HA    | 2.39                     | 0.53              |
| 25:a:61:GLU:HA    | 25:a:64:ILE:HG13  | 1.90                     | 0.53              |
| 28:d:212:LYS:HD2  | 28:d:212:LYS:C    | 2.34                     | 0.53              |
| 30:f:154:TRP:O    | 30:f:157:GLU:HG2  | 2.09                     | 0.53              |
| 30:f:301:HIS:CE1  | 30:f:305:LEU:HD23 | 2.43                     | 0.53              |
| 30:f:373:ALA:CB   | 30:f:748:LEU:HD21 | 2.39                     | 0.53              |
| 30:f:466:LEU:CB   | 30:f:485:LEU:HD21 | 2.37                     | 0.53              |
| 31:F:78:GLU:OE1   | 31:F:78:GLU:HA    | 2.09                     | 0.53              |
| 32:U:173:VAL:N    | 32:U:174:PRO:HD3  | 2.24                     | 0.53              |
| 32:U:264:VAL:CG1  | 32:U:329:LEU:HD21 | 2.39                     | 0.53              |
| 32:U:423:MET:HG3  | 32:U:446:LEU:HD11 | 1.90                     | 0.53              |
| 32:U:501:LEU:HB2  | 32:U:512:ALA:HB1  | 1.89                     | 0.53              |
| 32:U:609:ASP:OD1  | 32:U:609:ASP:C    | 2.52                     | 0.53              |
| 3:C:63:LEU:HD13   | 3:C:63:LEU:C      | 2.34                     | 0.52              |
| 3:C:235:PHE:HA    | 3:C:238:ALA:HB3   | 1.90                     | 0.52              |
| 4:D:130:VAL:HB    | 4:D:139:LEU:CD2   | 2.40                     | 0.52              |
| 4:D:146:GLU:OE1   | 4:D:147:ALA:N     | 2.42                     | 0.52              |
| 4:D:392:TYR:H     | 21:W:136:ILE:HD11 | 1.74                     | 0.52              |
| 5:E:72:LYS:O      | 5:E:72:LYS:HG2    | 2.08                     | 0.52              |
| 5:E:342:ASP:O     | 5:E:346:VAL:N     | 2.40                     | 0.52              |
| 12:M:39:ILE:HD12  | 12:M:193:VAL:CG2  | 2.39                     | 0.52              |
| 20:V:130:PHE:O    | 20:V:133:PRO:HG2  | 2.08                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 20:V:381:GLN:HG3  | 20:V:382:PHE:CD1  | 2.44                     | 0.52              |
| 21:W:121:LYS:HD2  | 21:W:121:LYS:C    | 2.33                     | 0.52              |
| 21:W:201:ARG:CD   | 21:W:204:ILE:HD11 | 2.38                     | 0.52              |
| 21:W:203:GLN:O    | 21:W:206:SER:OG   | 2.19                     | 0.52              |
| 21:W:372:ARG:O    | 25:a:326:GLU:HG2  | 2.09                     | 0.52              |
| 23:Y:29:PRO:CB    | 23:Y:32:ARG:HG2   | 2.27                     | 0.52              |
| 24:Z:38:VAL:HG23  | 24:Z:56:VAL:HG11  | 1.91                     | 0.52              |
| 25:a:342:ASP:N    | 25:a:342:ASP:OD1  | 2.40                     | 0.52              |
| 26:b:78:VAL:HG13  | 26:b:78:VAL:O     | 2.08                     | 0.52              |
| 26:b:179:LEU:HD13 | 26:b:181:ASP:H    | 1.74                     | 0.52              |
| 28:d:206:MET:N    | 28:d:206:MET:SD   | 2.82                     | 0.52              |
| 30:f:6:ARG:CD     | 30:f:6:ARG:H      | 2.22                     | 0.52              |
| 30:f:523:GLY:O    | 30:f:564:LEU:HD11 | 2.08                     | 0.52              |
| 30:f:646:MET:O    | 30:f:649:HIS:NE2  | 2.42                     | 0.52              |
| 30:f:680:ARG:HH11 | 30:f:761:MET:CE   | 2.21                     | 0.52              |
| 31:F:195:ILE:HA   | 31:F:236:LEU:HD21 | 1.92                     | 0.52              |
| 32:U:494:TYR:CD1  | 32:U:516:LEU:HD11 | 2.44                     | 0.52              |
| 32:U:678:ASP:OD1  | 32:U:679:PRO:HD2  | 2.10                     | 0.52              |
| 32:U:710:ARG:NH1  | 32:U:737:LEU:HD21 | 2.24                     | 0.52              |
| 32:U:712:LEU:O    | 32:U:716:VAL:HG13 | 2.09                     | 0.52              |
| 32:U:811:PHE:CZ   | 32:U:884:VAL:HA   | 2.44                     | 0.52              |
| 32:U:890:LYS:HZ2  | 32:U:891:VAL:HG12 | 1.74                     | 0.52              |
| 1:A:232:ARG:HB2   | 1:A:232:ARG:CZ    | 2.39                     | 0.52              |
| 1:A:394:MET:HE3   | 2:B:199:GLU:CG    | 2.34                     | 0.52              |
| 2:B:280:SER:C     | 2:B:281:ILE:HD13  | 2.34                     | 0.52              |
| 5:E:98:VAL:HB     | 5:E:107:ILE:CG2   | 2.38                     | 0.52              |
| 5:E:192:ASP:N     | 5:E:192:ASP:OD1   | 2.42                     | 0.52              |
| 20:V:379:LEU:HD11 | 20:V:395:ILE:HG21 | 1.90                     | 0.52              |
| 20:V:482:PHE:HE2  | 23:Y:377:LEU:CD1  | 2.15                     | 0.52              |
| 21:W:312:MET:HB3  | 21:W:365:ILE:CD1  | 2.38                     | 0.52              |
| 21:W:441:LYS:HB2  | 21:W:441:LYS:HZ3  | 1.74                     | 0.52              |
| 22:X:130:GLU:HB3  | 22:X:153:LEU:HD22 | 1.90                     | 0.52              |
| 22:X:200:ILE:HG22 | 22:X:203:PRO:HD3  | 1.90                     | 0.52              |
| 28:d:251:ARG:HH11 | 28:d:251:ARG:HG3  | 1.73                     | 0.52              |
| 31:F:404:GLY:HA2  | 31:F:415:LEU:HD21 | 1.90                     | 0.52              |
| 32:U:111:GLN:O    | 32:U:114:GLU:HG3  | 2.10                     | 0.52              |
| 32:U:872:GLU:HG2  | 32:U:872:GLU:O    | 2.09                     | 0.52              |
| 32:U:889:LEU:O    | 32:U:889:LEU:HD23 | 2.09                     | 0.52              |
| 2:B:116:ILE:HG12  | 2:B:117:ASP:N     | 2.24                     | 0.52              |
| 3:C:42:LEU:CD1    | 4:D:54:LEU:HD13   | 2.39                     | 0.52              |
| 3:C:360:LYS:O     | 3:C:360:LYS:CD    | 2.57                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:C:384:GLU:O     | 3:C:387:VAL:HG22  | 2.08                     | 0.52              |
| 5:E:286:ASP:OD1   | 5:E:287:PRO:HD2   | 2.09                     | 0.52              |
| 12:M:8:ASP:OD2    | 12:M:25:TYR:OH    | 2.22                     | 0.52              |
| 21:W:125:ILE:HG13 | 21:W:129:ARG:HH12 | 1.74                     | 0.52              |
| 21:W:157:GLY:CA   | 21:W:161:GLU:HG3  | 2.39                     | 0.52              |
| 21:W:259:GLU:HB3  | 21:W:262:LYS:HB3  | 1.90                     | 0.52              |
| 22:X:340:GLU:N    | 22:X:341:PRO:HD2  | 2.24                     | 0.52              |
| 22:X:396:THR:N    | 27:c:242:GLU:OE1  | 2.42                     | 0.52              |
| 25:a:33:LEU:HB2   | 26:b:18:ASN:HD22  | 1.75                     | 0.52              |
| 25:a:47:ASP:C     | 25:a:47:ASP:OD1   | 2.52                     | 0.52              |
| 25:a:230:ARG:O    | 25:a:230:ARG:CG   | 2.57                     | 0.52              |
| 26:b:13:SER:O     | 26:b:80:PRO:HB2   | 2.10                     | 0.52              |
| 26:b:141:ILE:HB   | 26:b:171:VAL:CG2  | 2.39                     | 0.52              |
| 30:f:75:LEU:HD12  | 30:f:76:GLU:N     | 2.24                     | 0.52              |
| 30:f:373:ALA:HA   | 30:f:748:LEU:HD21 | 1.91                     | 0.52              |
| 30:f:373:ALA:CA   | 30:f:748:LEU:HD21 | 2.39                     | 0.52              |
| 30:f:679:LEU:HD11 | 30:f:681:TYR:HE2  | 1.74                     | 0.52              |
| 32:U:167:ILE:HB   | 32:U:204:ILE:CG2  | 2.36                     | 0.52              |
| 32:U:422:LEU:HG   | 32:U:423:MET:HE2  | 1.90                     | 0.52              |
| 1:A:168:GLU:OE2   | 1:A:168:GLU:HA    | 2.09                     | 0.52              |
| 1:A:295:VAL:HG21  | 2:B:307:ARG:CZ    | 2.39                     | 0.52              |
| 3:C:82:LYS:HB3    | 3:C:82:LYS:NZ     | 2.25                     | 0.52              |
| 4:D:132:LEU:CD2   | 4:D:139:LEU:HD23  | 2.40                     | 0.52              |
| 4:D:140:VAL:O     | 4:D:140:VAL:HG12  | 2.09                     | 0.52              |
| 5:E:148:VAL:HG13  | 5:E:149:ILE:CD1   | 2.40                     | 0.52              |
| 5:E:235:ILE:O     | 5:E:235:ILE:HG13  | 2.09                     | 0.52              |
| 17:R:50:ALA:HA    | 36:R:301:LDZ:H22  | 1.92                     | 0.52              |
| 20:V:467:TYR:HE2  | 23:Y:362:LYS:HE2  | 1.74                     | 0.52              |
| 22:X:236:PHE:CE1  | 22:X:251:LEU:HG   | 2.45                     | 0.52              |
| 22:X:407:MET:HG3  | 24:Z:266:ILE:CD1  | 2.40                     | 0.52              |
| 23:Y:267:ARG:O    | 23:Y:270:VAL:HG12 | 2.10                     | 0.52              |
| 24:Z:40:LEU:HD11  | 24:Z:54:PHE:HD1   | 1.73                     | 0.52              |
| 25:a:205:LEU:HD23 | 25:a:205:LEU:H    | 1.75                     | 0.52              |
| 26:b:12:ASN:HD21  | 26:b:55:ALA:HB2   | 1.74                     | 0.52              |
| 27:c:151:VAL:CG2  | 27:c:152:LYS:H    | 2.22                     | 0.52              |
| 30:f:176:ALA:O    | 30:f:179:VAL:HG23 | 2.09                     | 0.52              |
| 30:f:440:ILE:CG1  | 30:f:441:LYS:HD2  | 2.39                     | 0.52              |
| 13:n:56:VAL:HG13  | 13:n:87:MET:HE3   | 1.92                     | 0.52              |
| 31:F:221:LYS:HD2  | 31:F:221:LYS:N    | 2.25                     | 0.52              |
| 32:U:173:VAL:HG13 | 32:U:176:MET:O    | 2.10                     | 0.52              |
| 32:U:201:LEU:O    | 32:U:204:ILE:HD11 | 2.10                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 32:U:264:VAL:HG13 | 32:U:329:LEU:HD21 | 1.92                     | 0.52              |
| 32:U:481:LEU:HD13 | 32:U:481:LEU:C    | 2.35                     | 0.52              |
| 2:B:136:LEU:HB3   | 2:B:138:PHE:CD2   | 2.45                     | 0.52              |
| 4:D:214:MET:CE    | 33:D:501:ATP:H2'  | 2.40                     | 0.52              |
| 5:E:172:LEU:HD23  | 5:E:299:ILE:HB    | 1.92                     | 0.52              |
| 19:T:27:LEU:HD22  | 19:T:184:TYR:HB2  | 1.91                     | 0.52              |
| 20:V:386:PHE:HB3  | 20:V:392:TYR:HB2  | 1.91                     | 0.52              |
| 22:X:343:SER:O    | 22:X:344:ARG:C    | 2.52                     | 0.52              |
| 23:Y:13:LYS:HB2   | 23:Y:13:LYS:NZ    | 2.24                     | 0.52              |
| 25:a:33:LEU:HD12  | 25:a:34:TRP:N     | 2.24                     | 0.52              |
| 26:b:14:GLU:HB3   | 26:b:82:GLY:H     | 1.74                     | 0.52              |
| 27:c:73:PHE:CD2   | 27:c:95:MET:HG2   | 2.44                     | 0.52              |
| 27:c:164:ASN:OD1  | 27:c:165:ALA:N    | 2.43                     | 0.52              |
| 28:d:212:LYS:HD2  | 28:d:213:ARG:N    | 2.24                     | 0.52              |
| 19:t:200:GLU:OE1  | 19:t:201:GLY:N    | 2.43                     | 0.52              |
| 32:U:472:ILE:HD12 | 32:U:473:VAL:N    | 2.25                     | 0.52              |
| 1:A:113:ILE:HD11  | 1:A:142:VAL:CG1   | 2.34                     | 0.52              |
| 5:E:319:PRO:O     | 5:E:320:ILE:HD13  | 2.08                     | 0.52              |
| 8:I:11:ILE:HD13   | 9:J:7:ILE:HD12    | 1.91                     | 0.52              |
| 20:V:135:LEU:HD22 | 20:V:135:LEU:N    | 2.25                     | 0.52              |
| 20:V:201:ARG:HA   | 20:V:201:ARG:HE   | 1.75                     | 0.52              |
| 20:V:278:GLU:OE1  | 20:V:278:GLU:HA   | 2.08                     | 0.52              |
| 21:W:118:LEU:C    | 21:W:118:LEU:HD13 | 2.34                     | 0.52              |
| 23:Y:31:HIS:C     | 23:Y:32:ARG:HD2   | 2.34                     | 0.52              |
| 23:Y:241:ILE:HG23 | 23:Y:261:PHE:CE1  | 2.45                     | 0.52              |
| 25:a:33:LEU:CD1   | 25:a:36:GLN:HG3   | 2.39                     | 0.52              |
| 27:c:110:GLY:HA3  | 27:c:141:VAL:O    | 2.09                     | 0.52              |
| 30:f:483:PHE:HE2  | 30:f:517:VAL:HG21 | 1.75                     | 0.52              |
| 30:f:610:GLN:HA   | 30:f:610:GLN:HE21 | 1.75                     | 0.52              |
| 18:s:114:ASP:OD2  | 18:s:114:ASP:N    | 2.36                     | 0.52              |
| 31:F:175:MET:HB2  | 31:F:250:LYS:O    | 2.09                     | 0.52              |
| 32:U:9:ILE:CD1    | 32:U:42:VAL:HG21  | 2.39                     | 0.52              |
| 32:U:712:LEU:HD13 | 32:U:712:LEU:C    | 2.34                     | 0.52              |
| 1:A:235:ALA:HB1   | 1:A:269:ALA:O     | 2.10                     | 0.52              |
| 2:B:187:ILE:HD13  | 2:B:235:LEU:HD23  | 1.91                     | 0.52              |
| 2:B:225:TYR:CZ    | 2:B:352:GLU:HB2   | 2.45                     | 0.52              |
| 2:B:260:LEU:HD23  | 2:B:299:SER:HB2   | 1.92                     | 0.52              |
| 2:B:355:LEU:HD13  | 2:B:389:ASP:HB2   | 1.90                     | 0.52              |
| 3:C:189:TYR:CE1   | 3:C:298:ILE:HD12  | 2.45                     | 0.52              |
| 3:C:282:GLY:O     | 3:C:284:GLU:N     | 2.43                     | 0.52              |
| 4:D:382:SER:HB2   | 4:D:399:PHE:CD1   | 2.45                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:E:270:LEU:CD2   | 5:E:273:VAL:HB    | 2.34                     | 0.52              |
| 5:E:291:ARG:HH21  | 5:E:294:ARG:NH1   | 2.07                     | 0.52              |
| 20:V:285:TRP:CD1  | 20:V:289:LEU:HD21 | 2.45                     | 0.52              |
| 21:W:279:PHE:HD1  | 21:W:280:ASP:H    | 1.58                     | 0.52              |
| 23:Y:300:ARG:HG3  | 23:Y:300:ARG:NH1  | 2.25                     | 0.52              |
| 24:Z:113:LYS:HE2  | 24:Z:117:PRO:O    | 2.10                     | 0.52              |
| 25:a:48:PRO:HB2   | 25:a:51:ALA:N     | 2.24                     | 0.52              |
| 25:a:357:CYS:O    | 25:a:360:VAL:HG12 | 2.09                     | 0.52              |
| 26:b:11:ASP:OD1   | 26:b:12:ASN:N     | 2.43                     | 0.52              |
| 28:d:64:LEU:HA    | 28:d:165:PHE:CE1  | 2.45                     | 0.52              |
| 28:d:198:LEU:HD12 | 28:d:200:PHE:CZ   | 2.45                     | 0.52              |
| 28:d:227:SER:O    | 28:d:228:GLN:HG2  | 2.10                     | 0.52              |
| 30:f:470:VAL:HA   | 30:f:478:ARG:HB2  | 1.90                     | 0.52              |
| 30:f:617:SER:HA   | 30:f:620:PHE:HE1  | 1.74                     | 0.52              |
| 32:U:177:LEU:O    | 32:U:177:LEU:HD23 | 2.10                     | 0.52              |
| 1:A:365:GLU:HA    | 1:A:366:ARG:NH1   | 2.25                     | 0.52              |
| 2:B:59:ARG:CB     | 30:f:184:LEU:HD22 | 2.39                     | 0.52              |
| 3:C:237:MET:O     | 3:C:237:MET:HG2   | 2.09                     | 0.52              |
| 4:D:203:LEU:HD22  | 4:D:322:LEU:HD21  | 1.92                     | 0.52              |
| 4:D:373:ALA:HB1   | 5:E:292:PRO:O     | 2.10                     | 0.52              |
| 20:V:349:ARG:NH2  | 29:e:37:HIS:O     | 2.43                     | 0.52              |
| 20:V:366:ALA:HB2  | 20:V:374:LYS:HG3  | 1.92                     | 0.52              |
| 21:W:422:ASN:O    | 21:W:426:ASN:HB2  | 2.10                     | 0.52              |
| 23:Y:212:GLU:HG2  | 23:Y:213:LEU:N    | 2.24                     | 0.52              |
| 24:Z:44:GLN:C     | 24:Z:45:LYS:HG2   | 2.34                     | 0.52              |
| 24:Z:230:LEU:HB3  | 25:a:349:MET:HE3  | 1.91                     | 0.52              |
| 25:a:135:ILE:HG13 | 25:a:155:PHE:HE2  | 1.75                     | 0.52              |
| 25:a:370:GLN:NE2  | 28:d:244:LYS:HB3  | 2.25                     | 0.52              |
| 26:b:25:ARG:NH1   | 26:b:144:GLY:O    | 2.42                     | 0.52              |
| 26:b:91:ARG:HH21  | 26:b:127:LEU:CD2  | 2.22                     | 0.52              |
| 26:b:91:ARG:HH21  | 26:b:127:LEU:HD21 | 1.75                     | 0.52              |
| 26:b:91:ARG:HH12  | 26:b:130:ARG:HH12 | 1.58                     | 0.52              |
| 28:d:193:GLU:O    | 28:d:197:ILE:HG12 | 2.10                     | 0.52              |
| 30:f:217:LEU:HD11 | 30:f:245:ASN:HD21 | 1.75                     | 0.52              |
| 30:f:456:ARG:O    | 30:f:456:ARG:HD2  | 2.09                     | 0.52              |
| 30:f:620:PHE:CZ   | 30:f:629:LYS:HD2  | 2.44                     | 0.52              |
| 30:f:780:PRO:HG3  | 30:f:803:PHE:CD2  | 2.44                     | 0.52              |
| 32:U:334:ALA:O    | 32:U:338:HIS:N    | 2.30                     | 0.52              |
| 32:U:443:LEU:HD22 | 32:U:443:LEU:N    | 2.25                     | 0.52              |
| 1:A:301:GLU:HG2   | 31:F:254:PRO:HG2  | 1.92                     | 0.52              |
| 1:A:424:SER:OG    | 1:A:425:ALA:N     | 2.42                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:C:57:ARG:NH2    | 32:U:649:ARG:HH12 | 2.04                     | 0.52              |
| 4:D:364:VAL:O     | 4:D:364:VAL:CG2   | 2.58                     | 0.52              |
| 4:D:417:TYR:OH    | 6:G:26:GLU:OE2    | 2.26                     | 0.52              |
| 5:E:50:LEU:HD13   | 31:F:82:VAL:CG1   | 2.37                     | 0.52              |
| 20:V:224:LEU:HB2  | 20:V:261:TYR:OH   | 2.09                     | 0.52              |
| 20:V:404:LYS:HD2  | 20:V:446:VAL:CG2  | 2.40                     | 0.52              |
| 20:V:404:LYS:HE3  | 20:V:446:VAL:HG21 | 1.91                     | 0.52              |
| 21:W:445:LEU:HB3  | 24:Z:226:ILE:HD11 | 1.92                     | 0.52              |
| 22:X:190:LEU:O    | 22:X:190:LEU:HD22 | 2.10                     | 0.52              |
| 22:X:372:LYS:O    | 22:X:372:LYS:CG   | 2.58                     | 0.52              |
| 24:Z:22:HIS:CE1   | 24:Z:55:ALA:HB1   | 2.44                     | 0.52              |
| 24:Z:213:GLU:C    | 24:Z:219:LYS:HZ2  | 2.18                     | 0.52              |
| 24:Z:263:ALA:HB1  | 27:c:288:VAL:HG13 | 1.91                     | 0.52              |
| 25:a:258:GLN:N    | 25:a:259:PRO:HD2  | 2.25                     | 0.52              |
| 25:a:340:VAL:C    | 25:a:341:LEU:HD23 | 2.35                     | 0.52              |
| 26:b:97:LEU:HB3   | 26:b:100:ARG:HH12 | 1.75                     | 0.52              |
| 26:b:129:LYS:O    | 26:b:132:LYS:HG2  | 2.10                     | 0.52              |
| 27:c:229:LEU:HD22 | 27:c:229:LEU:N    | 2.25                     | 0.52              |
| 30:f:271:MET:HE3  | 30:f:271:MET:H    | 1.74                     | 0.52              |
| 12:m:87:LEU:HD12  | 12:m:133:CYS:SG   | 2.49                     | 0.52              |
| 31:F:226:TYR:CE1  | 31:F:353:GLU:HA   | 2.45                     | 0.52              |
| 32:U:505:ASP:C    | 32:U:505:ASP:OD1  | 2.52                     | 0.52              |
| 32:U:536:ALA:HB1  | 32:U:545:LEU:HD11 | 1.92                     | 0.52              |
| 32:U:610:VAL:HG23 | 32:U:611:ASN:H    | 1.74                     | 0.52              |
| 32:U:801:GLN:HG2  | 32:U:878:LEU:H    | 1.75                     | 0.52              |
| 3:C:24:TYR:OH     | 4:D:41:TYR:HD1    | 1.93                     | 0.52              |
| 3:C:164:VAL:HG12  | 3:C:183:PRO:HG2   | 1.92                     | 0.52              |
| 4:D:285:VAL:HG21  | 5:E:255:ARG:CZ    | 2.39                     | 0.52              |
| 5:E:72:LYS:CB     | 5:E:78:ARG:HD3    | 2.40                     | 0.52              |
| 5:E:138:LEU:O     | 5:E:142:ILE:HG13  | 2.10                     | 0.52              |
| 20:V:318:GLN:HG2  | 20:V:319:HIS:H    | 1.75                     | 0.52              |
| 21:W:206:SER:HB2  | 21:W:230:MET:HE3  | 1.92                     | 0.52              |
| 22:X:366:SER:O    | 22:X:369:ILE:HG13 | 2.09                     | 0.52              |
| 22:X:409:LYS:HA   | 22:X:412:ASP:HB2  | 1.92                     | 0.52              |
| 24:Z:36:VAL:HG22  | 24:Z:96:HIS:CB    | 2.39                     | 0.52              |
| 27:c:292:MET:CE   | 28:d:253:LEU:HD13 | 2.37                     | 0.52              |
| 30:f:141:LYS:HD2  | 30:f:142:TYR:N    | 2.25                     | 0.52              |
| 30:f:416:MET:HE1  | 30:f:447:ALA:CA   | 2.40                     | 0.52              |
| 30:f:519:ALA:HB3  | 30:f:557:TRP:NE1  | 2.25                     | 0.52              |
| 30:f:603:SER:HB2  | 30:f:639:LYS:HD3  | 1.91                     | 0.52              |
| 30:f:672:LEU:HA   | 30:f:675:PHE:HE1  | 1.75                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 31:F:314:LEU:HD23 | 31:F:342:LEU:HD13 | 1.92                     | 0.52              |
| 32:U:181:LEU:O    | 32:U:181:LEU:HD22 | 2.10                     | 0.52              |
| 32:U:745:THR:HB   | 32:U:786:THR:CG2  | 2.40                     | 0.52              |
| 32:U:803:LYS:HE3  | 32:U:804:SER:O    | 2.10                     | 0.52              |
| 2:B:386:ALA:C     | 2:B:387:LYS:HD2   | 2.35                     | 0.51              |
| 3:C:176:GLU:C     | 3:C:176:GLU:OE1   | 2.53                     | 0.51              |
| 4:D:120:ASP:HB3   | 4:D:123:LEU:HD23  | 1.91                     | 0.51              |
| 4:D:130:VAL:HB    | 4:D:139:LEU:HD22  | 1.93                     | 0.51              |
| 4:D:130:VAL:HG23  | 4:D:132:LEU:HD21  | 1.92                     | 0.51              |
| 5:E:91:LYS:NZ     | 5:E:91:LYS:HB3    | 2.24                     | 0.51              |
| 5:E:352:MET:HA    | 5:E:352:MET:CE    | 2.33                     | 0.51              |
| 6:G:112:ASP:OD1   | 6:G:112:ASP:N     | 2.43                     | 0.51              |
| 19:T:74:GLU:OE2   | 19:T:82:SER:HA    | 2.09                     | 0.51              |
| 20:V:304:GLU:HG3  | 20:V:307:ARG:NE   | 2.25                     | 0.51              |
| 20:V:347:GLN:HE22 | 20:V:348:PHE:HE2  | 1.58                     | 0.51              |
| 20:V:355:ARG:HH12 | 20:V:358:MET:HG2  | 1.75                     | 0.51              |
| 21:W:263:TRP:HE1  | 21:W:295:LYS:HG2  | 1.75                     | 0.51              |
| 21:W:279:PHE:HD1  | 21:W:280:ASP:N    | 2.08                     | 0.51              |
| 22:X:316:ASP:C    | 22:X:316:ASP:OD2  | 2.53                     | 0.51              |
| 23:Y:202:LEU:HD22 | 23:Y:239:LYS:HZ3  | 1.75                     | 0.51              |
| 23:Y:300:ARG:HD3  | 29:e:52:PHE:CE1   | 2.44                     | 0.51              |
| 24:Z:262:LEU:O    | 24:Z:266:ILE:HG12 | 2.10                     | 0.51              |
| 25:a:35:HIS:NE2   | 26:b:17:ARG:HG2   | 2.25                     | 0.51              |
| 28:d:45:LYS:HB3   | 28:d:88:GLN:OE1   | 2.11                     | 0.51              |
| 30:f:119:LYS:HA   | 30:f:119:LYS:HE3  | 1.91                     | 0.51              |
| 30:f:551:LYS:HA   | 30:f:551:LYS:CE   | 2.40                     | 0.51              |
| 30:f:744:MET:HA   | 30:f:747:GLN:HE21 | 1.75                     | 0.51              |
| 9:j:42:VAL:HG22   | 9:j:210:VAL:HG12  | 1.91                     | 0.51              |
| 16:q:29:LYS:NZ    | 16:q:31:ASP:OD1   | 2.35                     | 0.51              |
| 31:F:220:PRO:C    | 31:F:221:LYS:HD2  | 2.36                     | 0.51              |
| 1:A:134:ILE:HD12  | 1:A:140:VAL:HG11  | 1.93                     | 0.51              |
| 2:B:216:ILE:H     | 2:B:216:ILE:HD12  | 1.75                     | 0.51              |
| 3:C:98:ASP:OD1    | 3:C:99:VAL:N      | 2.41                     | 0.51              |
| 3:C:149:GLU:CG    | 23:Y:133:ALA:HB1  | 2.40                     | 0.51              |
| 3:C:298:ILE:O     | 3:C:298:ILE:HG12  | 2.10                     | 0.51              |
| 4:D:168:GLY:HA3   | 33:D:501:ATP:HN62 | 1.74                     | 0.51              |
| 4:D:242:GLU:C     | 4:D:242:GLU:OE1   | 2.53                     | 0.51              |
| 5:E:69:PHE:O      | 5:E:80:VAL:HA     | 2.10                     | 0.51              |
| 5:E:190:GLN:O     | 5:E:191:LEU:HB2   | 2.10                     | 0.51              |
| 5:E:204:VAL:CG2   | 5:E:253:ILE:HD11  | 2.34                     | 0.51              |
| 36:N:301:LDZ:N16  | 36:N:301:LDZ:O32  | 2.43                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 20:V:281:ASN:C    | 20:V:281:ASN:OD1  | 2.53                     | 0.51              |
| 20:V:430:SER:OG   | 20:V:433:ASP:OD1  | 2.20                     | 0.51              |
| 23:Y:214:MET:HE2  | 23:Y:219:PHE:HA   | 1.92                     | 0.51              |
| 24:Z:22:HIS:HD2   | 24:Z:25:ARG:HD3   | 1.75                     | 0.51              |
| 25:a:104:VAL:HG23 | 25:a:104:VAL:O    | 2.09                     | 0.51              |
| 25:a:210:VAL:HG12 | 25:a:213:PHE:CE2  | 2.44                     | 0.51              |
| 26:b:48:ASN:HD21  | 26:b:64:LEU:CB    | 2.24                     | 0.51              |
| 27:c:59:GLY:HA3   | 27:c:69:VAL:HA    | 1.90                     | 0.51              |
| 28:d:52:ARG:HA    | 28:d:81:TYR:CD2   | 2.46                     | 0.51              |
| 28:d:181:CYS:SG   | 28:d:182:ILE:N    | 2.83                     | 0.51              |
| 29:e:60:LEU:HD22  | 29:e:60:LEU:H     | 1.75                     | 0.51              |
| 30:f:821:LEU:HD11 | 30:f:882:LEU:HD22 | 1.92                     | 0.51              |
| 32:U:676:THR:HG23 | 32:U:677:ASN:OD1  | 2.09                     | 0.51              |
| 32:U:792:ASN:CG   | 32:U:796:LYS:H    | 2.18                     | 0.51              |
| 1:A:196:LEU:CD1   | 30:f:348:ILE:HD13 | 2.28                     | 0.51              |
| 2:B:94:GLU:O      | 2:B:98:LYS:HD3    | 2.10                     | 0.51              |
| 2:B:411:ARG:HG2   | 2:B:413:LYS:H     | 1.74                     | 0.51              |
| 3:C:356:GLY:HA3   | 35:C:501:ADP:C8   | 2.45                     | 0.51              |
| 4:D:123:LEU:CB    | 4:D:142:VAL:HG11  | 2.39                     | 0.51              |
| 21:W:84:ASN:HD21  | 21:W:123:ARG:HB2  | 1.75                     | 0.51              |
| 21:W:105:VAL:O    | 21:W:109:CYS:N    | 2.42                     | 0.51              |
| 21:W:145:LEU:HD11 | 21:W:185:PHE:CD1  | 2.46                     | 0.51              |
| 23:Y:101:ARG:HH22 | 23:Y:105:MET:HE2  | 1.75                     | 0.51              |
| 23:Y:229:ILE:HB   | 23:Y:299:MET:HE1  | 1.91                     | 0.51              |
| 23:Y:240:VAL:HG23 | 23:Y:260:LEU:HD11 | 1.92                     | 0.51              |
| 26:b:179:LEU:HD13 | 26:b:180:ALA:N    | 2.25                     | 0.51              |
| 30:f:6:ARG:HB2    | 30:f:8:LYS:HZ3    | 1.75                     | 0.51              |
| 30:f:438:ASP:O    | 30:f:441:LYS:HG2  | 2.10                     | 0.51              |
| 30:f:530:CYS:O    | 30:f:534:VAL:HG22 | 2.09                     | 0.51              |
| 30:f:664:GLU:O    | 30:f:669:GLU:HG2  | 2.11                     | 0.51              |
| 30:f:681:TYR:CB   | 30:f:761:MET:HE3  | 2.22                     | 0.51              |
| 30:f:813:LYS:CD   | 30:f:882:LEU:HD21 | 2.36                     | 0.51              |
| 32:U:191:LYS:HE2  | 32:U:560:MET:HE1  | 1.92                     | 0.51              |
| 32:U:231:ASP:HA   | 32:U:234:GLU:HG3  | 1.91                     | 0.51              |
| 1:A:280:ILE:HA    | 1:A:295:VAL:CG1   | 2.35                     | 0.51              |
| 2:B:54:PRO:HG3    | 2:B:60:LEU:HD23   | 1.93                     | 0.51              |
| 2:B:112:LEU:HD12  | 2:B:113:GLU:N     | 2.25                     | 0.51              |
| 4:D:249:ASP:OD1   | 4:D:249:ASP:C     | 2.53                     | 0.51              |
| 5:E:244:SER:O     | 31:F:300:LYS:HA   | 2.10                     | 0.51              |
| 10:K:234:LEU:O    | 10:K:238:ILE:HG13 | 2.09                     | 0.51              |
| 11:L:88:MET:HE2   | 11:L:112:ILE:HD11 | 1.93                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 20:V:494:MET:HE1  | 24:Z:274:ASN:OD1  | 2.10                     | 0.51              |
| 22:X:258:LYS:HE2  | 22:X:266:ASP:OD2  | 2.10                     | 0.51              |
| 22:X:366:SER:HA   | 22:X:369:ILE:HD11 | 1.91                     | 0.51              |
| 23:Y:260:LEU:C    | 23:Y:260:LEU:HD23 | 2.34                     | 0.51              |
| 24:Z:38:VAL:HG21  | 24:Z:75:LEU:CD2   | 2.40                     | 0.51              |
| 24:Z:81:MET:CE    | 27:c:94:LYS:HD3   | 2.38                     | 0.51              |
| 24:Z:190:ARG:NH2  | 27:c:300:LEU:HD22 | 2.25                     | 0.51              |
| 25:a:304:VAL:HG13 | 25:a:305:ASN:OD1  | 2.10                     | 0.51              |
| 28:d:227:SER:C    | 28:d:228:GLN:HG2  | 2.36                     | 0.51              |
| 30:f:297:MET:HE1  | 30:f:456:ARG:HH21 | 1.74                     | 0.51              |
| 30:f:712:LYS:HE2  | 30:f:750:GLN:CD   | 2.35                     | 0.51              |
| 32:U:201:LEU:HD22 | 32:U:201:LEU:O    | 2.11                     | 0.51              |
| 32:U:520:MET:HE1  | 32:U:525:ASN:HB3  | 1.92                     | 0.51              |
| 2:B:59:ARG:NH2    | 30:f:184:LEU:HD13 | 2.25                     | 0.51              |
| 3:C:273:MET:O     | 3:C:276:LEU:N     | 2.43                     | 0.51              |
| 33:E:402:ATP:H5'1 | 31:F:344:ARG:NH1  | 2.26                     | 0.51              |
| 7:H:202:MET:SD    | 7:H:207:ILE:HG21  | 2.51                     | 0.51              |
| 9:J:69:VAL:HG12   | 9:J:104:VAL:HG12  | 1.93                     | 0.51              |
| 19:T:69:GLN:NE2   | 19:T:73:ASP:OD1   | 2.44                     | 0.51              |
| 21:W:51:GLU:HB3   | 21:W:66:ILE:HD12  | 1.92                     | 0.51              |
| 22:X:154:LEU:CD2  | 22:X:166:LEU:HD11 | 2.41                     | 0.51              |
| 24:Z:59:ASP:HB2   | 26:b:99:HIS:HE2   | 1.73                     | 0.51              |
| 25:a:78:GLU:O     | 25:a:82:HIS:ND1   | 2.43                     | 0.51              |
| 28:d:124:ALA:H    | 28:d:125:LYS:NZ   | 2.08                     | 0.51              |
| 6:g:69:LEU:HD23   | 6:g:79:VAL:HG23   | 1.92                     | 0.51              |
| 7:h:92:LEU:HD13   | 7:h:112:ARG:HB3   | 1.92                     | 0.51              |
| 7:h:159:ALA:HB1   | 7:h:173:LEU:HD13  | 1.92                     | 0.51              |
| 31:F:210:GLU:HA   | 31:F:213:GLU:OE2  | 2.11                     | 0.51              |
| 31:F:300:LYS:O    | 31:F:301:ALA:HB3  | 2.09                     | 0.51              |
| 2:B:85:MET:HG2    | 2:B:86:LYS:HD2    | 1.93                     | 0.51              |
| 2:B:155:LYS:HB2   | 2:B:155:LYS:NZ    | 2.25                     | 0.51              |
| 3:C:381:GLU:HG3   | 22:X:191:THR:HG23 | 1.93                     | 0.51              |
| 4:D:126:PRO:O     | 4:D:127:ASN:C     | 2.54                     | 0.51              |
| 5:E:50:LEU:HD11   | 31:F:82:VAL:HG21  | 1.92                     | 0.51              |
| 5:E:80:VAL:HG13   | 5:E:80:VAL:O      | 2.10                     | 0.51              |
| 20:V:116:ALA:HB1  | 20:V:167:LEU:HD21 | 1.91                     | 0.51              |
| 20:V:313:LEU:HD11 | 20:V:329:HIS:HE1  | 1.71                     | 0.51              |
| 21:W:353:ASP:O    | 21:W:357:ARG:HG2  | 2.10                     | 0.51              |
| 22:X:335:LEU:O    | 22:X:338:VAL:HG12 | 2.11                     | 0.51              |
| 24:Z:230:LEU:HD22 | 25:a:349:MET:HE3  | 1.92                     | 0.51              |
| 25:a:326:GLU:OE2  | 25:a:326:GLU:N    | 2.42                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 26:b:100:ARG:NH2  | 26:b:107:MET:SD   | 2.84                     | 0.51              |
| 30:f:72:ARG:HB3   | 30:f:73:PRO:HD3   | 1.93                     | 0.51              |
| 30:f:459:CYS:SG   | 30:f:461:PRO:HD3  | 2.50                     | 0.51              |
| 30:f:463:LEU:HD12 | 30:f:489:TYR:OH   | 2.11                     | 0.51              |
| 30:f:709:THR:O    | 30:f:712:LYS:HG3  | 2.10                     | 0.51              |
| 31:F:138:GLY:HA2  | 31:F:159:LEU:HD21 | 1.91                     | 0.51              |
| 32:U:164:GLU:O    | 32:U:167:ILE:HG23 | 2.10                     | 0.51              |
| 32:U:510:GLU:CG   | 32:U:543:LYS:HG2  | 2.40                     | 0.51              |
| 32:U:801:GLN:HA   | 32:U:878:LEU:O    | 2.10                     | 0.51              |
| 32:U:916:ASP:OD1  | 32:U:917:THR:N    | 2.44                     | 0.51              |
| 1:A:252:GLU:HG2   | 31:F:259:MET:HE3  | 1.91                     | 0.51              |
| 1:A:293:ASN:HB3   | 1:A:297:ARG:NH2   | 2.26                     | 0.51              |
| 1:A:303:ILE:HG13  | 1:A:336:ARG:CD    | 2.40                     | 0.51              |
| 2:B:91:LYS:O      | 2:B:91:LYS:HD3    | 2.11                     | 0.51              |
| 2:B:249:ARG:HD3   | 3:C:283:PHE:CE2   | 2.45                     | 0.51              |
| 3:C:149:GLU:HG2   | 23:Y:133:ALA:HB1  | 1.92                     | 0.51              |
| 3:C:174:LEU:HD23  | 3:C:174:LEU:O     | 2.10                     | 0.51              |
| 3:C:273:MET:HA    | 3:C:276:LEU:HB2   | 1.92                     | 0.51              |
| 21:W:98:LYS:HA    | 21:W:135:LYS:HZ1  | 1.75                     | 0.51              |
| 21:W:326:MET:HE2  | 21:W:326:MET:O    | 2.11                     | 0.51              |
| 21:W:351:TRP:HA   | 21:W:351:TRP:CE3  | 2.45                     | 0.51              |
| 21:W:373:ILE:HD12 | 25:a:326:GLU:HG3  | 1.88                     | 0.51              |
| 24:Z:94:TRP:HB3   | 24:Z:112:MET:SD   | 2.51                     | 0.51              |
| 25:a:72:ASN:CA    | 26:b:17:ARG:HH12  | 2.24                     | 0.51              |
| 25:a:86:GLN:C     | 25:a:88:THR:HG23  | 2.36                     | 0.51              |
| 25:a:302:ILE:CG2  | 25:a:306:GLU:HG2  | 2.40                     | 0.51              |
| 27:c:247:GLU:O    | 27:c:251:LEU:HB2  | 2.11                     | 0.51              |
| 27:c:256:ASN:C    | 27:c:256:ASN:OD1  | 2.53                     | 0.51              |
| 28:d:200:PHE:CB   | 28:d:203:PRO:HG3  | 2.40                     | 0.51              |
| 28:d:206:MET:O    | 28:d:210:ALA:N    | 2.27                     | 0.51              |
| 30:f:639:LYS:HG3  | 30:f:640:LYS:HE2  | 1.91                     | 0.51              |
| 30:f:828:ARG:NE   | 30:f:843:SER:HA   | 2.25                     | 0.51              |
| 30:f:848:GLN:OE1  | 30:f:850:VAL:HG22 | 2.10                     | 0.51              |
| 31:F:213:GLU:OE1  | 31:F:213:GLU:C    | 2.53                     | 0.51              |
| 31:F:222:GLY:HA3  | 31:F:348:LEU:HA   | 1.93                     | 0.51              |
| 1:A:197:HIS:HD2   | 30:f:345:PRO:HG2  | 1.76                     | 0.51              |
| 3:C:327:ASP:O     | 3:C:331:ILE:HG13  | 2.11                     | 0.51              |
| 4:D:216:ALA:CB    | 4:D:263:PHE:HE2   | 2.23                     | 0.51              |
| 4:D:354:LEU:HA    | 4:D:394:VAL:HG23  | 1.92                     | 0.51              |
| 5:E:130:VAL:CG1   | 5:E:186:ALA:HA    | 2.41                     | 0.51              |
| 5:E:270:LEU:HD21  | 5:E:273:VAL:O     | 2.11                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 20:V:104:THR:O    | 20:V:107:ARG:HG2  | 2.11                     | 0.51              |
| 21:W:372:ARG:NH1  | 25:a:327:VAL:HG21 | 2.24                     | 0.51              |
| 25:a:95:THR:O     | 25:a:99:LYS:HB3   | 2.11                     | 0.51              |
| 25:a:319:LEU:HD12 | 25:a:319:LEU:O    | 2.11                     | 0.51              |
| 28:d:96:HIS:HB2   | 28:d:132:TYR:HD2  | 1.75                     | 0.51              |
| 30:f:530:CYS:O    | 30:f:534:VAL:HG13 | 2.10                     | 0.51              |
| 30:f:760:PHE:CD1  | 30:f:806:VAL:HG11 | 2.46                     | 0.51              |
| 30:f:785:ARG:O    | 30:f:785:ARG:NE   | 2.38                     | 0.51              |
| 11:l:180:MET:HE2  | 11:l:180:MET:HA   | 1.91                     | 0.51              |
| 31:F:314:LEU:CD2  | 31:F:342:LEU:HD13 | 2.41                     | 0.51              |
| 32:U:567:ILE:HD11 | 32:U:585:THR:HG22 | 1.93                     | 0.51              |
| 32:U:660:CYS:SG   | 32:U:694:ILE:HD11 | 2.51                     | 0.51              |
| 2:B:116:ILE:HD13  | 2:B:132:TYR:OH    | 2.11                     | 0.51              |
| 2:B:371:ARG:HG2   | 2:B:371:ARG:NH1   | 2.25                     | 0.51              |
| 3:C:90:HIS:O      | 3:C:91:PRO:C      | 2.53                     | 0.51              |
| 4:D:339:ARG:HH22  | 4:D:343:LEU:CB    | 2.23                     | 0.51              |
| 5:E:173:TYR:CB    | 5:E:282:PRO:HG3   | 2.41                     | 0.51              |
| 11:L:121:GLN:HG3  | 11:L:121:GLN:O    | 2.10                     | 0.51              |
| 15:P:170:MET:O    | 15:P:174:VAL:HG22 | 2.11                     | 0.51              |
| 17:R:166:TYR:CE1  | 15:p:33:MET:HE1   | 2.45                     | 0.51              |
| 20:V:150:ARG:NH2  | 20:V:155:ALA:O    | 2.44                     | 0.51              |
| 20:V:449:ALA:HB3  | 20:V:459:GLN:O    | 2.09                     | 0.51              |
| 21:W:152:ILE:HD12 | 21:W:165:ILE:HB   | 1.93                     | 0.51              |
| 21:W:272:LEU:HD23 | 21:W:340:VAL:HG21 | 1.93                     | 0.51              |
| 21:W:333:LEU:HG   | 21:W:335:SER:H    | 1.76                     | 0.51              |
| 23:Y:377:LEU:HD12 | 23:Y:380:VAL:HG12 | 1.92                     | 0.51              |
| 26:b:8:VAL:N      | 26:b:50:GLY:O     | 2.44                     | 0.51              |
| 30:f:519:ALA:HB3  | 30:f:557:TRP:HE1  | 1.75                     | 0.51              |
| 9:j:140:GLY:O     | 9:j:213:ARG:NH1   | 2.44                     | 0.51              |
| 32:U:248:ILE:C    | 32:U:248:ILE:HD12 | 2.36                     | 0.51              |
| 32:U:745:THR:HB   | 32:U:786:THR:HG21 | 1.93                     | 0.51              |
| 1:A:127:ASP:OD1   | 1:A:128:GLN:HG2   | 2.11                     | 0.51              |
| 1:A:213:LEU:CD1   | 1:A:337:LEU:HD21  | 2.41                     | 0.51              |
| 3:C:63:LEU:HD22   | 4:D:82:ILE:HD13   | 1.92                     | 0.51              |
| 4:D:107:THR:HG22  | 5:E:77:PRO:HG3    | 1.92                     | 0.51              |
| 20:V:99:ARG:O     | 20:V:102:PRO:HD2  | 2.11                     | 0.51              |
| 20:V:150:ARG:O    | 20:V:155:ALA:HB2  | 2.11                     | 0.51              |
| 21:W:361:HIS:O    | 21:W:365:ILE:HG22 | 2.11                     | 0.51              |
| 22:X:301:ASP:OD2  | 22:X:301:ASP:C    | 2.54                     | 0.51              |
| 22:X:316:ASP:OD1  | 22:X:319:ILE:HG12 | 2.10                     | 0.51              |
| 24:Z:81:MET:CE    | 27:c:94:LYS:HB3   | 2.40                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 25:a:277:LEU:CD1  | 25:a:296:ILE:HD13 | 2.41                     | 0.51              |
| 26:b:107:MET:HE3  | 26:b:135:LYS:HB2  | 1.92                     | 0.51              |
| 26:b:113:VAL:HG22 | 26:b:114:GLY:H    | 1.76                     | 0.51              |
| 27:c:36:LEU:HD23  | 27:c:36:LEU:C     | 2.36                     | 0.51              |
| 30:f:729:MET:HE3  | 30:f:729:MET:CA   | 2.22                     | 0.51              |
| 30:f:826:GLN:HB3  | 30:f:846:VAL:HG13 | 1.92                     | 0.51              |
| 8:i:119:GLN:CG    | 9:j:78:ALA:HB1    | 2.41                     | 0.51              |
| 12:m:110:HIS:O    | 12:m:114:ARG:HG2  | 2.10                     | 0.51              |
| 13:n:60:VAL:HG23  | 13:n:87:MET:HE1   | 1.93                     | 0.51              |
| 19:t:54:SER:O     | 19:t:108:ASN:ND2  | 2.44                     | 0.51              |
| 31:F:164:LEU:H    | 31:F:164:LEU:HD12 | 1.76                     | 0.51              |
| 31:F:387:CYS:SG   | 31:F:421:MET:HE3  | 2.51                     | 0.51              |
| 2:B:116:ILE:HD13  | 2:B:132:TYR:CZ    | 2.46                     | 0.50              |
| 4:D:178:ARG:HB3   | 4:D:178:ARG:CZ    | 2.42                     | 0.50              |
| 6:G:5:SER:N       | 6:G:19:GLU:OE2    | 2.42                     | 0.50              |
| 6:G:174:GLU:OE1   | 6:G:174:GLU:N     | 2.32                     | 0.50              |
| 12:M:70:ASP:OD1   | 12:M:71:ARG:N     | 2.43                     | 0.50              |
| 18:S:64:LEU:O     | 18:S:68:ILE:HG13  | 2.11                     | 0.50              |
| 20:V:349:ARG:HA   | 20:V:354:LYS:CE   | 2.39                     | 0.50              |
| 21:W:201:ARG:HH21 | 21:W:205:ILE:HB   | 1.76                     | 0.50              |
| 21:W:268:LYS:HD2  | 21:W:301:LYS:HG3  | 1.92                     | 0.50              |
| 21:W:312:MET:CB   | 21:W:365:ILE:HD11 | 2.39                     | 0.50              |
| 23:Y:18:ARG:HD2   | 23:Y:22:LEU:CD2   | 2.41                     | 0.50              |
| 23:Y:202:LEU:O    | 23:Y:205:VAL:HG12 | 2.11                     | 0.50              |
| 24:Z:17:LEU:HG    | 27:c:213:GLU:OE1  | 2.11                     | 0.50              |
| 24:Z:213:GLU:OE1  | 24:Z:213:GLU:HA   | 2.10                     | 0.50              |
| 28:d:205:LYS:HG2  | 28:d:209:TYR:HD2  | 1.73                     | 0.50              |
| 30:f:304:PHE:HA   | 30:f:307:LEU:CD1  | 2.41                     | 0.50              |
| 30:f:661:ALA:HB3  | 30:f:662:MET:HE3  | 1.93                     | 0.50              |
| 32:U:34:PHE:CG    | 32:U:34:PHE:O     | 2.64                     | 0.50              |
| 32:U:632:GLN:C    | 32:U:632:GLN:CD   | 2.79                     | 0.50              |
| 1:A:139:ARG:HG3   | 1:A:155:PRO:HA    | 1.92                     | 0.50              |
| 5:E:233:ASP:O     | 5:E:234:GLU:C     | 2.55                     | 0.50              |
| 8:I:51:ASN:OD1    | 8:I:51:ASN:O      | 2.28                     | 0.50              |
| 9:J:91:CYS:SG     | 9:J:107:ILE:HD13  | 2.52                     | 0.50              |
| 13:N:85:LYS:NZ    | 13:N:86:GLU:OE2   | 2.35                     | 0.50              |
| 19:T:72:ILE:O     | 19:T:76:LEU:HD13  | 2.10                     | 0.50              |
| 20:V:68:ASP:O     | 20:V:72:LEU:HD23  | 2.09                     | 0.50              |
| 20:V:203:LEU:HD13 | 20:V:203:LEU:C    | 2.36                     | 0.50              |
| 20:V:479:ARG:NE   | 23:Y:370:ILE:HD11 | 2.26                     | 0.50              |
| 21:W:304:ASP:C    | 21:W:304:ASP:OD1  | 2.54                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:X:281:GLY:H    | 22:X:284:THR:HG22 | 1.76                     | 0.50              |
| 23:Y:96:GLY:HA2   | 23:Y:100:ILE:CG2  | 2.26                     | 0.50              |
| 23:Y:136:HIS:O    | 23:Y:140:ILE:HG12 | 2.11                     | 0.50              |
| 23:Y:307:LEU:CD2  | 23:Y:319:MET:HE3  | 2.38                     | 0.50              |
| 24:Z:10:VAL:O     | 24:Z:50:VAL:HG22  | 2.11                     | 0.50              |
| 24:Z:205:LEU:HD11 | 25:a:356:TRP:CZ3  | 2.46                     | 0.50              |
| 25:a:320:VAL:HG21 | 25:a:333:MET:HE1  | 1.93                     | 0.50              |
| 28:d:92:SER:H     | 28:d:95:MET:CG    | 2.24                     | 0.50              |
| 9:j:104:VAL:O     | 9:j:108:THR:HG22  | 2.11                     | 0.50              |
| 32:U:265:ILE:HG23 | 32:U:326:ILE:HD12 | 1.92                     | 0.50              |
| 1:A:196:LEU:HG    | 1:A:197:HIS:CD2   | 2.47                     | 0.50              |
| 1:A:235:ALA:HB1   | 1:A:269:ALA:C     | 2.36                     | 0.50              |
| 4:D:212:LYS:HZ3   | 33:D:501:ATP:PB   | 2.34                     | 0.50              |
| 5:E:242:ARG:NH2   | 5:E:286:ASP:OD2   | 2.44                     | 0.50              |
| 5:E:380:LEU:CD1   | 31:F:343:LEU:HD13 | 2.41                     | 0.50              |
| 20:V:83:GLU:OE1   | 20:V:160:LEU:HD12 | 2.10                     | 0.50              |
| 21:W:133:GLU:OE1  | 21:W:133:GLU:N    | 2.44                     | 0.50              |
| 21:W:165:ILE:HD13 | 21:W:189:GLN:HB3  | 1.93                     | 0.50              |
| 21:W:273:TYR:CB   | 21:W:276:LEU:HB2  | 2.40                     | 0.50              |
| 21:W:451:MET:HG3  | 21:W:451:MET:O    | 2.11                     | 0.50              |
| 24:Z:43:TRP:HB3   | 24:Z:48:LEU:HD13  | 1.94                     | 0.50              |
| 24:Z:214:LYS:HD2  | 24:Z:214:LYS:C    | 2.36                     | 0.50              |
| 27:c:242:GLU:OE2  | 27:c:246:LYS:NZ   | 2.39                     | 0.50              |
| 28:d:194:ALA:HA   | 28:d:197:ILE:HD13 | 1.93                     | 0.50              |
| 30:f:494:ARG:HG3  | 30:f:497:VAL:CG2  | 2.40                     | 0.50              |
| 30:f:560:LEU:HD23 | 30:f:594:LEU:HD21 | 1.93                     | 0.50              |
| 31:F:315:ASN:C    | 31:F:315:ASN:OD1  | 2.54                     | 0.50              |
| 32:U:177:LEU:HD11 | 32:U:204:ILE:HG12 | 1.92                     | 0.50              |
| 2:B:261:GLY:C     | 2:B:263:GLY:H     | 2.18                     | 0.50              |
| 3:C:19:GLY:N      | 32:U:146:LYS:HZ3  | 2.09                     | 0.50              |
| 3:C:149:GLU:OE1   | 3:C:149:GLU:HA    | 2.11                     | 0.50              |
| 3:C:235:PHE:O     | 3:C:239:ARG:HG2   | 2.11                     | 0.50              |
| 4:D:284:GLU:O     | 4:D:284:GLU:OE1   | 2.28                     | 0.50              |
| 5:E:264:MET:HE2   | 5:E:289:LEU:CD1   | 2.42                     | 0.50              |
| 5:E:277:MET:HE3   | 5:E:295:LEU:HD21  | 1.93                     | 0.50              |
| 5:E:327:ASP:OD2   | 5:E:329:GLU:N     | 2.43                     | 0.50              |
| 21:W:47:LEU:O     | 21:W:50:LEU:HB2   | 2.12                     | 0.50              |
| 22:X:166:LEU:O    | 22:X:170:GLN:HB2  | 2.12                     | 0.50              |
| 22:X:259:ILE:HD13 | 22:X:290:VAL:HG13 | 1.92                     | 0.50              |
| 23:Y:314:LEU:HD23 | 23:Y:314:LEU:O    | 2.12                     | 0.50              |
| 23:Y:320:ALA:CB   | 23:Y:327:VAL:HG22 | 2.41                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 27:c:272:ILE:O    | 27:c:275:VAL:HG13 | 2.12                     | 0.50              |
| 28:d:255:MET:HE2  | 28:d:256:ILE:C    | 2.35                     | 0.50              |
| 30:f:505:MET:CE   | 30:f:519:ALA:HA   | 2.42                     | 0.50              |
| 9:j:190:LEU:HD23  | 9:j:190:LEU:O     | 2.10                     | 0.50              |
| 12:m:232:ARG:O    | 12:m:236:GLU:HG3  | 2.11                     | 0.50              |
| 31:F:406:ILE:HD13 | 31:F:422:GLU:CD   | 2.37                     | 0.50              |
| 32:U:69:TYR:CD1   | 32:U:69:TYR:C     | 2.90                     | 0.50              |
| 32:U:252:LEU:HD12 | 32:U:256:ALA:HB2  | 1.94                     | 0.50              |
| 32:U:441:GLY:O    | 32:U:445:ALA:N    | 2.42                     | 0.50              |
| 32:U:554:LEU:HD12 | 32:U:588:MET:SD   | 2.52                     | 0.50              |
| 32:U:650:TYR:OH   | 32:U:685:GLN:NE2  | 2.44                     | 0.50              |
| 1:A:108:ASP:HB2   | 1:A:109:PRO:HD3   | 1.92                     | 0.50              |
| 2:B:106:PRO:HB3   | 3:C:121:TYR:HD1   | 1.76                     | 0.50              |
| 3:C:116:LEU:HD22  | 3:C:116:LEU:N     | 2.26                     | 0.50              |
| 3:C:130:LYS:HG3   | 3:C:131:VAL:N     | 2.26                     | 0.50              |
| 3:C:194:THR:HA    | 3:C:355:SER:HB2   | 1.93                     | 0.50              |
| 20:V:350:GLN:O    | 20:V:354:LYS:HG2  | 2.11                     | 0.50              |
| 20:V:428:LEU:HD23 | 20:V:434:ALA:CB   | 2.42                     | 0.50              |
| 20:V:466:ILE:HD11 | 20:V:471:GLU:CD   | 2.36                     | 0.50              |
| 21:W:70:VAL:HG11  | 21:W:90:LEU:HD11  | 1.94                     | 0.50              |
| 21:W:252:ASP:O    | 21:W:256:ILE:HD12 | 2.11                     | 0.50              |
| 22:X:407:MET:HA   | 22:X:410:VAL:HB   | 1.93                     | 0.50              |
| 23:Y:189:VAL:HG13 | 23:Y:287:LEU:CD2  | 2.39                     | 0.50              |
| 25:a:186:LYS:HD3  | 25:a:221:VAL:HG22 | 1.93                     | 0.50              |
| 25:a:291:LEU:HD13 | 25:a:333:MET:CG   | 2.41                     | 0.50              |
| 27:c:49:VAL:CG1   | 27:c:50:PRO:HD3   | 2.40                     | 0.50              |
| 27:c:180:ASN:HD21 | 32:U:725:MET:HG3  | 1.76                     | 0.50              |
| 28:d:63:ILE:HD11  | 28:d:166:PHE:CZ   | 2.47                     | 0.50              |
| 30:f:474:SER:HB3  | 30:f:477:MET:HE2  | 1.94                     | 0.50              |
| 7:h:18:LEU:HD23   | 7:h:21:ILE:HD12   | 1.92                     | 0.50              |
| 12:m:111:LEU:O    | 12:m:115:VAL:HG23 | 2.12                     | 0.50              |
| 16:q:164:LEU:HD12 | 16:q:194:ILE:HG21 | 1.92                     | 0.50              |
| 32:U:377:HIS:HB2  | 32:U:411:ILE:CD1  | 2.41                     | 0.50              |
| 32:U:597:LYS:HB3  | 32:U:597:LYS:NZ   | 2.25                     | 0.50              |
| 32:U:901:GLN:NE2  | 32:U:915:LYS:HB3  | 2.19                     | 0.50              |
| 1:A:68:SER:OG     | 1:A:69:ASP:N      | 2.44                     | 0.50              |
| 2:B:119:ASN:OD1   | 2:B:119:ASN:C     | 2.54                     | 0.50              |
| 2:B:294:ARG:NH1   | 2:B:294:ARG:CB    | 2.75                     | 0.50              |
| 3:C:248:MET:HE1   | 3:C:273:MET:CG    | 2.10                     | 0.50              |
| 11:L:210:VAL:HG13 | 11:L:229:VAL:HG11 | 1.93                     | 0.50              |
| 12:M:35:THR:HG22  | 12:M:50:GLU:OE1   | 2.12                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 20:V:83:GLU:O     | 20:V:87:SER:OG    | 2.19                     | 0.50              |
| 20:V:309:MET:HB2  | 20:V:332:LEU:HD12 | 1.94                     | 0.50              |
| 21:W:79:GLU:OE2   | 21:W:82:LEU:HD12  | 2.12                     | 0.50              |
| 21:W:171:VAL:HG12 | 21:W:172:GLU:N    | 2.26                     | 0.50              |
| 23:Y:224:VAL:HG22 | 23:Y:228:MET:HE3  | 1.94                     | 0.50              |
| 25:a:33:LEU:HD12  | 25:a:33:LEU:C     | 2.36                     | 0.50              |
| 25:a:217:LEU:HD11 | 25:a:238:TYR:CE1  | 2.47                     | 0.50              |
| 28:d:140:GLU:OE2  | 28:d:144:MET:HE3  | 2.11                     | 0.50              |
| 28:d:253:LEU:O    | 28:d:253:LEU:HG   | 2.12                     | 0.50              |
| 30:f:6:ARG:NE     | 30:f:6:ARG:H      | 2.10                     | 0.50              |
| 30:f:828:ARG:HB2  | 30:f:829:MET:CE   | 2.42                     | 0.50              |
| 16:q:3:TYR:OH     | 16:q:139:THR:HG21 | 2.11                     | 0.50              |
| 31:F:187:ASP:O    | 31:F:368:ILE:HG21 | 2.12                     | 0.50              |
| 32:U:349:ASP:N    | 32:U:349:ASP:OD1  | 2.45                     | 0.50              |
| 32:U:572:ARG:CZ   | 32:U:572:ARG:HB3  | 2.40                     | 0.50              |
| 1:A:75:PRO:HA     | 1:A:78:TRP:CD2    | 2.47                     | 0.50              |
| 1:A:219:GLY:HA3   | 2:B:343:ARG:HD2   | 1.92                     | 0.50              |
| 1:A:245:LEU:HB2   | 1:A:280:ILE:HG21  | 1.94                     | 0.50              |
| 1:A:267:LYS:HA    | 30:f:354:GLU:OE1  | 2.11                     | 0.50              |
| 2:B:256:ILE:O     | 2:B:256:ILE:HG13  | 2.10                     | 0.50              |
| 2:B:263:GLY:C     | 2:B:265:LYS:H     | 2.19                     | 0.50              |
| 2:B:332:ASN:C     | 2:B:333:ARG:HG2   | 2.37                     | 0.50              |
| 4:D:184:PRO:HG3   | 4:D:191:TYR:CE1   | 2.47                     | 0.50              |
| 5:E:184:ALA:O     | 5:E:187:VAL:HG22  | 2.11                     | 0.50              |
| 5:E:316:HIS:CD2   | 5:E:344:ARG:HB2   | 2.46                     | 0.50              |
| 5:E:356:ARG:O     | 5:E:357:ALA:HB3   | 2.12                     | 0.50              |
| 8:I:166:ASN:OD1   | 8:I:167:ASN:N     | 2.45                     | 0.50              |
| 20:V:139:MET:HE1  | 20:V:141:THR:HG22 | 1.93                     | 0.50              |
| 21:W:379:ALA:HB1  | 21:W:384:LEU:O    | 2.11                     | 0.50              |
| 22:X:350:ILE:HG23 | 22:X:361:VAL:HG21 | 1.94                     | 0.50              |
| 23:Y:23:ARG:O     | 23:Y:23:ARG:HD3   | 2.12                     | 0.50              |
| 23:Y:224:VAL:HG11 | 23:Y:256:VAL:HG11 | 1.94                     | 0.50              |
| 25:a:35:HIS:HB3   | 26:b:15:TYR:CZ    | 2.46                     | 0.50              |
| 25:a:162:TYR:C    | 25:a:162:TYR:CD2  | 2.90                     | 0.50              |
| 30:f:6:ARG:H      | 30:f:6:ARG:HE     | 1.58                     | 0.50              |
| 30:f:12:GLN:HB3   | 30:f:13:PRO:HD3   | 1.93                     | 0.50              |
| 30:f:559:PRO:O    | 30:f:563:GLY:N    | 2.36                     | 0.50              |
| 32:U:84:ALA:HB3   | 32:U:88:PHE:HD2   | 1.76                     | 0.50              |
| 32:U:208:LEU:O    | 32:U:211:PRO:HG3  | 2.12                     | 0.50              |
| 2:B:184:TYR:CE2   | 2:B:198:LYS:HE3   | 2.47                     | 0.50              |
| 3:C:172:PRO:C     | 3:C:174:LEU:H     | 2.20                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:C:193:GLY:O     | 3:C:356:GLY:N     | 2.45                     | 0.50              |
| 3:C:373:GLU:C     | 3:C:373:GLU:OE1   | 2.55                     | 0.50              |
| 4:D:264:ILE:CG2   | 4:D:267:ILE:HD13  | 2.42                     | 0.50              |
| 4:D:266:GLU:O     | 5:E:258:MET:HE1   | 2.12                     | 0.50              |
| 5:E:181:THR:OG1   | 33:E:402:ATP:O3G  | 2.25                     | 0.50              |
| 18:S:4:PRO:O      | 19:T:100:ARG:NH1  | 2.40                     | 0.50              |
| 20:V:228:ARG:HD3  | 20:V:257:ASN:ND2  | 2.27                     | 0.50              |
| 20:V:497:PRO:HG3  | 24:Z:278:ASN:OD1  | 2.12                     | 0.50              |
| 23:Y:176:ARG:NH1  | 23:Y:179:ARG:HH22 | 2.09                     | 0.50              |
| 23:Y:307:LEU:HD22 | 23:Y:319:MET:CE   | 2.39                     | 0.50              |
| 24:Z:139:ILE:HD12 | 24:Z:140:SER:H    | 1.77                     | 0.50              |
| 25:a:41:VAL:HA    | 25:a:44:PHE:CD2   | 2.47                     | 0.50              |
| 26:b:29:GLN:HE21  | 26:b:29:GLN:CA    | 2.17                     | 0.50              |
| 26:b:48:ASN:ND2   | 26:b:64:LEU:HB3   | 2.26                     | 0.50              |
| 27:c:102:THR:HG23 | 27:c:103:GLY:N    | 2.27                     | 0.50              |
| 28:d:60:GLN:O     | 28:d:64:LEU:HD13  | 2.11                     | 0.50              |
| 28:d:152:PHE:CE2  | 28:d:198:LEU:HB3  | 2.43                     | 0.50              |
| 30:f:165:GLU:HA   | 30:f:168:LYS:CE   | 2.39                     | 0.50              |
| 30:f:441:LYS:HD2  | 30:f:441:LYS:N    | 2.27                     | 0.50              |
| 6:g:49:VAL:HG22   | 6:g:219:VAL:HG12  | 1.94                     | 0.50              |
| 32:U:16:GLU:HG3   | 32:U:19:LEU:H     | 1.77                     | 0.50              |
| 1:A:77:LEU:CD1    | 30:f:694:LEU:HD12 | 2.41                     | 0.50              |
| 1:A:190:VAL:HG11  | 1:A:212:VAL:CG2   | 2.41                     | 0.50              |
| 1:A:308:GLY:O     | 1:A:309:PHE:HB3   | 2.11                     | 0.50              |
| 2:B:60:LEU:HA     | 2:B:63:LEU:CD2    | 2.40                     | 0.50              |
| 2:B:302:GLU:C     | 2:B:302:GLU:OE1   | 2.55                     | 0.50              |
| 3:C:258:ARG:NH2   | 3:C:263:SER:O     | 2.34                     | 0.50              |
| 4:D:149:SER:HG    | 4:D:246:MET:CG    | 2.24                     | 0.50              |
| 4:D:167:ILE:HD11  | 4:D:214:MET:HG2   | 1.94                     | 0.50              |
| 4:D:230:VAL:CG2   | 4:D:264:ILE:HA    | 2.41                     | 0.50              |
| 5:E:87:LEU:HD21   | 5:E:92:LEU:HD11   | 1.94                     | 0.50              |
| 5:E:349:GLU:OE2   | 31:F:350:ARG:NE   | 2.27                     | 0.50              |
| 21:W:28:LEU:HB3   | 21:W:29:PRO:HD3   | 1.94                     | 0.50              |
| 21:W:328:LEU:HD23 | 21:W:341:PHE:HB3  | 1.94                     | 0.50              |
| 22:X:256:LEU:O    | 22:X:260:MET:HG2  | 2.11                     | 0.50              |
| 22:X:366:SER:O    | 22:X:370:LEU:HG   | 2.12                     | 0.50              |
| 23:Y:149:LEU:N    | 23:Y:157:ILE:HD11 | 2.27                     | 0.50              |
| 24:Z:22:HIS:CE1   | 24:Z:35:VAL:HG12  | 2.46                     | 0.50              |
| 25:a:50:PHE:HD2   | 25:a:52:GLN:HB3   | 1.77                     | 0.50              |
| 25:a:158:LEU:C    | 25:a:158:LEU:HD13 | 2.36                     | 0.50              |
| 25:a:370:GLN:OE1  | 28:d:244:LYS:HG2  | 2.12                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 28:d:114:GLU:O    | 28:d:117:THR:HG22 | 2.12                     | 0.50              |
| 30:f:411:ALA:HB3  | 30:f:443:GLY:HA3  | 1.93                     | 0.50              |
| 30:f:531:ASN:OD1  | 30:f:531:ASN:N    | 2.43                     | 0.50              |
| 30:f:557:TRP:CD1  | 30:f:558:LEU:HD22 | 2.46                     | 0.50              |
| 30:f:631:LYS:O    | 30:f:635:LYS:HG2  | 2.12                     | 0.50              |
| 30:f:713:PHE:CZ   | 30:f:752:HIS:HB3  | 2.47                     | 0.50              |
| 12:m:220:THR:HG21 | 12:m:223:ARG:O    | 2.12                     | 0.50              |
| 31:F:272:PHE:CE1  | 31:F:283:ILE:HG21 | 2.47                     | 0.50              |
| 1:A:97:ARG:HH12   | 2:B:129:SER:HB2   | 1.77                     | 0.49              |
| 4:D:94:GLU:C      | 4:D:94:GLU:OE1    | 2.55                     | 0.49              |
| 4:D:95:ALA:O      | 27:c:272:ILE:HD11 | 2.12                     | 0.49              |
| 9:J:190:LEU:HD23  | 9:J:190:LEU:C     | 2.37                     | 0.49              |
| 17:R:108:ARG:CZ   | 17:R:108:ARG:HB2  | 2.41                     | 0.49              |
| 20:V:81:GLN:HA    | 20:V:84:LYS:HD2   | 1.94                     | 0.49              |
| 20:V:268:GLU:OE1  | 20:V:268:GLU:C    | 2.55                     | 0.49              |
| 20:V:302:TYR:OH   | 20:V:338:LEU:HD13 | 2.11                     | 0.49              |
| 20:V:471:GLU:HG3  | 20:V:472:PRO:N    | 2.27                     | 0.49              |
| 21:W:137:TYR:C    | 21:W:141:GLU:HB2  | 2.36                     | 0.49              |
| 21:W:445:LEU:HD23 | 21:W:445:LEU:O    | 2.12                     | 0.49              |
| 24:Z:17:LEU:HD11  | 27:c:217:LEU:HD12 | 1.93                     | 0.49              |
| 24:Z:25:ARG:HB2   | 27:c:104:ARG:HD2  | 1.94                     | 0.49              |
| 25:a:35:HIS:C     | 25:a:38:THR:H     | 2.19                     | 0.49              |
| 25:a:321:LYS:HB3  | 25:a:321:LYS:NZ   | 2.25                     | 0.49              |
| 30:f:7:ASP:O      | 30:f:10:PRO:HD2   | 2.12                     | 0.49              |
| 30:f:305:LEU:HD22 | 30:f:314:TYR:CD2  | 2.47                     | 0.49              |
| 30:f:426:LEU:HD22 | 30:f:426:LEU:H    | 1.77                     | 0.49              |
| 30:f:673:ARG:NH2  | 30:f:707:LEU:HD22 | 2.17                     | 0.49              |
| 32:U:9:ILE:HD11   | 32:U:42:VAL:HG21  | 1.94                     | 0.49              |
| 32:U:521:LEU:HD12 | 32:U:522:GLY:N    | 2.27                     | 0.49              |
| 32:U:573:ASP:O    | 32:U:579:ARG:HD3  | 2.12                     | 0.49              |
| 32:U:879:ASP:OD1  | 32:U:879:ASP:N    | 2.33                     | 0.49              |
| 1:A:273:PHE:CE2   | 1:A:275:ASP:HB2   | 2.47                     | 0.49              |
| 2:B:140:ASP:OD2   | 2:B:143:LEU:HG    | 2.12                     | 0.49              |
| 2:B:230:THR:HG22  | 2:B:230:THR:O     | 2.11                     | 0.49              |
| 3:C:189:TYR:O     | 3:C:317:PHE:HB2   | 2.12                     | 0.49              |
| 3:C:363:CYS:HA    | 3:C:383:PHE:CE1   | 2.47                     | 0.49              |
| 4:D:122:GLU:CD    | 27:c:278:GLN:HA   | 2.37                     | 0.49              |
| 20:V:106:ARG:H    | 20:V:106:ARG:NE   | 2.08                     | 0.49              |
| 21:W:71:VAL:HG21  | 21:W:104:MET:CG   | 2.41                     | 0.49              |
| 22:X:147:LEU:HD21 | 22:X:176:THR:OG1  | 2.12                     | 0.49              |
| 22:X:251:LEU:O    | 22:X:255:LEU:HG   | 2.12                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 23:Y:70:LEU:HG    | 23:Y:74:LYS:HZ1   | 1.75                     | 0.49              |
| 23:Y:223:THR:O    | 23:Y:227:SER:HB2  | 2.12                     | 0.49              |
| 25:a:144:ASN:C    | 25:a:145:LEU:HD23 | 2.37                     | 0.49              |
| 25:a:162:TYR:C    | 25:a:162:TYR:HD2  | 2.20                     | 0.49              |
| 27:c:41:MET:CE    | 27:c:143:VAL:HG11 | 2.41                     | 0.49              |
| 30:f:298:LEU:HD23 | 30:f:298:LEU:H    | 1.77                     | 0.49              |
| 10:k:234:LEU:O    | 10:k:238:ILE:HG13 | 2.11                     | 0.49              |
| 32:U:645:ASN:OD1  | 32:U:647:HIS:HB2  | 2.11                     | 0.49              |
| 1:A:351:ARG:HB2   | 1:A:385:ILE:HD11  | 1.94                     | 0.49              |
| 1:A:426:THR:N     | 1:A:427:PRO:HD2   | 2.27                     | 0.49              |
| 2:B:373:THR:O     | 2:B:413:LYS:HG2   | 2.13                     | 0.49              |
| 4:D:113:VAL:HB    | 4:D:138:ALA:HA    | 1.93                     | 0.49              |
| 4:D:339:ARG:CZ    | 4:D:339:ARG:O     | 2.60                     | 0.49              |
| 12:M:202:ASP:C    | 12:M:202:ASP:OD2  | 2.55                     | 0.49              |
| 21:W:59:ASP:CB    | 21:W:62:SER:HB2   | 2.39                     | 0.49              |
| 21:W:147:LYS:HB2  | 21:W:147:LYS:HZ1  | 1.75                     | 0.49              |
| 21:W:248:ARG:CD   | 21:W:290:ILE:HD11 | 2.21                     | 0.49              |
| 21:W:388:GLU:OE1  | 21:W:388:GLU:HA   | 2.11                     | 0.49              |
| 23:Y:90:ASP:O     | 23:Y:94:ASN:ND2   | 2.45                     | 0.49              |
| 23:Y:117:LYS:HZ3  | 23:Y:151:TYR:HD1  | 1.61                     | 0.49              |
| 24:Z:131:LEU:H    | 24:Z:131:LEU:CD2  | 2.26                     | 0.49              |
| 26:b:115:SER:HG   | 26:b:116:PRO:HD2  | 1.76                     | 0.49              |
| 30:f:292:LYS:O    | 30:f:292:LYS:HG3  | 2.11                     | 0.49              |
| 30:f:304:PHE:HA   | 30:f:307:LEU:HD11 | 1.94                     | 0.49              |
| 30:f:612:LEU:O    | 30:f:632:LYS:HD3  | 2.13                     | 0.49              |
| 8:i:187:LYS:HD3   | 8:i:187:LYS:N     | 2.27                     | 0.49              |
| 17:r:13:VAL:HG21  | 17:r:103:CYS:HB3  | 1.93                     | 0.49              |
| 31:F:241:ALA:HB2  | 31:F:248:PHE:CZ   | 2.47                     | 0.49              |
| 32:U:138:PHE:CD2  | 32:U:162:VAL:HG21 | 2.47                     | 0.49              |
| 32:U:520:MET:HE1  | 32:U:525:ASN:CB   | 2.42                     | 0.49              |
| 1:A:323:ARG:HH12  | 1:A:433:ASN:N     | 2.11                     | 0.49              |
| 3:C:351:MET:HE3   | 3:C:387:VAL:CG1   | 2.39                     | 0.49              |
| 5:E:299:ILE:N     | 5:E:299:ILE:HD12  | 2.28                     | 0.49              |
| 15:P:34:VAL:HG11  | 16:Q:117:TYR:CD2  | 2.47                     | 0.49              |
| 21:W:177:MET:HE1  | 21:W:181:GLU:HB3  | 1.95                     | 0.49              |
| 21:W:212:LYS:O    | 21:W:213:PHE:HD1  | 1.95                     | 0.49              |
| 23:Y:192:ARG:NH2  | 23:Y:291:HIS:HB3  | 2.27                     | 0.49              |
| 24:Z:121:LEU:C    | 24:Z:121:LEU:HD12 | 2.36                     | 0.49              |
| 26:b:32:ALA:O     | 26:b:36:VAL:HG12  | 2.11                     | 0.49              |
| 26:b:75:LEU:O     | 26:b:78:VAL:HB    | 2.12                     | 0.49              |
| 27:c:151:VAL:CG2  | 27:c:152:LYS:N    | 2.73                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 30:f:228:LYS:CE   | 30:f:233:LEU:HD12 | 2.43                     | 0.49              |
| 30:f:250:ARG:HH11 | 30:f:252:ALA:HB3  | 1.77                     | 0.49              |
| 30:f:428:GLN:O    | 30:f:431:LYS:HG2  | 2.13                     | 0.49              |
| 30:f:494:ARG:HB2  | 30:f:496:ASP:OD1  | 2.12                     | 0.49              |
| 30:f:761:MET:HA   | 30:f:761:MET:CE   | 2.39                     | 0.49              |
| 31:F:221:LYS:HE3  | 31:F:221:LYS:CA   | 2.36                     | 0.49              |
| 32:U:562:GLU:OE1  | 32:U:562:GLU:N    | 2.46                     | 0.49              |
| 32:U:710:ARG:NH2  | 32:U:738:ASP:OD1  | 2.44                     | 0.49              |
| 1:A:68:SER:CB     | 1:A:72:LEU:HD22   | 2.43                     | 0.49              |
| 1:A:264:ALA:HB1   | 1:A:315:ILE:CD1   | 2.43                     | 0.49              |
| 1:A:290:GLY:HA3   | 31:F:296:PHE:CE2  | 2.47                     | 0.49              |
| 2:B:246:THR:OG1   | 2:B:280:SER:HB3   | 2.13                     | 0.49              |
| 2:B:378:VAL:HG21  | 2:B:419:PHE:HD2   | 1.75                     | 0.49              |
| 4:D:89:ILE:CD1    | 5:E:70:ILE:HG23   | 2.42                     | 0.49              |
| 5:E:126:ASP:OD1   | 5:E:128:GLY:N     | 2.38                     | 0.49              |
| 14:O:8:VAL:HG12   | 14:O:124:PRO:O    | 2.12                     | 0.49              |
| 22:X:125:LEU:HD12 | 22:X:125:LEU:O    | 2.13                     | 0.49              |
| 22:X:151:SER:HB3  | 22:X:155:ARG:NH2  | 2.23                     | 0.49              |
| 26:b:2:VAL:HG13   | 26:b:2:VAL:O      | 2.11                     | 0.49              |
| 27:c:233:ASP:O    | 27:c:236:GLU:N    | 2.45                     | 0.49              |
| 28:d:20:GLY:HA2   | 28:d:23:LEU:HG    | 1.95                     | 0.49              |
| 28:d:118:GLU:O    | 28:d:121:ARG:HG2  | 2.13                     | 0.49              |
| 17:r:7:PHE:HB3    | 17:r:126:THR:HG22 | 1.94                     | 0.49              |
| 31:F:202:ILE:CD1  | 31:F:327:LYS:HB3  | 2.43                     | 0.49              |
| 32:U:231:ASP:O    | 32:U:234:GLU:HG3  | 2.12                     | 0.49              |
| 2:B:59:ARG:HA     | 2:B:59:ARG:NH1    | 2.27                     | 0.49              |
| 2:B:112:LEU:HB2   | 2:B:150:VAL:HG21  | 1.95                     | 0.49              |
| 2:B:246:THR:HG21  | 2:B:277:HIS:HB3   | 1.93                     | 0.49              |
| 2:B:332:ASN:OD1   | 2:B:332:ASN:N     | 2.42                     | 0.49              |
| 3:C:186:VAL:HG12  | 3:C:313:ARG:HB3   | 1.94                     | 0.49              |
| 5:E:349:GLU:OE1   | 5:E:349:GLU:HA    | 2.11                     | 0.49              |
| 20:V:262:SER:HB3  | 28:d:120:GLU:HB2  | 1.94                     | 0.49              |
| 20:V:288:TYR:O    | 20:V:292:THR:HG22 | 2.11                     | 0.49              |
| 21:W:55:ARG:HH22  | 21:W:93:ARG:NH2   | 2.09                     | 0.49              |
| 21:W:132:THR:OG1  | 21:W:133:GLU:OE1  | 2.28                     | 0.49              |
| 21:W:382:LEU:O    | 21:W:384:LEU:HD12 | 2.13                     | 0.49              |
| 21:W:449:GLU:OE1  | 21:W:450:GLU:N    | 2.45                     | 0.49              |
| 23:Y:16:ASP:OD1   | 23:Y:16:ASP:C     | 2.55                     | 0.49              |
| 23:Y:134:LEU:HA   | 23:Y:137:ARG:HD2  | 1.95                     | 0.49              |
| 23:Y:159:ARG:O    | 23:Y:163:LYS:HG2  | 2.13                     | 0.49              |
| 26:b:7:MET:HE2    | 26:b:96:ALA:HB3   | 1.93                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 26:b:108:ARG:NH1  | 26:b:137:ASN:HD21 | 2.07                     | 0.49              |
| 27:c:282:ARG:HG2  | 27:c:282:ARG:NH1  | 2.27                     | 0.49              |
| 28:d:33:LEU:HD22  | 28:d:34:ASN:OD1   | 2.11                     | 0.49              |
| 28:d:161:GLU:OE1  | 28:d:162:SER:N    | 2.46                     | 0.49              |
| 30:f:202:HIS:HA   | 30:f:205:CYS:SG   | 2.52                     | 0.49              |
| 30:f:682:GLY:H    | 30:f:688:ARG:HH21 | 1.61                     | 0.49              |
| 30:f:692:LEU:CD2  | 30:f:696:LEU:HD11 | 2.41                     | 0.49              |
| 15:p:9:ALA:HB1    | 15:p:145:MET:CE   | 2.43                     | 0.49              |
| 31:F:197:GLU:OE2  | 31:F:350:ARG:HD2  | 2.12                     | 0.49              |
| 31:F:369:HIS:CD2  | 31:F:397:LYS:HB2  | 2.48                     | 0.49              |
| 32:U:206:MET:HE2  | 32:U:206:MET:N    | 2.28                     | 0.49              |
| 32:U:234:GLU:C    | 32:U:234:GLU:OE1  | 2.56                     | 0.49              |
| 32:U:742:HIS:NE2  | 32:U:814:PRO:HG3  | 2.27                     | 0.49              |
| 32:U:811:PHE:CG   | 32:U:885:MET:HE1  | 2.48                     | 0.49              |
| 32:U:889:LEU:HD22 | 32:U:907:SER:O    | 2.12                     | 0.49              |
| 1:A:398:ARG:HD3   | 2:B:195:GLN:NE2   | 2.27                     | 0.49              |
| 2:B:394:ASP:OD1   | 3:C:308:PRO:HG2   | 2.13                     | 0.49              |
| 2:B:421:LYS:HA    | 2:B:424:GLU:HG3   | 1.94                     | 0.49              |
| 4:D:225:ALA:HB1   | 4:D:259:PRO:C     | 2.38                     | 0.49              |
| 4:D:231:VAL:HG22  | 5:E:262:ASN:ND2   | 2.28                     | 0.49              |
| 5:E:270:LEU:HD11  | 5:E:273:VAL:CG1   | 2.42                     | 0.49              |
| 5:E:327:ASP:OD1   | 5:E:330:ALA:HB2   | 2.13                     | 0.49              |
| 17:R:38:ILE:HG23  | 17:R:61:ALA:HA    | 1.94                     | 0.49              |
| 20:V:415:SER:CA   | 23:Y:346:LYS:NZ   | 2.75                     | 0.49              |
| 22:X:170:GLN:NE2  | 22:X:193:ALA:HA   | 2.28                     | 0.49              |
| 23:Y:104:MET:HE1  | 23:Y:130:LYS:CG   | 2.42                     | 0.49              |
| 23:Y:117:LYS:O    | 23:Y:121:LEU:N    | 2.37                     | 0.49              |
| 23:Y:279:GLU:OE1  | 23:Y:296:VAL:HG21 | 2.12                     | 0.49              |
| 24:Z:254:ASN:OD1  | 24:Z:254:ASN:C    | 2.55                     | 0.49              |
| 25:a:140:GLU:C    | 25:a:140:GLU:OE1  | 2.56                     | 0.49              |
| 25:a:280:MET:HG2  | 25:a:291:LEU:CD2  | 2.43                     | 0.49              |
| 28:d:124:ALA:H    | 28:d:125:LYS:HZ3  | 1.60                     | 0.49              |
| 30:f:192:VAL:CB   | 30:f:193:PRO:HD3  | 2.42                     | 0.49              |
| 30:f:608:LYS:HG2  | 30:f:639:LYS:HZ1  | 1.77                     | 0.49              |
| 30:f:657:ILE:HA   | 30:f:661:ALA:HB2  | 1.95                     | 0.49              |
| 30:f:761:MET:HE2  | 30:f:761:MET:CA   | 2.43                     | 0.49              |
| 7:h:85:LEU:HD12   | 7:h:131:VAL:HG21  | 1.94                     | 0.49              |
| 31:F:91:SER:HB3   | 31:F:126:THR:HA   | 1.94                     | 0.49              |
| 31:F:154:ASN:OD1  | 31:F:155:LYS:N    | 2.46                     | 0.49              |
| 32:U:792:ASN:CB   | 32:U:796:LYS:HB3  | 2.42                     | 0.49              |
| 1:A:268:LYS:HE3   | 30:f:354:GLU:HB3  | 1.94                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:223:ILE:HB    | 2:B:347:ILE:CD1   | 2.40                     | 0.49              |
| 2:B:231:GLY:N     | 33:B:501:ATP:O2B  | 2.41                     | 0.49              |
| 2:B:417:GLU:OE1   | 2:B:420:LYS:HE3   | 2.12                     | 0.49              |
| 5:E:116:ASP:OD1   | 5:E:117:PRO:HD2   | 2.13                     | 0.49              |
| 5:E:146:ARG:HG2   | 5:E:146:ARG:HH11  | 1.78                     | 0.49              |
| 11:L:88:MET:SD    | 11:L:112:ILE:HD11 | 2.52                     | 0.49              |
| 14:O:2:THR:HG23   | 14:O:34:LYS:HE3   | 1.94                     | 0.49              |
| 20:V:218:TYR:O    | 20:V:222:ASP:N    | 2.45                     | 0.49              |
| 21:W:366:MET:O    | 21:W:370:TYR:HB2  | 2.11                     | 0.49              |
| 21:W:374:THR:HG23 | 21:W:377:ARG:H    | 1.78                     | 0.49              |
| 22:X:287:LEU:O    | 22:X:290:VAL:HG12 | 2.13                     | 0.49              |
| 24:Z:134:PRO:CG   | 27:c:220:LEU:HD13 | 2.43                     | 0.49              |
| 25:a:196:ARG:HA   | 25:a:199:THR:CG2  | 2.43                     | 0.49              |
| 25:a:328:ASP:N    | 25:a:328:ASP:OD1  | 2.45                     | 0.49              |
| 26:b:23:PRO:HB2   | 26:b:27:GLN:HB2   | 1.94                     | 0.49              |
| 29:e:52:PHE:HA    | 29:e:55:GLN:HE21  | 1.76                     | 0.49              |
| 30:f:698:SER:OG   | 30:f:705:ASN:OD1  | 2.15                     | 0.49              |
| 30:f:787:LEU:HA   | 30:f:790:GLN:HB2  | 1.95                     | 0.49              |
| 6:g:73:THR:HG22   | 6:g:74:GLU:N      | 2.28                     | 0.49              |
| 6:g:196:GLU:O     | 6:g:200:THR:HG23  | 2.12                     | 0.49              |
| 8:i:44:LEU:C      | 8:i:44:LEU:HD12   | 2.38                     | 0.49              |
| 31:F:360:GLU:C    | 31:F:360:GLU:OE2  | 2.56                     | 0.49              |
| 32:U:333:MET:HE3  | 32:U:333:MET:N    | 2.21                     | 0.49              |
| 32:U:369:THR:HG21 | 32:U:392:TRP:HZ2  | 1.78                     | 0.49              |
| 32:U:748:LEU:H    | 32:U:748:LEU:CD1  | 2.24                     | 0.49              |
| 32:U:801:GLN:HG2  | 32:U:878:LEU:O    | 2.12                     | 0.49              |
| 2:B:363:ARG:HB3   | 2:B:363:ARG:CZ    | 2.43                     | 0.49              |
| 4:D:284:GLU:OE1   | 4:D:284:GLU:C     | 2.56                     | 0.49              |
| 5:E:60:VAL:HA     | 5:E:71:VAL:HG12   | 1.95                     | 0.49              |
| 5:E:215:ILE:HG22  | 5:E:263:GLN:HE22  | 1.77                     | 0.49              |
| 11:L:209:ASN:OD1  | 11:L:209:ASN:N    | 2.45                     | 0.49              |
| 19:T:92:LEU:HD21  | 19:T:110:MET:SD   | 2.53                     | 0.49              |
| 20:V:67:LEU:O     | 20:V:71:THR:HG22  | 2.13                     | 0.49              |
| 20:V:404:LYS:CE   | 20:V:446:VAL:HG21 | 2.43                     | 0.49              |
| 20:V:413:SER:HB2  | 23:Y:338:ILE:HB   | 1.94                     | 0.49              |
| 21:W:112:VAL:CG2  | 21:W:120:ILE:HD11 | 2.43                     | 0.49              |
| 21:W:125:ILE:HG13 | 21:W:129:ARG:NH1  | 2.28                     | 0.49              |
| 21:W:231:ILE:HD13 | 21:W:246:HIS:HB3  | 1.95                     | 0.49              |
| 21:W:243:ILE:HG13 | 21:W:273:TYR:CE1  | 2.47                     | 0.49              |
| 22:X:375:HIS:O    | 22:X:388:PHE:HB2  | 2.12                     | 0.49              |
| 22:X:416:ASN:O    | 22:X:420:LYS:HG3  | 2.13                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 23:Y:325:VAL:CG2  | 29:e:60:LEU:HD13  | 2.43                     | 0.49              |
| 23:Y:338:ILE:HD11 | 23:Y:343:LEU:HD22 | 1.94                     | 0.49              |
| 24:Z:39:LEU:HD11  | 24:Z:122:VAL:HG21 | 1.95                     | 0.49              |
| 24:Z:201:LEU:HD12 | 24:Z:205:LEU:HD23 | 1.93                     | 0.49              |
| 25:a:122:LYS:HE2  | 25:a:130:VAL:HG13 | 1.95                     | 0.49              |
| 25:a:302:ILE:HD12 | 25:a:302:ILE:N    | 2.27                     | 0.49              |
| 28:d:103:LEU:HD12 | 28:d:133:ILE:CD1  | 2.41                     | 0.49              |
| 30:f:216:MET:N    | 30:f:216:MET:SD   | 2.86                     | 0.49              |
| 30:f:321:MET:C    | 30:f:321:MET:SD   | 2.96                     | 0.49              |
| 30:f:425:GLY:O    | 30:f:429:ILE:HG12 | 2.12                     | 0.49              |
| 30:f:813:LYS:HD2  | 30:f:882:LEU:CD2  | 2.37                     | 0.49              |
| 30:f:817:VAL:O    | 30:f:817:VAL:HG12 | 2.13                     | 0.49              |
| 30:f:825:MET:SD   | 30:f:848:GLN:NE2  | 2.85                     | 0.49              |
| 9:j:116:GLN:HG3   | 10:k:83:ALA:HB1   | 1.94                     | 0.49              |
| 14:o:180:SER:OG   | 14:o:181:LYS:N    | 2.45                     | 0.49              |
| 32:U:25:HIS:HD1   | 32:U:59:PHE:HE2   | 1.61                     | 0.49              |
| 32:U:356:THR:HG22 | 32:U:717:ILE:CD1  | 2.43                     | 0.49              |
| 32:U:680:VAL:HG13 | 32:U:682:TYR:CE1  | 2.48                     | 0.49              |
| 1:A:80:LEU:O      | 1:A:80:LEU:HD22   | 2.13                     | 0.49              |
| 2:B:202:GLU:HA    | 2:B:202:GLU:OE2   | 2.12                     | 0.49              |
| 2:B:360:THR:O     | 2:B:364:ILE:HG12  | 2.13                     | 0.49              |
| 2:B:410:ARG:NH1   | 23:Y:94:ASN:HA    | 2.28                     | 0.49              |
| 3:C:149:GLU:OE1   | 3:C:149:GLU:CA    | 2.61                     | 0.49              |
| 3:C:189:TYR:HE2   | 3:C:316:GLU:CG    | 2.23                     | 0.49              |
| 4:D:200:ARG:O     | 4:D:200:ARG:CG    | 2.60                     | 0.49              |
| 4:D:269:ALA:O     | 4:D:270:ILE:HD13  | 2.12                     | 0.49              |
| 5:E:297:ARG:HG2   | 5:E:299:ILE:HD12  | 1.94                     | 0.49              |
| 5:E:363:VAL:HG22  | 5:E:366:ASP:OD1   | 2.12                     | 0.49              |
| 12:M:198:TYR:OH   | 12:M:236:GLU:OE1  | 2.30                     | 0.49              |
| 20:V:72:LEU:HA    | 20:V:75:ILE:CD1   | 2.41                     | 0.49              |
| 20:V:101:LEU:HD11 | 20:V:173:ILE:HD13 | 1.95                     | 0.49              |
| 20:V:332:LEU:HA   | 20:V:335:VAL:HG12 | 1.93                     | 0.49              |
| 21:W:48:LEU:HD12  | 21:W:90:LEU:HD21  | 1.93                     | 0.49              |
| 21:W:436:MET:HE3  | 27:c:226:MET:HB3  | 1.95                     | 0.49              |
| 21:W:448:LYS:O    | 21:W:452:ILE:HB   | 2.13                     | 0.49              |
| 22:X:142:ARG:HB2  | 22:X:146:ALA:CB   | 2.36                     | 0.49              |
| 22:X:421:LEU:C    | 22:X:421:LEU:HD13 | 2.38                     | 0.49              |
| 23:Y:116:ASP:HB3  | 23:Y:118:GLU:OE1  | 2.12                     | 0.49              |
| 24:Z:138:TYR:HE1  | 24:Z:157:HIS:HD2  | 1.61                     | 0.49              |
| 24:Z:138:TYR:CE1  | 24:Z:157:HIS:HD2  | 2.31                     | 0.49              |
| 25:a:280:MET:HE3  | 25:a:296:ILE:HG12 | 1.95                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 27:c:222:LYS:HD2  | 27:c:222:LYS:HA   | 1.58                     | 0.49              |
| 28:d:5:LEU:HD11   | 28:d:6:LYS:HZ2    | 1.77                     | 0.49              |
| 28:d:115:PHE:CE1  | 28:d:119:LEU:HD21 | 2.48                     | 0.49              |
| 29:e:58:ALA:O     | 29:e:61:GLU:HG3   | 2.13                     | 0.49              |
| 30:f:554:TYR:OH   | 30:f:788:MET:O    | 2.30                     | 0.49              |
| 30:f:641:GLU:OE1  | 30:f:763:ARG:NH2  | 2.35                     | 0.49              |
| 8:i:119:GLN:HA    | 8:i:122:THR:HG22  | 1.95                     | 0.49              |
| 11:l:35:THR:HG21  | 11:l:73:SER:OG    | 2.13                     | 0.49              |
| 18:s:148:LEU:HD23 | 18:s:178:VAL:HG12 | 1.95                     | 0.49              |
| 32:U:238:LYS:HD2  | 32:U:238:LYS:O    | 2.13                     | 0.49              |
| 32:U:251:ASP:OD1  | 32:U:251:ASP:C    | 2.56                     | 0.49              |
| 32:U:516:LEU:CB   | 32:U:532:MET:HE2  | 2.43                     | 0.49              |
| 32:U:536:ALA:HB1  | 32:U:545:LEU:CD1  | 2.43                     | 0.49              |
| 32:U:748:LEU:HD23 | 32:U:760:VAL:HG22 | 1.94                     | 0.49              |
| 2:B:125:THR:OG1   | 2:B:126:SER:N     | 2.46                     | 0.48              |
| 2:B:209:GLU:HA    | 2:B:212:GLU:OE2   | 2.13                     | 0.48              |
| 2:B:409:GLU:HA    | 2:B:409:GLU:OE2   | 2.13                     | 0.48              |
| 3:C:28:ILE:CD1    | 4:D:43:ARG:HG2    | 2.41                     | 0.48              |
| 3:C:152:GLY:HA3   | 3:C:328:ILE:HG13  | 1.94                     | 0.48              |
| 3:C:381:GLU:HG2   | 22:X:191:THR:CG2  | 2.43                     | 0.48              |
| 3:C:388:ALA:O     | 3:C:393:LYS:N     | 2.37                     | 0.48              |
| 4:D:71:GLU:OE2    | 32:U:644:TYR:HD1  | 1.96                     | 0.48              |
| 4:D:181:VAL:HG11  | 4:D:308:ILE:HD11  | 1.95                     | 0.48              |
| 5:E:161:ARG:NE    | 21:W:173:THR:HA   | 2.28                     | 0.48              |
| 5:E:272:ARG:HG3   | 5:E:272:ARG:NH1   | 2.28                     | 0.48              |
| 20:V:218:TYR:HA   | 20:V:221:LEU:HD12 | 1.95                     | 0.48              |
| 20:V:438:VAL:HG11 | 20:V:458:VAL:HG21 | 1.94                     | 0.48              |
| 20:V:467:TYR:CE2  | 23:Y:362:LYS:HE2  | 2.48                     | 0.48              |
| 21:W:130:MET:HE3  | 21:W:130:MET:C    | 2.38                     | 0.48              |
| 21:W:170:GLN:O    | 21:W:171:VAL:HB   | 2.13                     | 0.48              |
| 23:Y:227:SER:O    | 23:Y:231:LEU:HG   | 2.13                     | 0.48              |
| 25:a:216:LEU:C    | 25:a:216:LEU:HD23 | 2.38                     | 0.48              |
| 27:c:146:ASP:OD2  | 27:c:149:GLN:HG3  | 2.13                     | 0.48              |
| 27:c:216:MET:C    | 27:c:220:LEU:HG   | 2.38                     | 0.48              |
| 28:d:4:GLN:OE1    | 28:d:4:GLN:O      | 2.31                     | 0.48              |
| 28:d:104:LEU:HD23 | 28:d:104:LEU:C    | 2.38                     | 0.48              |
| 30:f:744:MET:CB   | 30:f:747:GLN:HE21 | 2.25                     | 0.48              |
| 31:F:195:ILE:HG12 | 31:F:236:LEU:HD13 | 1.95                     | 0.48              |
| 31:F:289:ASP:OD1  | 31:F:289:ASP:N    | 2.44                     | 0.48              |
| 32:U:160:LEU:O    | 32:U:164:GLU:N    | 2.36                     | 0.48              |
| 32:U:387:ARG:HA   | 32:U:390:LEU:HD21 | 1.93                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 32:U:401:LYS:O    | 32:U:405:THR:HG22 | 2.12                     | 0.48              |
| 2:B:54:PRO:O      | 2:B:56:THR:HG22   | 2.12                     | 0.48              |
| 2:B:90:GLU:N      | 2:B:94:GLU:HB3    | 2.18                     | 0.48              |
| 2:B:176:VAL:HG21  | 2:B:247:PHE:CD1   | 2.48                     | 0.48              |
| 2:B:397:ALA:HA    | 2:B:400:THR:CG2   | 2.42                     | 0.48              |
| 3:C:37:ASP:OD1    | 3:C:37:ASP:N      | 2.44                     | 0.48              |
| 3:C:300:ILE:C     | 3:C:300:ILE:HD12  | 2.37                     | 0.48              |
| 5:E:353:PHE:CZ    | 5:E:373:LYS:HE2   | 2.49                     | 0.48              |
| 7:H:48:GLU:OE1    | 7:H:50:LYS:HG3    | 2.14                     | 0.48              |
| 20:V:130:PHE:HD2  | 20:V:134:PHE:CE2  | 2.27                     | 0.48              |
| 20:V:334:VAL:HG21 | 20:V:395:ILE:HD11 | 1.95                     | 0.48              |
| 21:W:112:VAL:HG23 | 21:W:120:ILE:CD1  | 2.43                     | 0.48              |
| 21:W:124:LEU:CD2  | 21:W:147:LYS:HD2  | 2.43                     | 0.48              |
| 21:W:176:SER:OG   | 21:W:176:SER:O    | 2.27                     | 0.48              |
| 21:W:231:ILE:CD1  | 21:W:246:HIS:HB3  | 2.43                     | 0.48              |
| 21:W:286:LEU:HD13 | 21:W:286:LEU:O    | 2.13                     | 0.48              |
| 21:W:422:ASN:C    | 21:W:422:ASN:OD1  | 2.56                     | 0.48              |
| 24:Z:148:GLY:O    | 24:Z:149:THR:HG23 | 2.13                     | 0.48              |
| 25:a:324:ILE:CD1  | 25:a:331:VAL:HG22 | 2.43                     | 0.48              |
| 26:b:151:GLU:HA   | 26:b:154:THR:OG1  | 2.12                     | 0.48              |
| 30:f:180:GLN:O    | 30:f:183:PRO:HD2  | 2.12                     | 0.48              |
| 30:f:712:LYS:HD2  | 30:f:713:PHE:N    | 2.29                     | 0.48              |
| 30:f:828:ARG:HH21 | 30:f:861:THR:HG21 | 1.78                     | 0.48              |
| 16:q:161:ARG:HB3  | 16:q:161:ARG:NH1  | 2.29                     | 0.48              |
| 31:F:139:LEU:N    | 31:F:139:LEU:HD23 | 2.27                     | 0.48              |
| 1:A:174:TYR:H     | 1:A:232:ARG:NH2   | 2.11                     | 0.48              |
| 2:B:168:ASP:OD1   | 2:B:170:LEU:HB3   | 2.13                     | 0.48              |
| 2:B:286:GLU:OE2   | 3:C:278:ASN:ND2   | 2.39                     | 0.48              |
| 2:B:294:ARG:HB2   | 2:B:294:ARG:NH1   | 2.29                     | 0.48              |
| 2:B:338:ASP:OD1   | 2:B:339:PRO:HD2   | 2.14                     | 0.48              |
| 3:C:214:VAL:O     | 3:C:214:VAL:HG13  | 2.13                     | 0.48              |
| 5:E:331:ILE:HG12  | 5:E:371:VAL:CG2   | 2.44                     | 0.48              |
| 20:V:71:THR:O     | 20:V:74:ASP:HB2   | 2.13                     | 0.48              |
| 20:V:216:ARG:NH1  | 29:e:21:GLU:HA    | 2.28                     | 0.48              |
| 21:W:124:LEU:HD21 | 21:W:147:LYS:HD2  | 1.95                     | 0.48              |
| 21:W:180:LYS:O    | 21:W:183:VAL:HG12 | 2.12                     | 0.48              |
| 21:W:198:ASP:OD1  | 21:W:198:ASP:C    | 2.56                     | 0.48              |
| 21:W:305:LEU:HG   | 21:W:309:PHE:HE2  | 1.78                     | 0.48              |
| 23:Y:101:ARG:NH2  | 23:Y:140:ILE:HD11 | 2.29                     | 0.48              |
| 23:Y:297:ARG:HG2  | 23:Y:297:ARG:HH11 | 1.78                     | 0.48              |
| 25:a:33:LEU:HB2   | 26:b:18:ASN:ND2   | 2.27                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 25:a:112:ILE:CD1  | 25:a:151:VAL:HG11 | 2.44                     | 0.48              |
| 25:a:156:TYR:HA   | 25:a:159:SER:OG   | 2.13                     | 0.48              |
| 25:a:216:LEU:HD23 | 25:a:216:LEU:O    | 2.12                     | 0.48              |
| 25:a:281:THR:HG22 | 25:a:289:ARG:NH1  | 2.28                     | 0.48              |
| 28:d:78:LEU:HB2   | 28:d:82:TYR:HE1   | 1.78                     | 0.48              |
| 30:f:94:LYS:HA    | 30:f:98:PHE:HD1   | 1.77                     | 0.48              |
| 30:f:119:LYS:HG3  | 30:f:165:GLU:OE2  | 2.13                     | 0.48              |
| 30:f:655:LEU:O    | 30:f:660:ILE:HD12 | 2.13                     | 0.48              |
| 11:l:88:MET:SD    | 11:l:112:ILE:HD11 | 2.53                     | 0.48              |
| 1:A:85:GLN:HB2    | 1:A:88:GLN:OE1    | 2.14                     | 0.48              |
| 1:A:120:LYS:O     | 31:F:90:VAL:HB    | 2.12                     | 0.48              |
| 1:A:387:SER:CA    | 1:A:390:THR:HG22  | 2.39                     | 0.48              |
| 2:B:150:VAL:HG11  | 2:B:159:VAL:HG22  | 1.95                     | 0.48              |
| 2:B:375:ALA:C     | 2:B:376:ASP:OD1   | 2.56                     | 0.48              |
| 3:C:63:LEU:HD13   | 3:C:63:LEU:O      | 2.14                     | 0.48              |
| 3:C:127:LEU:HB3   | 3:C:128:PRO:HD2   | 1.95                     | 0.48              |
| 4:D:91:GLN:HE22   | 4:D:248:ARG:HD3   | 1.78                     | 0.48              |
| 4:D:98:GLN:HE22   | 4:D:121:ARG:HE    | 1.61                     | 0.48              |
| 5:E:197:LYS:HD2   | 5:E:197:LYS:C     | 2.37                     | 0.48              |
| 13:N:161:LEU:O    | 13:N:165:MET:HG3  | 2.13                     | 0.48              |
| 20:V:428:LEU:CD2  | 20:V:434:ALA:HA   | 2.44                     | 0.48              |
| 21:W:331:GLY:N    | 21:W:334:GLU:OE1  | 2.42                     | 0.48              |
| 21:W:403:PHE:HD2  | 21:W:417:ARG:NH2  | 2.11                     | 0.48              |
| 22:X:151:SER:O    | 22:X:155:ARG:NE   | 2.46                     | 0.48              |
| 23:Y:229:ILE:HD12 | 23:Y:229:ILE:O    | 2.14                     | 0.48              |
| 24:Z:274:ASN:HD22 | 27:c:281:LYS:NZ   | 2.11                     | 0.48              |
| 25:a:144:ASN:ND2  | 25:a:146:PRO:HB3  | 2.27                     | 0.48              |
| 25:a:144:ASN:HD21 | 25:a:146:PRO:HB3  | 1.78                     | 0.48              |
| 25:a:247:ARG:HH21 | 25:a:251:LEU:CD1  | 2.26                     | 0.48              |
| 30:f:154:TRP:HA   | 30:f:157:GLU:CD   | 2.38                     | 0.48              |
| 30:f:670:MET:HA   | 30:f:672:LEU:HD11 | 1.94                     | 0.48              |
| 31:F:69:MET:O     | 31:F:73:ILE:HG13  | 2.12                     | 0.48              |
| 31:F:204:LEU:C    | 31:F:204:LEU:HD23 | 2.38                     | 0.48              |
| 32:U:159:ARG:HH11 | 32:U:159:ARG:CB   | 2.25                     | 0.48              |
| 32:U:171:ASN:OD1  | 32:U:172:ASP:N    | 2.45                     | 0.48              |
| 32:U:765:VAL:HG13 | 32:U:775:LEU:HD21 | 1.96                     | 0.48              |
| 1:A:219:GLY:N     | 33:A:501:ATP:O1B  | 2.46                     | 0.48              |
| 1:A:399:ALA:O     | 1:A:400:ARG:HB2   | 2.14                     | 0.48              |
| 2:B:268:ARG:NH1   | 2:B:311:GLU:OE1   | 2.44                     | 0.48              |
| 3:C:115:ALA:O     | 3:C:123:LEU:HA    | 2.14                     | 0.48              |
| 3:C:145:ASP:OD1   | 3:C:145:ASP:N     | 2.47                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:C:287:LYS:H     | 3:C:287:LYS:HD2   | 1.78                     | 0.48              |
| 4:D:92:PHE:HE1    | 4:D:101:ALA:HB1   | 1.78                     | 0.48              |
| 4:D:131:ALA:HB2   | 4:D:143:LEU:HD11  | 1.95                     | 0.48              |
| 4:D:392:TYR:HB3   | 21:W:137:TYR:HE1  | 1.78                     | 0.48              |
| 5:E:197:LYS:HE2   | 31:F:320:PHE:CG   | 2.48                     | 0.48              |
| 13:N:166:GLU:OE1  | 13:N:166:GLU:HA   | 2.14                     | 0.48              |
| 21:W:307:LYS:HG2  | 21:W:315:MET:CE   | 2.41                     | 0.48              |
| 21:W:376:LYS:CA   | 21:W:376:LYS:HE2  | 2.43                     | 0.48              |
| 21:W:422:ASN:OD1  | 21:W:423:ASN:N    | 2.46                     | 0.48              |
| 26:b:83:LYS:HD2   | 26:b:84:ILE:N     | 2.23                     | 0.48              |
| 31:F:347:ARG:O    | 31:F:348:LEU:C    | 2.57                     | 0.48              |
| 32:U:98:GLU:OE1   | 32:U:99:THR:N     | 2.45                     | 0.48              |
| 32:U:579:ARG:HB3  | 32:U:614:VAL:HG21 | 1.95                     | 0.48              |
| 32:U:615:ARG:HH21 | 32:U:645:ASN:ND2  | 2.11                     | 0.48              |
| 32:U:901:GLN:HE21 | 32:U:915:LYS:CB   | 2.19                     | 0.48              |
| 2:B:75:GLU:HA     | 2:B:78:PHE:HB3    | 1.95                     | 0.48              |
| 2:B:79:ILE:HA     | 2:B:82:GLN:NE2    | 2.29                     | 0.48              |
| 2:B:170:LEU:HD21  | 2:B:269:GLU:HB3   | 1.96                     | 0.48              |
| 3:C:143:VAL:HG13  | 3:C:143:VAL:O     | 2.13                     | 0.48              |
| 4:D:108:GLY:C     | 4:D:109:SER:HG    | 2.15                     | 0.48              |
| 4:D:357:GLU:OE2   | 4:D:395:LEU:HA    | 2.12                     | 0.48              |
| 20:V:407:VAL:HA   | 20:V:410:ILE:CG2  | 2.42                     | 0.48              |
| 20:V:485:ASP:C    | 20:V:485:ASP:OD1  | 2.56                     | 0.48              |
| 21:W:98:LYS:CE    | 21:W:139:GLU:HB2  | 2.44                     | 0.48              |
| 21:W:241:LEU:CD1  | 21:W:245:LYS:HZ2  | 2.27                     | 0.48              |
| 21:W:317:TRP:HD1  | 21:W:358:VAL:HG11 | 1.77                     | 0.48              |
| 22:X:297:ARG:HH21 | 22:X:337:ARG:CB   | 2.27                     | 0.48              |
| 24:Z:16:LEU:HG    | 27:c:216:MET:HE3  | 1.95                     | 0.48              |
| 24:Z:105:ASP:O    | 24:Z:155:PHE:HE2  | 1.95                     | 0.48              |
| 25:a:186:LYS:HD2  | 25:a:221:VAL:HA   | 1.96                     | 0.48              |
| 28:d:161:GLU:OE1  | 28:d:163:TYR:N    | 2.31                     | 0.48              |
| 28:d:248:GLU:HA   | 28:d:248:GLU:OE1  | 2.12                     | 0.48              |
| 30:f:103:TYR:CZ   | 30:f:106:LEU:HD23 | 2.48                     | 0.48              |
| 30:f:240:VAL:HG13 | 30:f:241:PRO:CD   | 2.43                     | 0.48              |
| 30:f:578:ALA:O    | 30:f:582:VAL:HG13 | 2.13                     | 0.48              |
| 14:o:188:ARG:HB3  | 14:o:189:PRO:CD   | 2.44                     | 0.48              |
| 17:r:177:LEU:HB3  | 17:r:188:VAL:HG22 | 1.95                     | 0.48              |
| 32:U:173:VAL:O    | 32:U:173:VAL:HG12 | 2.13                     | 0.48              |
| 1:A:205:GLY:H     | 31:F:373:MET:HA   | 1.78                     | 0.48              |
| 1:A:242:GLY:O     | 1:A:280:ILE:HG23  | 2.13                     | 0.48              |
| 2:B:63:LEU:HD22   | 2:B:63:LEU:H      | 1.77                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:186:ASP:C     | 2:B:186:ASP:OD1   | 2.57                     | 0.48              |
| 2:B:256:ILE:HB    | 2:B:305:ILE:HD11  | 1.95                     | 0.48              |
| 4:D:125:LYS:CB    | 4:D:126:PRO:HD2   | 2.43                     | 0.48              |
| 5:E:170:CYS:HB3   | 5:E:276:ILE:HD12  | 1.96                     | 0.48              |
| 9:J:90:GLU:HA     | 9:J:90:GLU:OE2    | 2.12                     | 0.48              |
| 16:Q:141:SER:OG   | 17:r:139:VAL:HG23 | 2.14                     | 0.48              |
| 20:V:83:GLU:OE1   | 20:V:83:GLU:HA    | 2.12                     | 0.48              |
| 20:V:184:ALA:O    | 20:V:187:ILE:HG23 | 2.14                     | 0.48              |
| 20:V:352:SER:C    | 20:V:353:LEU:HD22 | 2.39                     | 0.48              |
| 20:V:359:PRO:HA   | 20:V:382:PHE:CE2  | 2.48                     | 0.48              |
| 25:a:226:ARG:HH12 | 25:a:230:ARG:CD   | 2.27                     | 0.48              |
| 26:b:23:PRO:C     | 26:b:24:THR:HG1   | 2.18                     | 0.48              |
| 26:b:91:ARG:O     | 26:b:94:HIS:HB3   | 2.14                     | 0.48              |
| 26:b:128:ALA:CB   | 26:b:160:LEU:HD21 | 2.43                     | 0.48              |
| 27:c:98:MET:HE3   | 27:c:98:MET:HB2   | 1.71                     | 0.48              |
| 27:c:116:PRO:HD2  | 27:c:118:PHE:CE2  | 2.49                     | 0.48              |
| 27:c:154:LYS:HA   | 27:c:154:LYS:CE   | 2.43                     | 0.48              |
| 27:c:250:GLU:OE2  | 27:c:254:ASN:ND2  | 2.47                     | 0.48              |
| 28:d:171:LEU:HA   | 28:d:174:ILE:CG2  | 2.44                     | 0.48              |
| 30:f:139:CYS:SG   | 30:f:188:VAL:HG11 | 2.54                     | 0.48              |
| 30:f:170:TRP:CZ3  | 30:f:173:LEU:HD13 | 2.49                     | 0.48              |
| 30:f:744:MET:HA   | 30:f:747:GLN:CG   | 2.44                     | 0.48              |
| 30:f:861:THR:OG1  | 30:f:862:ILE:N    | 2.46                     | 0.48              |
| 31:F:194:GLN:NE2  | 31:F:353:GLU:O    | 2.46                     | 0.48              |
| 32:U:398:ASN:O    | 32:U:437:TYR:HE2  | 1.96                     | 0.48              |
| 32:U:478:SER:HB2  | 32:U:511:ALA:HB1  | 1.94                     | 0.48              |
| 32:U:736:ILE:CD1  | 32:U:779:LEU:HD23 | 2.44                     | 0.48              |
| 32:U:756:HIS:NE2  | 32:U:758:PRO:HG2  | 2.29                     | 0.48              |
| 1:A:112:ILE:CD1   | 31:F:164:LEU:HD23 | 2.38                     | 0.48              |
| 6:G:174:GLU:H     | 6:G:174:GLU:CD    | 2.20                     | 0.48              |
| 7:H:82:TYR:O      | 7:H:86:VAL:HG23   | 2.13                     | 0.48              |
| 17:R:6:ALA:HB3    | 17:R:101:MET:CE   | 2.43                     | 0.48              |
| 20:V:193:GLN:OE1  | 20:V:193:GLN:CA   | 2.62                     | 0.48              |
| 20:V:240:LEU:HD22 | 20:V:240:LEU:N    | 2.29                     | 0.48              |
| 21:W:311:THR:O    | 21:W:312:MET:HB2  | 2.14                     | 0.48              |
| 22:X:221:GLU:O    | 22:X:223:LYS:NZ   | 2.45                     | 0.48              |
| 23:Y:232:GLU:OE1  | 23:Y:232:GLU:N    | 2.31                     | 0.48              |
| 24:Z:214:LYS:N    | 24:Z:219:LYS:HZ2  | 2.12                     | 0.48              |
| 25:a:109:GLU:O    | 25:a:112:ILE:HG12 | 2.13                     | 0.48              |
| 25:a:161:LYS:HA   | 25:a:161:LYS:CE   | 2.43                     | 0.48              |
| 27:c:48:GLY:C     | 27:c:50:PRO:HD2   | 2.39                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 30:f:790:GLN:HA   | 30:f:796:LEU:CD2  | 2.43                     | 0.48              |
| 31:F:138:GLY:CA   | 31:F:159:LEU:HD21 | 2.44                     | 0.48              |
| 32:U:265:ILE:HG13 | 32:U:329:LEU:HD23 | 1.95                     | 0.48              |
| 32:U:505:ASP:OD1  | 32:U:507:VAL:N    | 2.45                     | 0.48              |
| 32:U:653:ALA:HB2  | 32:U:675:MET:SD   | 2.53                     | 0.48              |
| 4:D:312:ASN:C     | 4:D:312:ASN:OD1   | 2.57                     | 0.48              |
| 4:D:377:SER:HB2   | 5:E:292:PRO:HB3   | 1.96                     | 0.48              |
| 7:H:85:LEU:HD13   | 7:H:117:MET:HE2   | 1.96                     | 0.48              |
| 20:V:107:ARG:HG3  | 20:V:107:ARG:O    | 2.13                     | 0.48              |
| 20:V:415:SER:HB2  | 23:Y:346:LYS:HZ2  | 1.78                     | 0.48              |
| 20:V:440:LYS:HD3  | 28:d:145:GLU:C    | 2.39                     | 0.48              |
| 21:W:117:ASP:OD1  | 21:W:118:LEU:N    | 2.44                     | 0.48              |
| 21:W:132:THR:OG1  | 21:W:133:GLU:N    | 2.46                     | 0.48              |
| 21:W:187:LEU:HD23 | 21:W:187:LEU:C    | 2.39                     | 0.48              |
| 24:Z:8:LYS:HG2    | 24:Z:47:VAL:HG22  | 1.95                     | 0.48              |
| 24:Z:106:ILE:HD13 | 24:Z:155:PHE:CE2  | 2.49                     | 0.48              |
| 24:Z:193:ASN:O    | 27:c:228:GLY:HA3  | 2.14                     | 0.48              |
| 25:a:34:TRP:CZ3   | 26:b:18:ASN:HA    | 2.49                     | 0.48              |
| 25:a:324:ILE:CD1  | 25:a:331:VAL:HG13 | 2.44                     | 0.48              |
| 27:c:55:GLY:HA3   | 27:c:112:TYR:HE1  | 1.77                     | 0.48              |
| 28:d:133:ILE:O    | 28:d:133:ILE:HG13 | 2.14                     | 0.48              |
| 30:f:426:LEU:HD22 | 30:f:426:LEU:N    | 2.29                     | 0.48              |
| 30:f:742:ALA:HA   | 30:f:745:LEU:HG   | 1.94                     | 0.48              |
| 6:g:10:ASP:OD1    | 6:g:11:ARG:N      | 2.47                     | 0.48              |
| 32:U:88:PHE:HZ    | 32:U:96:TYR:HH    | 1.59                     | 0.48              |
| 32:U:159:ARG:CB   | 32:U:159:ARG:NH1  | 2.77                     | 0.48              |
| 32:U:198:LEU:HD23 | 32:U:223:LEU:HD22 | 1.96                     | 0.48              |
| 32:U:247:GLN:HA   | 32:U:913:ILE:HD13 | 1.96                     | 0.48              |
| 32:U:486:MET:HE1  | 32:U:781:LEU:CD2  | 2.43                     | 0.48              |
| 32:U:521:LEU:HD12 | 32:U:522:GLY:H    | 1.79                     | 0.48              |
| 1:A:292:ASP:HB3   | 2:B:303:ARG:HD2   | 1.95                     | 0.48              |
| 1:A:309:PHE:CE1   | 31:F:238:ARG:HA   | 2.48                     | 0.48              |
| 2:B:385:MET:C     | 2:B:385:MET:HE3   | 2.39                     | 0.48              |
| 3:C:25:LEU:HA     | 3:C:28:ILE:HG22   | 1.96                     | 0.48              |
| 3:C:162:LYS:NZ    | 23:Y:98:SER:HB2   | 2.29                     | 0.48              |
| 5:E:55:GLN:OE1    | 5:E:108:MET:HE2   | 2.14                     | 0.48              |
| 5:E:248:SER:HA    | 5:E:251:ARG:HH22  | 1.78                     | 0.48              |
| 5:E:284:THR:HG22  | 31:F:297:ASP:HB2  | 1.94                     | 0.48              |
| 12:M:198:TYR:HB3  | 12:M:243:LEU:HD11 | 1.96                     | 0.48              |
| 20:V:192:MET:O    | 20:V:195:ILE:CD1  | 2.62                     | 0.48              |
| 20:V:254:LEU:HA   | 20:V:257:ASN:OD1  | 2.13                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 21:W:55:ARG:HH22  | 21:W:93:ARG:NE    | 2.12                     | 0.48              |
| 23:Y:48:ASN:OD1   | 23:Y:76:ALA:HB3   | 2.13                     | 0.48              |
| 23:Y:96:GLY:CA    | 23:Y:100:ILE:HG23 | 2.28                     | 0.48              |
| 24:Z:193:ASN:OD1  | 24:Z:194:GLN:HG2  | 2.13                     | 0.48              |
| 25:a:41:VAL:O     | 25:a:44:PHE:N     | 2.45                     | 0.48              |
| 25:a:77:VAL:HG21  | 25:a:113:LEU:HB3  | 1.95                     | 0.48              |
| 25:a:82:HIS:HD2   | 25:a:85:ARG:HH22  | 1.61                     | 0.48              |
| 25:a:142:LEU:O    | 25:a:143:ASN:HB3  | 2.14                     | 0.48              |
| 25:a:278:MET:C    | 25:a:280:MET:H    | 2.22                     | 0.48              |
| 27:c:132:SER:O    | 27:c:136:LEU:HD22 | 2.14                     | 0.48              |
| 30:f:445:LEU:HD11 | 30:f:466:LEU:HD11 | 1.95                     | 0.48              |
| 11:l:74:ILE:HG22  | 11:l:132:LEU:HD22 | 1.95                     | 0.48              |
| 32:U:54:PHE:C     | 32:U:56:SER:H     | 2.22                     | 0.48              |
| 32:U:145:HIS:O    | 32:U:145:HIS:CG   | 2.67                     | 0.48              |
| 32:U:247:GLN:HE22 | 32:U:904:LYS:CG   | 2.26                     | 0.48              |
| 32:U:587:ALA:HB2  | 32:U:621:SER:CB   | 2.44                     | 0.48              |
| 1:A:77:LEU:C      | 1:A:77:LEU:HD23   | 2.39                     | 0.47              |
| 1:A:83:ASP:HA     | 1:A:86:THR:CG2    | 2.44                     | 0.47              |
| 2:B:358:GLU:C     | 2:B:358:GLU:OE2   | 2.56                     | 0.47              |
| 3:C:339:THR:OG1   | 3:C:378:VAL:O     | 2.22                     | 0.47              |
| 4:D:207:PRO:HD2   | 4:D:333:PHE:O     | 2.13                     | 0.47              |
| 4:D:222:HIS:CD2   | 4:D:222:HIS:N     | 2.81                     | 0.47              |
| 20:V:161:PRO:HG3  | 20:V:198:GLN:HE22 | 1.79                     | 0.47              |
| 21:W:430:GLN:HA   | 21:W:430:GLN:OE1  | 2.14                     | 0.47              |
| 23:Y:18:ARG:NH1   | 23:Y:22:LEU:HD21  | 2.12                     | 0.47              |
| 23:Y:275:LEU:HD21 | 23:Y:296:VAL:CG1  | 2.36                     | 0.47              |
| 23:Y:307:LEU:HD23 | 23:Y:308:LEU:HD22 | 1.96                     | 0.47              |
| 24:Z:22:HIS:NE2   | 24:Z:55:ALA:HB1   | 2.29                     | 0.47              |
| 24:Z:126:VAL:C    | 24:Z:128:PRO:HD3  | 2.39                     | 0.47              |
| 25:a:141:MET:O    | 25:a:144:ASN:HB2  | 2.14                     | 0.47              |
| 25:a:226:ARG:NH1  | 25:a:230:ARG:HG2  | 2.28                     | 0.47              |
| 27:c:244:VAL:HG11 | 27:c:291:LEU:HG   | 1.95                     | 0.47              |
| 28:d:21:GLU:HG3   | 28:d:22:GLU:N     | 2.28                     | 0.47              |
| 30:f:25:ASP:OD1   | 30:f:25:ASP:N     | 2.47                     | 0.47              |
| 30:f:182:GLU:N    | 30:f:183:PRO:HD2  | 2.29                     | 0.47              |
| 30:f:404:ASP:N    | 30:f:404:ASP:OD1  | 2.46                     | 0.47              |
| 30:f:631:LYS:HA   | 30:f:634:LYS:CD   | 2.44                     | 0.47              |
| 30:f:872:VAL:O    | 30:f:874:LEU:HG   | 2.14                     | 0.47              |
| 31:F:86:LEU:HD13  | 31:F:86:LEU:O     | 2.14                     | 0.47              |
| 31:F:204:LEU:HD23 | 31:F:205:PRO:N    | 2.29                     | 0.47              |
| 32:U:213:PHE:C    | 32:U:216:VAL:HG12 | 2.39                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 32:U:450:HIS:HD1  | 32:U:457:ILE:CG1  | 2.23                     | 0.47              |
| 32:U:732:LEU:O    | 32:U:732:LEU:HD23 | 2.14                     | 0.47              |
| 32:U:874:ASN:N    | 32:U:874:ASN:OD1  | 2.46                     | 0.47              |
| 1:A:88:GLN:O      | 1:A:92:PRO:HG2    | 2.14                     | 0.47              |
| 3:C:219:LEU:HD22  | 4:D:289:LEU:CD2   | 2.43                     | 0.47              |
| 3:C:349:GLU:HA    | 3:C:349:GLU:OE2   | 2.12                     | 0.47              |
| 3:C:362:VAL:HG13  | 3:C:386:ALA:HB3   | 1.96                     | 0.47              |
| 5:E:104:THR:HG23  | 5:E:104:THR:O     | 2.13                     | 0.47              |
| 5:E:118:LEU:HB2   | 5:E:214:LEU:HD21  | 1.96                     | 0.47              |
| 5:E:146:ARG:HG2   | 5:E:146:ARG:NH1   | 2.28                     | 0.47              |
| 5:E:322:LYS:HB3   | 5:E:326:ILE:HD13  | 1.95                     | 0.47              |
| 20:V:122:THR:HG21 | 20:V:155:ALA:HB1  | 1.96                     | 0.47              |
| 20:V:358:MET:N    | 20:V:359:PRO:HD2  | 2.29                     | 0.47              |
| 21:W:51:GLU:O     | 21:W:54:THR:OG1   | 2.20                     | 0.47              |
| 21:W:102:ALA:O    | 21:W:105:VAL:HG22 | 2.15                     | 0.47              |
| 21:W:166:LEU:HD21 | 21:W:201:ARG:NH2  | 2.29                     | 0.47              |
| 21:W:307:LYS:HB2  | 21:W:307:LYS:HZ3  | 1.79                     | 0.47              |
| 23:Y:50:MET:HE3   | 23:Y:51:ALA:H     | 1.79                     | 0.47              |
| 25:a:156:TYR:O    | 25:a:160:SER:N    | 2.47                     | 0.47              |
| 28:d:241:GLU:C    | 28:d:241:GLU:OE1  | 2.57                     | 0.47              |
| 30:f:437:GLU:O    | 30:f:440:ILE:HG12 | 2.13                     | 0.47              |
| 31:F:215:LEU:O    | 31:F:215:LEU:HD23 | 2.14                     | 0.47              |
| 31:F:226:TYR:HE1  | 31:F:353:GLU:CD   | 2.22                     | 0.47              |
| 32:U:244:MET:HA   | 32:U:903:PHE:CE2  | 2.49                     | 0.47              |
| 32:U:554:LEU:HD11 | 32:U:761:VAL:CG2  | 2.34                     | 0.47              |
| 32:U:602:LEU:HD21 | 32:U:618:ALA:O    | 2.14                     | 0.47              |
| 2:B:369:THR:HG22  | 2:B:372:MET:CE    | 2.44                     | 0.47              |
| 3:C:127:LEU:HD13  | 4:D:102:ILE:HD11  | 1.97                     | 0.47              |
| 4:D:304:ASN:OD1   | 4:D:304:ASN:N     | 2.39                     | 0.47              |
| 5:E:261:LEU:HD12  | 5:E:294:ARG:NE    | 2.28                     | 0.47              |
| 20:V:90:GLU:OE1   | 20:V:92:ARG:HB2   | 2.14                     | 0.47              |
| 20:V:251:LEU:O    | 20:V:255:LEU:HB2  | 2.13                     | 0.47              |
| 20:V:334:VAL:HG22 | 20:V:395:ILE:HD11 | 1.96                     | 0.47              |
| 20:V:437:ILE:HA   | 28:d:146:GLY:HA3  | 1.96                     | 0.47              |
| 21:W:259:GLU:OE1  | 21:W:260:SER:N    | 2.46                     | 0.47              |
| 21:W:279:PHE:CD1  | 21:W:280:ASP:N    | 2.82                     | 0.47              |
| 21:W:280:ASP:OD2  | 21:W:282:GLU:HB3  | 2.14                     | 0.47              |
| 21:W:394:SER:HA   | 21:W:397:VAL:CG1  | 2.44                     | 0.47              |
| 24:Z:214:LYS:HE2  | 24:Z:214:LYS:HB3  | 1.68                     | 0.47              |
| 25:a:227:ASN:O    | 25:a:231:GLN:NE2  | 2.47                     | 0.47              |
| 25:a:244:ASN:O    | 25:a:272:ILE:HD11 | 2.14                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 26:b:110:ILE:HG22 | 26:b:139:ASP:CB   | 2.42                     | 0.47              |
| 26:b:140:ILE:HG22 | 26:b:170:LEU:CD1  | 2.44                     | 0.47              |
| 26:b:147:GLU:OE1  | 26:b:147:GLU:N    | 2.47                     | 0.47              |
| 29:e:60:LEU:HD22  | 29:e:60:LEU:N     | 2.29                     | 0.47              |
| 30:f:125:ILE:HG23 | 30:f:131:MET:HE1  | 1.94                     | 0.47              |
| 30:f:527:VAL:HG22 | 30:f:527:VAL:O    | 2.15                     | 0.47              |
| 11:l:35:THR:CG2   | 11:l:133:LEU:HD12 | 2.44                     | 0.47              |
| 32:U:672:LEU:HA   | 32:U:675:MET:HG2  | 1.95                     | 0.47              |
| 32:U:697:GLN:NE2  | 32:U:745:THR:OG1  | 2.48                     | 0.47              |
| 1:A:108:ASP:HB3   | 1:A:109:PRO:HD3   | 1.94                     | 0.47              |
| 2:B:357:ASP:OD1   | 2:B:357:ASP:C     | 2.56                     | 0.47              |
| 5:E:50:LEU:CD1    | 31:F:82:VAL:HG21  | 2.44                     | 0.47              |
| 5:E:258:MET:HE3   | 5:E:258:MET:HB3   | 1.71                     | 0.47              |
| 10:K:146:VAL:HG11 | 10:K:222:PRO:HA   | 1.95                     | 0.47              |
| 21:W:169:LEU:HD13 | 21:W:172:GLU:OE1  | 2.14                     | 0.47              |
| 23:Y:301:ILE:HD11 | 23:Y:337:PHE:CD1  | 2.49                     | 0.47              |
| 23:Y:304:TYR:OH   | 23:Y:333:GLU:OE1  | 2.19                     | 0.47              |
| 24:Z:43:TRP:HB3   | 24:Z:48:LEU:CD1   | 2.44                     | 0.47              |
| 27:c:26:ASP:HB2   | 27:c:65:TYR:CE1   | 2.50                     | 0.47              |
| 28:d:168:ASP:OD1  | 28:d:169:ILE:HG13 | 2.15                     | 0.47              |
| 28:d:196:ARG:HD2  | 28:d:196:ARG:O    | 2.14                     | 0.47              |
| 28:d:255:MET:HE1  | 28:d:257:VAL:HG12 | 1.97                     | 0.47              |
| 30:f:33:ARG:CZ    | 30:f:33:ARG:HA    | 2.45                     | 0.47              |
| 30:f:602:GLY:HA2  | 30:f:639:LYS:HB3  | 1.96                     | 0.47              |
| 32:U:131:GLU:OE1  | 32:U:131:GLU:O    | 2.33                     | 0.47              |
| 32:U:184:CYS:SG   | 32:U:185:MET:N    | 2.88                     | 0.47              |
| 32:U:364:VAL:HG21 | 32:U:773:PHE:HE2  | 1.79                     | 0.47              |
| 32:U:471:ASP:HA   | 32:U:474:ARG:HD3  | 1.95                     | 0.47              |
| 32:U:471:ASP:OD1  | 32:U:471:ASP:O    | 2.31                     | 0.47              |
| 32:U:673:GLU:O    | 32:U:676:THR:HG22 | 2.14                     | 0.47              |
| 32:U:772:TRP:NE1  | 32:U:774:PRO:HG2  | 2.29                     | 0.47              |
| 1:A:180:CYS:HB3   | 1:A:183:GLN:HB2   | 1.96                     | 0.47              |
| 2:B:212:GLU:CB    | 30:f:845:ARG:HG3  | 2.43                     | 0.47              |
| 2:B:309:MET:O     | 2:B:313:LEU:HG    | 2.15                     | 0.47              |
| 4:D:342:ARG:HD3   | 4:D:361:GLU:OE2   | 2.14                     | 0.47              |
| 5:E:363:VAL:HG23  | 5:E:365:GLU:H     | 1.79                     | 0.47              |
| 20:V:130:PHE:C    | 20:V:133:PRO:HD2  | 2.39                     | 0.47              |
| 21:W:55:ARG:NH2   | 21:W:93:ARG:HE    | 2.11                     | 0.47              |
| 22:X:350:ILE:CG2  | 22:X:361:VAL:HG21 | 2.45                     | 0.47              |
| 23:Y:330:ILE:O    | 23:Y:334:LEU:HB2  | 2.15                     | 0.47              |
| 24:Z:22:HIS:CE1   | 24:Z:35:VAL:CG1   | 2.98                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 24:Z:146:ASP:OD2  | 25:a:178:ARG:HA   | 2.14                     | 0.47              |
| 24:Z:181:ASP:OD1  | 24:Z:181:ASP:N    | 2.46                     | 0.47              |
| 25:a:45:VAL:HG23  | 25:a:46:GLN:OE1   | 2.14                     | 0.47              |
| 25:a:86:GLN:O     | 25:a:86:GLN:HG3   | 2.13                     | 0.47              |
| 26:b:48:ASN:ND2   | 26:b:64:LEU:CB    | 2.77                     | 0.47              |
| 26:b:71:ILE:O     | 26:b:75:LEU:HD23  | 2.14                     | 0.47              |
| 26:b:147:GLU:OE2  | 26:b:152:LYS:NZ   | 2.42                     | 0.47              |
| 26:b:186:SER:OG   | 26:b:187:PRO:HD3  | 2.13                     | 0.47              |
| 27:c:27:THR:O     | 27:c:27:THR:OG1   | 2.26                     | 0.47              |
| 28:d:101:LEU:HD23 | 28:d:166:PHE:CE2  | 2.49                     | 0.47              |
| 28:d:122:LEU:HD22 | 28:d:122:LEU:H    | 1.79                     | 0.47              |
| 30:f:828:ARG:NH2  | 30:f:861:THR:HG21 | 2.29                     | 0.47              |
| 30:f:828:ARG:HH12 | 30:f:831:VAL:HG13 | 1.78                     | 0.47              |
| 31:F:318:ASP:C    | 31:F:318:ASP:OD1  | 2.57                     | 0.47              |
| 31:F:431:LYS:HE3  | 31:F:431:LYS:HB3  | 1.79                     | 0.47              |
| 32:U:65:SER:OG    | 32:U:81:ALA:N     | 2.48                     | 0.47              |
| 32:U:84:ALA:CB    | 32:U:88:PHE:HD2   | 2.28                     | 0.47              |
| 32:U:236:LEU:N    | 32:U:236:LEU:HD23 | 2.30                     | 0.47              |
| 32:U:356:THR:HG22 | 32:U:717:ILE:HD12 | 1.96                     | 0.47              |
| 1:A:360:ARG:HG2   | 30:f:851:ASP:OD2  | 2.14                     | 0.47              |
| 2:B:295:TYR:CE2   | 3:C:271:ARG:HD3   | 2.49                     | 0.47              |
| 2:B:303:ARG:HB2   | 2:B:303:ARG:CZ    | 2.43                     | 0.47              |
| 3:C:89:VAL:HG22   | 3:C:93:GLY:O      | 2.14                     | 0.47              |
| 3:C:273:MET:CE    | 3:C:293:MET:SD    | 2.99                     | 0.47              |
| 4:D:171:ASP:OD1   | 4:D:171:ASP:N     | 2.48                     | 0.47              |
| 20:V:175:MET:HE3  | 20:V:175:MET:HB3  | 1.74                     | 0.47              |
| 21:W:75:TYR:HH    | 21:W:114:GLU:CD   | 2.18                     | 0.47              |
| 21:W:142:ARG:HG2  | 21:W:177:MET:HG3  | 1.96                     | 0.47              |
| 22:X:111:LEU:HD23 | 22:X:111:LEU:HA   | 1.78                     | 0.47              |
| 23:Y:241:ILE:CG2  | 23:Y:261:PHE:HE1  | 2.28                     | 0.47              |
| 24:Z:11:VAL:HG21  | 24:Z:135:THR:CG2  | 2.41                     | 0.47              |
| 24:Z:259:VAL:CG1  | 27:c:291:LEU:HD22 | 2.45                     | 0.47              |
| 25:a:115:LYS:HA   | 25:a:118:ILE:HG12 | 1.96                     | 0.47              |
| 26:b:63:THR:OG1   | 26:b:64:LEU:N     | 2.47                     | 0.47              |
| 26:b:187:PRO:CG   | 26:b:188:ILE:HD12 | 2.40                     | 0.47              |
| 27:c:266:THR:OG1  | 27:c:268:GLU:OE2  | 2.32                     | 0.47              |
| 27:c:266:THR:O    | 27:c:269:GLN:HB3  | 2.15                     | 0.47              |
| 28:d:130:ASN:OD1  | 28:d:132:TYR:HB2  | 2.15                     | 0.47              |
| 28:d:256:ILE:O    | 28:d:256:ILE:CD1  | 2.58                     | 0.47              |
| 14:o:10:LYS:NZ    | 14:o:10:LYS:HB3   | 2.29                     | 0.47              |
| 31:F:384:LEU:HD11 | 31:F:420:TYR:CG   | 2.49                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 32:U:904:LYS:CE   | 32:U:908:ILE:HD12 | 2.44                     | 0.47              |
| 1:A:70:THR:OG1    | 1:A:71:GLY:N      | 2.47                     | 0.47              |
| 1:A:73:ALA:HB2    | 2:B:140:ASP:HA    | 1.95                     | 0.47              |
| 1:A:174:TYR:H     | 1:A:232:ARG:HH22  | 1.62                     | 0.47              |
| 1:A:286:ASP:CB    | 31:F:337:ILE:HG22 | 2.45                     | 0.47              |
| 2:B:53:THR:HB     | 30:f:834:ASP:OD1  | 2.14                     | 0.47              |
| 2:B:74:MET:HE2    | 2:B:74:MET:O      | 2.14                     | 0.47              |
| 2:B:223:ILE:HG12  | 2:B:334:ILE:HD11  | 1.97                     | 0.47              |
| 2:B:423:LYS:HD2   | 2:B:423:LYS:C     | 2.40                     | 0.47              |
| 3:C:63:LEU:HD21   | 4:D:81:ARG:HD2    | 1.97                     | 0.47              |
| 3:C:142:LYS:NZ    | 4:D:325:GLY:HA3   | 2.30                     | 0.47              |
| 3:C:222:LYS:NZ    | 4:D:286:GLN:OE1   | 2.32                     | 0.47              |
| 3:C:248:MET:CE    | 3:C:273:MET:HE2   | 2.44                     | 0.47              |
| 3:C:277:LEU:CD1   | 3:C:310:ARG:HG3   | 2.41                     | 0.47              |
| 3:C:336:MET:CE    | 3:C:367:GLY:HA3   | 2.36                     | 0.47              |
| 4:D:403:TYR:CD2   | 4:D:407:ILE:HG12  | 2.50                     | 0.47              |
| 5:E:304:PRO:HD3   | 5:E:339:ASN:O     | 2.15                     | 0.47              |
| 5:E:305:ASN:C     | 5:E:305:ASN:OD1   | 2.56                     | 0.47              |
| 5:E:372:ARG:H     | 5:E:372:ARG:HD2   | 1.80                     | 0.47              |
| 5:E:376:ASP:C     | 5:E:376:ASP:OD1   | 2.58                     | 0.47              |
| 9:J:172:LEU:HD23  | 9:J:190:LEU:HD21  | 1.97                     | 0.47              |
| 11:L:72:ILE:HD11  | 11:L:85:CYS:SG    | 2.55                     | 0.47              |
| 12:M:236:GLU:O    | 12:M:240:LYS:HG2  | 2.15                     | 0.47              |
| 20:V:195:ILE:HD12 | 20:V:196:SER:H    | 1.79                     | 0.47              |
| 20:V:222:ASP:N    | 20:V:222:ASP:OD1  | 2.47                     | 0.47              |
| 20:V:333:ILE:HD11 | 20:V:360:TYR:CB   | 2.29                     | 0.47              |
| 20:V:364:THR:HG21 | 29:e:43:TRP:CH2   | 2.50                     | 0.47              |
| 20:V:407:VAL:HG12 | 20:V:447:ILE:HD13 | 1.96                     | 0.47              |
| 21:W:87:ILE:HD11  | 21:W:104:MET:HE3  | 1.97                     | 0.47              |
| 21:W:244:CYS:SG   | 21:W:273:TYR:HD1  | 2.38                     | 0.47              |
| 21:W:265:GLN:HG2  | 21:W:336:PRO:CD   | 2.45                     | 0.47              |
| 21:W:360:GLU:O    | 21:W:363:ILE:HG22 | 2.15                     | 0.47              |
| 23:Y:51:ALA:HB3   | 23:Y:52:PRO:HD3   | 1.96                     | 0.47              |
| 23:Y:202:LEU:HD13 | 23:Y:239:LYS:NZ   | 2.29                     | 0.47              |
| 23:Y:241:ILE:HD13 | 23:Y:264:TYR:CD2  | 2.50                     | 0.47              |
| 23:Y:300:ARG:HE   | 23:Y:333:GLU:CD   | 2.22                     | 0.47              |
| 24:Z:29:VAL:HB    | 24:Z:33:LYS:NZ    | 2.29                     | 0.47              |
| 25:a:33:LEU:HD11  | 25:a:36:GLN:CB    | 2.44                     | 0.47              |
| 25:a:76:LEU:O     | 25:a:80:ILE:HD13  | 2.14                     | 0.47              |
| 25:a:136:GLU:OE1  | 25:a:136:GLU:CA   | 2.62                     | 0.47              |
| 25:a:144:ASN:O    | 25:a:145:LEU:HG   | 2.15                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 25:a:196:ARG:HA   | 25:a:199:THR:HG22 | 1.96                     | 0.47              |
| 25:a:278:MET:HE3  | 25:a:278:MET:HB2  | 1.77                     | 0.47              |
| 25:a:361:LYS:O    | 25:a:361:LYS:HD3  | 2.15                     | 0.47              |
| 26:b:141:ILE:O    | 26:b:141:ILE:HG13 | 2.12                     | 0.47              |
| 27:c:167:MET:HA   | 27:c:167:MET:HE3  | 1.96                     | 0.47              |
| 28:d:13:SER:OG    | 28:d:16:LEU:HD12  | 2.15                     | 0.47              |
| 28:d:33:LEU:HD22  | 28:d:34:ASN:N     | 2.28                     | 0.47              |
| 28:d:97:GLN:NE2   | 28:d:160:ALA:HB1  | 2.30                     | 0.47              |
| 30:f:209:MET:SD   | 30:f:213:GLN:NE2  | 2.88                     | 0.47              |
| 30:f:445:LEU:O    | 30:f:445:LEU:HD23 | 2.15                     | 0.47              |
| 30:f:465:LEU:O    | 30:f:469:TYR:HE2  | 1.98                     | 0.47              |
| 30:f:648:ALA:O    | 30:f:652:VAL:HG22 | 2.15                     | 0.47              |
| 30:f:746:ARG:HD3  | 30:f:746:ARG:N    | 2.28                     | 0.47              |
| 30:f:830:LEU:HD11 | 30:f:860:LYS:O    | 2.14                     | 0.47              |
| 12:m:53:VAL:O     | 12:m:53:VAL:HG23  | 2.15                     | 0.47              |
| 14:o:25:MET:HE2   | 18:s:188:TYR:OH   | 2.14                     | 0.47              |
| 17:r:10:ARG:HH11  | 17:r:10:ARG:HG3   | 1.80                     | 0.47              |
| 31:F:191:LEU:O    | 31:F:195:ILE:HG13 | 2.15                     | 0.47              |
| 32:U:96:TYR:O     | 32:U:99:THR:HG22  | 2.15                     | 0.47              |
| 32:U:418:GLU:HG2  | 32:U:421:GLN:HE22 | 1.79                     | 0.47              |
| 32:U:644:TYR:H    | 32:U:644:TYR:HD2  | 1.61                     | 0.47              |
| 32:U:801:GLN:NE2  | 32:U:877:LEU:HD23 | 2.29                     | 0.47              |
| 1:A:292:ASP:OD1   | 1:A:292:ASP:C     | 2.57                     | 0.47              |
| 1:A:305:GLN:O     | 1:A:312:ARG:HG3   | 2.14                     | 0.47              |
| 2:B:204:PRO:HG3   | 2:B:211:TYR:CE2   | 2.50                     | 0.47              |
| 2:B:220:LYS:NZ    | 2:B:345:GLY:O     | 2.48                     | 0.47              |
| 3:C:85:VAL:HG11   | 3:C:108:VAL:HG11  | 1.96                     | 0.47              |
| 3:C:128:PRO:HD3   | 4:D:96:VAL:CG2    | 2.42                     | 0.47              |
| 3:C:351:MET:CB    | 3:C:391:MET:HE3   | 2.44                     | 0.47              |
| 4:D:118:THR:HG22  | 4:D:118:THR:O     | 2.15                     | 0.47              |
| 4:D:214:MET:HE3   | 4:D:214:MET:HB2   | 1.88                     | 0.47              |
| 9:J:35:VAL:HG13   | 9:J:191:VAL:HG22  | 1.96                     | 0.47              |
| 15:P:167:SER:CB   | 15:P:199:LEU:HD11 | 2.44                     | 0.47              |
| 20:V:192:MET:O    | 20:V:195:ILE:HD12 | 2.14                     | 0.47              |
| 20:V:203:LEU:HD22 | 20:V:206:VAL:CG2  | 2.44                     | 0.47              |
| 23:Y:15:PRO:HD2   | 23:Y:146:ARG:HD2  | 1.96                     | 0.47              |
| 24:Z:105:ASP:OD1  | 24:Z:108:ILE:HD12 | 2.14                     | 0.47              |
| 24:Z:190:ARG:NH1  | 27:c:297:VAL:HA   | 2.25                     | 0.47              |
| 24:Z:279:LYS:O    | 24:Z:282:ASN:OD1  | 2.33                     | 0.47              |
| 26:b:51:LEU:CD1   | 26:b:61:LEU:HD12  | 2.45                     | 0.47              |
| 26:b:79:GLN:CD    | 26:b:79:GLN:N     | 2.73                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 26:b:97:LEU:O     | 26:b:100:ARG:HB3  | 2.14                     | 0.47              |
| 28:d:13:SER:HB3   | 28:d:16:LEU:CG    | 2.44                     | 0.47              |
| 28:d:66:LYS:HB2   | 28:d:66:LYS:HE2   | 1.70                     | 0.47              |
| 28:d:251:ARG:O    | 28:d:255:MET:HG3  | 2.15                     | 0.47              |
| 6:g:188:ASP:OD1   | 6:g:188:ASP:N     | 2.47                     | 0.47              |
| 16:q:108:ASP:OD1  | 16:q:109:GLU:N    | 2.47                     | 0.47              |
| 31:F:222:GLY:HA2  | 31:F:328:VAL:O    | 2.15                     | 0.47              |
| 32:U:353:LEU:CD1  | 32:U:373:ASN:HB2  | 2.45                     | 0.47              |
| 32:U:793:LYS:HG3  | 32:U:794:ASP:N    | 2.29                     | 0.47              |
| 1:A:263:MET:HG2   | 1:A:267:LYS:CE    | 2.45                     | 0.47              |
| 1:A:303:ILE:HG13  | 1:A:336:ARG:HD3   | 1.97                     | 0.47              |
| 1:A:358:HIS:CE1   | 1:A:386:ARG:HG3   | 2.50                     | 0.47              |
| 2:B:114:GLU:OE1   | 2:B:122:ILE:HD13  | 2.14                     | 0.47              |
| 2:B:184:TYR:O     | 2:B:187:ILE:HG22  | 2.14                     | 0.47              |
| 2:B:375:ALA:O     | 2:B:376:ASP:OD1   | 2.33                     | 0.47              |
| 3:C:48:GLN:OE1    | 20:V:495:ARG:HD3  | 2.15                     | 0.47              |
| 5:E:257:LEU:O     | 5:E:261:LEU:HB2   | 2.15                     | 0.47              |
| 21:W:271:VAL:O    | 21:W:275:ILE:HD12 | 2.15                     | 0.47              |
| 23:Y:57:LEU:HD12  | 23:Y:58:CYS:N     | 2.30                     | 0.47              |
| 24:Z:190:ARG:NH2  | 27:c:297:VAL:HA   | 2.28                     | 0.47              |
| 27:c:104:ARG:HD3  | 27:c:104:ARG:N    | 2.29                     | 0.47              |
| 28:d:107:LEU:HD21 | 28:d:140:GLU:HA   | 1.96                     | 0.47              |
| 28:d:229:GLN:O    | 28:d:232:PRO:HD2  | 2.14                     | 0.47              |
| 30:f:882:LEU:HD12 | 30:f:882:LEU:O    | 2.15                     | 0.47              |
| 19:t:27:LEU:HD21  | 19:t:34:ALA:HB1   | 1.97                     | 0.47              |
| 31:F:153:VAL:HG12 | 31:F:159:LEU:H    | 1.80                     | 0.47              |
| 31:F:406:ILE:HG12 | 31:F:409:ARG:NH2  | 2.30                     | 0.47              |
| 32:U:387:ARG:HA   | 32:U:387:ARG:NE   | 2.30                     | 0.47              |
| 32:U:637:VAL:CG1  | 32:U:652:ALA:HB1  | 2.45                     | 0.47              |
| 32:U:789:ILE:HG13 | 32:U:911:ILE:CD1  | 2.45                     | 0.47              |
| 3:C:125:LYS:HB3   | 3:C:125:LYS:HE3   | 1.54                     | 0.47              |
| 4:D:228:ILE:HD11  | 4:D:253:LEU:HD23  | 1.97                     | 0.47              |
| 4:D:332:GLU:OE1   | 4:D:333:PHE:N     | 2.47                     | 0.47              |
| 5:E:84:ARG:HG2    | 5:E:86:GLN:OE1    | 2.15                     | 0.47              |
| 5:E:331:ILE:HD11  | 5:E:367:PHE:HB3   | 1.96                     | 0.47              |
| 6:G:112:ASP:OD2   | 14:O:73:ARG:NH2   | 2.48                     | 0.47              |
| 20:V:90:GLU:OE1   | 20:V:92:ARG:N     | 2.41                     | 0.47              |
| 20:V:209:LYS:HA   | 20:V:209:LYS:HD3  | 1.61                     | 0.47              |
| 21:W:89:LEU:HD23  | 21:W:93:ARG:HD2   | 1.97                     | 0.47              |
| 21:W:209:ILE:HG23 | 21:W:227:TYR:OH   | 2.15                     | 0.47              |
| 21:W:373:ILE:HD11 | 21:W:377:ARG:CG   | 2.33                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:X:338:VAL:HG13 | 22:X:339:ILE:CD1  | 2.43                     | 0.47              |
| 23:Y:114:ILE:HG22 | 23:Y:115:GLY:N    | 2.30                     | 0.47              |
| 24:Z:23:PHE:HB2   | 24:Z:126:VAL:HG21 | 1.96                     | 0.47              |
| 25:a:97:LEU:HD11  | 25:a:117:ALA:HB1  | 1.96                     | 0.47              |
| 26:b:119:ASP:OD1  | 26:b:152:LYS:HD2  | 2.14                     | 0.47              |
| 27:c:114:SER:OG   | 27:c:147:PRO:HD3  | 2.15                     | 0.47              |
| 30:f:138:GLU:CA   | 30:f:141:LYS:HE3  | 2.28                     | 0.47              |
| 30:f:828:ARG:HD2  | 30:f:829:MET:O    | 2.15                     | 0.47              |
| 31:F:291:ILE:HD12 | 31:F:306:VAL:HG12 | 1.96                     | 0.47              |
| 32:U:167:ILE:HD12 | 32:U:204:ILE:CG2  | 2.40                     | 0.47              |
| 32:U:369:THR:CG2  | 32:U:392:TRP:HZ2  | 2.27                     | 0.47              |
| 32:U:423:MET:HE2  | 32:U:423:MET:CA   | 2.45                     | 0.47              |
| 32:U:739:ALA:O    | 32:U:744:VAL:HG12 | 2.14                     | 0.47              |
| 1:A:254:ALA:HA    | 1:A:257:VAL:HG12  | 1.96                     | 0.46              |
| 3:C:391:MET:O     | 3:C:395:SER:OG    | 2.23                     | 0.46              |
| 5:E:245:GLU:OE1   | 31:F:301:ALA:HB2  | 2.14                     | 0.46              |
| 5:E:283:ASP:OD1   | 5:E:283:ASP:N     | 2.46                     | 0.46              |
| 5:E:383:LYS:O     | 5:E:384:LEU:HD22  | 2.15                     | 0.46              |
| 6:G:84:THR:OG1    | 12:M:156:VAL:HG22 | 2.15                     | 0.46              |
| 13:N:128:ILE:HD11 | 13:N:137:TYR:CD1  | 2.50                     | 0.46              |
| 20:V:208:ALA:HA   | 20:V:211:TYR:HD2  | 1.79                     | 0.46              |
| 20:V:300:LEU:HA   | 20:V:302:TYR:CE1  | 2.50                     | 0.46              |
| 20:V:333:ILE:CD1  | 20:V:360:TYR:HB3  | 2.28                     | 0.46              |
| 20:V:360:TYR:OH   | 20:V:391:THR:HG21 | 2.15                     | 0.46              |
| 21:W:112:VAL:HG21 | 21:W:124:LEU:HD23 | 1.97                     | 0.46              |
| 22:X:377:ILE:CG2  | 23:Y:358:ARG:HH12 | 2.28                     | 0.46              |
| 22:X:379:ASP:OD2  | 22:X:381:GLY:N    | 2.47                     | 0.46              |
| 22:X:406:ASN:ND2  | 27:c:253:LYS:HB2  | 2.29                     | 0.46              |
| 27:c:307:VAL:HG23 | 28:d:239:SER:OG   | 2.14                     | 0.46              |
| 28:d:11:ARG:HE    | 28:d:12:LYS:H     | 1.61                     | 0.46              |
| 30:f:480:GLY:HA2  | 30:f:483:PHE:CE1  | 2.50                     | 0.46              |
| 30:f:828:ARG:HB2  | 30:f:829:MET:HE1  | 1.97                     | 0.46              |
| 31:F:214:ASN:OD1  | 31:F:214:ASN:C    | 2.58                     | 0.46              |
| 32:U:244:MET:O    | 32:U:248:ILE:HG23 | 2.14                     | 0.46              |
| 32:U:250:PHE:HB3  | 32:U:911:ILE:HG21 | 1.97                     | 0.46              |
| 32:U:800:VAL:O    | 32:U:880:ASN:N    | 2.48                     | 0.46              |
| 1:A:83:ASP:HA     | 1:A:86:THR:HG23   | 1.97                     | 0.46              |
| 1:A:124:ASP:OD1   | 1:A:124:ASP:N     | 2.47                     | 0.46              |
| 1:A:307:ASP:C     | 1:A:307:ASP:OD1   | 2.58                     | 0.46              |
| 1:A:334:PRO:HB3   | 31:F:398:ALA:HB2  | 1.96                     | 0.46              |
| 2:B:160:ILE:HD12  | 2:B:160:ILE:N     | 2.30                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:C:205:HIS:O     | 3:C:205:HIS:ND1   | 2.40                     | 0.46              |
| 7:H:47:THR:HG21   | 7:H:74:VAL:HG21   | 1.97                     | 0.46              |
| 16:Q:172:ILE:O    | 16:q:174:ASN:N    | 2.45                     | 0.46              |
| 36:R:301:LDZ:H21  | 36:R:301:LDZ:C22  | 2.45                     | 0.46              |
| 20:V:203:LEU:HD22 | 20:V:203:LEU:O    | 2.15                     | 0.46              |
| 20:V:251:LEU:HD23 | 20:V:276:PHE:HD1  | 1.81                     | 0.46              |
| 21:W:41:GLN:O     | 21:W:45:GLU:OE1   | 2.32                     | 0.46              |
| 21:W:51:GLU:H     | 21:W:51:GLU:HG2   | 1.59                     | 0.46              |
| 21:W:105:VAL:HG21 | 21:W:140:ILE:CD1  | 2.28                     | 0.46              |
| 21:W:419:LYS:HZ1  | 21:W:423:ASN:HB3  | 1.79                     | 0.46              |
| 22:X:338:VAL:C    | 22:X:341:PRO:HD2  | 2.40                     | 0.46              |
| 22:X:360:ASP:N    | 22:X:360:ASP:OD1  | 2.44                     | 0.46              |
| 23:Y:371:LYS:HD3  | 23:Y:371:LYS:C    | 2.40                     | 0.46              |
| 24:Z:93:GLY:HA2   | 24:Z:119:SER:HB2  | 1.96                     | 0.46              |
| 27:c:61:PHE:CE1   | 27:c:139:ARG:HB2  | 2.50                     | 0.46              |
| 30:f:420:TRP:N    | 30:f:451:VAL:HG23 | 2.29                     | 0.46              |
| 30:f:477:MET:HE1  | 30:f:478:ARG:HB3  | 1.96                     | 0.46              |
| 9:j:26:VAL:HG23   | 9:j:74:ALA:O      | 2.15                     | 0.46              |
| 36:n:301:LDZ:H42  | 14:o:119:SER:OG   | 2.15                     | 0.46              |
| 14:o:100:VAL:HG13 | 14:o:126:VAL:HG21 | 1.97                     | 0.46              |
| 32:U:107:HIS:ND1  | 32:U:110:LYS:HE3  | 2.30                     | 0.46              |
| 32:U:247:GLN:HE22 | 32:U:904:LYS:CD   | 2.28                     | 0.46              |
| 32:U:247:GLN:HE21 | 32:U:904:LYS:HB2  | 1.79                     | 0.46              |
| 1:A:114:ASN:C     | 1:A:114:ASN:OD1   | 2.58                     | 0.46              |
| 1:A:286:ASP:HB2   | 31:F:337:ILE:HG22 | 1.96                     | 0.46              |
| 3:C:121:TYR:HD1   | 3:C:121:TYR:H     | 1.63                     | 0.46              |
| 3:C:128:PRO:CD    | 4:D:96:VAL:HG23   | 2.43                     | 0.46              |
| 4:D:109:SER:HB2   | 4:D:111:TYR:CE1   | 2.48                     | 0.46              |
| 17:R:18:ASP:OD1   | 17:R:34:LYS:NZ    | 2.48                     | 0.46              |
| 20:V:268:GLU:HG2  | 20:V:299:GLN:OE1  | 2.15                     | 0.46              |
| 22:X:236:PHE:HE1  | 22:X:251:LEU:CD1  | 2.29                     | 0.46              |
| 23:Y:199:GLU:C    | 23:Y:199:GLU:OE1  | 2.59                     | 0.46              |
| 23:Y:204:THR:HA   | 23:Y:207:THR:HG23 | 1.97                     | 0.46              |
| 23:Y:307:LEU:HD23 | 23:Y:307:LEU:C    | 2.40                     | 0.46              |
| 23:Y:383:LEU:O    | 23:Y:383:LEU:HD23 | 2.15                     | 0.46              |
| 25:a:25:LEU:CD2   | 25:a:37:LEU:HD11  | 2.44                     | 0.46              |
| 25:a:270:ARG:HD3  | 25:a:270:ARG:HA   | 1.73                     | 0.46              |
| 26:b:3:LEU:O      | 26:b:105:HIS:HA   | 2.15                     | 0.46              |
| 26:b:33:VAL:HA    | 26:b:36:VAL:HG12  | 1.97                     | 0.46              |
| 27:c:246:LYS:NZ   | 27:c:246:LYS:HB2  | 2.29                     | 0.46              |
| 28:d:52:ARG:HH22  | 28:d:89:LEU:CD2   | 2.28                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 30:f:62:ARG:HA    | 30:f:65:GLU:OE1   | 2.15                     | 0.46              |
| 30:f:603:SER:H    | 30:f:639:LYS:HD3  | 1.80                     | 0.46              |
| 9:j:134:VAL:HG12  | 9:j:144:LEU:HD13  | 1.96                     | 0.46              |
| 10:k:197:SER:O    | 10:k:201:ILE:HG13 | 2.15                     | 0.46              |
| 32:U:50:GLU:OE1   | 32:U:50:GLU:CA    | 2.62                     | 0.46              |
| 32:U:247:GLN:CA   | 32:U:913:ILE:HD13 | 2.46                     | 0.46              |
| 32:U:645:ASN:OD1  | 32:U:647:HIS:N    | 2.46                     | 0.46              |
| 1:A:73:ALA:HB3    | 1:A:78:TRP:HE1    | 1.80                     | 0.46              |
| 2:B:63:LEU:HB3    | 30:f:226:TYR:CG   | 2.51                     | 0.46              |
| 2:B:212:GLU:HA    | 30:f:845:ARG:CG   | 2.33                     | 0.46              |
| 2:B:239:VAL:O     | 2:B:243:THR:HB    | 2.16                     | 0.46              |
| 3:C:218:GLU:HA    | 3:C:221:GLN:HB2   | 1.96                     | 0.46              |
| 4:D:152:MET:SD    | 4:D:253:LEU:HD21  | 2.56                     | 0.46              |
| 5:E:135:ILE:O     | 5:E:135:ILE:HG12  | 2.15                     | 0.46              |
| 5:E:148:VAL:CG2   | 5:E:167:PRO:HB2   | 2.45                     | 0.46              |
| 5:E:280:ASN:C     | 5:E:281:ARG:HG2   | 2.40                     | 0.46              |
| 10:K:119:LEU:O    | 10:K:119:LEU:HD13 | 2.15                     | 0.46              |
| 11:L:229:VAL:HG12 | 11:L:229:VAL:O    | 2.15                     | 0.46              |
| 15:P:141:CYS:SG   | 15:P:145:MET:HE2  | 2.55                     | 0.46              |
| 19:T:193:THR:HG22 | 19:T:194:GLU:H    | 1.81                     | 0.46              |
| 21:W:43:VAL:O     | 21:W:46:THR:HG22  | 2.16                     | 0.46              |
| 21:W:134:GLY:C    | 21:W:136:ILE:HG23 | 2.41                     | 0.46              |
| 21:W:265:GLN:C    | 21:W:265:GLN:CD   | 2.83                     | 0.46              |
| 21:W:444:HIS:CE1  | 24:Z:157:HIS:CD2  | 3.03                     | 0.46              |
| 22:X:415:TYR:HE1  | 23:Y:383:LEU:HB2  | 1.80                     | 0.46              |
| 23:Y:229:ILE:CA   | 23:Y:299:MET:HE1  | 2.46                     | 0.46              |
| 24:Z:22:HIS:HD2   | 24:Z:25:ARG:CD    | 2.28                     | 0.46              |
| 24:Z:201:LEU:HD21 | 27:c:309:PHE:HE1  | 1.81                     | 0.46              |
| 25:a:98:GLU:OE1   | 25:a:98:GLU:HA    | 2.15                     | 0.46              |
| 25:a:112:ILE:HG13 | 25:a:151:VAL:HG11 | 1.97                     | 0.46              |
| 26:b:179:LEU:HD12 | 26:b:181:ASP:HB3  | 1.97                     | 0.46              |
| 27:c:88:ASP:OD1   | 27:c:88:ASP:C     | 2.59                     | 0.46              |
| 27:c:178:THR:HG21 | 32:U:399:TRP:CD1  | 2.51                     | 0.46              |
| 28:d:92:SER:N     | 28:d:95:MET:HG2   | 2.31                     | 0.46              |
| 28:d:135:HIS:HB3  | 28:d:136:PRO:HD3  | 1.97                     | 0.46              |
| 30:f:143:ARG:HD3  | 30:f:143:ARG:N    | 2.30                     | 0.46              |
| 30:f:292:LYS:O    | 30:f:292:LYS:NZ   | 2.44                     | 0.46              |
| 30:f:731:MET:C    | 30:f:731:MET:SD   | 2.98                     | 0.46              |
| 30:f:759:LEU:HB2  | 30:f:809:ILE:CD1  | 2.35                     | 0.46              |
| 6:g:201:CYS:O     | 6:g:205:VAL:HG13  | 2.15                     | 0.46              |
| 32:U:101:ILE:HA   | 32:U:104:CYS:SG   | 2.55                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:77:LEU:HD21   | 2:B:137:SER:O     | 2.16                     | 0.46              |
| 2:B:59:ARG:H      | 30:f:184:LEU:HD11 | 1.80                     | 0.46              |
| 2:B:421:LYS:HA    | 2:B:424:GLU:CG    | 2.46                     | 0.46              |
| 3:C:110:PRO:O     | 3:C:111:ASN:C     | 2.58                     | 0.46              |
| 3:C:369:TYR:HE2   | 3:C:389:LYS:HE2   | 1.80                     | 0.46              |
| 4:D:183:LEU:HD12  | 4:D:183:LEU:HA    | 1.78                     | 0.46              |
| 8:I:67:LYS:NZ     | 8:I:69:ASN:O      | 2.48                     | 0.46              |
| 19:T:22:ILE:HD12  | 19:T:50:MET:HG3   | 1.97                     | 0.46              |
| 20:V:298:ILE:HD13 | 20:V:298:ILE:N    | 2.30                     | 0.46              |
| 20:V:398:LEU:O    | 20:V:402:VAL:HG13 | 2.15                     | 0.46              |
| 21:W:228:ASN:OD1  | 21:W:228:ASN:C    | 2.59                     | 0.46              |
| 21:W:311:THR:C    | 21:W:313:GLU:H    | 2.22                     | 0.46              |
| 22:X:267:VAL:HG11 | 22:X:291:ALA:CB   | 2.46                     | 0.46              |
| 22:X:379:ASP:OD2  | 22:X:379:ASP:C    | 2.58                     | 0.46              |
| 24:Z:176:LEU:HD22 | 27:c:218:LEU:HB2  | 1.98                     | 0.46              |
| 25:a:174:LYS:CG   | 25:a:178:ARG:HH22 | 2.24                     | 0.46              |
| 25:a:210:VAL:HG12 | 25:a:213:PHE:HE2  | 1.80                     | 0.46              |
| 25:a:246:GLU:OE2  | 25:a:250:THR:HG21 | 2.16                     | 0.46              |
| 26:b:7:MET:HE1    | 26:b:52:ILE:HD11  | 1.98                     | 0.46              |
| 26:b:143:PHE:HE1  | 26:b:173:VAL:HG11 | 1.81                     | 0.46              |
| 27:c:54:MET:CE    | 27:c:75:MET:HB2   | 2.46                     | 0.46              |
| 27:c:175:ARG:O    | 27:c:176:GLN:C    | 2.59                     | 0.46              |
| 27:c:292:MET:HE2  | 28:d:253:LEU:CD2  | 2.42                     | 0.46              |
| 31:F:228:PRO:HB3  | 31:F:229:PRO:HD2  | 1.97                     | 0.46              |
| 32:U:166:THR:CG2  | 32:U:166:THR:O    | 2.63                     | 0.46              |
| 32:U:611:ASN:O    | 32:U:614:VAL:HG12 | 2.15                     | 0.46              |
| 32:U:744:VAL:CG2  | 32:U:783:TYR:HB3  | 2.42                     | 0.46              |
| 2:B:78:PHE:CD2    | 2:B:79:ILE:HG13   | 2.51                     | 0.46              |
| 3:C:32:GLN:OE1    | 3:C:32:GLN:HA     | 2.15                     | 0.46              |
| 5:E:161:ARG:NE    | 21:W:173:THR:O    | 2.48                     | 0.46              |
| 11:L:23:GLU:OE1   | 11:L:23:GLU:N     | 2.48                     | 0.46              |
| 20:V:318:GLN:HG2  | 20:V:319:HIS:N    | 2.30                     | 0.46              |
| 21:W:118:LEU:O    | 21:W:118:LEU:HD22 | 2.15                     | 0.46              |
| 21:W:179:LYS:HE3  | 21:W:212:LYS:HD2  | 1.98                     | 0.46              |
| 23:Y:46:ARG:HH11  | 23:Y:46:ARG:HG3   | 1.79                     | 0.46              |
| 24:Z:74:TYR:OH    | 27:c:102:THR:HG21 | 2.15                     | 0.46              |
| 25:a:61:GLU:HA    | 25:a:64:ILE:HD11  | 1.97                     | 0.46              |
| 26:b:160:LEU:N    | 26:b:160:LEU:HD23 | 2.31                     | 0.46              |
| 27:c:211:GLU:HB2  | 32:U:574:LYS:NZ   | 2.29                     | 0.46              |
| 28:d:71:PHE:C     | 28:d:71:PHE:CD2   | 2.93                     | 0.46              |
| 30:f:206:ASP:OD1  | 30:f:207:LEU:N    | 2.48                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 8:i:167:ASN:HB2   | 8:i:200:THR:HG23  | 1.97                     | 0.46              |
| 16:q:19:ARG:NH1   | 16:q:193:ASN:OD1  | 2.49                     | 0.46              |
| 31:F:291:ILE:CD1  | 31:F:306:VAL:HG12 | 2.46                     | 0.46              |
| 32:U:137:MET:HE1  | 32:U:140:ARG:HE   | 1.80                     | 0.46              |
| 32:U:420:LEU:HD22 | 32:U:460:TYR:CE2  | 2.50                     | 0.46              |
| 1:A:213:LEU:HA    | 1:A:319:MET:O     | 2.16                     | 0.46              |
| 1:A:304:ASN:O     | 1:A:308:GLY:HA3   | 2.15                     | 0.46              |
| 2:B:148:CYS:SG    | 2:B:149:SER:N     | 2.89                     | 0.46              |
| 3:C:19:GLY:HA3    | 32:U:146:LYS:NZ   | 2.31                     | 0.46              |
| 3:C:148:TYR:CZ    | 3:C:162:LYS:HE2   | 2.51                     | 0.46              |
| 4:D:39:ASP:O      | 4:D:42:SER:OG     | 2.29                     | 0.46              |
| 5:E:84:ARG:CD     | 27:c:50:PRO:HG3   | 2.43                     | 0.46              |
| 5:E:316:HIS:CD2   | 5:E:344:ARG:HG3   | 2.51                     | 0.46              |
| 6:G:155:ASP:OD1   | 6:G:159:TYR:N     | 2.48                     | 0.46              |
| 11:L:33:SER:H     | 31:F:439:ALA:HB2  | 1.81                     | 0.46              |
| 11:L:212:ILE:CD1  | 11:L:229:VAL:HG13 | 2.44                     | 0.46              |
| 13:N:149:THR:HG22 | 13:N:150:LYS:N    | 2.29                     | 0.46              |
| 14:O:8:VAL:O      | 14:O:8:VAL:HG13   | 2.15                     | 0.46              |
| 20:V:261:TYR:N    | 20:V:261:TYR:CD2  | 2.83                     | 0.46              |
| 20:V:309:MET:HE1  | 20:V:331:LEU:HD23 | 1.98                     | 0.46              |
| 21:W:107:GLN:HE21 | 21:W:111:TYR:HE1  | 1.63                     | 0.46              |
| 21:W:220:GLU:HG3  | 21:W:221:LYS:HE3  | 1.97                     | 0.46              |
| 21:W:333:LEU:HD23 | 21:W:334:GLU:N    | 2.28                     | 0.46              |
| 23:Y:117:LYS:NZ   | 23:Y:151:TYR:HD1  | 2.14                     | 0.46              |
| 25:a:207:GLY:O    | 25:a:271:LYS:HE2  | 2.16                     | 0.46              |
| 27:c:41:MET:HE3   | 27:c:143:VAL:HG11 | 1.97                     | 0.46              |
| 28:d:52:ARG:HH22  | 28:d:89:LEU:CD1   | 2.28                     | 0.46              |
| 30:f:463:LEU:N    | 30:f:489:TYR:OH   | 2.48                     | 0.46              |
| 6:g:113:MET:HE2   | 6:g:113:MET:HA    | 1.97                     | 0.46              |
| 6:g:123:GLN:NE2   | 7:h:84:VAL:HG21   | 2.31                     | 0.46              |
| 11:l:40:SER:HB3   | 11:l:187:LEU:HD22 | 1.98                     | 0.46              |
| 16:q:119:ASP:OD1  | 16:q:119:ASP:N    | 2.49                     | 0.46              |
| 17:r:190:SER:O    | 17:r:190:SER:OG   | 2.31                     | 0.46              |
| 31:F:141:ASP:OD2  | 31:F:144:LYS:NZ   | 2.36                     | 0.46              |
| 32:U:773:PHE:N    | 32:U:774:PRO:HD2  | 2.31                     | 0.46              |
| 32:U:811:PHE:CZ   | 32:U:884:VAL:HG22 | 2.50                     | 0.46              |
| 1:A:219:GLY:CA    | 2:B:343:ARG:HD2   | 2.46                     | 0.46              |
| 2:B:341:LEU:O     | 2:B:341:LEU:HD23  | 2.16                     | 0.46              |
| 4:D:339:ARG:NH2   | 4:D:343:LEU:HG    | 2.30                     | 0.46              |
| 20:V:109:ASN:H    | 20:V:112:VAL:HB   | 1.81                     | 0.46              |
| 20:V:324:PHE:HB2  | 29:e:22:PHE:CG    | 2.51                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 20:V:434:ALA:O    | 20:V:438:VAL:HG23 | 2.15                     | 0.46              |
| 21:W:71:VAL:HG21  | 21:W:104:MET:HG2  | 1.98                     | 0.46              |
| 21:W:106:GLN:HG2  | 21:W:106:GLN:H    | 1.51                     | 0.46              |
| 22:X:323:LEU:HD23 | 22:X:323:LEU:HA   | 1.80                     | 0.46              |
| 23:Y:68:ASP:HA    | 23:Y:71:ASN:ND2   | 2.31                     | 0.46              |
| 23:Y:81:LEU:HD23  | 23:Y:81:LEU:N     | 2.31                     | 0.46              |
| 23:Y:377:LEU:HD12 | 23:Y:380:VAL:CG1  | 2.45                     | 0.46              |
| 24:Z:72:HIS:CE1   | 24:Z:111:LEU:HD21 | 2.51                     | 0.46              |
| 25:a:76:LEU:HA    | 25:a:79:ILE:HG22  | 1.97                     | 0.46              |
| 25:a:313:LYS:NZ   | 25:a:317:VAL:HG13 | 2.31                     | 0.46              |
| 26:b:18:ASN:O     | 26:b:25:ARG:HG3   | 2.14                     | 0.46              |
| 26:b:54:LEU:HB3   | 26:b:84:ILE:HG13  | 1.98                     | 0.46              |
| 26:b:143:PHE:CE1  | 26:b:173:VAL:HG11 | 2.51                     | 0.46              |
| 28:d:50:LEU:HD22  | 28:d:50:LEU:N     | 2.26                     | 0.46              |
| 28:d:71:PHE:CE1   | 28:d:166:PHE:HZ   | 2.26                     | 0.46              |
| 30:f:278:VAL:HG12 | 30:f:280:ASP:H    | 1.81                     | 0.46              |
| 30:f:682:GLY:H    | 30:f:688:ARG:NH2  | 2.14                     | 0.46              |
| 30:f:825:MET:HE3  | 30:f:825:MET:H    | 1.81                     | 0.46              |
| 9:j:50:VAL:O      | 9:j:51:ALA:HB3    | 2.15                     | 0.46              |
| 31:F:207:ASN:C    | 31:F:208:HIS:HD1  | 2.24                     | 0.46              |
| 31:F:251:LEU:HD12 | 31:F:251:LEU:HA   | 1.75                     | 0.46              |
| 32:U:620:GLU:HG3  | 32:U:654:MET:HB3  | 1.97                     | 0.46              |
| 32:U:757:MET:N    | 32:U:758:PRO:HD2  | 2.31                     | 0.46              |
| 2:B:96:ARG:O      | 2:B:99:VAL:HG12   | 2.16                     | 0.46              |
| 2:B:164:MET:SD    | 2:B:164:MET:O     | 2.74                     | 0.46              |
| 2:B:309:MET:HE2   | 2:B:309:MET:HB2   | 1.88                     | 0.46              |
| 2:B:390:LEU:CD2   | 2:B:395:ILE:HD11  | 2.38                     | 0.46              |
| 3:C:53:ASN:HA     | 4:D:68:LEU:HD21   | 1.96                     | 0.46              |
| 4:D:100:THR:HG22  | 4:D:101:ALA:N     | 2.31                     | 0.46              |
| 4:D:190:LEU:HD23  | 4:D:190:LEU:HA    | 1.71                     | 0.46              |
| 5:E:40:TYR:HA     | 31:F:72:LYS:HD3   | 1.98                     | 0.46              |
| 5:E:300:HIS:HD1   | 5:E:300:HIS:C     | 2.16                     | 0.46              |
| 20:V:75:ILE:O     | 20:V:79:VAL:HG12  | 2.16                     | 0.46              |
| 21:W:124:LEU:C    | 21:W:124:LEU:HD13 | 2.41                     | 0.46              |
| 21:W:125:ILE:CG1  | 21:W:129:ARG:HH12 | 2.29                     | 0.46              |
| 21:W:216:GLU:CD   | 21:W:216:GLU:H    | 2.24                     | 0.46              |
| 24:Z:14:LEU:HD12  | 24:Z:14:LEU:O     | 2.16                     | 0.46              |
| 24:Z:96:HIS:HE1   | 24:Z:98:GLY:HA3   | 1.79                     | 0.46              |
| 25:a:57:ILE:HD12  | 25:a:57:ILE:O     | 2.16                     | 0.46              |
| 25:a:287:ASN:OD1  | 25:a:288:HIS:ND1  | 2.48                     | 0.46              |
| 25:a:354:GLU:OE1  | 25:a:354:GLU:HA   | 2.16                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 26:b:149:ASN:ND2  | 26:b:151:GLU:OE2  | 2.49                     | 0.46              |
| 27:c:261:GLU:O    | 27:c:264:LYS:HG2  | 2.15                     | 0.46              |
| 30:f:143:ARG:NH1  | 30:f:189:LYS:HA   | 2.29                     | 0.46              |
| 30:f:268:LEU:HA   | 30:f:272:LEU:CD1  | 2.46                     | 0.46              |
| 30:f:370:MET:HE3  | 30:f:370:MET:CA   | 2.22                     | 0.46              |
| 30:f:472:HIS:HE1  | 30:f:474:SER:HB2  | 1.81                     | 0.46              |
| 7:h:85:LEU:HD11   | 7:h:117:MET:HE3   | 1.98                     | 0.46              |
| 10:k:50:VAL:HG11  | 10:k:66:LYS:HB2   | 1.98                     | 0.46              |
| 32:U:257:SER:OG   | 32:U:260:PHE:HB2  | 2.15                     | 0.46              |
| 32:U:373:ASN:ND2  | 32:U:386:LEU:HD11 | 2.30                     | 0.46              |
| 32:U:443:LEU:H    | 32:U:443:LEU:CD2  | 2.29                     | 0.46              |
| 32:U:475:HIS:CG   | 32:U:511:ALA:HB2  | 2.51                     | 0.46              |
| 1:A:176:ASP:HA    | 1:A:357:ILE:HG12  | 1.98                     | 0.46              |
| 1:A:213:LEU:HB2   | 1:A:337:LEU:HG    | 1.97                     | 0.46              |
| 1:A:213:LEU:HD23  | 1:A:214:LEU:N     | 2.31                     | 0.46              |
| 1:A:328:ASP:C     | 1:A:330:ALA:H     | 2.24                     | 0.46              |
| 2:B:57:GLN:HB2    | 30:f:181:ARG:NH1  | 2.30                     | 0.46              |
| 2:B:120:HIS:C     | 2:B:135:ILE:HD11  | 2.41                     | 0.46              |
| 3:C:85:VAL:HG23   | 3:C:87:VAL:HG13   | 1.98                     | 0.46              |
| 3:C:185:GLY:HA2   | 3:C:291:VAL:O     | 2.15                     | 0.46              |
| 4:D:269:ALA:C     | 4:D:270:ILE:HD13  | 2.41                     | 0.46              |
| 5:E:55:GLN:CD     | 5:E:108:MET:HE2   | 2.41                     | 0.46              |
| 5:E:190:GLN:N     | 5:E:190:GLN:OE1   | 2.49                     | 0.46              |
| 9:J:40:ILE:HD11   | 9:J:210:VAL:HG13  | 1.98                     | 0.46              |
| 15:P:3:MET:HE1    | 15:P:105:GLU:HG3  | 1.98                     | 0.46              |
| 20:V:192:MET:HE1  | 20:V:211:TYR:HA   | 1.97                     | 0.46              |
| 20:V:283:ASN:ND2  | 29:e:17:ASP:HB2   | 2.30                     | 0.46              |
| 20:V:448:GLU:OE1  | 20:V:461:LYS:HD2  | 2.16                     | 0.46              |
| 21:W:401:THR:HG22 | 21:W:402:ILE:CD1  | 2.44                     | 0.46              |
| 22:X:142:ARG:O    | 22:X:146:ALA:HB3  | 2.16                     | 0.46              |
| 23:Y:202:LEU:HD22 | 23:Y:239:LYS:NZ   | 2.31                     | 0.46              |
| 23:Y:222:TYR:O    | 23:Y:226:VAL:HG22 | 2.16                     | 0.46              |
| 25:a:84:VAL:HA    | 25:a:87:MET:CG    | 2.46                     | 0.46              |
| 26:b:141:ILE:O    | 26:b:141:ILE:CG1  | 2.64                     | 0.46              |
| 28:d:3:GLU:HB3    | 28:d:6:LYS:HE2    | 1.97                     | 0.46              |
| 28:d:170:LEU:HA   | 28:d:173:THR:HG22 | 1.98                     | 0.46              |
| 30:f:64:GLY:O     | 30:f:68:THR:OG1   | 2.24                     | 0.46              |
| 30:f:318:THR:O    | 30:f:321:MET:HG3  | 2.15                     | 0.46              |
| 30:f:351:THR:O    | 30:f:351:THR:HG23 | 2.15                     | 0.46              |
| 30:f:524:MET:SD   | 30:f:524:MET:C    | 2.99                     | 0.46              |
| 30:f:664:GLU:CD   | 30:f:666:ILE:H    | 2.24                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 30:f:680:ARG:HD2  | 30:f:761:MET:HE1  | 1.96                     | 0.46              |
| 30:f:680:ARG:HH22 | 30:f:762:VAL:HG22 | 1.80                     | 0.46              |
| 30:f:784:ASP:O    | 30:f:787:LEU:HG   | 2.16                     | 0.46              |
| 11:l:19:ILE:O     | 11:l:23:GLU:OE1   | 2.34                     | 0.46              |
| 11:l:33:SER:OG    | 11:l:49:LEU:O     | 2.17                     | 0.46              |
| 13:n:15:LEU:HD21  | 13:n:102:ALA:HB3  | 1.98                     | 0.46              |
| 31:F:140:VAL:HG21 | 31:F:160:ILE:CG2  | 2.46                     | 0.46              |
| 31:F:339:ASP:OD1  | 31:F:340:PRO:HD2  | 2.16                     | 0.46              |
| 31:F:388:THR:HG23 | 31:F:424:ILE:HD13 | 1.97                     | 0.46              |
| 32:U:894:MET:HB2  | 32:U:906:LEU:HD23 | 1.98                     | 0.46              |
| 1:A:214:LEU:HD23  | 1:A:341:ILE:HB    | 1.98                     | 0.45              |
| 1:A:428:ARG:NE    | 1:A:428:ARG:O     | 2.50                     | 0.45              |
| 2:B:71:TYR:CE1    | 30:f:654:VAL:HG21 | 2.51                     | 0.45              |
| 3:C:149:GLU:OE2   | 23:Y:136:HIS:ND1  | 2.39                     | 0.45              |
| 4:D:164:TYR:CD1   | 4:D:174:LYS:HD2   | 2.51                     | 0.45              |
| 4:D:275:PHE:HA    | 4:D:282:ASP:OD2   | 2.16                     | 0.45              |
| 4:D:380:GLN:NE2   | 5:E:167:PRO:HA    | 2.32                     | 0.45              |
| 5:E:218:MET:HE2   | 5:E:218:MET:HB2   | 1.80                     | 0.45              |
| 5:E:320:ILE:HD12  | 31:F:217:ILE:HG12 | 1.97                     | 0.45              |
| 20:V:105:SER:O    | 20:V:108:LEU:HD12 | 2.14                     | 0.45              |
| 20:V:168:GLN:O    | 20:V:172:VAL:HG22 | 2.16                     | 0.45              |
| 20:V:348:PHE:CD1  | 20:V:361:PHE:HB2  | 2.51                     | 0.45              |
| 21:W:274:VAL:CG1  | 21:W:287:VAL:HG12 | 2.45                     | 0.45              |
| 23:Y:24:PHE:O     | 23:Y:29:PRO:HD2   | 2.16                     | 0.45              |
| 23:Y:117:LYS:CE   | 23:Y:151:TYR:HD1  | 2.29                     | 0.45              |
| 24:Z:162:ILE:HG21 | 27:c:221:HIS:HA   | 1.97                     | 0.45              |
| 24:Z:201:LEU:HD21 | 27:c:309:PHE:CE1  | 2.51                     | 0.45              |
| 25:a:124:ASN:OD1  | 25:a:124:ASN:N    | 2.37                     | 0.45              |
| 25:a:340:VAL:O    | 25:a:341:LEU:HD23 | 2.16                     | 0.45              |
| 28:d:63:ILE:HG23  | 28:d:64:LEU:HD12  | 1.98                     | 0.45              |
| 30:f:65:GLU:HG3   | 30:f:66:LYS:HD2   | 1.98                     | 0.45              |
| 30:f:221:ILE:CG2  | 30:f:768:LEU:HD21 | 2.43                     | 0.45              |
| 30:f:445:LEU:HD23 | 30:f:445:LEU:C    | 2.40                     | 0.45              |
| 6:g:73:THR:HG22   | 6:g:74:GLU:H      | 1.81                     | 0.45              |
| 12:m:115:VAL:O    | 12:m:119:VAL:HG23 | 2.17                     | 0.45              |
| 32:U:510:GLU:CD   | 32:U:543:LYS:HG2  | 2.40                     | 0.45              |
| 32:U:719:ASP:CG   | 32:U:721:HIS:H    | 2.22                     | 0.45              |
| 1:A:184:ILE:O     | 1:A:188:ARG:HG3   | 2.16                     | 0.45              |
| 1:A:330:ALA:O     | 1:A:336:ARG:HD2   | 2.16                     | 0.45              |
| 2:B:108:SER:O     | 2:B:151:LEU:HA    | 2.17                     | 0.45              |
| 33:B:501:ATP:H3'  | 33:B:501:ATP:PA   | 2.57                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:D:191:TYR:CD1   | 4:D:198:PRO:HG3   | 2.43                     | 0.45              |
| 4:D:192:LYS:HD2   | 4:D:192:LYS:O     | 2.15                     | 0.45              |
| 4:D:263:PHE:HD1   | 4:D:264:ILE:N     | 2.15                     | 0.45              |
| 4:D:391:ARG:HH22  | 4:D:395:LEU:HG    | 1.81                     | 0.45              |
| 5:E:270:LEU:HD23  | 5:E:270:LEU:O     | 2.17                     | 0.45              |
| 5:E:378:LYS:HG3   | 5:E:378:LYS:O     | 2.15                     | 0.45              |
| 17:R:6:ALA:HB3    | 17:R:101:MET:HE1  | 1.97                     | 0.45              |
| 19:T:92:LEU:O     | 19:T:96:MET:HG2   | 2.16                     | 0.45              |
| 20:V:268:GLU:OE1  | 20:V:269:LYS:HD3  | 2.16                     | 0.45              |
| 21:W:133:GLU:CA   | 21:W:136:ILE:HG21 | 2.44                     | 0.45              |
| 22:X:373:LYS:HB2  | 22:X:373:LYS:HE3  | 1.84                     | 0.45              |
| 23:Y:15:PRO:HB3   | 23:Y:147:ILE:HG23 | 1.97                     | 0.45              |
| 23:Y:277:VAL:O    | 23:Y:280:GLN:HG3  | 2.16                     | 0.45              |
| 24:Z:182:THR:C    | 24:Z:183:THR:HG1  | 2.21                     | 0.45              |
| 25:a:157:ASP:O    | 25:a:160:SER:OG   | 2.23                     | 0.45              |
| 26:b:138:VAL:HG22 | 26:b:139:ASP:N    | 2.31                     | 0.45              |
| 27:c:62:VAL:HG23  | 27:c:63:ASP:H     | 1.81                     | 0.45              |
| 27:c:67:VAL:HG11  | 27:c:141:VAL:HG21 | 1.97                     | 0.45              |
| 27:c:223:LYS:HE2  | 27:c:223:LYS:HB3  | 1.85                     | 0.45              |
| 27:c:286:GLU:OE2  | 27:c:286:GLU:HA   | 2.16                     | 0.45              |
| 28:d:1:MET:HE2    | 28:d:32:GLU:HG2   | 1.98                     | 0.45              |
| 30:f:579:ALA:O    | 30:f:582:VAL:HG22 | 2.15                     | 0.45              |
| 30:f:608:LYS:HE2  | 30:f:639:LYS:HE3  | 1.97                     | 0.45              |
| 30:f:766:GLN:NE2  | 30:f:769:THR:HB   | 2.30                     | 0.45              |
| 30:f:827:PRO:HB3  | 30:f:860:LYS:HZ1  | 1.80                     | 0.45              |
| 12:m:20:VAL:O     | 12:m:20:VAL:HG12  | 2.17                     | 0.45              |
| 12:m:141:SER:O    | 12:m:145:GLY:N    | 2.40                     | 0.45              |
| 15:p:9:ALA:HB1    | 15:p:145:MET:HE1  | 1.98                     | 0.45              |
| 31:F:134:LEU:N    | 31:F:134:LEU:HD23 | 2.30                     | 0.45              |
| 31:F:153:VAL:CG1  | 31:F:159:LEU:H    | 2.29                     | 0.45              |
| 32:U:201:LEU:HD13 | 32:U:201:LEU:C    | 2.42                     | 0.45              |
| 32:U:560:MET:HE3  | 32:U:560:MET:HB2  | 1.87                     | 0.45              |
| 32:U:588:MET:HE3  | 32:U:588:MET:HB3  | 1.67                     | 0.45              |
| 2:B:292:THR:CG2   | 2:B:333:ARG:HH22  | 2.28                     | 0.45              |
| 4:D:263:PHE:HE1   | 4:D:265:ASP:HA    | 1.81                     | 0.45              |
| 5:E:158:LEU:CD2   | 21:W:137:TYR:HE2  | 2.28                     | 0.45              |
| 5:E:307:GLN:OE1   | 5:E:307:GLN:CA    | 2.63                     | 0.45              |
| 16:Q:29:LYS:NZ    | 17:R:123:SER:O    | 2.41                     | 0.45              |
| 20:V:85:ALA:HA    | 20:V:93:PHE:HD2   | 1.81                     | 0.45              |
| 20:V:289:LEU:HA   | 20:V:292:THR:HG22 | 1.98                     | 0.45              |
| 20:V:407:VAL:CA   | 20:V:410:ILE:HG22 | 2.45                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 21:W:79:GLU:O     | 21:W:83:LEU:N     | 2.48                     | 0.45              |
| 21:W:131:VAL:O    | 21:W:132:THR:C    | 2.59                     | 0.45              |
| 21:W:145:LEU:HD13 | 21:W:174:TYR:CD2  | 2.52                     | 0.45              |
| 21:W:151:THR:HA   | 21:W:154:GLU:HG3  | 1.96                     | 0.45              |
| 21:W:168:GLU:C    | 21:W:168:GLU:OE1  | 2.58                     | 0.45              |
| 21:W:406:VAL:O    | 22:X:342:PHE:HB2  | 2.17                     | 0.45              |
| 21:W:415:PHE:N    | 21:W:415:PHE:CD1  | 2.84                     | 0.45              |
| 22:X:118:LYS:HG2  | 22:X:126:ARG:HH11 | 1.81                     | 0.45              |
| 24:Z:124:ILE:HG22 | 24:Z:135:THR:OG1  | 2.16                     | 0.45              |
| 26:b:121:GLU:O    | 26:b:122:LYS:C    | 2.60                     | 0.45              |
| 28:d:63:ILE:HD12  | 28:d:63:ILE:HA    | 1.82                     | 0.45              |
| 28:d:65:ARG:HA    | 28:d:66:LYS:NZ    | 2.30                     | 0.45              |
| 28:d:71:PHE:CE2   | 28:d:75:MET:CE    | 2.97                     | 0.45              |
| 30:f:139:CYS:HA   | 30:f:143:ARG:NH2  | 2.23                     | 0.45              |
| 30:f:350:LYS:HD3  | 30:f:350:LYS:HA   | 1.56                     | 0.45              |
| 30:f:476:THR:O    | 30:f:479:LEU:HB3  | 2.16                     | 0.45              |
| 30:f:557:TRP:CA   | 30:f:560:LEU:HG   | 2.45                     | 0.45              |
| 30:f:693:ALA:HA   | 30:f:696:LEU:HG   | 1.99                     | 0.45              |
| 30:f:813:LYS:CB   | 30:f:882:LEU:HD21 | 2.46                     | 0.45              |
| 17:r:36:ILE:HD13  | 17:r:57:GLU:CB    | 2.47                     | 0.45              |
| 18:s:16:ALA:HB2   | 18:s:121:VAL:HG23 | 1.98                     | 0.45              |
| 31:F:177:VAL:CG2  | 31:F:248:PHE:HB3  | 2.46                     | 0.45              |
| 31:F:325:GLN:OE1  | 31:F:325:GLN:HA   | 2.15                     | 0.45              |
| 32:U:234:GLU:O    | 32:U:237:VAL:CG1  | 2.62                     | 0.45              |
| 32:U:241:ASN:HB3  | 32:U:244:MET:HE1  | 1.97                     | 0.45              |
| 32:U:884:VAL:HG12 | 32:U:889:LEU:HA   | 1.96                     | 0.45              |
| 1:A:204:LEU:HD12  | 1:A:204:LEU:HA    | 1.86                     | 0.45              |
| 2:B:263:GLY:O     | 2:B:265:LYS:N     | 2.43                     | 0.45              |
| 3:C:77:VAL:HG21   | 3:C:86:LEU:HD23   | 1.94                     | 0.45              |
| 4:D:153:MET:CE    | 5:E:267:PHE:HE2   | 2.28                     | 0.45              |
| 4:D:234:GLU:HA    | 5:E:216:ARG:NH1   | 2.30                     | 0.45              |
| 4:D:267:ILE:HG23  | 4:D:317:LEU:HD21  | 1.99                     | 0.45              |
| 4:D:292:LEU:HD22  | 4:D:296:MET:CE    | 2.46                     | 0.45              |
| 4:D:397:LYS:HG2   | 4:D:397:LYS:O     | 2.14                     | 0.45              |
| 15:P:12:ALA:HB3   | 15:P:136:VAL:HG22 | 1.98                     | 0.45              |
| 20:V:231:LEU:H    | 20:V:231:LEU:HD22 | 1.82                     | 0.45              |
| 21:W:121:LYS:HE3  | 21:W:121:LYS:HB3  | 1.74                     | 0.45              |
| 21:W:312:MET:HG3  | 21:W:365:ILE:HD11 | 1.97                     | 0.45              |
| 23:Y:278:VAL:CA   | 23:Y:281:GLU:HG3  | 2.38                     | 0.45              |
| 25:a:293:PHE:HE1  | 25:a:331:VAL:HG22 | 1.80                     | 0.45              |
| 28:d:125:LYS:N    | 28:d:125:LYS:HD3  | 2.30                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 28:d:234:ASP:OD1  | 28:d:235:THR:N    | 2.50                     | 0.45              |
| 30:f:460:ASP:OD1  | 30:f:489:TYR:OH   | 2.31                     | 0.45              |
| 30:f:557:TRP:HA   | 30:f:560:LEU:HD11 | 1.97                     | 0.45              |
| 30:f:760:PHE:HA   | 30:f:806:VAL:HG11 | 1.98                     | 0.45              |
| 30:f:778:LEU:HD23 | 30:f:778:LEU:N    | 2.31                     | 0.45              |
| 32:U:131:GLU:CD   | 32:U:135:ASN:HD21 | 2.23                     | 0.45              |
| 32:U:135:ASN:HA   | 32:U:138:PHE:HB2  | 1.99                     | 0.45              |
| 32:U:166:THR:HG23 | 32:U:169:GLU:OE1  | 2.15                     | 0.45              |
| 32:U:238:LYS:HD2  | 32:U:238:LYS:C    | 2.42                     | 0.45              |
| 32:U:260:PHE:O    | 32:U:263:SER:OG   | 2.26                     | 0.45              |
| 32:U:513:GLY:HA3  | 32:U:548:LEU:HD23 | 1.99                     | 0.45              |
| 32:U:772:TRP:HB3  | 32:U:775:LEU:HB2  | 1.98                     | 0.45              |
| 1:A:91:GLN:CB     | 1:A:92:PRO:HD3    | 2.47                     | 0.45              |
| 2:B:150:VAL:HG12  | 2:B:152:LEU:HD23  | 1.98                     | 0.45              |
| 3:C:101:LYS:HD3   | 3:C:102:ASN:OD1   | 2.16                     | 0.45              |
| 3:C:389:LYS:HG3   | 3:C:393:LYS:HE3   | 1.99                     | 0.45              |
| 4:D:155:THR:O     | 4:D:158:GLN:HG3   | 2.17                     | 0.45              |
| 5:E:262:ASN:C     | 5:E:262:ASN:OD1   | 2.60                     | 0.45              |
| 5:E:265:ASP:C     | 5:E:265:ASP:OD2   | 2.60                     | 0.45              |
| 5:E:340:GLY:O     | 33:E:402:ATP:H1'  | 2.16                     | 0.45              |
| 16:Q:101:ASN:C    | 16:Q:102:LEU:HD12 | 2.42                     | 0.45              |
| 17:R:183:ASP:OD1  | 17:R:183:ASP:N    | 2.43                     | 0.45              |
| 20:V:309:MET:CB   | 20:V:332:LEU:HD12 | 2.47                     | 0.45              |
| 21:W:451:MET:HE3  | 24:Z:100:LYS:C    | 2.41                     | 0.45              |
| 24:Z:230:LEU:CB   | 25:a:349:MET:HE3  | 2.47                     | 0.45              |
| 25:a:122:LYS:HD2  | 25:a:125:ILE:HG13 | 1.99                     | 0.45              |
| 26:b:11:ASP:OD2   | 26:b:16:MET:HE3   | 2.17                     | 0.45              |
| 26:b:185:SER:O    | 26:b:189:LEU:HB2  | 2.16                     | 0.45              |
| 27:c:71:ASP:OD1   | 27:c:71:ASP:C     | 2.59                     | 0.45              |
| 27:c:281:LYS:O    | 27:c:281:LYS:HD2  | 2.16                     | 0.45              |
| 27:c:302:ALA:O    | 27:c:306:THR:HG23 | 2.17                     | 0.45              |
| 28:d:83:PHE:O     | 28:d:83:PHE:CG    | 2.70                     | 0.45              |
| 29:e:42:ASN:ND2   | 29:e:44:ASP:HB2   | 2.28                     | 0.45              |
| 30:f:127:SER:O    | 30:f:127:SER:OG   | 2.34                     | 0.45              |
| 30:f:246:SER:HA   | 30:f:256:PHE:CE1  | 2.52                     | 0.45              |
| 30:f:261:ARG:CA   | 30:f:267:ARG:HH12 | 2.20                     | 0.45              |
| 30:f:655:LEU:HD22 | 30:f:659:LEU:HD11 | 1.99                     | 0.45              |
| 11:l:122:ARG:CZ   | 11:l:122:ARG:HB2  | 2.46                     | 0.45              |
| 14:o:164:ILE:HG23 | 14:o:171:GLY:HA2  | 1.99                     | 0.45              |
| 15:p:112:ASP:OD2  | 15:p:115:THR:HG22 | 2.16                     | 0.45              |
| 17:r:10:ARG:HG3   | 17:r:10:ARG:NH1   | 2.31                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 31:F:194:GLN:NE2  | 31:F:355:PRO:HD3  | 2.31                     | 0.45              |
| 1:A:190:VAL:HG11  | 1:A:212:VAL:HG21  | 1.99                     | 0.45              |
| 3:C:71:SER:HB3    | 3:C:116:LEU:O     | 2.16                     | 0.45              |
| 4:D:97:ASP:HA     | 27:c:272:ILE:HD12 | 1.99                     | 0.45              |
| 6:G:193:GLN:OE1   | 6:G:193:GLN:N     | 2.50                     | 0.45              |
| 19:T:74:GLU:OE1   | 19:T:83:TYR:CD2   | 2.70                     | 0.45              |
| 20:V:101:LEU:N    | 20:V:102:PRO:HD2  | 2.32                     | 0.45              |
| 20:V:106:ARG:HD2  | 20:V:106:ARG:C    | 2.42                     | 0.45              |
| 22:X:163:LYS:HD2  | 22:X:196:THR:HG23 | 1.98                     | 0.45              |
| 23:Y:46:ARG:HH11  | 23:Y:46:ARG:CG    | 2.30                     | 0.45              |
| 23:Y:338:ILE:HD13 | 23:Y:338:ILE:N    | 2.32                     | 0.45              |
| 24:Z:151:THR:HG23 | 25:a:146:PRO:HG2  | 1.97                     | 0.45              |
| 24:Z:199:LYS:HE3  | 25:a:364:GLU:CG   | 2.46                     | 0.45              |
| 25:a:148:VAL:CG1  | 25:a:149:THR:H    | 2.27                     | 0.45              |
| 26:b:25:ARG:HA    | 26:b:28:ALA:HB3   | 1.99                     | 0.45              |
| 28:d:182:ILE:O    | 28:d:182:ILE:HG22 | 2.17                     | 0.45              |
| 30:f:7:ASP:OD1    | 30:f:7:ASP:N      | 2.49                     | 0.45              |
| 30:f:94:LYS:HA    | 30:f:98:PHE:CD1   | 2.52                     | 0.45              |
| 30:f:197:ALA:O    | 30:f:201:GLU:HG3  | 2.16                     | 0.45              |
| 30:f:316:ASP:O    | 30:f:320:ILE:HG12 | 2.15                     | 0.45              |
| 31:F:133:PHE:O    | 31:F:133:PHE:CG   | 2.67                     | 0.45              |
| 32:U:167:ILE:HG13 | 32:U:168:LEU:N    | 2.31                     | 0.45              |
| 32:U:368:ALA:HB2  | 32:U:728:PHE:HD1  | 1.82                     | 0.45              |
| 32:U:573:ASP:OD1  | 32:U:575:ASP:HB2  | 2.16                     | 0.45              |
| 32:U:798:PRO:C    | 32:U:880:ASN:HD22 | 2.25                     | 0.45              |
| 1:A:127:ASP:OD1   | 1:A:128:GLN:N     | 2.50                     | 0.45              |
| 3:C:371:LEU:CD2   | 4:D:191:TYR:HE2   | 2.30                     | 0.45              |
| 4:D:60:TYR:CD1    | 32:U:603:LEU:HD12 | 2.51                     | 0.45              |
| 9:J:191:VAL:HG11  | 9:J:208:LEU:HD21  | 1.99                     | 0.45              |
| 10:K:20:ARG:HE    | 31:F:435:LEU:CD2  | 2.28                     | 0.45              |
| 17:R:38:ILE:HG22  | 17:R:39:ASN:OD1   | 2.17                     | 0.45              |
| 20:V:160:LEU:HD22 | 20:V:161:PRO:HD2  | 1.98                     | 0.45              |
| 20:V:164:GLU:O    | 20:V:168:GLN:HG2  | 2.17                     | 0.45              |
| 20:V:411:SER:CB   | 20:V:447:ILE:HG21 | 2.46                     | 0.45              |
| 21:W:215:GLN:HG2  | 21:W:223:LYS:HE3  | 1.99                     | 0.45              |
| 22:X:160:MET:N    | 22:X:160:MET:SD   | 2.89                     | 0.45              |
| 24:Z:205:LEU:CD1  | 25:a:353:LEU:HD22 | 2.45                     | 0.45              |
| 25:a:95:THR:O     | 25:a:99:LYS:N     | 2.48                     | 0.45              |
| 25:a:140:GLU:OE1  | 25:a:140:GLU:O    | 2.34                     | 0.45              |
| 26:b:7:MET:CB     | 26:b:109:ILE:HG22 | 2.42                     | 0.45              |
| 28:d:166:PHE:HA   | 28:d:169:ILE:CD1  | 2.46                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 29:e:48:VAL:O     | 29:e:48:VAL:CG1   | 2.60                     | 0.45              |
| 30:f:8:LYS:HD3    | 30:f:9:ALA:N      | 2.30                     | 0.45              |
| 30:f:262:PHE:O    | 30:f:264:GLU:N    | 2.45                     | 0.45              |
| 12:m:186:CYS:O    | 12:m:190:VAL:HG23 | 2.17                     | 0.45              |
| 13:n:52:ASP:O     | 13:n:56:VAL:HG23  | 2.17                     | 0.45              |
| 14:o:144:ARG:NH1  | 14:o:144:ARG:HB3  | 2.32                     | 0.45              |
| 19:t:48:SER:C     | 19:t:49:THR:HG1   | 2.23                     | 0.45              |
| 32:U:159:ARG:NH1  | 32:U:159:ARG:HB3  | 2.32                     | 0.45              |
| 32:U:725:MET:HE3  | 32:U:725:MET:O    | 2.17                     | 0.45              |
| 1:A:192:GLU:OE2   | 1:A:232:ARG:HB3   | 2.17                     | 0.45              |
| 1:A:197:HIS:CE1   | 30:f:343:LYS:HG3  | 2.51                     | 0.45              |
| 1:A:405:THR:HG21  | 1:A:407:LYS:NZ    | 2.32                     | 0.45              |
| 2:B:369:THR:HA    | 2:B:372:MET:HE2   | 1.99                     | 0.45              |
| 3:C:158:ILE:O     | 3:C:161:ILE:HG22  | 2.17                     | 0.45              |
| 6:G:203:SER:O     | 6:G:207:SER:N     | 2.49                     | 0.45              |
| 20:V:126:ALA:O    | 20:V:129:ASP:HB2  | 2.17                     | 0.45              |
| 20:V:254:LEU:HD12 | 20:V:270:LEU:HD13 | 1.99                     | 0.45              |
| 21:W:281:ASN:OD1  | 21:W:281:ASN:N    | 2.48                     | 0.45              |
| 22:X:271:VAL:HG11 | 22:X:288:LYS:HE2  | 1.98                     | 0.45              |
| 22:X:278:ARG:O    | 22:X:278:ARG:HG2  | 2.17                     | 0.45              |
| 22:X:415:TYR:OH   | 23:Y:379:ARG:O    | 2.35                     | 0.45              |
| 23:Y:46:ARG:O     | 23:Y:47:ASP:HB2   | 2.17                     | 0.45              |
| 23:Y:274:SER:O    | 23:Y:277:VAL:HG12 | 2.16                     | 0.45              |
| 26:b:88:THR:HA    | 26:b:91:ARG:CD    | 2.45                     | 0.45              |
| 27:c:35:SER:HB3   | 27:c:213:GLU:CD   | 2.41                     | 0.45              |
| 27:c:44:HIS:CE1   | 27:c:53:VAL:HB    | 2.51                     | 0.45              |
| 27:c:46:ARG:O     | 27:c:46:ARG:HD2   | 2.16                     | 0.45              |
| 27:c:248:MET:CE   | 27:c:288:VAL:HG22 | 2.47                     | 0.45              |
| 11:l:84:LEU:O     | 11:l:88:MET:HG3   | 2.17                     | 0.45              |
| 16:q:43:LEU:HD12  | 16:q:183:ILE:HD11 | 1.97                     | 0.45              |
| 2:B:290:ILE:HG23  | 2:B:290:ILE:O     | 2.15                     | 0.45              |
| 3:C:51:GLU:C      | 3:C:51:GLU:OE2    | 2.59                     | 0.45              |
| 4:D:410:ASP:OD1   | 4:D:411:GLU:N     | 2.50                     | 0.45              |
| 8:I:8:ARG:HB3     | 8:I:11:ILE:HG13   | 1.98                     | 0.45              |
| 9:J:31:THR:OG1    | 9:J:163:ARG:O     | 2.27                     | 0.45              |
| 14:O:77:VAL:HG13  | 14:O:101:LEU:HD22 | 1.99                     | 0.45              |
| 20:V:325:LYS:HA   | 20:V:328:VAL:CG1  | 2.47                     | 0.45              |
| 20:V:392:TYR:C    | 20:V:392:TYR:CD2  | 2.95                     | 0.45              |
| 21:W:42:GLU:HA    | 21:W:45:GLU:OE2   | 2.17                     | 0.45              |
| 21:W:103:LYS:HA   | 21:W:106:GLN:HG3  | 1.99                     | 0.45              |
| 22:X:277:LEU:HD12 | 22:X:278:ARG:H    | 1.81                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:X:404:ILE:O    | 23:Y:376:LEU:HD12 | 2.17                     | 0.45              |
| 22:X:413:SER:HB2  | 27:c:260:GLU:OE1  | 2.17                     | 0.45              |
| 23:Y:13:LYS:O     | 23:Y:13:LYS:CG    | 2.65                     | 0.45              |
| 23:Y:80:GLU:OE1   | 23:Y:80:GLU:HA    | 2.17                     | 0.45              |
| 23:Y:222:TYR:OH   | 23:Y:285:ASP:OD1  | 2.32                     | 0.45              |
| 25:a:174:LYS:HE3  | 25:a:178:ARG:HH12 | 1.82                     | 0.45              |
| 25:a:185:ILE:O    | 25:a:185:ILE:CD1  | 2.64                     | 0.45              |
| 25:a:361:LYS:HD2  | 25:a:365:MET:CE   | 2.46                     | 0.45              |
| 27:c:75:MET:CE    | 27:c:88:ASP:H     | 2.28                     | 0.45              |
| 27:c:121:TRP:HZ3  | 27:c:123:SER:HB2  | 1.82                     | 0.45              |
| 28:d:52:ARG:HG3   | 28:d:81:TYR:HB3   | 1.98                     | 0.45              |
| 28:d:207:THR:O    | 28:d:211:LYS:HG2  | 2.17                     | 0.45              |
| 30:f:138:GLU:HA   | 30:f:141:LYS:CE   | 2.30                     | 0.45              |
| 30:f:679:LEU:CD2  | 30:f:688:ARG:HH22 | 2.30                     | 0.45              |
| 10:k:70:ILE:HD11  | 10:k:89:ILE:HD12  | 1.98                     | 0.45              |
| 13:n:27:ILE:O     | 19:t:179:ARG:NH1  | 2.47                     | 0.45              |
| 31:F:171:ARG:NH1  | 31:F:258:GLN:OE1  | 2.50                     | 0.45              |
| 32:U:98:GLU:CA    | 32:U:101:ILE:HG22 | 2.44                     | 0.45              |
| 32:U:218:GLN:O    | 32:U:221:ILE:HG22 | 2.16                     | 0.45              |
| 32:U:242:LEU:HD12 | 32:U:246:TYR:CD1  | 2.52                     | 0.45              |
| 32:U:631:GLU:O    | 32:U:634:PRO:HD2  | 2.17                     | 0.45              |
| 2:B:114:GLU:HG2   | 2:B:115:ILE:H     | 1.82                     | 0.45              |
| 2:B:418:ASP:O     | 2:B:422:SER:HB2   | 2.16                     | 0.45              |
| 3:C:23:TYR:HD2    | 32:U:102:ALA:HA   | 1.81                     | 0.45              |
| 3:C:277:LEU:HA    | 3:C:277:LEU:HD23  | 1.72                     | 0.45              |
| 3:C:325:ARG:NH1   | 3:C:353:GLY:H     | 2.15                     | 0.45              |
| 4:D:53:PHE:HE1    | 32:U:632:GLN:CG   | 2.30                     | 0.45              |
| 4:D:58:GLU:OE1    | 4:D:58:GLU:O      | 2.35                     | 0.45              |
| 4:D:109:SER:CB    | 4:D:111:TYR:HE1   | 2.29                     | 0.45              |
| 4:D:393:ILE:CG1   | 21:W:133:GLU:CB   | 2.92                     | 0.45              |
| 5:E:281:ARG:HD2   | 5:E:386:TYR:HD2   | 1.82                     | 0.45              |
| 5:E:300:HIS:HE1   | 5:E:302:ASP:OD2   | 2.00                     | 0.45              |
| 8:I:90:LEU:HD21   | 8:I:114:LEU:HB2   | 1.98                     | 0.45              |
| 12:M:232:ARG:HB3  | 12:M:232:ARG:CZ   | 2.46                     | 0.45              |
| 20:V:71:THR:HG23  | 20:V:72:LEU:HD23  | 1.99                     | 0.45              |
| 20:V:83:GLU:O     | 20:V:86:VAL:HG23  | 2.17                     | 0.45              |
| 20:V:203:LEU:HD13 | 20:V:203:LEU:O    | 2.15                     | 0.45              |
| 20:V:285:TRP:NE1  | 20:V:289:LEU:HD21 | 2.32                     | 0.45              |
| 21:W:357:ARG:HA   | 21:W:357:ARG:HE   | 1.82                     | 0.45              |
| 21:W:376:LYS:HD2  | 21:W:386:VAL:HG11 | 1.99                     | 0.45              |
| 23:Y:92:GLU:OE1   | 23:Y:92:GLU:HA    | 2.18                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 25:a:280:MET:HG2  | 25:a:291:LEU:HD21 | 1.99                     | 0.45              |
| 26:b:115:SER:O    | 26:b:116:PRO:C    | 2.60                     | 0.45              |
| 27:c:114:SER:HA   | 27:c:145:VAL:O    | 2.16                     | 0.45              |
| 27:c:175:ARG:C    | 27:c:176:GLN:HG3  | 2.43                     | 0.45              |
| 28:d:161:GLU:OE2  | 28:d:163:TYR:HD1  | 2.00                     | 0.45              |
| 30:f:159:VAL:HG13 | 30:f:160:ARG:NH1  | 2.21                     | 0.45              |
| 30:f:679:LEU:CD2  | 30:f:688:ARG:HH12 | 2.29                     | 0.45              |
| 30:f:828:ARG:CZ   | 30:f:861:THR:HG21 | 2.47                     | 0.45              |
| 31:F:223:VAL:CG1  | 31:F:352:ILE:HD11 | 2.47                     | 0.45              |
| 31:F:374:ASN:O    | 31:F:375:VAL:HG23 | 2.17                     | 0.45              |
| 32:U:84:ALA:HB3   | 32:U:88:PHE:CD2   | 2.52                     | 0.45              |
| 32:U:342:LEU:HD22 | 32:U:743:ASN:ND2  | 2.32                     | 0.45              |
| 32:U:546:ARG:HD3  | 32:U:771:PHE:CD1  | 2.52                     | 0.45              |
| 2:B:202:GLU:OE1   | 2:B:243:THR:HA    | 2.17                     | 0.44              |
| 3:C:24:TYR:HE1    | 4:D:41:TYR:N      | 2.14                     | 0.44              |
| 4:D:115:ILE:CG2   | 4:D:139:LEU:HD12  | 2.44                     | 0.44              |
| 4:D:194:ILE:CG2   | 4:D:196:ILE:HG23  | 2.46                     | 0.44              |
| 4:D:335:LEU:HD13  | 4:D:371:SER:CA    | 2.48                     | 0.44              |
| 5:E:134:GLU:HA    | 5:E:315:ILE:HG21  | 1.99                     | 0.44              |
| 5:E:143:ARG:HG3   | 5:E:143:ARG:NH1   | 2.31                     | 0.44              |
| 5:E:345:ASN:HD21  | 31:F:349:ASP:CG   | 2.25                     | 0.44              |
| 7:H:10:THR:HG23   | 7:H:20:GLN:HB2    | 1.99                     | 0.44              |
| 16:Q:3:TYR:N      | 16:Q:18:ASP:OD2   | 2.50                     | 0.44              |
| 21:W:149:LEU:HD22 | 21:W:185:PHE:CE2  | 2.52                     | 0.44              |
| 21:W:441:LYS:HB2  | 21:W:441:LYS:NZ   | 2.30                     | 0.44              |
| 22:X:268:GLN:HA   | 22:X:268:GLN:OE1  | 2.17                     | 0.44              |
| 23:Y:224:VAL:HG11 | 23:Y:256:VAL:CG1  | 2.47                     | 0.44              |
| 25:a:12:GLN:O     | 25:a:19:PRO:HG3   | 2.17                     | 0.44              |
| 25:a:174:LYS:CD   | 25:a:178:ARG:HH12 | 2.30                     | 0.44              |
| 25:a:236:THR:O    | 25:a:239:ALA:HB3  | 2.18                     | 0.44              |
| 27:c:44:HIS:NE2   | 27:c:53:VAL:HB    | 2.32                     | 0.44              |
| 27:c:286:GLU:OE2  | 27:c:286:GLU:CA   | 2.65                     | 0.44              |
| 28:d:3:GLU:O      | 28:d:25:ARG:HD3   | 2.16                     | 0.44              |
| 30:f:680:ARG:HD3  | 30:f:680:ARG:O    | 2.17                     | 0.44              |
| 30:f:686:LEU:HD12 | 30:f:687:ARG:NE   | 2.30                     | 0.44              |
| 8:i:33:THR:OG1    | 8:i:166:ASN:O     | 2.34                     | 0.44              |
| 8:i:90:LEU:HG     | 8:i:114:LEU:HD13  | 1.99                     | 0.44              |
| 10:k:209:LYS:O    | 10:k:214:ASN:ND2  | 2.45                     | 0.44              |
| 11:l:210:VAL:CG1  | 11:l:229:VAL:HG21 | 2.46                     | 0.44              |
| 14:o:27:VAL:HG22  | 18:s:185:ARG:HA   | 1.99                     | 0.44              |
| 18:s:172:MET:O    | 18:s:176:LYS:HG3  | 2.17                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 31:F:392:ASN:CG   | 31:F:395:GLN:HE21 | 2.22                     | 0.44              |
| 32:U:9:ILE:CG2    | 32:U:27:LEU:HD11  | 2.47                     | 0.44              |
| 32:U:529:ILE:HD13 | 32:U:529:ILE:HA   | 1.77                     | 0.44              |
| 1:A:196:LEU:HG    | 1:A:197:HIS:CE1   | 2.52                     | 0.44              |
| 3:C:190:GLY:O     | 3:C:296:ASN:HA    | 2.17                     | 0.44              |
| 4:D:144:PRO:CD    | 5:E:64:LEU:HD21   | 2.47                     | 0.44              |
| 4:D:263:PHE:CD1   | 4:D:263:PHE:C     | 2.95                     | 0.44              |
| 5:E:112:PRO:HD2   | 31:F:97:LEU:HD21  | 1.99                     | 0.44              |
| 20:V:309:MET:CE   | 20:V:331:LEU:HD23 | 2.47                     | 0.44              |
| 20:V:404:LYS:HD3  | 20:V:404:LYS:HA   | 1.69                     | 0.44              |
| 20:V:496:PHE:N    | 20:V:497:PRO:CD   | 2.81                     | 0.44              |
| 20:V:497:PRO:N    | 20:V:498:PRO:CD   | 2.80                     | 0.44              |
| 22:X:226:LYS:HD2  | 22:X:226:LYS:HA   | 1.80                     | 0.44              |
| 22:X:344:ARG:HB3  | 22:X:386:ILE:HG23 | 1.99                     | 0.44              |
| 23:Y:330:ILE:CD1  | 23:Y:334:LEU:HG   | 2.48                     | 0.44              |
| 25:a:197:ALA:HA   | 25:a:222:LEU:CD1  | 2.19                     | 0.44              |
| 30:f:144:LEU:C    | 30:f:144:LEU:HD12 | 2.42                     | 0.44              |
| 30:f:324:VAL:O    | 30:f:328:SER:OG   | 2.32                     | 0.44              |
| 30:f:394:ASP:OD1  | 30:f:394:ASP:N    | 2.47                     | 0.44              |
| 30:f:860:LYS:HD3  | 30:f:860:LYS:HA   | 1.69                     | 0.44              |
| 30:f:887:PHE:CD1  | 30:f:888:LEU:HG   | 2.53                     | 0.44              |
| 13:n:2:THR:HG23   | 13:n:34:LYS:NZ    | 2.32                     | 0.44              |
| 31:F:154:ASN:OD1  | 31:F:154:ASN:C    | 2.60                     | 0.44              |
| 31:F:300:LYS:O    | 31:F:300:LYS:HG2  | 2.17                     | 0.44              |
| 32:U:87:LEU:O     | 32:U:87:LEU:HD12  | 2.18                     | 0.44              |
| 32:U:324:LYS:HE2  | 32:U:325:MET:CE   | 2.46                     | 0.44              |
| 32:U:380:THR:HG23 | 32:U:382:SER:N    | 2.30                     | 0.44              |
| 1:A:195:LEU:HD13  | 1:A:235:ALA:HB2   | 1.98                     | 0.44              |
| 2:B:130:GLU:OE1   | 2:B:130:GLU:N     | 2.51                     | 0.44              |
| 2:B:139:VAL:HG23  | 2:B:141:LYS:HG2   | 1.99                     | 0.44              |
| 2:B:170:LEU:HD11  | 2:B:174:MET:HE1   | 1.99                     | 0.44              |
| 2:B:211:TYR:HA    | 2:B:216:ILE:HD12  | 1.99                     | 0.44              |
| 4:D:181:VAL:HG21  | 4:D:308:ILE:HD11  | 2.00                     | 0.44              |
| 5:E:215:ILE:HD12  | 5:E:256:THR:HG23  | 2.00                     | 0.44              |
| 7:H:67:ILE:HD11   | 7:H:73:LEU:HD13   | 1.99                     | 0.44              |
| 20:V:127:THR:HB   | 20:V:131:LEU:CD1  | 2.47                     | 0.44              |
| 20:V:415:SER:HB2  | 23:Y:346:LYS:NZ   | 2.32                     | 0.44              |
| 21:W:107:GLN:NE2  | 21:W:111:TYR:HE1  | 2.15                     | 0.44              |
| 21:W:254:PRO:CD   | 21:W:262:LYS:HZ3  | 2.31                     | 0.44              |
| 22:X:122:ARG:HG2  | 22:X:125:LEU:HB3  | 1.96                     | 0.44              |
| 22:X:347:ILE:HG22 | 22:X:358:LYS:HE2  | 2.00                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 25:a:122:LYS:CD   | 25:a:125:ILE:HG13 | 2.47                     | 0.44              |
| 25:a:218:MET:O    | 25:a:218:MET:HG3  | 2.16                     | 0.44              |
| 25:a:311:VAL:O    | 25:a:315:LEU:HD12 | 2.17                     | 0.44              |
| 30:f:144:LEU:HD12 | 30:f:145:VAL:N    | 2.32                     | 0.44              |
| 30:f:369:ARG:CZ   | 30:f:744:MET:HB3  | 2.47                     | 0.44              |
| 30:f:536:SER:HA   | 30:f:539:LEU:CD1  | 2.31                     | 0.44              |
| 30:f:723:TYR:CE2  | 30:f:727:PHE:HZ   | 2.35                     | 0.44              |
| 7:h:67:ILE:HD11   | 7:h:73:LEU:HD12   | 1.99                     | 0.44              |
| 31:F:283:ILE:HG23 | 31:F:328:VAL:HG22 | 1.98                     | 0.44              |
| 32:U:9:ILE:HD13   | 32:U:42:VAL:CG1   | 2.40                     | 0.44              |
| 32:U:108:TYR:HE2  | 32:U:126:ILE:CG2  | 2.30                     | 0.44              |
| 32:U:118:LEU:HD21 | 32:U:122:GLU:CD   | 2.42                     | 0.44              |
| 32:U:205:TYR:O    | 32:U:211:PRO:HB3  | 2.17                     | 0.44              |
| 32:U:412:HIS:HB3  | 32:U:449:ILE:HD12 | 1.98                     | 0.44              |
| 1:A:174:TYR:CE2   | 1:A:188:ARG:HD3   | 2.52                     | 0.44              |
| 3:C:49:ARG:HB2    | 4:D:65:GLN:OE1    | 2.17                     | 0.44              |
| 4:D:210:CYS:SG    | 4:D:335:LEU:HD22  | 2.57                     | 0.44              |
| 5:E:366:ASP:OD1   | 5:E:366:ASP:N     | 2.50                     | 0.44              |
| 19:T:22:ILE:HD12  | 19:T:50:MET:SD    | 2.58                     | 0.44              |
| 20:V:240:LEU:HD22 | 20:V:240:LEU:H    | 1.83                     | 0.44              |
| 20:V:454:GLU:OE1  | 20:V:454:GLU:C    | 2.60                     | 0.44              |
| 22:X:200:ILE:HD12 | 22:X:200:ILE:N    | 2.32                     | 0.44              |
| 23:Y:80:GLU:OE2   | 23:Y:84:LEU:HD21  | 2.16                     | 0.44              |
| 25:a:34:TRP:O     | 25:a:38:THR:N     | 2.50                     | 0.44              |
| 25:a:58:LYS:O     | 25:a:62:ASN:N     | 2.40                     | 0.44              |
| 26:b:85:THR:O     | 26:b:85:THR:CG2   | 2.65                     | 0.44              |
| 27:c:251:LEU:HD12 | 27:c:251:LEU:HA   | 1.72                     | 0.44              |
| 28:d:9:TRP:HA     | 28:d:18:LYS:HZ1   | 1.83                     | 0.44              |
| 30:f:160:ARG:HA   | 30:f:160:ARG:NH1  | 2.31                     | 0.44              |
| 16:q:38:MET:CE    | 16:q:44:LEU:HD22  | 2.47                     | 0.44              |
| 31:F:97:LEU:HD12  | 31:F:97:LEU:HA    | 1.86                     | 0.44              |
| 32:U:176:MET:O    | 32:U:177:LEU:HB3  | 2.17                     | 0.44              |
| 32:U:427:LEU:HB2  | 32:U:430:ASP:OD2  | 2.18                     | 0.44              |
| 32:U:437:TYR:HE1  | 32:U:472:ILE:CB   | 2.26                     | 0.44              |
| 32:U:693:LEU:HD23 | 32:U:736:ILE:HG21 | 2.00                     | 0.44              |
| 1:A:123:VAL:CG1   | 1:A:147:TYR:O     | 2.66                     | 0.44              |
| 3:C:246:ILE:HB    | 3:C:291:VAL:HG12  | 1.99                     | 0.44              |
| 5:E:310:LEU:HD12  | 5:E:310:LEU:C     | 2.42                     | 0.44              |
| 5:E:369:LYS:HA    | 5:E:372:ARG:HD3   | 1.98                     | 0.44              |
| 5:E:383:LYS:C     | 5:E:384:LEU:HD22  | 2.43                     | 0.44              |
| 8:I:174:MET:O     | 8:I:177:GLN:OE1   | 2.36                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 10:K:53:ARG:O     | 10:K:53:ARG:HG2   | 2.18                     | 0.44              |
| 20:V:357:LEU:O    | 20:V:361:PHE:N    | 2.45                     | 0.44              |
| 21:W:145:LEU:HB2  | 21:W:174:TYR:CE2  | 2.53                     | 0.44              |
| 21:W:276:LEU:O    | 21:W:357:ARG:HD2  | 2.17                     | 0.44              |
| 22:X:106:GLU:OE2  | 22:X:106:GLU:C    | 2.61                     | 0.44              |
| 22:X:357:SER:O    | 22:X:361:VAL:HG12 | 2.17                     | 0.44              |
| 23:Y:31:HIS:ND1   | 23:Y:32:ARG:HD2   | 2.32                     | 0.44              |
| 23:Y:111:LEU:HD23 | 23:Y:111:LEU:HA   | 1.82                     | 0.44              |
| 24:Z:13:PRO:HD2   | 24:Z:168:GLU:OE1  | 2.18                     | 0.44              |
| 24:Z:57:PRO:HG2   | 24:Z:71:ASP:HB2   | 1.99                     | 0.44              |
| 24:Z:224:HIS:CE1  | 25:a:340:VAL:HG11 | 2.52                     | 0.44              |
| 24:Z:232:ASP:OD1  | 25:a:338:PRO:HG3  | 2.18                     | 0.44              |
| 24:Z:242:LEU:HG   | 24:Z:243:GLN:OE1  | 2.17                     | 0.44              |
| 27:c:245:VAL:HG23 | 27:c:291:LEU:HD11 | 1.99                     | 0.44              |
| 30:f:699:VAL:O    | 30:f:699:VAL:HG12 | 2.17                     | 0.44              |
| 14:o:115:TYR:CZ   | 14:o:128:MET:HE2  | 2.53                     | 0.44              |
| 32:U:350:LEU:CB   | 32:U:351:MET:HE2  | 2.47                     | 0.44              |
| 32:U:757:MET:SD   | 32:U:757:MET:C    | 3.01                     | 0.44              |
| 32:U:892:LEU:H    | 32:U:892:LEU:CD2  | 2.30                     | 0.44              |
| 3:C:120:SER:O     | 3:C:121:TYR:C     | 2.61                     | 0.44              |
| 4:D:192:LYS:CD    | 4:D:192:LYS:C     | 2.91                     | 0.44              |
| 5:E:349:GLU:HB3   | 5:E:370:ALA:HB1   | 1.99                     | 0.44              |
| 13:N:139:TYR:O    | 13:N:143:THR:HG22 | 2.17                     | 0.44              |
| 20:V:72:LEU:HD23  | 20:V:112:VAL:HG22 | 1.97                     | 0.44              |
| 20:V:236:ARG:HD2  | 32:U:70:HIS:CD2   | 2.53                     | 0.44              |
| 20:V:356:SER:O    | 20:V:359:PRO:HD2  | 2.18                     | 0.44              |
| 20:V:494:MET:O    | 20:V:497:PRO:HG2  | 2.17                     | 0.44              |
| 21:W:145:LEU:CD2  | 21:W:177:MET:HE3  | 2.47                     | 0.44              |
| 21:W:272:LEU:HD12 | 21:W:272:LEU:HA   | 1.67                     | 0.44              |
| 21:W:328:LEU:HD21 | 21:W:341:PHE:HB3  | 2.00                     | 0.44              |
| 22:X:405:GLN:O    | 22:X:408:SER:HB3  | 2.17                     | 0.44              |
| 23:Y:97:GLU:O     | 23:Y:100:ILE:HG13 | 2.18                     | 0.44              |
| 23:Y:138:LEU:CA   | 23:Y:141:VAL:HG12 | 2.45                     | 0.44              |
| 25:a:41:VAL:O     | 25:a:44:PHE:HB2   | 2.18                     | 0.44              |
| 25:a:373:ASP:N    | 25:a:373:ASP:OD1  | 2.50                     | 0.44              |
| 28:d:206:MET:CA   | 28:d:209:TYR:HB2  | 2.36                     | 0.44              |
| 30:f:670:MET:SD   | 30:f:707:LEU:HD11 | 2.58                     | 0.44              |
| 19:t:107:TRP:O    | 19:t:108:ASN:ND2  | 2.48                     | 0.44              |
| 31:F:259:MET:HG3  | 31:F:260:PHE:N    | 2.31                     | 0.44              |
| 31:F:391:PHE:CZ   | 31:F:428:GLN:HG2  | 2.52                     | 0.44              |
| 32:U:46:GLU:HG2   | 32:U:80:TYR:HE2   | 1.83                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 32:U:226:PRO:HB3  | 32:U:263:SER:OG   | 2.17                     | 0.44              |
| 32:U:458:ILE:CD1  | 32:U:490:ARG:HH22 | 2.30                     | 0.44              |
| 32:U:524:LYS:HB2  | 32:U:524:LYS:HE3  | 1.72                     | 0.44              |
| 32:U:603:LEU:HD21 | 32:U:622:LEU:HD11 | 2.00                     | 0.44              |
| 32:U:697:GLN:OE1  | 32:U:745:THR:HB   | 2.17                     | 0.44              |
| 2:B:139:VAL:HG12  | 2:B:161:GLY:HA2   | 1.99                     | 0.44              |
| 2:B:242:GLN:O     | 2:B:242:GLN:HG3   | 2.17                     | 0.44              |
| 2:B:317:ASP:C     | 2:B:317:ASP:OD2   | 2.61                     | 0.44              |
| 2:B:409:GLU:OE2   | 2:B:409:GLU:CA    | 2.65                     | 0.44              |
| 3:C:158:ILE:HG12  | 3:C:199:LEU:HD21  | 2.00                     | 0.44              |
| 3:C:194:THR:CA    | 3:C:355:SER:HB2   | 2.48                     | 0.44              |
| 3:C:339:THR:HG22  | 3:C:340:ARG:H     | 1.83                     | 0.44              |
| 3:C:340:ARG:NH2   | 23:Y:211:TYR:OH   | 2.51                     | 0.44              |
| 4:D:345:PHE:O     | 4:D:349:THR:OG1   | 2.17                     | 0.44              |
| 5:E:229:ILE:HA    | 5:E:274:LYS:O     | 2.18                     | 0.44              |
| 7:H:195:LYS:HE2   | 7:H:202:MET:CE    | 2.48                     | 0.44              |
| 11:L:10:VAL:HG22  | 11:L:10:VAL:O     | 2.17                     | 0.44              |
| 15:P:177:ASP:OD1  | 15:P:177:ASP:C    | 2.60                     | 0.44              |
| 19:T:67:LEU:HD13  | 19:T:91:TRP:CZ3   | 2.53                     | 0.44              |
| 20:V:125:ASN:OD1  | 20:V:126:ALA:N    | 2.43                     | 0.44              |
| 20:V:162:GLU:OE2  | 20:V:203:LEU:HA   | 2.18                     | 0.44              |
| 20:V:349:ARG:CA   | 20:V:354:LYS:HE2  | 2.44                     | 0.44              |
| 20:V:416:ARG:HH12 | 23:Y:350:VAL:HG22 | 1.82                     | 0.44              |
| 21:W:312:MET:HA   | 21:W:312:MET:CE   | 2.45                     | 0.44              |
| 21:W:371:THR:O    | 21:W:372:ARG:HG2  | 2.18                     | 0.44              |
| 22:X:407:MET:HE2  | 24:Z:266:ILE:CD1  | 2.44                     | 0.44              |
| 25:a:50:PHE:CD2   | 25:a:52:GLN:HB3   | 2.52                     | 0.44              |
| 26:b:137:ASN:O    | 26:b:137:ASN:OD1  | 2.36                     | 0.44              |
| 27:c:175:ARG:HD2  | 27:c:201:TYR:CD2  | 2.52                     | 0.44              |
| 27:c:208:ARG:HD2  | 27:c:208:ARG:C    | 2.43                     | 0.44              |
| 28:d:185:ALA:HA   | 28:d:224:SER:O    | 2.18                     | 0.44              |
| 30:f:113:MET:SD   | 30:f:113:MET:C    | 3.01                     | 0.44              |
| 17:r:183:ASP:OD1  | 17:r:183:ASP:N    | 2.49                     | 0.44              |
| 19:t:66:VAL:O     | 19:t:70:MET:HG3   | 2.18                     | 0.44              |
| 31:F:336:ASP:OD1  | 31:F:336:ASP:N    | 2.50                     | 0.44              |
| 32:U:712:LEU:O    | 32:U:715:LYS:HG2  | 2.17                     | 0.44              |
| 2:B:337:LEU:HD23  | 2:B:337:LEU:H     | 1.83                     | 0.44              |
| 4:D:189:GLU:OE2   | 4:D:190:LEU:N     | 2.51                     | 0.44              |
| 4:D:192:LYS:HE2   | 4:D:193:GLN:N     | 2.33                     | 0.44              |
| 4:D:329:ARG:HD3   | 4:D:329:ARG:HA    | 1.80                     | 0.44              |
| 7:H:230:ALA:CB    | 22:X:90:ARG:HH12  | 2.30                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 13:N:94:ASP:OD1   | 13:N:94:ASP:N     | 2.50                     | 0.44              |
| 20:V:127:THR:O    | 20:V:131:LEU:N    | 2.39                     | 0.44              |
| 20:V:172:VAL:HG12 | 20:V:187:ILE:HG23 | 2.00                     | 0.44              |
| 20:V:432:GLU:CD   | 20:V:432:GLU:N    | 2.73                     | 0.44              |
| 20:V:435:GLU:O    | 20:V:439:ALA:N    | 2.38                     | 0.44              |
| 22:X:97:LEU:HD22  | 22:X:97:LEU:N     | 2.33                     | 0.44              |
| 22:X:106:GLU:OE2  | 22:X:107:VAL:N    | 2.51                     | 0.44              |
| 22:X:132:ARG:CD   | 22:X:136:LEU:HD23 | 2.48                     | 0.44              |
| 23:Y:113:ARG:HD3  | 23:Y:113:ARG:C    | 2.43                     | 0.44              |
| 23:Y:298:GLU:OE1  | 23:Y:298:GLU:HA   | 2.18                     | 0.44              |
| 25:a:273:GLN:HE21 | 25:a:302:ILE:CD1  | 2.26                     | 0.44              |
| 27:c:49:VAL:CG2   | 27:c:148:ILE:HD11 | 2.44                     | 0.44              |
| 27:c:193:ILE:HG22 | 27:c:194:HIS:CD2  | 2.47                     | 0.44              |
| 28:d:97:GLN:CD    | 28:d:160:ALA:HB1  | 2.43                     | 0.44              |
| 30:f:20:ALA:HB3   | 30:f:21:PRO:HD3   | 2.00                     | 0.44              |
| 30:f:630:ASP:O    | 30:f:634:LYS:HG2  | 2.18                     | 0.44              |
| 6:g:123:GLN:HA    | 6:g:126:THR:HG22  | 2.00                     | 0.44              |
| 9:j:217:LEU:HD21  | 9:j:219:ILE:HD11  | 2.00                     | 0.44              |
| 13:n:128:ILE:HD11 | 13:n:137:TYR:CD1  | 2.53                     | 0.44              |
| 31:F:188:ILE:CG1  | 31:F:235:LEU:HD23 | 2.31                     | 0.44              |
| 31:F:275:ALA:HB1  | 31:F:281:SER:OG   | 2.18                     | 0.44              |
| 32:U:655:ALA:O    | 32:U:659:CYS:HB3  | 2.18                     | 0.44              |
| 2:B:331:THR:HG21  | 2:B:334:ILE:HD12  | 2.00                     | 0.44              |
| 2:B:342:ILE:O     | 2:B:342:ILE:HG22  | 2.18                     | 0.44              |
| 2:B:372:MET:SD    | 3:C:180:ILE:HD11  | 2.58                     | 0.44              |
| 2:B:372:MET:HG3   | 3:C:178:LEU:O     | 2.17                     | 0.44              |
| 3:C:297:ARG:CB    | 3:C:300:ILE:HG13  | 2.47                     | 0.44              |
| 3:C:301:LEU:HA    | 3:C:301:LEU:HD23  | 1.85                     | 0.44              |
| 3:C:313:ARG:HG3   | 3:C:314:LYS:N     | 2.32                     | 0.44              |
| 4:D:105:SER:OG    | 4:D:107:THR:HG23  | 2.16                     | 0.44              |
| 4:D:153:MET:HE3   | 4:D:227:PHE:HD2   | 1.83                     | 0.44              |
| 4:D:163:MET:HA    | 4:D:222:HIS:NE2   | 2.32                     | 0.44              |
| 4:D:392:TYR:HD1   | 21:W:137:TYR:CE1  | 2.34                     | 0.44              |
| 5:E:211:SER:OG    | 5:E:256:THR:OG1   | 2.12                     | 0.44              |
| 5:E:326:ILE:HG22  | 5:E:328:TYR:CE1   | 2.53                     | 0.44              |
| 5:E:384:LEU:HD12  | 5:E:386:TYR:CE1   | 2.42                     | 0.44              |
| 14:O:188:ARG:HB3  | 14:O:189:PRO:CD   | 2.48                     | 0.44              |
| 20:V:289:LEU:HD23 | 20:V:289:LEU:N    | 2.32                     | 0.44              |
| 20:V:318:GLN:OE1  | 20:V:318:GLN:N    | 2.49                     | 0.44              |
| 21:W:94:ARG:O     | 21:W:94:ARG:HG3   | 2.17                     | 0.44              |
| 21:W:145:LEU:HB2  | 21:W:174:TYR:CD2  | 2.53                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 21:W:169:LEU:CD1  | 21:W:173:THR:HG23 | 2.41                     | 0.44              |
| 22:X:344:ARG:HA   | 22:X:385:LEU:O    | 2.18                     | 0.44              |
| 25:a:37:LEU:HD23  | 25:a:37:LEU:O     | 2.18                     | 0.44              |
| 25:a:55:GLY:O     | 25:a:58:LYS:HG2   | 2.18                     | 0.44              |
| 26:b:33:VAL:O     | 26:b:36:VAL:CG1   | 2.66                     | 0.44              |
| 27:c:270:LEU:HD13 | 27:c:273:LYS:HE2  | 1.99                     | 0.44              |
| 28:d:194:ALA:HA   | 28:d:197:ILE:HD11 | 2.00                     | 0.44              |
| 28:d:198:LEU:HD12 | 28:d:200:PHE:CE1  | 2.53                     | 0.44              |
| 30:f:16:SER:HB2   | 30:f:17:PRO:HD3   | 1.99                     | 0.44              |
| 30:f:477:MET:HE3  | 30:f:478:ARG:H    | 1.83                     | 0.44              |
| 30:f:631:LYS:HA   | 30:f:634:LYS:CG   | 2.47                     | 0.44              |
| 9:j:116:GLN:HA    | 9:j:119:THR:HG22  | 2.00                     | 0.44              |
| 31:F:213:GLU:OE1  | 31:F:214:ASN:N    | 2.51                     | 0.44              |
| 31:F:226:TYR:CD1  | 31:F:226:TYR:C    | 2.96                     | 0.44              |
| 31:F:310:MET:HE2  | 31:F:310:MET:HB3  | 1.73                     | 0.44              |
| 32:U:398:ASN:O    | 32:U:437:TYR:CE2  | 2.71                     | 0.44              |
| 32:U:424:ALA:HA   | 32:U:427:LEU:CD1  | 2.48                     | 0.44              |
| 32:U:577:ILE:HD13 | 32:U:580:ARG:HD3  | 1.99                     | 0.44              |
| 1:A:205:GLY:CA    | 31:F:373:MET:HB3  | 2.48                     | 0.43              |
| 1:A:329:PRO:O     | 31:F:229:PRO:HB3  | 2.18                     | 0.43              |
| 3:C:60:ARG:HE     | 3:C:60:ARG:HB2    | 1.60                     | 0.43              |
| 3:C:199:LEU:O     | 3:C:199:LEU:HD13  | 2.18                     | 0.43              |
| 3:C:326:LEU:HD13  | 3:C:345:ARG:HA    | 2.00                     | 0.43              |
| 4:D:185:LEU:HD11  | 4:D:306:LYS:CG    | 2.48                     | 0.43              |
| 4:D:246:MET:O     | 4:D:250:VAL:HG23  | 2.18                     | 0.43              |
| 4:D:381:GLU:O     | 4:D:385:LEU:HD23  | 2.18                     | 0.43              |
| 5:E:154:THR:HG23  | 5:E:155:ASN:OD1   | 2.17                     | 0.43              |
| 5:E:171:LEU:HB2   | 5:E:295:LEU:HD13  | 1.98                     | 0.43              |
| 5:E:235:ILE:HG23  | 5:E:285:LEU:HD21  | 1.99                     | 0.43              |
| 5:E:273:VAL:O     | 5:E:273:VAL:HG12  | 2.18                     | 0.43              |
| 5:E:372:ARG:H     | 5:E:372:ARG:CD    | 2.31                     | 0.43              |
| 8:I:174:MET:HA    | 8:I:177:GLN:OE1   | 2.17                     | 0.43              |
| 9:J:144:LEU:HD13  | 9:J:144:LEU:C     | 2.43                     | 0.43              |
| 20:V:234:ARG:CB   | 20:V:250:LEU:HD11 | 2.46                     | 0.43              |
| 21:W:60:MET:HE1   | 21:W:99:GLN:OE1   | 2.18                     | 0.43              |
| 21:W:161:GLU:H    | 21:W:161:GLU:HG2  | 1.66                     | 0.43              |
| 23:Y:229:ILE:HA   | 23:Y:299:MET:HE1  | 1.99                     | 0.43              |
| 24:Z:275:LEU:C    | 24:Z:275:LEU:HD13 | 2.43                     | 0.43              |
| 25:a:99:LYS:CG    | 25:a:103:LYS:HZ1  | 2.31                     | 0.43              |
| 25:a:100:THR:HA   | 25:a:103:LYS:NZ   | 2.33                     | 0.43              |
| 25:a:104:VAL:C    | 25:a:105:LYS:HG2  | 2.43                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 26:b:25:ARG:HH11  | 26:b:144:GLY:HA2  | 1.83                     | 0.43              |
| 26:b:161:ASN:HA   | 26:b:165:GLY:O    | 2.18                     | 0.43              |
| 28:d:203:PRO:HG2  | 28:d:206:MET:CE   | 2.48                     | 0.43              |
| 30:f:125:ILE:CG2  | 30:f:129:LEU:HB2  | 2.31                     | 0.43              |
| 30:f:263:PRO:O    | 30:f:266:LEU:HD22 | 2.17                     | 0.43              |
| 30:f:408:LEU:HB2  | 30:f:439:TYR:OH   | 2.18                     | 0.43              |
| 30:f:554:TYR:HD1  | 30:f:557:TRP:CZ3  | 2.35                     | 0.43              |
| 30:f:656:GLY:HA2  | 30:f:660:ILE:CD1  | 2.41                     | 0.43              |
| 14:o:91:TYR:CD2   | 14:o:95:ILE:HD12  | 2.53                     | 0.43              |
| 32:U:19:LEU:HA    | 32:U:22:PHE:CD2   | 2.52                     | 0.43              |
| 32:U:235:LYS:NZ   | 32:U:238:LYS:HE2  | 2.32                     | 0.43              |
| 32:U:559:ARG:C    | 32:U:560:MET:HG3  | 2.42                     | 0.43              |
| 32:U:592:GLY:HA2  | 32:U:627:PHE:CD1  | 2.52                     | 0.43              |
| 32:U:629:THR:O    | 32:U:629:THR:OG1  | 2.36                     | 0.43              |
| 1:A:189:GLU:OE2   | 31:F:409:ARG:NH1  | 2.51                     | 0.43              |
| 1:A:238:ILE:HG21  | 1:A:260:LEU:HD22  | 1.99                     | 0.43              |
| 1:A:295:VAL:HG21  | 2:B:307:ARG:NH2   | 2.33                     | 0.43              |
| 1:A:424:SER:OG    | 1:A:427:PRO:HD2   | 2.18                     | 0.43              |
| 2:B:74:MET:SD     | 2:B:75:GLU:HG2    | 2.58                     | 0.43              |
| 2:B:195:GLN:O     | 2:B:199:GLU:HB3   | 2.19                     | 0.43              |
| 2:B:257:GLN:HG3   | 2:B:262:ASP:O     | 2.18                     | 0.43              |
| 4:D:192:LYS:HD2   | 4:D:192:LYS:C     | 2.42                     | 0.43              |
| 4:D:263:PHE:HD1   | 4:D:263:PHE:C     | 2.26                     | 0.43              |
| 18:S:145:LEU:HD21 | 18:S:182:ALA:HB2  | 1.99                     | 0.43              |
| 20:V:203:LEU:HD22 | 20:V:206:VAL:HG22 | 1.99                     | 0.43              |
| 20:V:251:LEU:HD12 | 20:V:251:LEU:HA   | 1.75                     | 0.43              |
| 21:W:35:ALA:CB    | 21:W:43:VAL:HG21  | 2.47                     | 0.43              |
| 21:W:118:LEU:HD21 | 21:W:121:LYS:CE   | 2.48                     | 0.43              |
| 22:X:311:ALA:HB3  | 22:X:312:GLU:OE1  | 2.18                     | 0.43              |
| 23:Y:227:SER:OG   | 23:Y:240:VAL:HG11 | 2.18                     | 0.43              |
| 24:Z:201:LEU:HD23 | 27:c:308:VAL:HG11 | 2.00                     | 0.43              |
| 25:a:34:TRP:HZ3   | 26:b:18:ASN:HA    | 1.82                     | 0.43              |
| 25:a:37:LEU:HA    | 25:a:40:GLN:CD    | 2.43                     | 0.43              |
| 25:a:40:GLN:CD    | 25:a:40:GLN:H     | 2.23                     | 0.43              |
| 25:a:302:ILE:HG22 | 25:a:303:THR:N    | 2.33                     | 0.43              |
| 30:f:281:ILE:CD1  | 30:f:286:LYS:HD3  | 2.48                     | 0.43              |
| 30:f:620:PHE:CD2  | 30:f:620:PHE:C    | 2.96                     | 0.43              |
| 30:f:821:LEU:CD2  | 30:f:882:LEU:HD13 | 2.40                     | 0.43              |
| 30:f:827:PRO:HB3  | 30:f:860:LYS:HE3  | 1.99                     | 0.43              |
| 30:f:842:VAL:HG21 | 30:f:862:ILE:CG1  | 2.49                     | 0.43              |
| 6:g:75:ASN:N      | 6:g:75:ASN:OD1    | 2.50                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 11:l:38:LEU:HD23  | 11:l:38:LEU:N     | 2.33                     | 0.43              |
| 19:t:136:SER:O    | 19:t:137:LEU:HD12 | 2.17                     | 0.43              |
| 31:F:218:GLN:H    | 31:F:218:GLN:HG3  | 1.62                     | 0.43              |
| 32:U:269:ARG:NH2  | 32:U:326:ILE:HG21 | 2.32                     | 0.43              |
| 1:A:121:PHE:CZ    | 1:A:147:TYR:HE2   | 2.36                     | 0.43              |
| 2:B:61:LYS:HA     | 2:B:64:LYS:HE2    | 2.00                     | 0.43              |
| 2:B:68:ILE:HG22   | 2:B:72:LEU:HD23   | 2.00                     | 0.43              |
| 2:B:82:GLN:HA     | 2:B:85:MET:SD     | 2.58                     | 0.43              |
| 4:D:153:MET:CE    | 4:D:227:PHE:HD2   | 2.30                     | 0.43              |
| 11:L:188:VAL:HG11 | 11:L:232:PHE:CD1  | 2.53                     | 0.43              |
| 14:O:77:VAL:CG1   | 14:O:101:LEU:HD22 | 2.48                     | 0.43              |
| 21:W:129:ARG:O    | 21:W:132:THR:HG22 | 2.18                     | 0.43              |
| 21:W:239:SER:HG   | 21:W:242:SER:HB3  | 1.84                     | 0.43              |
| 22:X:339:ILE:HD12 | 22:X:342:PHE:HE1  | 1.82                     | 0.43              |
| 23:Y:313:SER:HB2  | 23:Y:353:ILE:HD11 | 1.99                     | 0.43              |
| 24:Z:8:LYS:HB2    | 24:Z:8:LYS:HE2    | 1.54                     | 0.43              |
| 24:Z:204:LYS:O    | 24:Z:208:ILE:HG13 | 2.19                     | 0.43              |
| 25:a:184:ASP:OD1  | 25:a:185:ILE:N    | 2.52                     | 0.43              |
| 26:b:101:GLN:O    | 26:b:102:GLY:C    | 2.60                     | 0.43              |
| 30:f:6:ARG:H      | 30:f:6:ARG:HD2    | 1.83                     | 0.43              |
| 30:f:242:GLU:HB2  | 30:f:243:PRO:HD3  | 2.01                     | 0.43              |
| 30:f:680:ARG:O    | 30:f:680:ARG:CD   | 2.65                     | 0.43              |
| 7:h:85:LEU:HD11   | 7:h:117:MET:CE    | 2.49                     | 0.43              |
| 7:h:189:THR:O     | 7:h:193:THR:HG22  | 2.17                     | 0.43              |
| 13:n:19:SER:O     | 13:n:19:SER:OG    | 2.36                     | 0.43              |
| 31:F:206:MET:HB2  | 31:F:206:MET:HE3  | 1.82                     | 0.43              |
| 31:F:438:TYR:O    | 31:F:439:ALA:HB3  | 2.18                     | 0.43              |
| 32:U:88:PHE:HB3   | 32:U:89:ASN:OD1   | 2.18                     | 0.43              |
| 1:A:167:GLU:OE2   | 1:A:168:GLU:HB2   | 2.18                     | 0.43              |
| 1:A:398:ARG:HD3   | 2:B:195:GLN:CD    | 2.43                     | 0.43              |
| 2:B:303:ARG:HG2   | 2:B:307:ARG:NH1   | 2.32                     | 0.43              |
| 3:C:117:ARG:CZ    | 3:C:124:HIS:HE1   | 2.32                     | 0.43              |
| 5:E:55:GLN:O      | 31:F:132:TYR:HA   | 2.19                     | 0.43              |
| 7:H:107:ALA:O     | 7:H:111:GLN:HG3   | 2.18                     | 0.43              |
| 20:V:172:VAL:HG13 | 20:V:187:ILE:HG13 | 2.00                     | 0.43              |
| 20:V:273:LYS:HZ1  | 32:U:40:GLU:HB3   | 1.81                     | 0.43              |
| 20:V:300:LEU:HD12 | 20:V:300:LEU:N    | 2.33                     | 0.43              |
| 20:V:416:ARG:CB   | 20:V:416:ARG:NH1  | 2.81                     | 0.43              |
| 21:W:98:LYS:HG3   | 21:W:139:GLU:CD   | 2.43                     | 0.43              |
| 21:W:133:GLU:CA   | 21:W:136:ILE:HD13 | 2.47                     | 0.43              |
| 21:W:268:LYS:NZ   | 21:W:301:LYS:HE3  | 2.22                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:X:395:LYS:HB3  | 27:c:242:GLU:OE1  | 2.18                     | 0.43              |
| 23:Y:366:TYR:CA   | 23:Y:369:THR:HG22 | 2.47                     | 0.43              |
| 24:Z:29:VAL:HB    | 24:Z:33:LYS:HZ2   | 1.83                     | 0.43              |
| 24:Z:94:TRP:HH2   | 24:Z:105:ASP:CG   | 2.26                     | 0.43              |
| 24:Z:143:GLU:O    | 24:Z:152:SER:HB3  | 2.19                     | 0.43              |
| 25:a:100:THR:O    | 25:a:104:VAL:HG22 | 2.18                     | 0.43              |
| 25:a:129:GLN:O    | 25:a:129:GLN:HG2  | 2.16                     | 0.43              |
| 26:b:10:VAL:CG1   | 26:b:11:ASP:N     | 2.82                     | 0.43              |
| 28:d:75:MET:SD    | 28:d:102:ASN:HB2  | 2.59                     | 0.43              |
| 28:d:194:ALA:C    | 28:d:197:ILE:HG12 | 2.43                     | 0.43              |
| 29:e:30:LEU:HD12  | 29:e:32:GLU:CD    | 2.44                     | 0.43              |
| 30:f:7:ASP:C      | 30:f:10:PRO:HD2   | 2.43                     | 0.43              |
| 30:f:261:ARG:HB2  | 30:f:267:ARG:HH22 | 1.84                     | 0.43              |
| 30:f:507:ASP:CG   | 30:f:509:LYS:HG2  | 2.43                     | 0.43              |
| 30:f:581:GLU:O    | 30:f:588:ARG:HD2  | 2.18                     | 0.43              |
| 30:f:605:ASN:ND2  | 30:f:608:LYS:HB3  | 2.23                     | 0.43              |
| 30:f:672:LEU:CD1  | 30:f:707:LEU:HD12 | 2.47                     | 0.43              |
| 31:F:202:ILE:HD12 | 31:F:327:LYS:HB3  | 2.00                     | 0.43              |
| 32:U:107:HIS:O    | 32:U:110:LYS:HG2  | 2.19                     | 0.43              |
| 32:U:151:ILE:HG21 | 32:U:179:TYR:OH   | 2.18                     | 0.43              |
| 32:U:669:ILE:HD12 | 32:U:669:ILE:HA   | 1.91                     | 0.43              |
| 2:B:283:PHE:HD1   | 2:B:328:ILE:O     | 2.01                     | 0.43              |
| 3:C:287:LYS:O     | 3:C:287:LYS:HG2   | 2.18                     | 0.43              |
| 4:D:119:ILE:HD11  | 4:D:141:ASP:N     | 2.34                     | 0.43              |
| 4:D:125:LYS:HG2   | 4:D:126:PRO:HD2   | 2.00                     | 0.43              |
| 4:D:418:LYS:HB3   | 4:D:418:LYS:HE2   | 1.80                     | 0.43              |
| 5:E:238:ILE:HD12  | 5:E:253:ILE:HD12  | 2.01                     | 0.43              |
| 6:G:123:GLN:HG3   | 7:H:80:PRO:HB2    | 2.00                     | 0.43              |
| 7:H:47:THR:HG21   | 7:H:74:VAL:CG2    | 2.48                     | 0.43              |
| 10:K:217:LEU:HD23 | 10:K:218:ALA:N    | 2.33                     | 0.43              |
| 15:P:33:MET:O     | 17:r:167:ARG:NH1  | 2.51                     | 0.43              |
| 20:V:276:PHE:CD2  | 20:V:277:PRO:HD2  | 2.53                     | 0.43              |
| 20:V:373:ALA:HB3  | 20:V:427:GLN:NE2  | 2.33                     | 0.43              |
| 20:V:428:LEU:HD11 | 20:V:437:ILE:CD1  | 2.49                     | 0.43              |
| 21:W:72:LYS:HA    | 21:W:111:TYR:OH   | 2.17                     | 0.43              |
| 21:W:98:LYS:HG3   | 21:W:139:GLU:CG   | 2.48                     | 0.43              |
| 21:W:144:ARG:HG2  | 21:W:144:ARG:HH11 | 1.82                     | 0.43              |
| 21:W:199:TYR:HE1  | 21:W:236:HIS:CD2  | 2.37                     | 0.43              |
| 22:X:97:LEU:HD11  | 22:X:106:GLU:CG   | 2.49                     | 0.43              |
| 22:X:118:LYS:HZ2  | 22:X:118:LYS:CB   | 2.31                     | 0.43              |
| 22:X:283:GLN:OE1  | 22:X:283:GLN:CA   | 2.63                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:X:395:LYS:C    | 22:X:397:TYR:H    | 2.24                     | 0.43              |
| 25:a:65:SER:HA    | 25:a:68:GLU:HB2   | 2.00                     | 0.43              |
| 25:a:173:TYR:C    | 25:a:173:TYR:CD1  | 2.96                     | 0.43              |
| 25:a:198:PHE:HZ   | 25:a:257:GLN:HB2  | 1.83                     | 0.43              |
| 26:b:51:LEU:O     | 26:b:51:LEU:HG    | 2.18                     | 0.43              |
| 30:f:267:ARG:HA   | 30:f:271:MET:CE   | 2.44                     | 0.43              |
| 30:f:480:GLY:HA2  | 30:f:483:PHE:HE1  | 1.84                     | 0.43              |
| 30:f:483:PHE:CE2  | 30:f:517:VAL:HG21 | 2.53                     | 0.43              |
| 30:f:789:SER:HA   | 30:f:793:VAL:CB   | 2.47                     | 0.43              |
| 12:m:33:SER:OG    | 12:m:34:SER:N     | 2.51                     | 0.43              |
| 15:p:87:MET:SD    | 15:p:129:PRO:HB3  | 2.58                     | 0.43              |
| 31:F:122:ALA:HB2  | 31:F:137:ILE:HD13 | 1.98                     | 0.43              |
| 31:F:164:LEU:HD12 | 31:F:164:LEU:N    | 2.34                     | 0.43              |
| 32:U:8:ILE:C      | 32:U:10:SER:H     | 2.26                     | 0.43              |
| 32:U:195:ASN:HB2  | 32:U:223:LEU:CD1  | 2.48                     | 0.43              |
| 32:U:554:LEU:HA   | 32:U:588:MET:HE2  | 2.01                     | 0.43              |
| 1:A:197:HIS:CD2   | 30:f:345:PRO:HG2  | 2.54                     | 0.43              |
| 2:B:85:MET:SD     | 2:B:85:MET:N      | 2.91                     | 0.43              |
| 2:B:144:LEU:HD13  | 2:B:144:LEU:HA    | 1.87                     | 0.43              |
| 2:B:250:VAL:O     | 2:B:284:ILE:HA    | 2.19                     | 0.43              |
| 2:B:324:ASP:C     | 2:B:324:ASP:OD1   | 2.62                     | 0.43              |
| 3:C:105:ILE:HD12  | 3:C:108:VAL:HB    | 2.01                     | 0.43              |
| 4:D:97:ASP:OD1    | 4:D:97:ASP:N      | 2.52                     | 0.43              |
| 4:D:145:PRO:HG2   | 4:D:256:GLU:OE2   | 2.18                     | 0.43              |
| 4:D:185:LEU:HD11  | 4:D:306:LYS:HG3   | 2.01                     | 0.43              |
| 5:E:152:PRO:C     | 5:E:153:LEU:HD23  | 2.44                     | 0.43              |
| 8:I:118:LYS:O     | 8:I:122:THR:HG22  | 2.18                     | 0.43              |
| 20:V:254:LEU:HD11 | 20:V:270:LEU:HD13 | 2.01                     | 0.43              |
| 22:X:152:GLN:O    | 22:X:155:ARG:HG2  | 2.17                     | 0.43              |
| 22:X:401:LEU:O    | 22:X:401:LEU:HD13 | 2.18                     | 0.43              |
| 24:Z:97:THR:O     | 24:Z:98:GLY:C     | 2.61                     | 0.43              |
| 27:c:192:LEU:HA   | 27:c:196:LEU:HB3  | 1.99                     | 0.43              |
| 27:c:292:MET:HE2  | 27:c:292:MET:HB3  | 1.92                     | 0.43              |
| 30:f:65:GLU:CB    | 30:f:97:LYS:HE2   | 2.44                     | 0.43              |
| 30:f:448:CYS:O    | 30:f:451:VAL:HG12 | 2.19                     | 0.43              |
| 30:f:633:GLU:HA   | 30:f:636:ASP:OD1  | 2.18                     | 0.43              |
| 36:n:301:LDZ:H40  | 14:o:115:TYR:CG   | 2.53                     | 0.43              |
| 14:o:184:LEU:HD13 | 14:o:184:LEU:C    | 2.43                     | 0.43              |
| 31:F:194:GLN:HG2  | 31:F:352:ILE:HG22 | 2.01                     | 0.43              |
| 32:U:7:GLY:N      | 32:U:37:GLU:OE1   | 2.51                     | 0.43              |
| 32:U:24:LEU:HD23  | 32:U:24:LEU:C     | 2.42                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 32:U:620:GLU:CG   | 32:U:654:MET:HB3  | 2.48                     | 0.43              |
| 32:U:807:LYS:O    | 32:U:810:THR:HG22 | 2.19                     | 0.43              |
| 1:A:402:LYS:HB2   | 1:A:402:LYS:HE2   | 1.70                     | 0.43              |
| 2:B:264:PRO:HB3   | 2:B:311:GLU:HB2   | 2.01                     | 0.43              |
| 3:C:161:ILE:HG12  | 3:C:203:VAL:HG21  | 2.00                     | 0.43              |
| 3:C:198:LEU:HD13  | 3:C:198:LEU:C     | 2.44                     | 0.43              |
| 3:C:300:ILE:C     | 3:C:300:ILE:CD1   | 2.92                     | 0.43              |
| 3:C:300:ILE:HD12  | 3:C:301:LEU:N     | 2.34                     | 0.43              |
| 4:D:176:GLU:OE2   | 4:D:329:ARG:NH1   | 2.46                     | 0.43              |
| 4:D:343:LEU:HD23  | 4:D:343:LEU:HA    | 1.76                     | 0.43              |
| 7:H:79:GLY:N      | 7:H:80:PRO:HD2    | 2.33                     | 0.43              |
| 20:V:227:VAL:O    | 20:V:231:LEU:HD22 | 2.19                     | 0.43              |
| 20:V:281:ASN:OD1  | 20:V:283:ASN:N    | 2.38                     | 0.43              |
| 20:V:459:GLN:HG3  | 20:V:460:SER:N    | 2.34                     | 0.43              |
| 20:V:482:PHE:CE2  | 23:Y:377:LEU:HD21 | 2.54                     | 0.43              |
| 21:W:152:ILE:CD1  | 21:W:165:ILE:HB   | 2.48                     | 0.43              |
| 21:W:241:LEU:HD13 | 21:W:241:LEU:C    | 2.44                     | 0.43              |
| 21:W:319:THR:HA   | 21:W:322:GLU:HG3  | 2.00                     | 0.43              |
| 21:W:406:VAL:CG1  | 22:X:342:PHE:HB3  | 2.36                     | 0.43              |
| 22:X:409:LYS:HD2  | 27:c:256:ASN:HD22 | 1.83                     | 0.43              |
| 23:Y:59:LYS:HD3   | 23:Y:59:LYS:C     | 2.44                     | 0.43              |
| 24:Z:11:VAL:HG12  | 24:Z:15:VAL:HG11  | 2.01                     | 0.43              |
| 24:Z:111:LEU:HD13 | 24:Z:111:LEU:C    | 2.43                     | 0.43              |
| 24:Z:259:VAL:HG21 | 27:c:241:ASN:HD22 | 1.82                     | 0.43              |
| 25:a:268:LEU:O    | 25:a:272:ILE:HG22 | 2.19                     | 0.43              |
| 25:a:374:ILE:O    | 25:a:375:LEU:HD23 | 2.18                     | 0.43              |
| 26:b:142:ASN:ND2  | 26:b:146:GLU:OE1  | 2.52                     | 0.43              |
| 27:c:31:VAL:CG2   | 27:c:203:ILE:HG21 | 2.45                     | 0.43              |
| 30:f:61:GLU:OE1   | 30:f:61:GLU:HA    | 2.19                     | 0.43              |
| 30:f:694:LEU:HD23 | 30:f:695:ALA:N    | 2.31                     | 0.43              |
| 30:f:707:LEU:HG   | 30:f:785:ARG:NH1  | 2.32                     | 0.43              |
| 9:j:195:LEU:HD23  | 9:j:206:ILE:HG12  | 2.01                     | 0.43              |
| 13:n:56:VAL:HG12  | 13:n:84:PHE:CE1   | 2.54                     | 0.43              |
| 31:F:202:ILE:O    | 31:F:206:MET:HE3  | 2.19                     | 0.43              |
| 2:B:184:TYR:CE2   | 2:B:198:LYS:CE    | 3.02                     | 0.43              |
| 2:B:258:LYS:O     | 2:B:299:SER:OG    | 2.35                     | 0.43              |
| 3:C:31:LEU:O      | 3:C:34:ILE:HG22   | 2.17                     | 0.43              |
| 3:C:127:LEU:HB3   | 3:C:128:PRO:CD    | 2.48                     | 0.43              |
| 4:D:378:ILE:HD13  | 4:D:403:TYR:CD1   | 2.53                     | 0.43              |
| 5:E:243:PHE:CZ    | 31:F:304:ARG:CZ   | 3.02                     | 0.43              |
| 6:G:120:ASP:OD1   | 7:H:83:ARG:NH1    | 2.52                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:G:163:PHE:CG    | 6:G:166:THR:OG1   | 2.70                     | 0.43              |
| 8:I:11:ILE:HG22   | 8:I:12:PHE:N      | 2.34                     | 0.43              |
| 16:Q:184:ASP:OD2  | 16:Q:184:ASP:C    | 2.62                     | 0.43              |
| 20:V:256:ARG:HD2  | 20:V:256:ARG:C    | 2.44                     | 0.43              |
| 20:V:487:HIS:ND1  | 24:Z:271:ALA:HB2  | 2.33                     | 0.43              |
| 21:W:54:THR:O     | 21:W:58:SER:N     | 2.51                     | 0.43              |
| 21:W:177:MET:SD   | 21:W:178:GLU:N    | 2.92                     | 0.43              |
| 21:W:413:ILE:CD1  | 21:W:415:PHE:HE1  | 2.31                     | 0.43              |
| 22:X:325:LYS:HD3  | 22:X:325:LYS:C    | 2.43                     | 0.43              |
| 23:Y:143:TYR:O    | 23:Y:147:ILE:HG13 | 2.18                     | 0.43              |
| 23:Y:144:LEU:O    | 23:Y:147:ILE:HD12 | 2.17                     | 0.43              |
| 23:Y:189:VAL:CG1  | 23:Y:287:LEU:HD11 | 2.49                     | 0.43              |
| 23:Y:307:LEU:HD21 | 23:Y:314:LEU:HD11 | 2.00                     | 0.43              |
| 25:a:33:LEU:HA    | 26:b:18:ASN:HB2   | 2.00                     | 0.43              |
| 25:a:48:PRO:CG    | 25:a:51:ALA:HA    | 2.49                     | 0.43              |
| 25:a:118:ILE:HD13 | 25:a:118:ILE:N    | 2.33                     | 0.43              |
| 25:a:276:CYS:SG   | 25:a:299:SER:OG   | 2.72                     | 0.43              |
| 26:b:23:PRO:C     | 26:b:24:THR:OG1   | 2.62                     | 0.43              |
| 26:b:91:ARG:HH12  | 26:b:130:ARG:NH1  | 2.17                     | 0.43              |
| 28:d:5:LEU:O      | 28:d:5:LEU:HD12   | 2.19                     | 0.43              |
| 30:f:445:LEU:HD22 | 30:f:481:SER:CA   | 2.48                     | 0.43              |
| 30:f:460:ASP:OD1  | 30:f:463:LEU:HD12 | 2.19                     | 0.43              |
| 30:f:679:LEU:HD23 | 30:f:679:LEU:C    | 2.44                     | 0.43              |
| 30:f:746:ARG:HA   | 30:f:750:GLN:CD   | 2.43                     | 0.43              |
| 30:f:789:SER:HA   | 30:f:793:VAL:CG1  | 2.48                     | 0.43              |
| 31:F:128:THR:HG22 | 31:F:128:THR:O    | 2.18                     | 0.43              |
| 32:U:103:LYS:HZ2  | 32:U:103:LYS:HB2  | 1.84                     | 0.43              |
| 32:U:365:CYS:HA   | 32:U:368:ALA:HB3  | 2.00                     | 0.43              |
| 32:U:609:ASP:CG   | 32:U:614:VAL:HG11 | 2.43                     | 0.43              |
| 32:U:756:HIS:CD2  | 32:U:758:PRO:HG2  | 2.53                     | 0.43              |
| 32:U:793:LYS:HG3  | 32:U:794:ASP:OD1  | 2.18                     | 0.43              |
| 1:A:210:LYS:HB2   | 1:A:312:ARG:HH22  | 1.84                     | 0.43              |
| 2:B:214:MET:HB3   | 2:B:214:MET:HE3   | 1.78                     | 0.43              |
| 3:C:20:LEU:C      | 3:C:22:GLN:H      | 2.25                     | 0.43              |
| 3:C:25:LEU:HD23   | 3:C:28:ILE:HG21   | 2.01                     | 0.43              |
| 3:C:42:LEU:HD13   | 4:D:54:LEU:CD1    | 2.49                     | 0.43              |
| 3:C:146:SER:HA    | 3:C:150:MET:CE    | 2.25                     | 0.43              |
| 3:C:249:ASP:OD1   | 3:C:250:GLU:O     | 2.37                     | 0.43              |
| 3:C:390:VAL:O     | 3:C:394:ASP:HB3   | 2.18                     | 0.43              |
| 4:D:46:LYS:HB3    | 4:D:46:LYS:HE2    | 1.76                     | 0.43              |
| 4:D:78:GLU:O      | 4:D:78:GLU:HG2    | 2.19                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:D:131:ALA:C     | 4:D:132:LEU:HD23  | 2.44                     | 0.43              |
| 4:D:191:TYR:CE2   | 4:D:196:ILE:HD11  | 2.54                     | 0.43              |
| 4:D:330:LYS:HD3   | 4:D:330:LYS:N     | 2.34                     | 0.43              |
| 5:E:203:ILE:O     | 5:E:203:ILE:HG13  | 2.18                     | 0.43              |
| 5:E:282:PRO:O     | 5:E:388:PRO:HA    | 2.19                     | 0.43              |
| 5:E:331:ILE:CD1   | 5:E:367:PHE:HD2   | 2.32                     | 0.43              |
| 11:L:164:ARG:HB2  | 11:L:164:ARG:CZ   | 2.49                     | 0.43              |
| 20:V:103:SER:O    | 20:V:106:ARG:NE   | 2.51                     | 0.43              |
| 21:W:149:LEU:HD13 | 21:W:185:PHE:CE2  | 2.54                     | 0.43              |
| 21:W:308:LEU:HD22 | 21:W:315:MET:CE   | 2.44                     | 0.43              |
| 21:W:310:THR:HG22 | 21:W:311:THR:N    | 2.34                     | 0.43              |
| 21:W:416:GLN:OE1  | 21:W:416:GLN:HA   | 2.19                     | 0.43              |
| 23:Y:180:LEU:HD12 | 23:Y:180:LEU:C    | 2.43                     | 0.43              |
| 23:Y:228:MET:SD   | 23:Y:259:TYR:HE1  | 2.42                     | 0.43              |
| 24:Z:29:VAL:HG11  | 24:Z:33:LYS:CE    | 2.49                     | 0.43              |
| 27:c:95:MET:HE2   | 27:c:95:MET:HB2   | 1.90                     | 0.43              |
| 27:c:125:VAL:O    | 27:c:129:THR:HG22 | 2.18                     | 0.43              |
| 27:c:161:ARG:HG2  | 27:c:162:LEU:H    | 1.83                     | 0.43              |
| 28:d:35:PHE:CD1   | 28:d:35:PHE:C     | 2.97                     | 0.43              |
| 28:d:141:GLN:O    | 28:d:145:GLU:HG2  | 2.19                     | 0.43              |
| 30:f:180:GLN:CB   | 30:f:219:LYS:HD3  | 2.49                     | 0.43              |
| 30:f:601:ALA:O    | 30:f:639:LYS:HB3  | 2.19                     | 0.43              |
| 12:m:175:GLU:OE1  | 12:m:175:GLU:HA   | 2.19                     | 0.43              |
| 19:t:63:LEU:HD22  | 19:t:92:LEU:HD11  | 2.01                     | 0.43              |
| 31:F:297:ASP:OD1  | 31:F:298:SER:N    | 2.52                     | 0.43              |
| 32:U:103:LYS:HB2  | 32:U:103:LYS:NZ   | 2.33                     | 0.43              |
| 32:U:112:CYS:SG   | 32:U:113:VAL:N    | 2.91                     | 0.43              |
| 32:U:154:ALA:HB2  | 32:U:162:VAL:HG13 | 2.00                     | 0.43              |
| 32:U:428:PRO:O    | 32:U:432:SER:HB2  | 2.19                     | 0.43              |
| 32:U:623:GLY:HA3  | 32:U:658:ILE:CD1  | 2.47                     | 0.43              |
| 32:U:661:ALA:HB1  | 32:U:693:LEU:HB3  | 1.99                     | 0.43              |
| 1:A:134:ILE:HA    | 1:A:138:MET:SD    | 2.59                     | 0.43              |
| 1:A:172:VAL:CG1   | 1:A:227:ARG:HG2   | 2.49                     | 0.43              |
| 1:A:268:LYS:H     | 30:f:354:GLU:HG2  | 1.84                     | 0.43              |
| 1:A:323:ARG:HH12  | 1:A:433:ASN:HA    | 1.82                     | 0.43              |
| 1:A:424:SER:O     | 2:B:339:PRO:HB2   | 2.19                     | 0.43              |
| 2:B:130:GLU:N     | 2:B:130:GLU:CD    | 2.77                     | 0.43              |
| 2:B:364:ILE:HG22  | 2:B:395:ILE:HG21  | 1.99                     | 0.43              |
| 3:C:164:VAL:CG2   | 3:C:186:VAL:HG11  | 2.39                     | 0.43              |
| 4:D:186:THR:OG1   | 4:D:187:HIS:N     | 2.51                     | 0.43              |
| 4:D:336:PRO:CD    | 4:D:371:SER:HA    | 2.38                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:E:144:GLU:OE2   | 5:E:297:ARG:NH1   | 2.49                     | 0.43              |
| 5:E:363:VAL:HG23  | 5:E:365:GLU:N     | 2.34                     | 0.43              |
| 8:I:122:THR:O     | 8:I:122:THR:OG1   | 2.37                     | 0.43              |
| 10:K:74:ILE:CD1   | 10:K:109:VAL:HG22 | 2.49                     | 0.43              |
| 13:N:57:ALA:O     | 13:N:61:THR:OG1   | 2.36                     | 0.43              |
| 14:O:184:LEU:C    | 14:O:184:LEU:HD13 | 2.44                     | 0.43              |
| 20:V:338:LEU:HD11 | 20:V:397:ARG:HD2  | 2.01                     | 0.43              |
| 21:W:68:VAL:O     | 21:W:72:LYS:N     | 2.33                     | 0.43              |
| 21:W:142:ARG:HD3  | 21:W:142:ARG:C    | 2.44                     | 0.43              |
| 21:W:312:MET:HG3  | 21:W:369:TYR:OH   | 2.19                     | 0.43              |
| 21:W:326:MET:C    | 21:W:326:MET:SD   | 3.01                     | 0.43              |
| 22:X:340:GLU:OE1  | 22:X:340:GLU:O    | 2.36                     | 0.43              |
| 23:Y:235:ASP:HA   | 23:Y:238:GLU:OE2  | 2.19                     | 0.43              |
| 23:Y:292:TYR:O    | 23:Y:296:VAL:HG23 | 2.17                     | 0.43              |
| 24:Z:109:ASN:ND2  | 24:Z:155:PHE:HE1  | 2.17                     | 0.43              |
| 24:Z:237:LEU:HD23 | 24:Z:237:LEU:HA   | 1.81                     | 0.43              |
| 25:a:69:HIS:ND1   | 25:a:69:HIS:O     | 2.52                     | 0.43              |
| 27:c:161:ARG:HG2  | 27:c:162:LEU:N    | 2.34                     | 0.43              |
| 28:d:75:MET:O     | 28:d:78:LEU:HD12  | 2.18                     | 0.43              |
| 30:f:416:MET:N    | 30:f:416:MET:SD   | 2.92                     | 0.43              |
| 30:f:524:MET:SD   | 30:f:525:ILE:N    | 2.92                     | 0.43              |
| 30:f:569:LYS:HG2  | 30:f:573:ILE:HG21 | 2.01                     | 0.43              |
| 8:i:53:HIS:HB3    | 8:i:56:LEU:HD13   | 2.00                     | 0.43              |
| 11:l:70:ILE:HD13  | 11:l:108:LEU:CD2  | 2.48                     | 0.43              |
| 17:r:173:GLY:O    | 17:r:193:VAL:HG23 | 2.19                     | 0.43              |
| 18:s:75:TYR:CD1   | 18:s:83:MET:HG3   | 2.54                     | 0.43              |
| 32:U:19:LEU:O     | 32:U:19:LEU:HD12  | 2.19                     | 0.43              |
| 32:U:54:PHE:C     | 32:U:56:SER:N     | 2.77                     | 0.43              |
| 32:U:225:ASP:OD1  | 32:U:227:GLN:NE2  | 2.52                     | 0.43              |
| 32:U:620:GLU:OE1  | 32:U:770:TRP:HH2  | 2.02                     | 0.43              |
| 1:A:268:LYS:HE3   | 30:f:354:GLU:HB2  | 1.98                     | 0.42              |
| 1:A:332:MET:HE3   | 1:A:332:MET:HB3   | 1.82                     | 0.42              |
| 1:A:423:PHE:O     | 1:A:424:SER:O     | 2.36                     | 0.42              |
| 2:B:114:GLU:OE2   | 2:B:116:ILE:N     | 2.52                     | 0.42              |
| 2:B:120:HIS:O     | 2:B:135:ILE:HD11  | 2.18                     | 0.42              |
| 2:B:186:ASP:OD1   | 2:B:186:ASP:O     | 2.36                     | 0.42              |
| 3:C:255:GLY:HA2   | 3:C:297:ARG:HH22  | 1.83                     | 0.42              |
| 4:D:354:LEU:HA    | 4:D:354:LEU:HD12  | 1.80                     | 0.42              |
| 9:J:190:LEU:HD23  | 9:J:190:LEU:O     | 2.19                     | 0.42              |
| 10:K:121:LEU:HD21 | 11:L:77:LEU:HD21  | 2.01                     | 0.42              |
| 20:V:79:VAL:HG11  | 20:V:120:PHE:HE1  | 1.85                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 20:V:99:ARG:NE    | 29:e:17:ASP:OD2   | 2.52                     | 0.42              |
| 20:V:132:LEU:N    | 20:V:133:PRO:HD2  | 2.35                     | 0.42              |
| 20:V:256:ARG:NH1  | 20:V:256:ARG:HG2  | 2.34                     | 0.42              |
| 21:W:89:LEU:HD21  | 21:W:93:ARG:HH11  | 1.82                     | 0.42              |
| 23:Y:240:VAL:HG21 | 23:Y:260:LEU:HD11 | 2.00                     | 0.42              |
| 25:a:186:LYS:HB3  | 25:a:187:ASP:H    | 1.57                     | 0.42              |
| 27:c:55:GLY:O     | 27:c:56:LEU:HD23  | 2.18                     | 0.42              |
| 27:c:163:ILE:HD12 | 27:c:163:ILE:C    | 2.43                     | 0.42              |
| 30:f:457:ASN:HD22 | 30:f:461:PRO:HD3  | 1.83                     | 0.42              |
| 30:f:657:ILE:O    | 30:f:661:ALA:HB3  | 2.19                     | 0.42              |
| 31:F:326:VAL:HG13 | 31:F:326:VAL:O    | 2.19                     | 0.42              |
| 32:U:234:GLU:CA   | 32:U:237:VAL:HG12 | 2.45                     | 0.42              |
| 32:U:247:GLN:HA   | 32:U:913:ILE:CD1  | 2.49                     | 0.42              |
| 32:U:669:ILE:HD11 | 32:U:709:PHE:CZ   | 2.54                     | 0.42              |
| 1:A:222:LYS:HE3   | 33:A:501:ATP:O2B  | 2.19                     | 0.42              |
| 1:A:245:LEU:HA    | 1:A:256:MET:HE2   | 2.01                     | 0.42              |
| 2:B:285:ASP:OD1   | 2:B:286:GLU:HG3   | 2.19                     | 0.42              |
| 4:D:320:ALA:O     | 4:D:326:ARG:NH1   | 2.52                     | 0.42              |
| 5:E:178:THR:OG1   | 5:E:180:LYS:NZ    | 2.52                     | 0.42              |
| 5:E:299:ILE:HD12  | 5:E:299:ILE:H     | 1.84                     | 0.42              |
| 10:K:12:VAL:HG23  | 10:K:13:ASN:CG    | 2.44                     | 0.42              |
| 14:O:175:ASP:OD1  | 14:O:188:ARG:O    | 2.37                     | 0.42              |
| 20:V:467:TYR:HE2  | 23:Y:362:LYS:CE   | 2.31                     | 0.42              |
| 21:W:63:THR:HA    | 21:W:66:ILE:HD11  | 2.00                     | 0.42              |
| 22:X:377:ILE:HG22 | 23:Y:309:GLU:O    | 2.19                     | 0.42              |
| 23:Y:156:LEU:O    | 23:Y:160:ASN:OD1  | 2.36                     | 0.42              |
| 24:Z:16:LEU:HD21  | 27:c:220:LEU:HD12 | 2.00                     | 0.42              |
| 24:Z:61:ASP:OD1   | 24:Z:63:LYS:O     | 2.37                     | 0.42              |
| 24:Z:133:LEU:HD12 | 24:Z:133:LEU:HA   | 1.81                     | 0.42              |
| 24:Z:144:VAL:HA   | 24:Z:152:SER:CB   | 2.35                     | 0.42              |
| 24:Z:199:LYS:HA   | 24:Z:199:LYS:CE   | 2.48                     | 0.42              |
| 26:b:33:VAL:HG23  | 26:b:34:ASN:N     | 2.34                     | 0.42              |
| 26:b:161:ASN:HB3  | 26:b:165:GLY:O    | 2.19                     | 0.42              |
| 27:c:219:ASN:O    | 27:c:223:LYS:CD   | 2.67                     | 0.42              |
| 27:c:248:MET:HE3  | 27:c:288:VAL:HG22 | 2.01                     | 0.42              |
| 28:d:242:LEU:HD23 | 28:d:242:LEU:HA   | 1.73                     | 0.42              |
| 30:f:513:GLU:O    | 30:f:517:VAL:HG13 | 2.18                     | 0.42              |
| 30:f:607:LEU:O    | 30:f:611:GLN:OE1  | 2.37                     | 0.42              |
| 30:f:617:SER:HA   | 30:f:620:PHE:CD1  | 2.54                     | 0.42              |
| 31:F:196:GLN:HA   | 31:F:199:VAL:HG22 | 2.00                     | 0.42              |
| 32:U:169:GLU:OE2  | 32:U:176:MET:HG2  | 2.19                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 32:U:247:GLN:NE2  | 32:U:904:LYS:CB   | 2.81                     | 0.42              |
| 32:U:805:ASN:OD1  | 32:U:805:ASN:N    | 2.51                     | 0.42              |
| 1:A:176:ASP:OD1   | 1:A:176:ASP:N     | 2.52                     | 0.42              |
| 2:B:208:PRO:O     | 2:B:212:GLU:HG3   | 2.19                     | 0.42              |
| 3:C:89:VAL:HG23   | 3:C:92:GLU:CB     | 2.49                     | 0.42              |
| 3:C:224:ILE:HG13  | 3:C:225:GLY:H     | 1.84                     | 0.42              |
| 4:D:123:LEU:H     | 4:D:123:LEU:HD22  | 1.85                     | 0.42              |
| 5:E:297:ARG:HG2   | 5:E:299:ILE:HD11  | 2.01                     | 0.42              |
| 5:E:339:ASN:OD1   | 5:E:340:GLY:N     | 2.49                     | 0.42              |
| 6:G:211:LYS:HG3   | 6:G:212:PRO:N     | 2.34                     | 0.42              |
| 14:O:64:LEU:HD22  | 14:O:75:PRO:CB    | 2.49                     | 0.42              |
| 15:P:33:MET:HE1   | 17:r:166:TYR:CE1  | 2.54                     | 0.42              |
| 20:V:71:THR:C     | 20:V:75:ILE:HD12  | 2.44                     | 0.42              |
| 20:V:245:ASP:OD1  | 20:V:245:ASP:C    | 2.62                     | 0.42              |
| 20:V:256:ARG:HG2  | 20:V:256:ARG:HH11 | 1.84                     | 0.42              |
| 20:V:339:LEU:HD12 | 20:V:339:LEU:HA   | 1.84                     | 0.42              |
| 20:V:415:SER:CA   | 23:Y:346:LYS:HZ2  | 2.32                     | 0.42              |
| 21:W:375:MET:HE3  | 21:W:375:MET:HA   | 2.01                     | 0.42              |
| 21:W:403:PHE:HD1  | 21:W:404:ALA:N    | 2.17                     | 0.42              |
| 21:W:407:ASP:OD1  | 21:W:407:ASP:C    | 2.62                     | 0.42              |
| 21:W:456:GLN:HA   | 24:Z:103:LYS:CE   | 2.50                     | 0.42              |
| 25:a:304:VAL:O    | 25:a:307:VAL:HG12 | 2.20                     | 0.42              |
| 26:b:25:ARG:NH1   | 26:b:144:GLY:HA2  | 2.35                     | 0.42              |
| 26:b:79:GLN:CD    | 26:b:79:GLN:H     | 2.27                     | 0.42              |
| 27:c:49:VAL:N     | 27:c:50:PRO:CD    | 2.83                     | 0.42              |
| 30:f:245:ASN:ND2  | 30:f:259:PHE:HE2  | 2.17                     | 0.42              |
| 30:f:603:SER:N    | 30:f:639:LYS:HD3  | 2.34                     | 0.42              |
| 30:f:639:LYS:CG   | 30:f:640:LYS:HE2  | 2.49                     | 0.42              |
| 30:f:680:ARG:HA   | 30:f:715:HIS:HB2  | 2.01                     | 0.42              |
| 30:f:712:LYS:HA   | 30:f:715:HIS:CE1  | 2.54                     | 0.42              |
| 13:n:3:THR:HG21   | 13:n:164:ALA:CB   | 2.49                     | 0.42              |
| 31:F:245:LYS:HE2  | 31:F:245:LYS:H    | 1.83                     | 0.42              |
| 32:U:131:GLU:O    | 32:U:135:ASN:ND2  | 2.44                     | 0.42              |
| 32:U:792:ASN:OD1  | 32:U:796:LYS:N    | 2.52                     | 0.42              |
| 1:A:139:ARG:C     | 1:A:153:LEU:HB2   | 2.44                     | 0.42              |
| 1:A:297:ARG:NH1   | 31:F:306:VAL:HG11 | 2.34                     | 0.42              |
| 2:B:178:LYS:CD    | 2:B:178:LYS:N     | 2.83                     | 0.42              |
| 2:B:209:GLU:C     | 2:B:212:GLU:HB2   | 2.45                     | 0.42              |
| 2:B:256:ILE:O     | 2:B:256:ILE:CG1   | 2.68                     | 0.42              |
| 2:B:288:ASP:C     | 2:B:288:ASP:OD1   | 2.62                     | 0.42              |
| 3:C:24:TYR:HE2    | 32:U:153:ILE:CD1  | 2.30                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:C:173:GLU:HA    | 3:C:176:GLU:OE2   | 2.19                     | 0.42              |
| 5:E:76:GLY:HA3    | 5:E:77:PRO:HD3    | 1.76                     | 0.42              |
| 5:E:338:PHE:HZ    | 5:E:375:ALA:HB2   | 1.84                     | 0.42              |
| 8:I:99:LEU:HD12   | 15:P:64:GLN:HB3   | 2.01                     | 0.42              |
| 16:Q:164:LEU:O    | 16:Q:168:GLN:HG2  | 2.20                     | 0.42              |
| 20:V:346:LEU:HD12 | 20:V:346:LEU:O    | 2.20                     | 0.42              |
| 20:V:451:ILE:HG12 | 20:V:452:ASN:N    | 2.34                     | 0.42              |
| 21:W:74:CYS:SG    | 21:W:83:LEU:HB2   | 2.59                     | 0.42              |
| 21:W:425:LEU:HD12 | 21:W:425:LEU:HA   | 1.80                     | 0.42              |
| 23:Y:239:LYS:HB3  | 23:Y:239:LYS:NZ   | 2.26                     | 0.42              |
| 23:Y:283:LYS:HG3  | 23:Y:292:TYR:CD2  | 2.54                     | 0.42              |
| 27:c:168:MET:HG3  | 27:c:169:VAL:N    | 2.34                     | 0.42              |
| 28:d:3:GLU:OE1    | 28:d:3:GLU:CA     | 2.67                     | 0.42              |
| 30:f:228:LYS:HE2  | 30:f:228:LYS:HB2  | 1.73                     | 0.42              |
| 30:f:233:LEU:HD23 | 30:f:233:LEU:HA   | 1.77                     | 0.42              |
| 12:m:71:ARG:HH11  | 12:m:71:ARG:HG3   | 1.84                     | 0.42              |
| 12:m:75:MET:HE2   | 12:m:77:VAL:CG1   | 2.50                     | 0.42              |
| 14:o:31:ASN:OD1   | 14:o:188:ARG:NH2  | 2.52                     | 0.42              |
| 31:F:241:ALA:HB2  | 31:F:248:PHE:CE2  | 2.53                     | 0.42              |
| 32:U:136:LYS:HB2  | 32:U:136:LYS:HE3  | 1.77                     | 0.42              |
| 32:U:212:ASP:C    | 32:U:212:ASP:OD1  | 2.62                     | 0.42              |
| 32:U:650:TYR:HE2  | 32:U:685:GLN:HE21 | 1.67                     | 0.42              |
| 1:A:135:GLU:OE1   | 1:A:138:MET:HE1   | 2.19                     | 0.42              |
| 2:B:253:SER:HB2   | 3:C:275:GLU:OE2   | 2.20                     | 0.42              |
| 2:B:288:ASP:O     | 2:B:288:ASP:OD1   | 2.37                     | 0.42              |
| 2:B:397:ALA:CA    | 2:B:400:THR:HG22  | 2.49                     | 0.42              |
| 2:B:412:MET:CE    | 2:B:413:LYS:HG3   | 2.49                     | 0.42              |
| 3:C:115:ALA:C     | 3:C:116:LEU:HD22  | 2.45                     | 0.42              |
| 3:C:224:ILE:HD12  | 3:C:233:GLU:OE1   | 2.20                     | 0.42              |
| 3:C:226:GLU:H     | 3:C:226:GLU:HG3   | 1.63                     | 0.42              |
| 3:C:250:GLU:HG2   | 3:C:251:ILE:H     | 1.84                     | 0.42              |
| 4:D:125:LYS:HB3   | 4:D:126:PRO:HD2   | 2.01                     | 0.42              |
| 4:D:415:GLU:OE1   | 4:D:415:GLU:CA    | 2.67                     | 0.42              |
| 5:E:116:ASP:OD1   | 5:E:117:PRO:CD    | 2.68                     | 0.42              |
| 5:E:245:GLU:O     | 5:E:245:GLU:CG    | 2.67                     | 0.42              |
| 10:K:231:LYS:O    | 10:K:235:GLU:HG3  | 2.19                     | 0.42              |
| 14:O:3:THR:HG23   | 14:O:3:THR:O      | 2.18                     | 0.42              |
| 14:O:192:VAL:O    | 14:O:192:VAL:HG12 | 2.19                     | 0.42              |
| 15:P:36:THR:O     | 15:P:36:THR:CG2   | 2.67                     | 0.42              |
| 15:P:141:CYS:HB3  | 15:P:177:ASP:HB2  | 2.02                     | 0.42              |
| 16:Q:13:VAL:O     | 16:Q:13:VAL:HG13  | 2.19                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 20:V:79:VAL:HG11  | 20:V:120:PHE:CE1  | 2.54                     | 0.42              |
| 20:V:338:LEU:O    | 20:V:401:ASN:ND2  | 2.52                     | 0.42              |
| 21:W:326:MET:SD   | 21:W:327:GLU:N    | 2.92                     | 0.42              |
| 21:W:373:ILE:HD12 | 21:W:374:THR:N    | 2.35                     | 0.42              |
| 22:X:171:LEU:HD11 | 22:X:210:LEU:HA   | 2.00                     | 0.42              |
| 23:Y:118:GLU:O    | 23:Y:122:THR:HG22 | 2.20                     | 0.42              |
| 23:Y:236:LEU:HB3  | 23:Y:241:ILE:HD11 | 2.02                     | 0.42              |
| 25:a:77:VAL:CG1   | 25:a:113:LEU:HD13 | 2.48                     | 0.42              |
| 27:c:63:ASP:OD2   | 32:U:541:HIS:HA   | 2.19                     | 0.42              |
| 28:d:52:ARG:O     | 28:d:56:GLU:HG3   | 2.20                     | 0.42              |
| 28:d:235:THR:CA   | 28:d:238:PRO:HD2  | 2.49                     | 0.42              |
| 30:f:655:LEU:HA   | 30:f:659:LEU:HD12 | 2.00                     | 0.42              |
| 30:f:671:ALA:O    | 30:f:674:THR:HG22 | 2.19                     | 0.42              |
| 30:f:821:LEU:HD21 | 30:f:882:LEU:CD2  | 2.49                     | 0.42              |
| 14:o:135:ALA:HB1  | 14:o:159:ALA:HB1  | 2.02                     | 0.42              |
| 19:t:43:MET:SD    | 19:t:64:LYS:HG2   | 2.59                     | 0.42              |
| 31:F:187:ASP:O    | 31:F:187:ASP:OD1  | 2.37                     | 0.42              |
| 32:U:465:LEU:HB3  | 32:U:496:LEU:HD21 | 2.01                     | 0.42              |
| 32:U:775:LEU:O    | 32:U:775:LEU:CD2  | 2.67                     | 0.42              |
| 1:A:153:LEU:CD2   | 1:A:154:PRO:HD2   | 2.48                     | 0.42              |
| 2:B:94:GLU:HG3    | 2:B:98:LYS:HZ3    | 1.84                     | 0.42              |
| 2:B:133:VAL:HB    | 2:B:158:ALA:HA    | 2.01                     | 0.42              |
| 2:B:139:VAL:HG11  | 2:B:159:VAL:HG12  | 2.01                     | 0.42              |
| 2:B:201:VAL:HG11  | 2:B:328:ILE:HD11  | 2.01                     | 0.42              |
| 2:B:347:ILE:O     | 2:B:347:ILE:CG1   | 2.67                     | 0.42              |
| 2:B:355:LEU:HD23  | 2:B:355:LEU:HA    | 1.84                     | 0.42              |
| 4:D:133:HIS:HB3   | 4:D:136:SER:O     | 2.19                     | 0.42              |
| 5:E:241:ARG:N     | 31:F:304:ARG:HH12 | 2.06                     | 0.42              |
| 5:E:328:TYR:O     | 5:E:332:VAL:HG23  | 2.20                     | 0.42              |
| 7:H:159:ALA:O     | 8:I:55:LEU:HD13   | 2.20                     | 0.42              |
| 12:M:108:LEU:HD23 | 12:M:147:GLN:HB3  | 2.00                     | 0.42              |
| 21:W:87:ILE:HD11  | 21:W:104:MET:CE   | 2.50                     | 0.42              |
| 21:W:370:TYR:CE1  | 25:a:326:GLU:OE1  | 2.72                     | 0.42              |
| 22:X:422:THR:HA   | 24:Z:283:ARG:NE   | 2.34                     | 0.42              |
| 23:Y:214:MET:HE1  | 23:Y:222:TYR:CG   | 2.54                     | 0.42              |
| 24:Z:134:PRO:HG2  | 27:c:220:LEU:HD13 | 2.02                     | 0.42              |
| 24:Z:165:GLU:HG3  | 24:Z:166:GLU:H    | 1.83                     | 0.42              |
| 25:a:186:LYS:C    | 25:a:188:LEU:HD22 | 2.44                     | 0.42              |
| 26:b:21:PHE:HA    | 26:b:177:PRO:HA   | 2.00                     | 0.42              |
| 28:d:71:PHE:HZ    | 28:d:101:LEU:HD22 | 1.84                     | 0.42              |
| 28:d:89:LEU:HD13  | 28:d:91:GLU:O     | 2.20                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 28:d:155:LYS:HD3  | 28:d:167:ILE:CG2  | 2.49                     | 0.42              |
| 30:f:222:ASP:OD1  | 30:f:222:ASP:N    | 2.49                     | 0.42              |
| 30:f:320:ILE:HA   | 30:f:324:VAL:HG21 | 2.00                     | 0.42              |
| 30:f:513:GLU:OE2  | 30:f:514:VAL:HG23 | 2.19                     | 0.42              |
| 30:f:631:LYS:O    | 30:f:635:LYS:HD3  | 2.19                     | 0.42              |
| 31:F:168:TYR:HD2  | 31:F:173:LYS:HZ1  | 1.68                     | 0.42              |
| 31:F:198:LEU:CD1  | 31:F:223:VAL:HG11 | 2.44                     | 0.42              |
| 1:A:365:GLU:C     | 1:A:366:ARG:HD3   | 2.44                     | 0.42              |
| 2:B:68:ILE:HD12   | 2:B:68:ILE:N      | 2.31                     | 0.42              |
| 3:C:138:MET:HA    | 3:C:138:MET:CE    | 2.50                     | 0.42              |
| 3:C:391:MET:HE2   | 3:C:391:MET:HB2   | 1.79                     | 0.42              |
| 4:D:98:GLN:OE1    | 4:D:98:GLN:HA     | 2.18                     | 0.42              |
| 4:D:339:ARG:HH22  | 4:D:343:LEU:CG    | 2.31                     | 0.42              |
| 4:D:392:TYR:CZ    | 21:W:136:ILE:HD12 | 2.54                     | 0.42              |
| 5:E:122:MET:HE1   | 5:E:218:MET:SD    | 2.60                     | 0.42              |
| 5:E:197:LYS:HE2   | 31:F:320:PHE:CD1  | 2.55                     | 0.42              |
| 5:E:261:LEU:HD21  | 5:E:288:ALA:CB    | 2.49                     | 0.42              |
| 16:Q:15:VAL:HG23  | 16:Q:35:MET:HE2   | 2.01                     | 0.42              |
| 21:W:359:VAL:CG2  | 21:W:382:LEU:HD22 | 2.49                     | 0.42              |
| 22:X:114:ILE:O    | 22:X:118:LYS:HG3  | 2.19                     | 0.42              |
| 22:X:397:TYR:HE2  | 23:Y:369:THR:HG21 | 1.85                     | 0.42              |
| 25:a:180:LEU:HD11 | 25:a:222:LEU:CD2  | 2.50                     | 0.42              |
| 26:b:16:MET:HG3   | 26:b:16:MET:O     | 2.18                     | 0.42              |
| 26:b:161:ASN:O    | 26:b:165:GLY:N    | 2.50                     | 0.42              |
| 28:d:95:MET:CA    | 28:d:95:MET:CE    | 2.92                     | 0.42              |
| 30:f:304:PHE:CZ   | 30:f:311:VAL:HG11 | 2.54                     | 0.42              |
| 30:f:507:ASP:OD1  | 30:f:509:LYS:HG2  | 2.19                     | 0.42              |
| 12:m:50:GLU:OE2   | 12:m:201:HIS:ND1  | 2.45                     | 0.42              |
| 18:s:83:MET:HE2   | 18:s:88:ILE:HG12  | 2.01                     | 0.42              |
| 32:U:458:ILE:HD11 | 32:U:485:ALA:HB2  | 2.02                     | 0.42              |
| 32:U:789:ILE:HD12 | 32:U:911:ILE:HD13 | 2.02                     | 0.42              |
| 1:A:121:PHE:CD2   | 1:A:121:PHE:N     | 2.88                     | 0.42              |
| 1:A:347:ASP:OD1   | 1:A:347:ASP:N     | 2.39                     | 0.42              |
| 2:B:136:LEU:HD13  | 2:B:136:LEU:HA    | 1.92                     | 0.42              |
| 2:B:156:VAL:O     | 2:B:156:VAL:HG12  | 2.19                     | 0.42              |
| 2:B:223:ILE:HA    | 2:B:329:MET:O     | 2.20                     | 0.42              |
| 2:B:333:ARG:O     | 2:B:336:THR:HG22  | 2.19                     | 0.42              |
| 2:B:359:LYS:NZ    | 2:B:359:LYS:HB3   | 2.35                     | 0.42              |
| 3:C:19:GLY:HA3    | 32:U:146:LYS:HE3  | 1.99                     | 0.42              |
| 3:C:214:VAL:CG1   | 3:C:248:MET:HG2   | 2.50                     | 0.42              |
| 3:C:250:GLU:CG    | 3:C:269:VAL:HG21  | 2.40                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:C:359:VAL:C     | 3:C:361:GLY:H     | 2.27                     | 0.42              |
| 4:D:125:LYS:HE2   | 4:D:125:LYS:HB2   | 1.80                     | 0.42              |
| 4:D:227:PHE:CD1   | 4:D:261:ILE:HB    | 2.55                     | 0.42              |
| 4:D:244:PRO:HA    | 4:D:247:VAL:HG12  | 2.02                     | 0.42              |
| 4:D:290:LEU:HD23  | 4:D:290:LEU:HA    | 1.81                     | 0.42              |
| 5:E:66:GLU:HB3    | 5:E:67:GLU:OE2    | 2.20                     | 0.42              |
| 5:E:342:ASP:O     | 5:E:346:VAL:HG23  | 2.19                     | 0.42              |
| 12:M:179:LEU:O    | 12:M:180:GLN:C    | 2.63                     | 0.42              |
| 18:S:80:ASN:OD1   | 18:S:80:ASN:N     | 2.52                     | 0.42              |
| 20:V:230:PHE:C    | 20:V:230:PHE:CD1  | 2.97                     | 0.42              |
| 20:V:232:HIS:CE1  | 20:V:254:LEU:HD21 | 2.55                     | 0.42              |
| 20:V:349:ARG:HA   | 20:V:354:LYS:HD3  | 2.02                     | 0.42              |
| 20:V:407:VAL:O    | 20:V:410:ILE:HG22 | 2.20                     | 0.42              |
| 21:W:45:GLU:HA    | 21:W:48:LEU:HD23  | 2.01                     | 0.42              |
| 21:W:121:LYS:HD2  | 21:W:122:LEU:N    | 2.35                     | 0.42              |
| 21:W:254:PRO:CA   | 21:W:262:LYS:HZ3  | 2.33                     | 0.42              |
| 22:X:358:LYS:HA   | 22:X:361:VAL:CG1  | 2.49                     | 0.42              |
| 22:X:393:VAL:O    | 22:X:393:VAL:HG22 | 2.20                     | 0.42              |
| 23:Y:117:LYS:HB2  | 23:Y:121:LEU:HD11 | 2.02                     | 0.42              |
| 23:Y:281:GLU:OE1  | 23:Y:282:MET:N    | 2.52                     | 0.42              |
| 23:Y:379:ARG:HG2  | 23:Y:379:ARG:NH1  | 2.32                     | 0.42              |
| 24:Z:34:ARG:HH12  | 24:Z:102:HIS:HB2  | 1.84                     | 0.42              |
| 25:a:68:GLU:HG2   | 25:a:70:ARG:HG2   | 2.01                     | 0.42              |
| 25:a:166:ILE:O    | 25:a:166:ILE:HG13 | 2.20                     | 0.42              |
| 25:a:288:HIS:O    | 25:a:289:ARG:C    | 2.62                     | 0.42              |
| 26:b:16:MET:O     | 26:b:16:MET:CG    | 2.68                     | 0.42              |
| 26:b:101:GLN:HG3  | 26:b:102:GLY:H    | 1.85                     | 0.42              |
| 26:b:110:ILE:CD1  | 26:b:110:ILE:O    | 2.64                     | 0.42              |
| 26:b:128:ALA:HB2  | 26:b:156:PHE:CD1  | 2.55                     | 0.42              |
| 26:b:135:LYS:N    | 26:b:135:LYS:CD   | 2.82                     | 0.42              |
| 27:c:208:ARG:C    | 27:c:208:ARG:CD   | 2.93                     | 0.42              |
| 27:c:261:GLU:OE1  | 27:c:261:GLU:N    | 2.52                     | 0.42              |
| 28:d:52:ARG:HA    | 28:d:81:TYR:CE2   | 2.54                     | 0.42              |
| 28:d:53:ASP:O     | 28:d:57:ILE:HG22  | 2.20                     | 0.42              |
| 29:e:19:PHE:N     | 29:e:19:PHE:CD1   | 2.83                     | 0.42              |
| 29:e:37:HIS:O     | 29:e:37:HIS:ND1   | 2.53                     | 0.42              |
| 30:f:32:GLU:HB3   | 30:f:33:ARG:HH21  | 1.85                     | 0.42              |
| 30:f:505:MET:HE1  | 30:f:519:ALA:HA   | 2.01                     | 0.42              |
| 12:m:35:THR:HG21  | 12:m:200:VAL:HG21 | 2.01                     | 0.42              |
| 12:m:51:LYS:NZ    | 12:m:62:SER:O     | 2.49                     | 0.42              |
| 19:t:189:ILE:HD12 | 19:t:203:LEU:HD12 | 2.01                     | 0.42              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 31:F:198:LEU:HD22 | 31:F:236:LEU:HG  | 2.02                     | 0.42              |
| 31:F:221:LYS:NZ   | 31:F:327:LYS:HE3 | 2.34                     | 0.42              |
| 31:F:358:ASN:O    | 31:F:362:ARG:NH1 | 2.50                     | 0.42              |
| 31:F:382:GLU:OE1  | 31:F:382:GLU:CA  | 2.63                     | 0.42              |
| 32:U:805:ASN:OD1  | 32:U:893:THR:OG1 | 2.36                     | 0.42              |
| 1:A:110:LYS:HE3   | 1:A:110:LYS:HB2  | 1.81                     | 0.42              |
| 1:A:277:ILE:HG23  | 1:A:277:ILE:O    | 2.20                     | 0.42              |
| 2:B:116:ILE:CG1   | 2:B:117:ASP:H    | 2.33                     | 0.42              |
| 2:B:150:VAL:HG12  | 2:B:152:LEU:CD2  | 2.50                     | 0.42              |
| 2:B:249:ARG:HG3   | 2:B:283:PHE:HD2  | 1.85                     | 0.42              |
| 3:C:49:ARG:NE     | 4:D:64:GLU:OE1   | 2.46                     | 0.42              |
| 3:C:75:GLU:OE1    | 3:C:76:VAL:N     | 2.53                     | 0.42              |
| 3:C:165:ILE:CD1   | 3:C:290:LYS:HD3  | 2.50                     | 0.42              |
| 3:C:373:GLU:OE1   | 3:C:373:GLU:O    | 2.38                     | 0.42              |
| 3:C:392:GLN:OE1   | 22:X:199:ALA:HB2 | 2.20                     | 0.42              |
| 4:D:412:GLN:O     | 4:D:413:GLU:HB2  | 2.19                     | 0.42              |
| 5:E:135:ILE:HD12  | 5:E:183:LEU:HB2  | 2.02                     | 0.42              |
| 5:E:158:LEU:HD22  | 21:W:137:TYR:HE2 | 1.85                     | 0.42              |
| 5:E:300:HIS:ND1   | 5:E:300:HIS:C    | 2.75                     | 0.42              |
| 5:E:304:PRO:CD    | 5:E:339:ASN:O    | 2.68                     | 0.42              |
| 6:G:50:ILE:HG21   | 6:G:79:VAL:HB    | 2.02                     | 0.42              |
| 6:G:201:CYS:O     | 6:G:205:VAL:HG13 | 2.20                     | 0.42              |
| 11:L:200:PRO:O    | 11:L:202:GLU:N   | 2.53                     | 0.42              |
| 14:O:36:HIS:CB    | 14:O:57:THR:HG21 | 2.50                     | 0.42              |
| 20:V:83:GLU:HA    | 20:V:86:VAL:CG2  | 2.49                     | 0.42              |
| 21:W:282:GLU:HA   | 21:W:282:GLU:OE1 | 2.20                     | 0.42              |
| 21:W:417:ARG:H    | 21:W:417:ARG:HG2 | 1.71                     | 0.42              |
| 24:Z:164:ALA:HB1  | 24:Z:169:GLU:HG2 | 1.98                     | 0.42              |
| 25:a:48:PRO:HG2   | 25:a:51:ALA:HB2  | 2.02                     | 0.42              |
| 25:a:325:ASP:OD1  | 25:a:325:ASP:N   | 2.52                     | 0.42              |
| 26:b:6:THR:O      | 26:b:49:VAL:HA   | 2.20                     | 0.42              |
| 26:b:119:ASP:HB2  | 26:b:124:LEU:CD2 | 2.49                     | 0.42              |
| 26:b:134:GLU:O    | 26:b:135:LYS:C   | 2.62                     | 0.42              |
| 26:b:153:LEU:O    | 26:b:156:PHE:N   | 2.47                     | 0.42              |
| 26:b:188:ILE:H    | 26:b:188:ILE:CD1 | 2.30                     | 0.42              |
| 27:c:53:VAL:O     | 27:c:113:HIS:HA  | 2.20                     | 0.42              |
| 28:d:1:MET:O      | 28:d:1:MET:HG2   | 2.20                     | 0.42              |
| 28:d:75:MET:HA    | 28:d:78:LEU:CD1  | 2.48                     | 0.42              |
| 29:e:21:GLU:HG3   | 29:e:22:PHE:N    | 2.34                     | 0.42              |
| 30:f:297:MET:HE1  | 30:f:456:ARG:NH2 | 2.34                     | 0.42              |
| 30:f:519:ALA:HA   | 30:f:522:CYS:SG  | 2.59                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:h:218:ARG:NH2   | 7:h:224:GLU:OE1   | 2.45                     | 0.42              |
| 17:r:5:LEU:C      | 17:r:5:LEU:HD12   | 2.45                     | 0.42              |
| 32:U:358:ASP:OD1  | 32:U:359:ALA:N    | 2.52                     | 0.42              |
| 32:U:549:ALA:HA   | 32:U:581:SER:OG   | 2.20                     | 0.42              |
| 32:U:552:ILE:CD1  | 32:U:566:LEU:HD21 | 2.42                     | 0.42              |
| 1:A:123:VAL:HG12  | 1:A:147:TYR:O     | 2.19                     | 0.42              |
| 1:A:170:PRO:CB    | 1:A:227:ARG:HG3   | 2.50                     | 0.42              |
| 1:A:255:ARG:NH1   | 1:A:255:ARG:HB3   | 2.35                     | 0.42              |
| 1:A:263:MET:HG2   | 1:A:267:LYS:HE2   | 2.01                     | 0.42              |
| 1:A:301:GLU:OE1   | 1:A:305:GLN:HG3   | 2.20                     | 0.42              |
| 1:A:394:MET:HE2   | 2:B:219:PRO:CD    | 2.49                     | 0.42              |
| 2:B:156:VAL:O     | 2:B:157:HIS:C     | 2.62                     | 0.42              |
| 2:B:234:LEU:HD12  | 2:B:234:LEU:O     | 2.20                     | 0.42              |
| 3:C:137:LEU:HD23  | 3:C:138:MET:CE    | 2.46                     | 0.42              |
| 4:D:230:VAL:HG22  | 4:D:264:ILE:HA    | 2.00                     | 0.42              |
| 4:D:264:ILE:HG21  | 4:D:267:ILE:HD13  | 2.02                     | 0.42              |
| 4:D:303:VAL:O     | 4:D:303:VAL:HG13  | 2.18                     | 0.42              |
| 5:E:264:MET:SD    | 5:E:275:MET:SD    | 3.17                     | 0.42              |
| 10:K:20:ARG:NH1   | 31:F:433:ALA:O    | 2.52                     | 0.42              |
| 10:K:141:LEU:HD12 | 10:K:156:MET:CE   | 2.50                     | 0.42              |
| 13:N:93:GLU:OE2   | 13:N:93:GLU:HA    | 2.19                     | 0.42              |
| 21:W:55:ARG:HH12  | 21:W:93:ARG:HB3   | 1.84                     | 0.42              |
| 21:W:131:VAL:HG13 | 21:W:132:THR:N    | 2.34                     | 0.42              |
| 21:W:265:GLN:HG2  | 21:W:336:PRO:HG3  | 2.01                     | 0.42              |
| 21:W:291:SER:OG   | 21:W:305:LEU:HD21 | 2.20                     | 0.42              |
| 21:W:359:VAL:HG22 | 21:W:382:LEU:HD13 | 2.01                     | 0.42              |
| 21:W:382:LEU:C    | 21:W:384:LEU:HD12 | 2.45                     | 0.42              |
| 23:Y:279:GLU:OE1  | 23:Y:292:TYR:HD2  | 2.02                     | 0.42              |
| 23:Y:308:LEU:HD11 | 23:Y:314:LEU:HD21 | 2.01                     | 0.42              |
| 24:Z:250:TYR:CA   | 24:Z:253:THR:HG22 | 2.46                     | 0.42              |
| 25:a:37:LEU:HA    | 25:a:40:GLN:HE22  | 1.84                     | 0.42              |
| 25:a:61:GLU:HA    | 25:a:64:ILE:CD1   | 2.50                     | 0.42              |
| 25:a:77:VAL:O     | 25:a:81:LEU:HD23  | 2.19                     | 0.42              |
| 25:a:79:ILE:CG2   | 25:a:80:ILE:CD1   | 2.98                     | 0.42              |
| 25:a:90:PRO:CB    | 25:a:121:LEU:HD11 | 2.43                     | 0.42              |
| 25:a:156:TYR:O    | 25:a:160:SER:HB3  | 2.19                     | 0.42              |
| 25:a:244:ASN:C    | 25:a:272:ILE:HD11 | 2.45                     | 0.42              |
| 27:c:120:CYS:HA   | 27:c:144:VAL:HG11 | 2.01                     | 0.42              |
| 28:d:50:LEU:H     | 28:d:50:LEU:CD2   | 2.28                     | 0.42              |
| 30:f:127:SER:HA   | 30:f:131:MET:SD   | 2.60                     | 0.42              |
| 30:f:209:MET:HE2  | 30:f:213:GLN:HE21 | 1.85                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 30:f:241:PRO:HA   | 30:f:244:GLU:OE1  | 2.20                     | 0.42              |
| 30:f:270:LEU:HB2  | 30:f:271:MET:HE1  | 1.98                     | 0.42              |
| 30:f:557:TRP:C    | 30:f:560:LEU:HG   | 2.45                     | 0.42              |
| 30:f:827:PRO:HB3  | 30:f:860:LYS:CE   | 2.50                     | 0.42              |
| 9:j:93:SER:O      | 9:j:97:THR:HG23   | 2.20                     | 0.42              |
| 15:p:93:LEU:O     | 15:p:93:LEU:HD23  | 2.19                     | 0.42              |
| 18:s:12:ILE:HG21  | 18:s:109:ILE:HB   | 2.02                     | 0.42              |
| 18:s:186:ASP:OD1  | 18:s:187:VAL:N    | 2.53                     | 0.42              |
| 32:U:208:LEU:HD12 | 32:U:209:GLU:H    | 1.85                     | 0.42              |
| 32:U:475:HIS:CE1  | 32:U:511:ALA:H    | 2.38                     | 0.42              |
| 32:U:475:HIS:HA   | 32:U:511:ALA:CB   | 2.50                     | 0.42              |
| 1:A:87:LEU:HA     | 1:A:87:LEU:HD23   | 1.77                     | 0.41              |
| 1:A:183:GLN:HG3   | 1:A:341:ILE:HG23  | 2.02                     | 0.41              |
| 2:B:175:LYS:HD2   | 2:B:175:LYS:HA    | 1.90                     | 0.41              |
| 2:B:175:LYS:O     | 2:B:176:VAL:C     | 2.63                     | 0.41              |
| 2:B:393:ALA:HB1   | 3:C:307:ARG:NH1   | 2.35                     | 0.41              |
| 3:C:76:VAL:O      | 3:C:76:VAL:CG1    | 2.66                     | 0.41              |
| 4:D:77:GLU:HG2    | 27:c:152:LYS:HG3  | 2.02                     | 0.41              |
| 4:D:145:PRO:HB2   | 4:D:256:GLU:HG3   | 2.02                     | 0.41              |
| 4:D:168:GLY:N     | 33:D:501:ATP:HN62 | 2.18                     | 0.41              |
| 4:D:200:ARG:NH1   | 4:D:200:ARG:CG    | 2.81                     | 0.41              |
| 5:E:66:GLU:OE1    | 5:E:66:GLU:HA     | 2.19                     | 0.41              |
| 5:E:291:ARG:HG2   | 5:E:292:PRO:O     | 2.20                     | 0.41              |
| 7:H:74:VAL:HG22   | 7:H:75:TYR:N      | 2.34                     | 0.41              |
| 20:V:236:ARG:O    | 20:V:240:LEU:HD23 | 2.19                     | 0.41              |
| 20:V:258:TYR:CE1  | 20:V:266:GLN:HG3  | 2.54                     | 0.41              |
| 20:V:496:PHE:H    | 20:V:497:PRO:HD2  | 1.82                     | 0.41              |
| 21:W:62:SER:O     | 21:W:66:ILE:HG12  | 2.20                     | 0.41              |
| 21:W:94:ARG:HA    | 21:W:94:ARG:NE    | 2.35                     | 0.41              |
| 22:X:262:ASN:C    | 22:X:264:PRO:HD3  | 2.45                     | 0.41              |
| 24:Z:73:ASP:HB2   | 26:b:63:THR:CG2   | 2.50                     | 0.41              |
| 24:Z:256:GLN:HG2  | 27:c:237:HIS:HE1  | 1.84                     | 0.41              |
| 25:a:31:LYS:O     | 25:a:32:LYS:HB2   | 2.19                     | 0.41              |
| 26:b:7:MET:CE     | 26:b:52:ILE:CD1   | 2.97                     | 0.41              |
| 27:c:68:ARG:O     | 27:c:68:ARG:HG3   | 2.19                     | 0.41              |
| 28:d:44:THR:OG1   | 28:d:44:THR:O     | 2.38                     | 0.41              |
| 28:d:55:LEU:HD12  | 28:d:55:LEU:HA    | 1.76                     | 0.41              |
| 28:d:181:CYS:HA   | 28:d:184:LYS:NZ   | 2.35                     | 0.41              |
| 30:f:346:ASP:OD1  | 30:f:346:ASP:N    | 2.53                     | 0.41              |
| 30:f:474:SER:HB3  | 30:f:477:MET:CE   | 2.50                     | 0.41              |
| 30:f:670:MET:HA   | 30:f:672:LEU:CD1  | 2.49                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 15:p:57:THR:HG23  | 15:p:58:ASP:N     | 2.35                     | 0.41              |
| 31:F:366:MET:CE   | 31:F:399:VAL:HG11 | 2.50                     | 0.41              |
| 31:F:379:VAL:O    | 31:F:379:VAL:HG12 | 2.20                     | 0.41              |
| 32:U:505:ASP:OD1  | 32:U:506:ALA:N    | 2.52                     | 0.41              |
| 32:U:537:GLN:OE1  | 32:U:537:GLN:HA   | 2.19                     | 0.41              |
| 1:A:99:THR:OG1    | 1:A:113:ILE:HG12  | 2.20                     | 0.41              |
| 1:A:108:ASP:CB    | 1:A:109:PRO:CD    | 2.97                     | 0.41              |
| 1:A:397:ILE:CG1   | 2:B:210:TYR:HB3   | 2.50                     | 0.41              |
| 2:B:209:GLU:O     | 2:B:212:GLU:HB2   | 2.21                     | 0.41              |
| 2:B:245:ALA:HB1   | 2:B:279:PRO:O     | 2.19                     | 0.41              |
| 3:C:44:ARG:NH1    | 3:C:44:ARG:C      | 2.76                     | 0.41              |
| 4:D:226:ALA:O     | 4:D:260:ALA:HA    | 2.19                     | 0.41              |
| 5:E:242:ARG:NE    | 5:E:286:ASP:OD2   | 2.52                     | 0.41              |
| 5:E:353:PHE:HE2   | 5:E:369:LYS:O     | 2.03                     | 0.41              |
| 12:M:17:ASP:OD1   | 12:M:17:ASP:N     | 2.45                     | 0.41              |
| 14:O:136:MET:O    | 14:O:140:GLU:HG2  | 2.20                     | 0.41              |
| 21:W:88:MET:HE3   | 21:W:88:MET:HB3   | 1.84                     | 0.41              |
| 21:W:378:MET:CE   | 21:W:393:LEU:HD22 | 2.50                     | 0.41              |
| 22:X:171:LEU:HD23 | 22:X:171:LEU:HA   | 1.90                     | 0.41              |
| 22:X:256:LEU:HD13 | 22:X:319:ILE:HD13 | 1.95                     | 0.41              |
| 22:X:327:TYR:CD2  | 22:X:327:TYR:C    | 2.97                     | 0.41              |
| 23:Y:45:VAL:HG23  | 23:Y:46:ARG:N     | 2.35                     | 0.41              |
| 23:Y:117:LYS:HE2  | 23:Y:151:TYR:HD1  | 1.81                     | 0.41              |
| 23:Y:149:LEU:CA   | 23:Y:157:ILE:HD11 | 2.50                     | 0.41              |
| 23:Y:193:ASP:OD2  | 23:Y:193:ASP:C    | 2.64                     | 0.41              |
| 23:Y:205:VAL:HA   | 23:Y:219:PHE:HE1  | 1.84                     | 0.41              |
| 24:Z:39:LEU:HD23  | 24:Z:39:LEU:HA    | 1.83                     | 0.41              |
| 24:Z:88:ARG:HD2   | 24:Z:88:ARG:C     | 2.43                     | 0.41              |
| 24:Z:131:LEU:HD23 | 24:Z:132:GLY:H    | 1.85                     | 0.41              |
| 25:a:34:TRP:HZ3   | 26:b:19:GLY:N     | 2.17                     | 0.41              |
| 26:b:19:GLY:N     | 26:b:24:THR:HG22  | 2.35                     | 0.41              |
| 26:b:120:ASN:OD1  | 26:b:120:ASN:C    | 2.63                     | 0.41              |
| 28:d:25:ARG:HG3   | 28:d:54:ILE:HD13  | 2.01                     | 0.41              |
| 28:d:34:ASN:OD1   | 28:d:34:ASN:N     | 2.40                     | 0.41              |
| 28:d:130:ASN:C    | 28:d:132:TYR:N    | 2.77                     | 0.41              |
| 28:d:171:LEU:N    | 28:d:171:LEU:HD23 | 2.34                     | 0.41              |
| 30:f:65:GLU:HB3   | 30:f:97:LYS:CE    | 2.49                     | 0.41              |
| 30:f:83:ARG:HG3   | 30:f:84:SER:N     | 2.35                     | 0.41              |
| 30:f:524:MET:HE2  | 30:f:524:MET:C    | 2.45                     | 0.41              |
| 30:f:736:THR:OG1  | 30:f:746:ARG:NH2  | 2.49                     | 0.41              |
| 30:f:746:ARG:HA   | 30:f:750:GLN:OE1  | 2.20                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 30:f:760:PHE:HD1  | 30:f:806:VAL:HG11 | 1.82                     | 0.41              |
| 9:j:5:ARG:O       | 9:j:123:GLY:N     | 2.51                     | 0.41              |
| 10:k:180:SER:HB2  | 10:k:201:ILE:HD13 | 2.02                     | 0.41              |
| 31:F:405:MET:HE3  | 31:F:405:MET:HB3  | 1.86                     | 0.41              |
| 32:U:61:ALA:HA    | 32:U:64:ALA:HB3   | 2.02                     | 0.41              |
| 32:U:449:ILE:HG12 | 32:U:450:HIS:CD2  | 2.50                     | 0.41              |
| 32:U:514:LEU:CD1  | 32:U:550:VAL:HB   | 2.50                     | 0.41              |
| 32:U:524:LYS:O    | 32:U:524:LYS:HG3  | 2.20                     | 0.41              |
| 1:A:222:LYS:N     | 33:A:501:ATP:O2B  | 2.54                     | 0.41              |
| 1:A:309:PHE:CE1   | 31:F:238:ARG:HG3  | 2.55                     | 0.41              |
| 2:B:170:LEU:HD11  | 2:B:174:MET:CE    | 2.49                     | 0.41              |
| 2:B:212:GLU:CG    | 30:f:845:ARG:HG3  | 2.49                     | 0.41              |
| 4:D:154:LEU:O     | 4:D:155:THR:C     | 2.63                     | 0.41              |
| 4:D:172:ILE:HG23  | 4:D:173:GLN:OE1   | 2.21                     | 0.41              |
| 4:D:339:ARG:HH12  | 4:D:343:LEU:HD12  | 1.86                     | 0.41              |
| 5:E:173:TYR:CG    | 5:E:282:PRO:HG3   | 2.55                     | 0.41              |
| 5:E:322:LYS:HE3   | 5:E:322:LYS:HB2   | 1.84                     | 0.41              |
| 9:J:144:LEU:HD13  | 9:J:145:TYR:N     | 2.35                     | 0.41              |
| 13:N:136:ILE:O    | 13:N:140:VAL:HG13 | 2.20                     | 0.41              |
| 16:Q:96:THR:O     | 16:Q:96:THR:OG1   | 2.26                     | 0.41              |
| 20:V:349:ARG:CG   | 20:V:354:LYS:HE2  | 2.50                     | 0.41              |
| 21:W:74:CYS:HB3   | 21:W:83:LEU:HD13  | 2.01                     | 0.41              |
| 21:W:112:VAL:HG23 | 21:W:120:ILE:CG1  | 2.49                     | 0.41              |
| 21:W:169:LEU:HG   | 21:W:173:THR:OG1  | 2.20                     | 0.41              |
| 21:W:229:LEU:H    | 21:W:229:LEU:CD2  | 2.27                     | 0.41              |
| 22:X:200:ILE:N    | 22:X:200:ILE:CD1  | 2.84                     | 0.41              |
| 22:X:339:ILE:C    | 22:X:341:PRO:HD2  | 2.45                     | 0.41              |
| 22:X:358:LYS:HA   | 22:X:361:VAL:HG12 | 2.02                     | 0.41              |
| 23:Y:178:ASN:HD22 | 23:Y:178:ASN:HA   | 1.56                     | 0.41              |
| 23:Y:236:LEU:HD22 | 23:Y:240:VAL:CG2  | 2.50                     | 0.41              |
| 23:Y:275:LEU:CA   | 23:Y:278:VAL:HG12 | 2.50                     | 0.41              |
| 24:Z:278:ASN:OD1  | 24:Z:278:ASN:C    | 2.63                     | 0.41              |
| 26:b:126:LYS:HA   | 26:b:129:LYS:HB2  | 2.02                     | 0.41              |
| 28:d:79:LYS:HB3   | 28:d:79:LYS:HE3   | 1.85                     | 0.41              |
| 30:f:106:LEU:CD1  | 30:f:109:ILE:HG21 | 2.51                     | 0.41              |
| 30:f:190:GLU:CD   | 30:f:197:ALA:HB2  | 2.46                     | 0.41              |
| 30:f:275:MET:N    | 30:f:275:MET:SD   | 2.92                     | 0.41              |
| 30:f:680:ARG:HD3  | 30:f:760:PHE:HE2  | 1.82                     | 0.41              |
| 8:i:37:ILE:HD12   | 8:i:193:ALA:HB2   | 2.03                     | 0.41              |
| 15:p:44:MET:HE2   | 15:p:66:LEU:CD2   | 2.51                     | 0.41              |
| 31:F:326:VAL:O    | 31:F:326:VAL:CG1  | 2.68                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 32:U:147:TYR:CE2  | 32:U:169:GLU:HB2  | 2.55                     | 0.41              |
| 32:U:339:LEU:HD22 | 32:U:414:GLY:O    | 2.20                     | 0.41              |
| 32:U:475:HIS:CE1  | 32:U:510:GLU:HB2  | 2.54                     | 0.41              |
| 32:U:505:ASP:O    | 32:U:508:THR:HG22 | 2.20                     | 0.41              |
| 32:U:672:LEU:HD11 | 32:U:690:ALA:HB1  | 2.03                     | 0.41              |
| 32:U:695:MET:HA   | 32:U:698:GLN:OE1  | 2.20                     | 0.41              |
| 32:U:800:VAL:HG22 | 32:U:880:ASN:HD21 | 1.82                     | 0.41              |
| 32:U:803:LYS:NZ   | 32:U:875:PHE:HB3  | 2.34                     | 0.41              |
| 2:B:67:ARG:HB3    | 30:f:646:MET:CE   | 2.50                     | 0.41              |
| 2:B:343:ARG:HE    | 2:B:346:ARG:HH12  | 1.68                     | 0.41              |
| 3:C:24:TYR:CE2    | 32:U:153:ILE:HD11 | 2.47                     | 0.41              |
| 3:C:57:ARG:HH22   | 32:U:649:ARG:NH1  | 2.09                     | 0.41              |
| 3:C:329:LEU:HD22  | 3:C:344:LEU:HD13  | 2.03                     | 0.41              |
| 4:D:403:TYR:CZ    | 4:D:407:ILE:HG21  | 2.55                     | 0.41              |
| 5:E:88:ASP:OD1    | 5:E:88:ASP:O      | 2.37                     | 0.41              |
| 5:E:302:ASP:OD1   | 5:E:303:LEU:N     | 2.54                     | 0.41              |
| 6:G:7:ALA:N       | 6:G:10:ASP:OD2    | 2.42                     | 0.41              |
| 17:R:2:THR:OG1    | 36:R:301:LDZ:O33  | 2.36                     | 0.41              |
| 20:V:208:ALA:O    | 20:V:211:TYR:HB2  | 2.20                     | 0.41              |
| 21:W:67:LEU:HD11  | 21:W:90:LEU:HB3   | 2.02                     | 0.41              |
| 21:W:78:LYS:N     | 21:W:78:LYS:HD2   | 2.35                     | 0.41              |
| 21:W:132:THR:HG23 | 21:W:133:GLU:N    | 2.35                     | 0.41              |
| 22:X:167:VAL:HG12 | 22:X:206:LEU:HD13 | 2.02                     | 0.41              |
| 22:X:304:LYS:HG3  | 22:X:305:ALA:N    | 2.35                     | 0.41              |
| 22:X:395:LYS:HD3  | 22:X:395:LYS:HA   | 1.76                     | 0.41              |
| 24:Z:11:VAL:HG13  | 24:Z:50:VAL:HG21  | 2.01                     | 0.41              |
| 24:Z:206:LEU:HA   | 24:Z:206:LEU:HD23 | 1.81                     | 0.41              |
| 25:a:184:ASP:C    | 25:a:185:ILE:HG13 | 2.45                     | 0.41              |
| 26:b:180:ALA:O    | 26:b:181:ASP:OD1  | 2.37                     | 0.41              |
| 27:c:269:GLN:O    | 27:c:272:ILE:HG22 | 2.20                     | 0.41              |
| 27:c:299:CYS:O    | 27:c:303:MET:HE1  | 2.20                     | 0.41              |
| 28:d:180:GLY:O    | 28:d:183:GLU:HB2  | 2.21                     | 0.41              |
| 30:f:706:ILE:HG12 | 30:f:745:LEU:HD13 | 2.03                     | 0.41              |
| 30:f:789:SER:O    | 30:f:796:LEU:HD22 | 2.21                     | 0.41              |
| 17:r:52:ASP:OD1   | 17:r:52:ASP:N     | 2.50                     | 0.41              |
| 31:F:365:ILE:HG13 | 35:F:501:ADP:N1   | 2.35                     | 0.41              |
| 32:U:241:ASN:OD1  | 32:U:243:LEU:N    | 2.42                     | 0.41              |
| 32:U:252:LEU:HD12 | 32:U:252:LEU:O    | 2.21                     | 0.41              |
| 32:U:352:ILE:HG21 | 32:U:376:MET:CE   | 2.43                     | 0.41              |
| 32:U:422:LEU:HG   | 32:U:423:MET:HE3  | 1.94                     | 0.41              |
| 32:U:554:LEU:HD12 | 32:U:554:LEU:HA   | 1.91                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 32:U:705:LYS:O    | 32:U:708:GLN:HG3  | 2.20                     | 0.41              |
| 32:U:800:VAL:HG22 | 32:U:880:ASN:CG   | 2.45                     | 0.41              |
| 1:A:156:LYS:HD3   | 1:A:157:ILE:N     | 2.36                     | 0.41              |
| 1:A:183:GLN:N     | 1:A:183:GLN:OE1   | 2.53                     | 0.41              |
| 1:A:337:LEU:HD12  | 1:A:337:LEU:HA    | 1.83                     | 0.41              |
| 2:B:176:VAL:HG21  | 2:B:247:PHE:HD1   | 1.85                     | 0.41              |
| 2:B:212:GLU:HG2   | 30:f:845:ARG:CG   | 2.49                     | 0.41              |
| 2:B:220:LYS:HZ3   | 2:B:220:LYS:HB3   | 1.86                     | 0.41              |
| 2:B:233:THR:O     | 2:B:237:LYS:HG2   | 2.21                     | 0.41              |
| 2:B:400:THR:HA    | 3:C:180:ILE:HG23  | 2.02                     | 0.41              |
| 2:B:408:ARG:HE    | 3:C:163:GLU:CD    | 2.28                     | 0.41              |
| 4:D:122:GLU:OE2   | 27:c:279:ASP:N    | 2.54                     | 0.41              |
| 4:D:153:MET:HE2   | 4:D:229:ARG:HB2   | 2.01                     | 0.41              |
| 5:E:47:LEU:O      | 5:E:51:GLN:NE2    | 2.54                     | 0.41              |
| 20:V:166:TYR:CD1  | 20:V:166:TYR:C    | 2.98                     | 0.41              |
| 21:W:326:MET:HE2  | 21:W:326:MET:C    | 2.46                     | 0.41              |
| 21:W:372:ARG:NH2  | 25:a:327:VAL:HG21 | 2.34                     | 0.41              |
| 22:X:339:ILE:HD11 | 22:X:350:ILE:HD12 | 1.99                     | 0.41              |
| 22:X:405:GLN:HG3  | 22:X:406:ASN:N    | 2.36                     | 0.41              |
| 23:Y:149:LEU:HA   | 23:Y:157:ILE:HD11 | 2.03                     | 0.41              |
| 23:Y:214:MET:HE3  | 23:Y:214:MET:HB2  | 1.94                     | 0.41              |
| 25:a:78:GLU:O     | 25:a:81:LEU:HG    | 2.20                     | 0.41              |
| 25:a:132:LYS:HA   | 25:a:135:ILE:HG22 | 2.02                     | 0.41              |
| 25:a:361:LYS:HD3  | 25:a:361:LYS:C    | 2.45                     | 0.41              |
| 26:b:44:ASN:C     | 26:b:46:GLU:H     | 2.27                     | 0.41              |
| 26:b:179:LEU:CD1  | 26:b:181:ASP:H    | 2.33                     | 0.41              |
| 28:d:67:ASP:HB2   | 28:d:70:SER:HB2   | 2.02                     | 0.41              |
| 30:f:56:LEU:HD23  | 30:f:56:LEU:HA    | 1.90                     | 0.41              |
| 30:f:438:ASP:C    | 30:f:441:LYS:HG2  | 2.46                     | 0.41              |
| 30:f:687:ARG:C    | 30:f:691:PRO:HG2  | 2.46                     | 0.41              |
| 15:p:33:MET:HG3   | 15:p:182:MET:HE3  | 2.02                     | 0.41              |
| 32:U:31:VAL:O     | 32:U:31:VAL:HG13  | 2.20                     | 0.41              |
| 32:U:345:ASN:OD1  | 32:U:345:ASN:N    | 2.52                     | 0.41              |
| 32:U:365:CYS:O    | 32:U:369:THR:N    | 2.47                     | 0.41              |
| 32:U:600:ARG:HG2  | 32:U:600:ARG:HH11 | 1.86                     | 0.41              |
| 32:U:804:SER:HA   | 32:U:892:LEU:HA   | 2.01                     | 0.41              |
| 1:A:259:GLU:OE1   | 1:A:259:GLU:CA    | 2.66                     | 0.41              |
| 3:C:80:MET:HB2    | 3:C:84:LYS:O      | 2.20                     | 0.41              |
| 3:C:115:ALA:C     | 3:C:116:LEU:HD13  | 2.46                     | 0.41              |
| 4:D:322:LEU:HD23  | 4:D:327:LEU:HD21  | 2.03                     | 0.41              |
| 5:E:270:LEU:HD23  | 5:E:270:LEU:C     | 2.45                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 11:L:70:ILE:HG12  | 11:L:105:VAL:HG22 | 2.03                     | 0.41              |
| 12:M:202:ASP:OD2  | 12:M:204:VAL:N    | 2.53                     | 0.41              |
| 18:S:148:LEU:HD12 | 18:S:178:VAL:CG1  | 2.51                     | 0.41              |
| 21:W:254:PRO:HA   | 21:W:257:GLN:C    | 2.44                     | 0.41              |
| 21:W:307:LYS:O    | 21:W:315:MET:HE3  | 2.21                     | 0.41              |
| 21:W:326:MET:CE   | 21:W:331:GLY:HA3  | 2.48                     | 0.41              |
| 22:X:96:PHE:CE2   | 22:X:109:LEU:HD23 | 2.55                     | 0.41              |
| 23:Y:150:PHE:HD1  | 23:Y:150:PHE:O    | 2.04                     | 0.41              |
| 23:Y:258:GLN:O    | 23:Y:262:SER:HB3  | 2.20                     | 0.41              |
| 23:Y:282:MET:CG   | 23:Y:288:PHE:HB3  | 2.37                     | 0.41              |
| 23:Y:325:VAL:HG22 | 29:e:60:LEU:HD13  | 2.03                     | 0.41              |
| 24:Z:19:VAL:HG13  | 24:Z:95:TYR:HE2   | 1.86                     | 0.41              |
| 24:Z:214:LYS:HE3  | 25:a:346:ILE:HD13 | 2.02                     | 0.41              |
| 24:Z:261:TYR:C    | 24:Z:261:TYR:CD1  | 2.99                     | 0.41              |
| 25:a:115:LYS:HA   | 25:a:115:LYS:HD3  | 1.89                     | 0.41              |
| 25:a:300:ALA:HB3  | 25:a:302:ILE:HD13 | 2.02                     | 0.41              |
| 26:b:117:VAL:HB   | 26:b:146:GLU:OE2  | 2.19                     | 0.41              |
| 26:b:135:LYS:HE3  | 26:b:135:LYS:CA   | 2.41                     | 0.41              |
| 30:f:174:ASP:HB2  | 30:f:178:LYS:HD2  | 2.01                     | 0.41              |
| 30:f:462:ALA:HB3  | 30:f:489:TYR:CE1  | 2.56                     | 0.41              |
| 30:f:631:LYS:HA   | 30:f:634:LYS:HD3  | 2.03                     | 0.41              |
| 30:f:670:MET:C    | 30:f:672:LEU:HD12 | 2.45                     | 0.41              |
| 30:f:771:LEU:O    | 30:f:775:THR:HG23 | 2.20                     | 0.41              |
| 30:f:776:LEU:O    | 30:f:778:LEU:HD23 | 2.21                     | 0.41              |
| 31:F:357:PRO:O    | 31:F:362:ARG:NH1  | 2.54                     | 0.41              |
| 32:U:15:ASP:H     | 32:U:20:LYS:NZ    | 2.18                     | 0.41              |
| 32:U:322:THR:HG22 | 32:U:322:THR:O    | 2.19                     | 0.41              |
| 32:U:567:ILE:HD11 | 32:U:585:THR:CG2  | 2.50                     | 0.41              |
| 32:U:616:ARG:HD2  | 32:U:770:TRP:CZ2  | 2.55                     | 0.41              |
| 32:U:680:VAL:HB   | 32:U:683:VAL:CG1  | 2.50                     | 0.41              |
| 1:A:319:MET:HE1   | 1:A:337:LEU:HD22  | 2.01                     | 0.41              |
| 2:B:123:VAL:HG13  | 2:B:133:VAL:CG2   | 2.50                     | 0.41              |
| 2:B:249:ARG:HG3   | 2:B:283:PHE:CD2   | 2.55                     | 0.41              |
| 3:C:24:TYR:HE1    | 4:D:40:LEU:C      | 2.29                     | 0.41              |
| 3:C:293:MET:CE    | 3:C:295:THR:HB    | 2.50                     | 0.41              |
| 4:D:97:ASP:OD1    | 4:D:100:THR:HB    | 2.21                     | 0.41              |
| 4:D:352:MET:CE    | 4:D:394:VAL:HG21  | 2.51                     | 0.41              |
| 5:E:177:GLY:HA2   | 31:F:344:ARG:CD   | 2.50                     | 0.41              |
| 5:E:200:SER:OG    | 5:E:234:GLU:O     | 2.28                     | 0.41              |
| 6:G:17:SER:OG     | 6:G:18:PRO:HD2    | 2.21                     | 0.41              |
| 8:I:119:GLN:HA    | 8:I:122:THR:HG22  | 2.03                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 14:O:56:THR:HG23  | 14:O:87:MET:HE1   | 2.02                     | 0.41              |
| 20:V:289:LEU:O    | 20:V:292:THR:HG22 | 2.21                     | 0.41              |
| 21:W:248:ARG:O    | 21:W:251:TYR:HB3  | 2.21                     | 0.41              |
| 22:X:253:TYR:N    | 22:X:253:TYR:CD1  | 2.88                     | 0.41              |
| 23:Y:15:PRO:HD3   | 23:Y:143:TYR:CE1  | 2.53                     | 0.41              |
| 23:Y:239:LYS:HE2  | 23:Y:239:LYS:CA   | 2.45                     | 0.41              |
| 25:a:39:LEU:HD23  | 25:a:39:LEU:H     | 1.85                     | 0.41              |
| 25:a:135:ILE:CD1  | 25:a:159:SER:HB3  | 2.50                     | 0.41              |
| 25:a:185:ILE:HD12 | 25:a:186:LYS:O    | 2.21                     | 0.41              |
| 27:c:54:MET:HE3   | 27:c:75:MET:HB2   | 2.03                     | 0.41              |
| 27:c:211:GLU:HB2  | 32:U:574:LYS:HZ2  | 1.85                     | 0.41              |
| 28:d:9:TRP:H      | 28:d:9:TRP:HE3    | 1.67                     | 0.41              |
| 28:d:68:ILE:HB    | 28:d:69:PRO:HD3   | 2.02                     | 0.41              |
| 29:e:39:TRP:HE3   | 29:e:41:ASP:OD1   | 2.03                     | 0.41              |
| 30:f:141:LYS:O    | 30:f:144:LEU:HG   | 2.20                     | 0.41              |
| 30:f:292:LYS:O    | 30:f:292:LYS:CG   | 2.69                     | 0.41              |
| 30:f:669:GLU:OE1  | 30:f:669:GLU:HA   | 2.20                     | 0.41              |
| 30:f:742:ALA:O    | 30:f:746:ARG:NE   | 2.54                     | 0.41              |
| 8:i:40:ASN:OD1    | 8:i:40:ASN:N      | 2.54                     | 0.41              |
| 15:p:148:MET:HE2  | 18:s:147:PRO:C    | 2.45                     | 0.41              |
| 18:s:68:ILE:HD11  | 18:s:92:LEU:HD13  | 2.02                     | 0.41              |
| 31:F:138:GLY:HA3  | 31:F:159:LEU:CD2  | 2.50                     | 0.41              |
| 32:U:182:LYS:HZ1  | 32:U:183:LEU:N    | 2.19                     | 0.41              |
| 32:U:380:THR:C    | 32:U:381:THR:HG23 | 2.45                     | 0.41              |
| 32:U:765:VAL:CG1  | 32:U:775:LEU:CD2  | 2.98                     | 0.41              |
| 1:A:109:PRO:HB2   | 1:A:110:LYS:H     | 1.55                     | 0.41              |
| 1:A:187:LEU:O     | 1:A:187:LEU:HG    | 2.21                     | 0.41              |
| 1:A:222:LYS:HB2   | 1:A:222:LYS:HE3   | 1.84                     | 0.41              |
| 3:C:329:LEU:CD2   | 3:C:344:LEU:HD22  | 2.49                     | 0.41              |
| 4:D:263:PHE:HA    | 4:D:308:ILE:O     | 2.21                     | 0.41              |
| 4:D:378:ILE:HD13  | 4:D:403:TYR:HD1   | 1.85                     | 0.41              |
| 5:E:349:GLU:HG3   | 5:E:373:LYS:CE    | 2.50                     | 0.41              |
| 6:G:75:ASN:OD1    | 6:G:75:ASN:N      | 2.54                     | 0.41              |
| 15:P:192:ASP:OD1  | 15:P:192:ASP:C    | 2.63                     | 0.41              |
| 20:V:298:ILE:HG22 | 20:V:298:ILE:O    | 2.19                     | 0.41              |
| 20:V:306:ARG:CD   | 20:V:336:GLU:HG3  | 2.42                     | 0.41              |
| 20:V:381:GLN:HE21 | 20:V:381:GLN:C    | 2.25                     | 0.41              |
| 20:V:400:HIS:CD2  | 28:d:145:GLU:HB3  | 2.46                     | 0.41              |
| 21:W:214:PHE:HA   | 21:W:216:GLU:OE1  | 2.20                     | 0.41              |
| 21:W:393:LEU:HD12 | 21:W:393:LEU:HA   | 1.90                     | 0.41              |
| 23:Y:326:GLY:HA2  | 29:e:63:HIS:NE2   | 2.36                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 24:Z:214:LYS:HB2  | 24:Z:219:LYS:HD2  | 2.02                     | 0.41              |
| 25:a:82:HIS:HD2   | 25:a:85:ARG:NH2   | 2.17                     | 0.41              |
| 25:a:274:LEU:HA   | 25:a:274:LEU:HD12 | 1.83                     | 0.41              |
| 26:b:183:LEU:O    | 26:b:183:LEU:HD22 | 2.21                     | 0.41              |
| 27:c:161:ARG:O    | 27:c:200:TYR:HB2  | 2.20                     | 0.41              |
| 28:d:11:ARG:NE    | 28:d:11:ARG:HA    | 2.36                     | 0.41              |
| 28:d:63:ILE:HG13  | 28:d:165:PHE:CD2  | 2.55                     | 0.41              |
| 28:d:169:ILE:HG13 | 28:d:169:ILE:H    | 1.67                     | 0.41              |
| 28:d:255:MET:HE2  | 28:d:256:ILE:O    | 2.21                     | 0.41              |
| 29:e:16:ASP:OD1   | 29:e:16:ASP:N     | 2.53                     | 0.41              |
| 30:f:554:TYR:HD1  | 30:f:557:TRP:HZ3  | 1.67                     | 0.41              |
| 30:f:729:MET:HE3  | 30:f:732:VAL:HB   | 2.02                     | 0.41              |
| 11:l:212:ILE:CG2  | 11:l:214:ILE:HD11 | 2.49                     | 0.41              |
| 13:n:2:THR:HG23   | 13:n:34:LYS:HZ3   | 1.86                     | 0.41              |
| 31:F:89:LEU:HD21  | 31:F:126:THR:CB   | 2.48                     | 0.41              |
| 32:U:142:LEU:HD13 | 32:U:147:TYR:CE1  | 2.53                     | 0.41              |
| 32:U:247:GLN:NE2  | 32:U:904:LYS:CD   | 2.76                     | 0.41              |
| 32:U:329:LEU:HA   | 32:U:329:LEU:HD12 | 1.71                     | 0.41              |
| 1:A:205:GLY:C     | 31:F:373:MET:HB3  | 2.46                     | 0.41              |
| 1:A:333:ARG:NH1   | 1:A:336:ARG:HG2   | 2.35                     | 0.41              |
| 1:A:411:GLU:HA    | 1:A:411:GLU:OE1   | 2.21                     | 0.41              |
| 2:B:107:MET:HE3   | 2:B:107:MET:HB2   | 2.01                     | 0.41              |
| 2:B:116:ILE:HG23  | 2:B:120:HIS:C     | 2.46                     | 0.41              |
| 2:B:162:VAL:CG1   | 2:B:163:LEU:N     | 2.83                     | 0.41              |
| 2:B:174:MET:SD    | 2:B:270:LEU:HD13  | 2.61                     | 0.41              |
| 2:B:176:VAL:HG22  | 2:B:247:PHE:O     | 2.20                     | 0.41              |
| 2:B:225:TYR:HA    | 2:B:331:THR:O     | 2.21                     | 0.41              |
| 2:B:256:ILE:HD11  | 2:B:295:TYR:CD1   | 2.56                     | 0.41              |
| 2:B:293:LYS:HD2   | 2:B:295:TYR:OH    | 2.20                     | 0.41              |
| 2:B:349:ARG:HG2   | 2:B:349:ARG:HH11  | 1.84                     | 0.41              |
| 2:B:362:LYS:N     | 2:B:384:ILE:HD11  | 2.35                     | 0.41              |
| 2:B:363:ARG:NH1   | 2:B:363:ARG:HB3   | 2.35                     | 0.41              |
| 3:C:20:LEU:HA     | 3:C:20:LEU:HD22   | 1.87                     | 0.41              |
| 3:C:189:TYR:HA    | 3:C:295:THR:O     | 2.21                     | 0.41              |
| 4:D:214:MET:HE1   | 33:D:501:ATP:H2'  | 2.03                     | 0.41              |
| 4:D:251:PHE:CE2   | 4:D:292:LEU:HD23  | 2.52                     | 0.41              |
| 4:D:276:ASP:HB3   | 5:E:248:SER:HB2   | 2.02                     | 0.41              |
| 5:E:135:ILE:CD1   | 5:E:183:LEU:HB2   | 2.51                     | 0.41              |
| 8:I:174:MET:HE3   | 8:I:196:VAL:HA    | 2.02                     | 0.41              |
| 8:I:194:ILE:HD12  | 8:I:237:ILE:HD13  | 2.02                     | 0.41              |
| 10:K:171:GLY:N    | 10:K:174:SER:OG   | 2.54                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 14:O:109:PRO:O    | 14:O:110:HIS:ND1  | 2.54                     | 0.41              |
| 14:O:166:ASN:OD1  | 19:T:148:PRO:HA   | 2.21                     | 0.41              |
| 16:Q:167:LEU:HD23 | 16:Q:171:PHE:HB2  | 2.03                     | 0.41              |
| 18:S:26:ASP:OD1   | 18:S:42:LYS:HE3   | 2.21                     | 0.41              |
| 19:T:79:ASP:OD2   | 11:l:107:ARG:NE   | 2.54                     | 0.41              |
| 20:V:299:GLN:O    | 20:V:300:LEU:HB2  | 2.21                     | 0.41              |
| 21:W:184:GLU:C    | 21:W:184:GLU:CD   | 2.88                     | 0.41              |
| 21:W:251:TYR:HD1  | 21:W:254:PRO:HG2  | 1.86                     | 0.41              |
| 21:W:307:LYS:HG2  | 21:W:307:LYS:O    | 2.20                     | 0.41              |
| 22:X:165:LEU:HD12 | 22:X:165:LEU:HA   | 1.90                     | 0.41              |
| 22:X:328:ASP:OD1  | 22:X:328:ASP:C    | 2.63                     | 0.41              |
| 22:X:364:LYS:O    | 22:X:368:MET:HG3  | 2.21                     | 0.41              |
| 22:X:406:ASN:HD22 | 27:c:253:LYS:HB2  | 1.86                     | 0.41              |
| 22:X:412:ASP:OD1  | 23:Y:379:ARG:NH1  | 2.54                     | 0.41              |
| 23:Y:42:MET:HA    | 23:Y:42:MET:CE    | 2.51                     | 0.41              |
| 23:Y:134:LEU:HA   | 23:Y:137:ARG:HG3  | 2.03                     | 0.41              |
| 23:Y:178:ASN:OD1  | 23:Y:207:THR:HG21 | 2.21                     | 0.41              |
| 23:Y:217:LYS:HZ3  | 23:Y:217:LYS:HB2  | 1.86                     | 0.41              |
| 23:Y:221:THR:O    | 23:Y:224:VAL:HG12 | 2.20                     | 0.41              |
| 23:Y:283:LYS:HG2  | 23:Y:292:TYR:CD1  | 2.56                     | 0.41              |
| 24:Z:11:VAL:CG2   | 24:Z:135:THR:HG21 | 2.44                     | 0.41              |
| 24:Z:16:LEU:HG    | 27:c:216:MET:CE   | 2.49                     | 0.41              |
| 24:Z:81:MET:HE1   | 27:c:94:LYS:NZ    | 2.35                     | 0.41              |
| 24:Z:135:THR:HG22 | 24:Z:135:THR:O    | 2.21                     | 0.41              |
| 24:Z:215:VAL:HG23 | 24:Z:216:ALA:N    | 2.36                     | 0.41              |
| 24:Z:272:LEU:HD12 | 24:Z:272:LEU:HA   | 1.76                     | 0.41              |
| 25:a:229:ASP:OD1  | 25:a:229:ASP:C    | 2.64                     | 0.41              |
| 26:b:70:ARG:O     | 26:b:74:LYS:HB2   | 2.21                     | 0.41              |
| 27:c:126:ASP:HA   | 27:c:129:THR:HG22 | 2.01                     | 0.41              |
| 27:c:139:ARG:HG3  | 27:c:139:ARG:NH1  | 2.34                     | 0.41              |
| 27:c:291:LEU:HA   | 27:c:291:LEU:HD23 | 1.74                     | 0.41              |
| 28:d:78:LEU:CD1   | 28:d:79:LYS:N     | 2.79                     | 0.41              |
| 30:f:171:GLN:OE1  | 30:f:179:VAL:HG13 | 2.21                     | 0.41              |
| 30:f:265:ALA:HA   | 30:f:267:ARG:HH11 | 1.85                     | 0.41              |
| 30:f:305:LEU:HD13 | 30:f:305:LEU:O    | 2.21                     | 0.41              |
| 30:f:407:MET:HE3  | 30:f:439:TYR:CE2  | 2.56                     | 0.41              |
| 30:f:478:ARG:O    | 30:f:482:ILE:HG23 | 2.20                     | 0.41              |
| 30:f:499:THR:O    | 30:f:503:PRO:HD3  | 2.20                     | 0.41              |
| 30:f:626:GLU:O    | 30:f:627:GLU:HG2  | 2.21                     | 0.41              |
| 30:f:635:LYS:HG2  | 30:f:635:LYS:H    | 1.61                     | 0.41              |
| 30:f:638:ASP:C    | 30:f:639:LYS:HG3  | 2.45                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 30:f:660:ILE:HG23 | 30:f:669:GLU:OE1  | 2.21                     | 0.41              |
| 30:f:703:ARG:HA   | 30:f:706:ILE:CD1  | 2.34                     | 0.41              |
| 30:f:707:LEU:HD21 | 30:f:785:ARG:HD2  | 2.03                     | 0.41              |
| 10:k:199:LEU:HD21 | 10:k:217:LEU:HD13 | 2.03                     | 0.41              |
| 10:k:201:ILE:O    | 10:k:205:VAL:HG22 | 2.20                     | 0.41              |
| 11:l:214:ILE:HD13 | 11:l:214:ILE:N    | 2.36                     | 0.41              |
| 15:p:25:ARG:HG3   | 15:p:25:ARG:HH11  | 1.86                     | 0.41              |
| 15:p:87:MET:HE3   | 15:p:119:PHE:HZ   | 1.85                     | 0.41              |
| 15:p:148:MET:HE3  | 15:p:172:ASN:HB3  | 2.03                     | 0.41              |
| 31:F:181:PRO:O    | 31:F:242:ALA:HB2  | 2.21                     | 0.41              |
| 31:F:200:GLU:O    | 31:F:200:GLU:HG3  | 2.21                     | 0.41              |
| 31:F:234:THR:HB   | 35:F:501:ADP:O2A  | 2.21                     | 0.41              |
| 31:F:294:LYS:HG3  | 31:F:295:ARG:O    | 2.21                     | 0.41              |
| 31:F:437:TYR:CD2  | 31:F:437:TYR:C    | 2.98                     | 0.41              |
| 32:U:8:ILE:C      | 32:U:10:SER:N     | 2.79                     | 0.41              |
| 32:U:137:MET:CE   | 32:U:137:MET:CA   | 2.89                     | 0.41              |
| 32:U:177:LEU:CD1  | 32:U:204:ILE:HG12 | 2.51                     | 0.41              |
| 32:U:201:LEU:O    | 32:U:204:ILE:CD1  | 2.69                     | 0.41              |
| 32:U:247:GLN:HG3  | 32:U:913:ILE:HD13 | 1.97                     | 0.41              |
| 32:U:321:GLN:HG2  | 32:U:322:THR:N    | 2.36                     | 0.41              |
| 32:U:418:GLU:HG2  | 32:U:421:GLN:CD   | 2.45                     | 0.41              |
| 32:U:514:LEU:HD12 | 32:U:514:LEU:HA   | 1.81                     | 0.41              |
| 32:U:705:LYS:HA   | 32:U:708:GLN:HG2  | 2.03                     | 0.41              |
| 1:A:189:GLU:CB    | 31:F:405:MET:HE1  | 2.47                     | 0.41              |
| 1:A:234:ASP:OD2   | 30:f:348:ILE:HB   | 2.21                     | 0.41              |
| 2:B:211:TYR:HB3   | 2:B:216:ILE:O     | 2.20                     | 0.41              |
| 3:C:362:VAL:HG21  | 3:C:387:VAL:HG12  | 2.02                     | 0.41              |
| 4:D:215:LEU:HD23  | 4:D:215:LEU:C     | 2.45                     | 0.41              |
| 5:E:316:HIS:CG    | 5:E:344:ARG:HG3   | 2.56                     | 0.41              |
| 5:E:380:LEU:HD13  | 31:F:335:VAL:HG11 | 2.03                     | 0.41              |
| 8:I:3:ARG:NE      | 11:L:123:TYR:OH   | 2.46                     | 0.41              |
| 14:O:188:ARG:HB3  | 14:O:189:PRO:HD3  | 2.02                     | 0.41              |
| 20:V:185:GLN:HA   | 20:V:188:SER:OG   | 2.21                     | 0.41              |
| 21:W:105:VAL:HG11 | 21:W:140:ILE:HD13 | 2.03                     | 0.41              |
| 21:W:247:TYR:HD1  | 21:W:250:ILE:HD11 | 1.86                     | 0.41              |
| 21:W:310:THR:O    | 21:W:311:THR:OG1  | 2.36                     | 0.41              |
| 21:W:321:VAL:CG1  | 21:W:322:GLU:N    | 2.83                     | 0.41              |
| 21:W:369:TYR:HD2  | 25:a:312:MET:HG2  | 1.85                     | 0.41              |
| 21:W:370:TYR:OH   | 25:a:308:GLU:HG2  | 2.21                     | 0.41              |
| 22:X:141:LYS:HD3  | 22:X:179:ALA:HB1  | 2.03                     | 0.41              |
| 23:Y:189:VAL:HG13 | 23:Y:287:LEU:HD11 | 2.01                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 24:Z:38:VAL:HG11  | 24:Z:75:LEU:HD11  | 2.03                     | 0.41              |
| 25:a:181:GLY:N    | 25:a:184:ASP:OD2  | 2.54                     | 0.41              |
| 27:c:49:VAL:CG1   | 27:c:50:PRO:CD    | 2.99                     | 0.41              |
| 28:d:101:LEU:HG   | 28:d:163:TYR:CE1  | 2.56                     | 0.41              |
| 30:f:257:ARG:HH11 | 30:f:289:VAL:HG21 | 1.85                     | 0.41              |
| 30:f:298:LEU:HG   | 30:f:299:GLY:N    | 2.36                     | 0.41              |
| 30:f:546:SER:OG   | 30:f:550:LEU:HD23 | 2.21                     | 0.41              |
| 15:p:148:MET:HE3  | 15:p:172:ASN:CB   | 2.51                     | 0.41              |
| 31:F:295:ARG:NE   | 31:F:339:ASP:OD2  | 2.46                     | 0.41              |
| 32:U:17:PRO:HB2   | 32:U:55:ARG:NH2   | 2.35                     | 0.41              |
| 32:U:253:TYR:HA   | 32:U:261:LEU:HD11 | 2.03                     | 0.41              |
| 32:U:390:LEU:O    | 32:U:393:LEU:N    | 2.54                     | 0.41              |
| 32:U:406:ALA:HB2  | 32:U:444:TYR:HD2  | 1.86                     | 0.41              |
| 32:U:450:HIS:CE1  | 32:U:457:ILE:HG12 | 2.56                     | 0.41              |
| 32:U:471:ASP:OD1  | 32:U:471:ASP:C    | 2.63                     | 0.41              |
| 32:U:786:THR:HB   | 32:U:886:PRO:HD3  | 2.03                     | 0.41              |
| 1:A:73:ALA:CB     | 2:B:140:ASP:HA    | 2.51                     | 0.40              |
| 1:A:177:VAL:O     | 1:A:177:VAL:HG23  | 2.21                     | 0.40              |
| 1:A:418:LYS:HE3   | 1:A:418:LYS:HB3   | 1.62                     | 0.40              |
| 2:B:234:LEU:HD22  | 33:B:501:ATP:H2'  | 2.02                     | 0.40              |
| 3:C:38:LYS:HB2    | 3:C:38:LYS:HE2    | 1.86                     | 0.40              |
| 3:C:78:ARG:HG2    | 3:C:79:ALA:O      | 2.20                     | 0.40              |
| 3:C:176:GLU:OE1   | 3:C:177:ALA:N     | 2.54                     | 0.40              |
| 3:C:315:ILE:HG22  | 3:C:316:GLU:N     | 2.36                     | 0.40              |
| 3:C:389:LYS:HE2   | 3:C:389:LYS:HB2   | 1.88                     | 0.40              |
| 5:E:316:HIS:HD2   | 5:E:344:ARG:HB2   | 1.84                     | 0.40              |
| 5:E:380:LEU:HD12  | 31:F:343:LEU:HD13 | 2.02                     | 0.40              |
| 9:J:116:GLN:NE2   | 10:K:84:ASP:OD1   | 2.51                     | 0.40              |
| 10:K:225:ASN:OD1  | 10:K:225:ASN:N    | 2.46                     | 0.40              |
| 17:R:6:ALA:HA     | 17:R:14:ILE:O     | 2.20                     | 0.40              |
| 17:R:150:VAL:HG12 | 17:R:154:TYR:CE2  | 2.56                     | 0.40              |
| 21:W:340:VAL:HG12 | 21:W:341:PHE:CD2  | 2.57                     | 0.40              |
| 21:W:403:PHE:C    | 21:W:403:PHE:CD1  | 2.98                     | 0.40              |
| 21:W:450:GLU:O    | 21:W:454:ASN:HB3  | 2.21                     | 0.40              |
| 23:Y:74:LYS:NZ    | 23:Y:74:LYS:HB3   | 2.36                     | 0.40              |
| 24:Z:280:ILE:HD12 | 24:Z:280:ILE:O    | 2.21                     | 0.40              |
| 26:b:25:ARG:NH1   | 26:b:144:GLY:CA   | 2.84                     | 0.40              |
| 26:b:157:VAL:HG21 | 26:b:170:LEU:HD13 | 2.02                     | 0.40              |
| 27:c:77:GLN:OE1   | 27:c:77:GLN:CA    | 2.69                     | 0.40              |
| 27:c:209:LYS:HE2  | 27:c:209:LYS:HB2  | 1.89                     | 0.40              |
| 28:d:1:MET:HG3    | 28:d:2:TYR:CD1    | 2.46                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 28:d:137:VAL:HG12 | 28:d:141:GLN:NE2  | 2.36                     | 0.40              |
| 30:f:126:ILE:O    | 30:f:131:MET:HE2  | 2.21                     | 0.40              |
| 30:f:479:LEU:HD13 | 30:f:514:VAL:CG2  | 2.29                     | 0.40              |
| 30:f:796:LEU:HD21 | 30:f:799:VAL:HG21 | 2.02                     | 0.40              |
| 30:f:804:LEU:HD21 | 30:f:806:VAL:HG22 | 2.02                     | 0.40              |
| 30:f:838:ARG:HG2  | 30:f:839:PRO:HD2  | 2.03                     | 0.40              |
| 9:j:91:CYS:SG     | 9:j:107:ILE:HD13  | 2.61                     | 0.40              |
| 16:q:157:VAL:O    | 16:q:161:ARG:HG3  | 2.21                     | 0.40              |
| 32:U:339:LEU:HD12 | 32:U:339:LEU:HA   | 1.84                     | 0.40              |
| 32:U:458:ILE:HD13 | 32:U:490:ARG:HH22 | 1.84                     | 0.40              |
| 32:U:671:LEU:O    | 32:U:674:PRO:HD2  | 2.20                     | 0.40              |
| 1:A:104:ALA:O     | 1:A:105:ASP:C     | 2.63                     | 0.40              |
| 1:A:303:ILE:HD11  | 1:A:330:ALA:CB    | 2.52                     | 0.40              |
| 1:A:361:SER:HA    | 30:f:849:ALA:HB3  | 2.02                     | 0.40              |
| 2:B:127:VAL:CG2   | 2:B:128:GLY:N     | 2.81                     | 0.40              |
| 2:B:151:LEU:HD11  | 2:B:163:LEU:HB2   | 2.02                     | 0.40              |
| 2:B:247:PHE:C     | 2:B:248:LEU:HD23  | 2.46                     | 0.40              |
| 4:D:87:LEU:CD2    | 4:D:133:HIS:HA    | 2.51                     | 0.40              |
| 4:D:98:GLN:HE22   | 4:D:121:ARG:NE    | 2.19                     | 0.40              |
| 4:D:311:THR:OG1   | 4:D:312:ASN:N     | 2.55                     | 0.40              |
| 5:E:113:ARG:HG3   | 5:E:113:ARG:NH1   | 2.36                     | 0.40              |
| 5:E:155:ASN:OD1   | 5:E:155:ASN:N     | 2.53                     | 0.40              |
| 7:H:33:PRO:HD2    | 7:H:48:GLU:HG2    | 2.03                     | 0.40              |
| 8:I:83:ALA:O      | 8:I:87:THR:HG23   | 2.21                     | 0.40              |
| 18:S:186:ASP:HB3  | 18:S:189:THR:HG22 | 2.03                     | 0.40              |
| 20:V:224:LEU:O    | 20:V:227:VAL:HG12 | 2.21                     | 0.40              |
| 21:W:235:GLN:HG3  | 21:W:235:GLN:O    | 2.20                     | 0.40              |
| 22:X:134:VAL:HB   | 22:X:149:LEU:HD12 | 2.03                     | 0.40              |
| 22:X:229:TYR:HB2  | 22:X:257:CYS:SG   | 2.61                     | 0.40              |
| 22:X:364:LYS:HD2  | 22:X:368:MET:HG3  | 2.04                     | 0.40              |
| 22:X:385:LEU:O    | 22:X:387:ILE:HD13 | 2.21                     | 0.40              |
| 23:Y:23:ARG:HD3   | 23:Y:23:ARG:C     | 2.46                     | 0.40              |
| 24:Z:11:VAL:CG1   | 24:Z:15:VAL:HG11  | 2.51                     | 0.40              |
| 24:Z:247:LYS:NZ   | 24:Z:247:LYS:CB   | 2.83                     | 0.40              |
| 26:b:72:LEU:HD23  | 26:b:72:LEU:N     | 2.37                     | 0.40              |
| 26:b:111:ALA:CB   | 26:b:140:ILE:HG13 | 2.52                     | 0.40              |
| 27:c:60:GLU:N     | 27:c:60:GLU:CD    | 2.79                     | 0.40              |
| 30:f:608:LYS:HD2  | 30:f:608:LYS:C    | 2.46                     | 0.40              |
| 30:f:746:ARG:O    | 30:f:750:GLN:HB2  | 2.21                     | 0.40              |
| 30:f:821:LEU:HD11 | 30:f:882:LEU:HD21 | 2.02                     | 0.40              |
| 9:j:33:VAL:CG2    | 9:j:168:VAL:HG11  | 2.51                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 15:p:11:MET:HE3   | 15:p:170:MET:HE2  | 2.03                     | 0.40              |
| 15:p:182:MET:HE2  | 15:p:182:MET:HB2  | 1.98                     | 0.40              |
| 31:F:93:VAL:HB    | 31:F:149:ASP:OD1  | 2.21                     | 0.40              |
| 31:F:399:VAL:CG2  | 31:F:427:VAL:HG11 | 2.51                     | 0.40              |
| 31:F:410:ARG:O    | 31:F:411:GLY:C    | 2.64                     | 0.40              |
| 1:A:359:ALA:HA    | 1:A:362:MET:SD    | 2.61                     | 0.40              |
| 2:B:135:ILE:HB    | 2:B:141:LYS:NZ    | 2.36                     | 0.40              |
| 3:C:42:LEU:HD23   | 3:C:42:LEU:C      | 2.46                     | 0.40              |
| 3:C:306:LEU:HD23  | 3:C:306:LEU:HA    | 1.83                     | 0.40              |
| 5:E:281:ARG:NH1   | 5:E:283:ASP:OD1   | 2.54                     | 0.40              |
| 5:E:362:VAL:HG23  | 31:F:215:LEU:HD11 | 2.03                     | 0.40              |
| 8:I:140:ASP:OD2   | 8:I:146:GLN:NE2   | 2.46                     | 0.40              |
| 18:S:148:LEU:C    | 18:S:148:LEU:HD13 | 2.46                     | 0.40              |
| 21:W:48:LEU:CD1   | 21:W:90:LEU:HD21  | 2.51                     | 0.40              |
| 21:W:94:ARG:O     | 21:W:94:ARG:CG    | 2.68                     | 0.40              |
| 21:W:97:LEU:O     | 21:W:100:ALA:N    | 2.52                     | 0.40              |
| 21:W:98:LYS:HE3   | 21:W:139:GLU:HB2  | 2.03                     | 0.40              |
| 21:W:123:ARG:NH1  | 21:W:124:LEU:HA   | 2.35                     | 0.40              |
| 21:W:142:ARG:C    | 21:W:142:ARG:CD   | 2.94                     | 0.40              |
| 22:X:340:GLU:N    | 22:X:341:PRO:CD   | 2.84                     | 0.40              |
| 23:Y:19:ILE:CG2   | 23:Y:150:PHE:HZ   | 2.34                     | 0.40              |
| 23:Y:134:LEU:HA   | 23:Y:137:ARG:CD   | 2.50                     | 0.40              |
| 23:Y:316:LEU:CD1  | 23:Y:327:VAL:HG13 | 2.51                     | 0.40              |
| 23:Y:333:GLU:HG3  | 23:Y:337:PHE:CE2  | 2.56                     | 0.40              |
| 24:Z:23:PHE:HE2   | 24:Z:127:LYS:HE2  | 1.85                     | 0.40              |
| 24:Z:176:LEU:O    | 24:Z:177:ARG:C    | 2.65                     | 0.40              |
| 25:a:99:LYS:HG3   | 25:a:103:LYS:HZ1  | 1.85                     | 0.40              |
| 25:a:166:ILE:HG23 | 25:a:168:ASN:OD1  | 2.22                     | 0.40              |
| 28:d:190:LEU:HD11 | 28:d:192:THR:HB   | 2.03                     | 0.40              |
| 30:f:3:GLU:HG3    | 30:f:7:ASP:HA     | 2.04                     | 0.40              |
| 30:f:79:ARG:HH11  | 30:f:80:ARG:HD3   | 1.85                     | 0.40              |
| 30:f:520:LEU:C    | 30:f:520:LEU:HD13 | 2.46                     | 0.40              |
| 30:f:852:VAL:HG22 | 30:f:853:VAL:N    | 2.36                     | 0.40              |
| 7:h:64:VAL:HG12   | 7:h:217:PHE:HZ    | 1.85                     | 0.40              |
| 9:j:89:VAL:HG22   | 16:q:66:LEU:HD21  | 2.03                     | 0.40              |
| 10:k:12:VAL:HG23  | 10:k:13:ASN:OD1   | 2.21                     | 0.40              |
| 12:m:87:LEU:HD13  | 12:m:135:PHE:CE1  | 2.57                     | 0.40              |
| 31:F:96:LEU:HD13  | 31:F:145:LEU:O    | 2.21                     | 0.40              |
| 31:F:154:ASN:HB3  | 31:F:157:SER:O    | 2.21                     | 0.40              |
| 31:F:200:GLU:HA   | 31:F:204:LEU:HB3  | 2.03                     | 0.40              |
| 32:U:350:LEU:HD21 | 32:U:384:GLN:HE22 | 1.86                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 32:U:460:TYR:CD1  | 32:U:460:TYR:C    | 2.99                     | 0.40              |
| 32:U:501:LEU:O    | 32:U:501:LEU:HD12 | 2.21                     | 0.40              |
| 32:U:578:LEU:HD23 | 32:U:578:LEU:HA   | 1.76                     | 0.40              |
| 32:U:633:CYS:HB3  | 32:U:634:PRO:HD3  | 2.02                     | 0.40              |
| 1:A:235:ALA:HB2   | 1:A:269:ALA:HB1   | 2.04                     | 0.40              |
| 9:J:209:ALA:HB1   | 9:J:217:LEU:HD11  | 2.03                     | 0.40              |
| 11:L:84:LEU:O     | 11:L:88:MET:HG3   | 2.21                     | 0.40              |
| 20:V:159:LEU:HD22 | 20:V:163:VAL:CG1  | 2.46                     | 0.40              |
| 20:V:235:LEU:O    | 20:V:235:LEU:HD12 | 2.21                     | 0.40              |
| 20:V:333:ILE:HG13 | 20:V:334:VAL:N    | 2.36                     | 0.40              |
| 20:V:338:LEU:HA   | 20:V:401:ASN:HD22 | 1.87                     | 0.40              |
| 21:W:107:GLN:O    | 21:W:111:TYR:CD1  | 2.75                     | 0.40              |
| 21:W:130:MET:C    | 21:W:130:MET:SD   | 3.04                     | 0.40              |
| 22:X:187:ARG:HD3  | 22:X:187:ARG:HA   | 1.71                     | 0.40              |
| 23:Y:144:LEU:CA   | 23:Y:147:ILE:HD11 | 2.38                     | 0.40              |
| 23:Y:283:LYS:O    | 23:Y:289:ALA:HB2  | 2.21                     | 0.40              |
| 26:b:33:VAL:HG12  | 26:b:112:PHE:CE2  | 2.46                     | 0.40              |
| 30:f:554:TYR:OH   | 30:f:788:MET:HG2  | 2.21                     | 0.40              |
| 30:f:606:VAL:HG23 | 30:f:607:LEU:HD22 | 2.04                     | 0.40              |
| 30:f:633:GLU:H    | 30:f:633:GLU:HG3  | 1.66                     | 0.40              |
| 30:f:721:VAL:HG22 | 30:f:723:TYR:H    | 1.85                     | 0.40              |
| 8:i:184:MET:HE3   | 8:i:184:MET:HB3   | 2.02                     | 0.40              |
| 32:U:224:ASP:O    | 32:U:224:ASP:CG   | 2.64                     | 0.40              |
| 32:U:227:GLN:O    | 32:U:231:ASP:OD1  | 2.39                     | 0.40              |
| 32:U:250:PHE:HD2  | 32:U:911:ILE:CG2  | 2.34                     | 0.40              |
| 32:U:649:ARG:HD2  | 32:U:678:ASP:OD2  | 2.21                     | 0.40              |
| 1:A:267:LYS:HA    | 30:f:354:GLU:CD   | 2.46                     | 0.40              |
| 1:A:351:ARG:HB2   | 1:A:385:ILE:CD1   | 2.51                     | 0.40              |
| 1:A:365:GLU:O     | 1:A:365:GLU:CD    | 2.65                     | 0.40              |
| 1:A:365:GLU:O     | 1:A:365:GLU:OE2   | 2.39                     | 0.40              |
| 2:B:112:LEU:HB2   | 2:B:150:VAL:CG2   | 2.50                     | 0.40              |
| 2:B:118:ASP:CG    | 30:f:697:ILE:HG21 | 2.47                     | 0.40              |
| 2:B:355:LEU:CD1   | 2:B:389:ASP:HB2   | 2.51                     | 0.40              |
| 4:D:168:GLY:H     | 33:D:501:ATP:N6   | 2.19                     | 0.40              |
| 4:D:169:GLY:HA3   | 4:D:343:LEU:HD13  | 2.04                     | 0.40              |
| 5:E:65:THR:HG23   | 5:E:68:LYS:HB2    | 2.02                     | 0.40              |
| 5:E:154:THR:C     | 5:E:156:PRO:HD3   | 2.47                     | 0.40              |
| 6:G:166:THR:CG2   | 6:G:167:ALA:N     | 2.84                     | 0.40              |
| 8:I:66:TYR:CD2    | 8:I:87:THR:HG21   | 2.57                     | 0.40              |
| 10:K:230:THR:OG1  | 10:K:233:GLU:OE1  | 2.29                     | 0.40              |
| 15:P:76:LYS:HB3   | 15:P:76:LYS:NZ    | 2.37                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 20:V:184:ALA:HA   | 20:V:187:ILE:CG2  | 2.52                     | 0.40              |
| 20:V:311:ASN:HA   | 20:V:314:ARG:NH1  | 2.34                     | 0.40              |
| 20:V:371:ASN:CB   | 20:V:427:GLN:HE21 | 2.27                     | 0.40              |
| 21:W:191:ARG:O    | 21:W:191:ARG:HD2  | 2.22                     | 0.40              |
| 21:W:253:THR:HG22 | 21:W:257:GLN:HG3  | 2.02                     | 0.40              |
| 23:Y:167:LEU:HA   | 23:Y:170:GLU:OE2  | 2.21                     | 0.40              |
| 23:Y:316:LEU:C    | 23:Y:316:LEU:HD12 | 2.47                     | 0.40              |
| 24:Z:17:LEU:CG    | 27:c:213:GLU:OE1  | 2.69                     | 0.40              |
| 24:Z:187:LEU:HD22 | 28:d:254:GLU:OE2  | 2.21                     | 0.40              |
| 24:Z:276:ILE:HD13 | 24:Z:276:ILE:HA   | 1.84                     | 0.40              |
| 25:a:29:TYR:HE2   | 25:a:60:TYR:CE1   | 2.40                     | 0.40              |
| 25:a:103:LYS:HG3  | 25:a:104:VAL:HG13 | 2.03                     | 0.40              |
| 25:a:198:PHE:CD1  | 25:a:198:PHE:C    | 3.00                     | 0.40              |
| 25:a:244:ASN:ND2  | 25:a:247:ARG:HG3  | 2.37                     | 0.40              |
| 27:c:147:PRO:C    | 27:c:148:ILE:HD13 | 2.47                     | 0.40              |
| 27:c:194:HIS:CD2  | 27:c:194:HIS:N    | 2.88                     | 0.40              |
| 27:c:267:PRO:O    | 27:c:271:ALA:N    | 2.41                     | 0.40              |
| 28:d:185:ALA:HB2  | 28:d:226:ALA:HB3  | 2.03                     | 0.40              |
| 28:d:188:LYS:HG3  | 28:d:222:TYR:H    | 1.86                     | 0.40              |
| 30:f:143:ARG:NH2  | 30:f:188:VAL:HG12 | 2.37                     | 0.40              |
| 15:p:76:LYS:NZ    | 15:p:76:LYS:HB3   | 2.37                     | 0.40              |
| 16:q:154:GLU:O    | 16:q:158:GLU:HG2  | 2.21                     | 0.40              |
| 31:F:175:MET:SD   | 31:F:251:LEU:HD13 | 2.62                     | 0.40              |
| 31:F:204:LEU:HB3  | 31:F:205:PRO:HD3  | 2.03                     | 0.40              |
| 32:U:69:TYR:O     | 32:U:69:TYR:HD1   | 2.04                     | 0.40              |
| 32:U:561:GLU:OE1  | 32:U:561:GLU:HA   | 2.22                     | 0.40              |
| 32:U:673:GLU:N    | 32:U:674:PRO:HD2  | 2.37                     | 0.40              |
| 32:U:901:GLN:NE2  | 32:U:915:LYS:HD3  | 2.36                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

| Mol | Chain | Analysed      | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|---------------|------------|----------|----------|-------------|-----|
| 1   | A     | 364/433 (84%) | 306 (84%)  | 52 (14%) | 6 (2%)   | 7           | 27  |
| 2   | B     | 386/440 (88%) | 335 (87%)  | 50 (13%) | 1 (0%)   | 36          | 65  |
| 3   | C     | 377/406 (93%) | 329 (87%)  | 44 (12%) | 4 (1%)   | 11          | 36  |
| 4   | D     | 378/418 (90%) | 332 (88%)  | 45 (12%) | 1 (0%)   | 36          | 65  |
| 5   | E     | 373/403 (93%) | 331 (89%)  | 41 (11%) | 1 (0%)   | 36          | 65  |
| 6   | G     | 238/246 (97%) | 225 (94%)  | 13 (6%)  | 0        | 100         | 100 |
| 6   | g     | 238/246 (97%) | 232 (98%)  | 6 (2%)   | 0        | 100         | 100 |
| 7   | H     | 227/234 (97%) | 220 (97%)  | 7 (3%)   | 0        | 100         | 100 |
| 7   | h     | 227/234 (97%) | 225 (99%)  | 2 (1%)   | 0        | 100         | 100 |
| 8   | I     | 245/261 (94%) | 239 (98%)  | 6 (2%)   | 0        | 100         | 100 |
| 8   | i     | 245/261 (94%) | 242 (99%)  | 3 (1%)   | 0        | 100         | 100 |
| 9   | J     | 230/248 (93%) | 221 (96%)  | 9 (4%)   | 0        | 100         | 100 |
| 9   | j     | 230/248 (93%) | 221 (96%)  | 9 (4%)   | 0        | 100         | 100 |
| 10  | K     | 231/241 (96%) | 225 (97%)  | 6 (3%)   | 0        | 100         | 100 |
| 10  | k     | 231/241 (96%) | 227 (98%)  | 4 (2%)   | 0        | 100         | 100 |
| 11  | L     | 231/263 (88%) | 220 (95%)  | 10 (4%)  | 1 (0%)   | 30          | 59  |
| 11  | l     | 231/263 (88%) | 224 (97%)  | 7 (3%)   | 0        | 100         | 100 |
| 12  | M     | 237/255 (93%) | 233 (98%)  | 4 (2%)   | 0        | 100         | 100 |
| 12  | m     | 237/255 (93%) | 233 (98%)  | 4 (2%)   | 0        | 100         | 100 |
| 13  | N     | 200/239 (84%) | 196 (98%)  | 4 (2%)   | 0        | 100         | 100 |
| 13  | n     | 200/239 (84%) | 195 (98%)  | 5 (2%)   | 0        | 100         | 100 |
| 14  | O     | 218/277 (79%) | 213 (98%)  | 5 (2%)   | 0        | 100         | 100 |
| 14  | o     | 218/277 (79%) | 211 (97%)  | 7 (3%)   | 0        | 100         | 100 |
| 15  | P     | 202/205 (98%) | 196 (97%)  | 6 (3%)   | 0        | 100         | 100 |
| 15  | p     | 202/205 (98%) | 194 (96%)  | 8 (4%)   | 0        | 100         | 100 |
| 16  | Q     | 194/201 (96%) | 188 (97%)  | 5 (3%)   | 1 (0%)   | 24          | 54  |
| 16  | q     | 194/201 (96%) | 186 (96%)  | 8 (4%)   | 0        | 100         | 100 |
| 17  | R     | 198/263 (75%) | 197 (100%) | 1 (0%)   | 0        | 100         | 100 |
| 17  | r     | 198/263 (75%) | 194 (98%)  | 4 (2%)   | 0        | 100         | 100 |
| 18  | S     | 210/241 (87%) | 205 (98%)  | 5 (2%)   | 0        | 100         | 100 |
| 18  | s     | 210/241 (87%) | 209 (100%) | 1 (0%)   | 0        | 100         | 100 |
| 19  | T     | 210/264 (80%) | 199 (95%)  | 11 (5%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed          | Favoured    | Allowed  | Outliers | Percentiles |     |
|-----|-------|-------------------|-------------|----------|----------|-------------|-----|
| 19  | t     | 210/264 (80%)     | 198 (94%)   | 12 (6%)  | 0        | 100         | 100 |
| 20  | V     | 470/534 (88%)     | 450 (96%)   | 20 (4%)  | 0        | 100         | 100 |
| 21  | W     | 444/456 (97%)     | 409 (92%)   | 34 (8%)  | 1 (0%)   | 43          | 72  |
| 22  | X     | 332/422 (79%)     | 315 (95%)   | 17 (5%)  | 0        | 100         | 100 |
| 23  | Y     | 376/389 (97%)     | 355 (94%)   | 21 (6%)  | 0        | 100         | 100 |
| 24  | Z     | 284/324 (88%)     | 252 (89%)   | 31 (11%) | 1 (0%)   | 30          | 59  |
| 25  | a     | 371/376 (99%)     | 327 (88%)   | 44 (12%) | 0        | 100         | 100 |
| 26  | b     | 189/377 (50%)     | 146 (77%)   | 40 (21%) | 3 (2%)   | 7           | 27  |
| 27  | c     | 285/310 (92%)     | 254 (89%)   | 30 (10%) | 1 (0%)   | 30          | 59  |
| 28  | d     | 255/350 (73%)     | 220 (86%)   | 35 (14%) | 0        | 100         | 100 |
| 29  | e     | 48/70 (69%)       | 42 (88%)    | 6 (12%)  | 0        | 100         | 100 |
| 30  | f     | 887/908 (98%)     | 840 (95%)   | 47 (5%)  | 0        | 100         | 100 |
| 31  | F     | 372/439 (85%)     | 334 (90%)   | 37 (10%) | 1 (0%)   | 36          | 65  |
| 32  | U     | 802/953 (84%)     | 752 (94%)   | 49 (6%)  | 1 (0%)   | 48          | 77  |
| All | All   | 13135/14884 (88%) | 12297 (94%) | 815 (6%) | 23 (0%)  | 44          | 72  |

All (23) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 108 | ASP  |
| 1   | A     | 109 | PRO  |
| 1   | A     | 424 | SER  |
| 3   | C     | 91  | PRO  |
| 4   | D     | 413 | GLU  |
| 5   | E     | 227 | PRO  |
| 21  | W     | 137 | TYR  |
| 26  | b     | 22  | LEU  |
| 26  | b     | 122 | LYS  |
| 31  | F     | 255 | GLN  |
| 1   | A     | 107 | GLU  |
| 1   | A     | 193 | THR  |
| 2   | B     | 278 | ALA  |
| 26  | b     | 181 | ASP  |
| 1   | A     | 91  | GLN  |
| 3   | C     | 242 | ALA  |
| 11  | L     | 201 | ALA  |
| 3   | C     | 117 | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 24  | Z     | 222 | ILE  |
| 27  | c     | 156 | VAL  |
| 32  | U     | 815 | ALA  |
| 3   | C     | 251 | ILE  |
| 16  | Q     | 25  | ILE  |

### 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   | A     | 310/372 (83%) | 296 (96%)  | 14 (4%)  | 24          | 58  |
| 2   | B     | 341/385 (89%) | 312 (92%)  | 29 (8%)  | 10          | 31  |
| 3   | C     | 325/352 (92%) | 315 (97%)  | 10 (3%)  | 35          | 69  |
| 4   | D     | 333/366 (91%) | 316 (95%)  | 17 (5%)  | 21          | 53  |
| 5   | E     | 298/353 (84%) | 282 (95%)  | 16 (5%)  | 20          | 51  |
| 6   | G     | 165/210 (79%) | 161 (98%)  | 4 (2%)   | 43          | 75  |
| 6   | g     | 168/210 (80%) | 166 (99%)  | 2 (1%)   | 63          | 86  |
| 7   | H     | 150/191 (78%) | 148 (99%)  | 2 (1%)   | 61          | 86  |
| 7   | h     | 150/191 (78%) | 149 (99%)  | 1 (1%)   | 76          | 92  |
| 8   | I     | 166/221 (75%) | 160 (96%)  | 6 (4%)   | 31          | 65  |
| 8   | i     | 160/221 (72%) | 155 (97%)  | 5 (3%)   | 35          | 69  |
| 9   | J     | 136/211 (64%) | 134 (98%)  | 2 (2%)   | 57          | 84  |
| 9   | j     | 136/211 (64%) | 133 (98%)  | 3 (2%)   | 45          | 77  |
| 10  | K     | 159/203 (78%) | 156 (98%)  | 3 (2%)   | 50          | 79  |
| 10  | k     | 158/203 (78%) | 154 (98%)  | 4 (2%)   | 42          | 74  |
| 11  | L     | 161/224 (72%) | 155 (96%)  | 6 (4%)   | 30          | 64  |
| 11  | l     | 161/224 (72%) | 161 (100%) | 0        | 100         | 100 |
| 12  | M     | 162/212 (76%) | 158 (98%)  | 4 (2%)   | 42          | 74  |
| 12  | m     | 163/212 (77%) | 159 (98%)  | 4 (2%)   | 42          | 74  |
| 13  | N     | 141/181 (78%) | 136 (96%)  | 5 (4%)   | 32          | 66  |

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| Mol | Chain | Analysed          | Rotameric  | Outliers | Percentiles |    |
|-----|-------|-------------------|------------|----------|-------------|----|
| 13  | n     | 140/181 (77%)     | 138 (99%)  | 2 (1%)   | 59          | 85 |
| 14  | O     | 158/228 (69%)     | 153 (97%)  | 5 (3%)   | 34          | 68 |
| 14  | o     | 157/228 (69%)     | 156 (99%)  | 1 (1%)   | 78          | 93 |
| 15  | P     | 159/174 (91%)     | 158 (99%)  | 1 (1%)   | 78          | 93 |
| 15  | p     | 156/174 (90%)     | 154 (99%)  | 2 (1%)   | 61          | 86 |
| 16  | Q     | 149/171 (87%)     | 146 (98%)  | 3 (2%)   | 48          | 78 |
| 16  | q     | 148/171 (86%)     | 147 (99%)  | 1 (1%)   | 76          | 92 |
| 17  | R     | 139/202 (69%)     | 135 (97%)  | 4 (3%)   | 37          | 71 |
| 17  | r     | 138/202 (68%)     | 132 (96%)  | 6 (4%)   | 26          | 60 |
| 18  | S     | 158/199 (79%)     | 156 (99%)  | 2 (1%)   | 61          | 86 |
| 18  | s     | 159/199 (80%)     | 157 (99%)  | 2 (1%)   | 61          | 86 |
| 19  | T     | 151/215 (70%)     | 150 (99%)  | 1 (1%)   | 76          | 92 |
| 19  | t     | 149/215 (69%)     | 148 (99%)  | 1 (1%)   | 76          | 92 |
| 20  | V     | 391/460 (85%)     | 372 (95%)  | 19 (5%)  | 22          | 54 |
| 21  | W     | 410/416 (99%)     | 390 (95%)  | 20 (5%)  | 22          | 54 |
| 22  | X     | 291/362 (80%)     | 279 (96%)  | 12 (4%)  | 27          | 61 |
| 23  | Y     | 334/344 (97%)     | 318 (95%)  | 16 (5%)  | 23          | 55 |
| 24  | Z     | 257/295 (87%)     | 237 (92%)  | 20 (8%)  | 11          | 35 |
| 25  | a     | 333/336 (99%)     | 317 (95%)  | 16 (5%)  | 23          | 55 |
| 26  | b     | 167/312 (54%)     | 158 (95%)  | 9 (5%)   | 20          | 51 |
| 27  | c     | 252/268 (94%)     | 232 (92%)  | 20 (8%)  | 11          | 34 |
| 28  | d     | 231/294 (79%)     | 217 (94%)  | 14 (6%)  | 17          | 46 |
| 29  | e     | 44/63 (70%)       | 42 (96%)   | 2 (4%)   | 24          | 58 |
| 30  | f     | 745/763 (98%)     | 730 (98%)  | 15 (2%)  | 48          | 78 |
| 31  | F     | 296/379 (78%)     | 271 (92%)  | 25 (8%)  | 10          | 31 |
| 32  | U     | 688/816 (84%)     | 657 (96%)  | 31 (4%)  | 24          | 58 |
| All | All   | 10343/12620 (82%) | 9956 (96%) | 387 (4%) | 31          | 64 |

All (387) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 79  | ASP  |
| 1   | A     | 90  | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 106 | SER  |
| 1   | A     | 171 | ASP  |
| 1   | A     | 189 | GLU  |
| 1   | A     | 190 | VAL  |
| 1   | A     | 191 | VAL  |
| 1   | A     | 193 | THR  |
| 1   | A     | 240 | VAL  |
| 1   | A     | 267 | LYS  |
| 1   | A     | 322 | ASN  |
| 1   | A     | 347 | ASP  |
| 1   | A     | 367 | ASP  |
| 1   | A     | 405 | THR  |
| 2   | B     | 63  | LEU  |
| 2   | B     | 75  | GLU  |
| 2   | B     | 78  | PHE  |
| 2   | B     | 99  | VAL  |
| 2   | B     | 102 | LEU  |
| 2   | B     | 107 | MET  |
| 2   | B     | 109 | VAL  |
| 2   | B     | 175 | LYS  |
| 2   | B     | 184 | TYR  |
| 2   | B     | 214 | MET  |
| 2   | B     | 216 | ILE  |
| 2   | B     | 239 | VAL  |
| 2   | B     | 243 | THR  |
| 2   | B     | 249 | ARG  |
| 2   | B     | 254 | GLU  |
| 2   | B     | 257 | GLN  |
| 2   | B     | 269 | GLU  |
| 2   | B     | 309 | MET  |
| 2   | B     | 319 | PHE  |
| 2   | B     | 322 | ARG  |
| 2   | B     | 332 | ASN  |
| 2   | B     | 335 | GLU  |
| 2   | B     | 362 | LYS  |
| 2   | B     | 367 | ILE  |
| 2   | B     | 383 | LEU  |
| 2   | B     | 384 | ILE  |
| 2   | B     | 385 | MET  |
| 2   | B     | 412 | MET  |
| 2   | B     | 423 | LYS  |
| 3   | C     | 24  | TYR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | C     | 94  | LYS  |
| 3   | C     | 122 | THR  |
| 3   | C     | 145 | ASP  |
| 3   | C     | 178 | LEU  |
| 3   | C     | 188 | LEU  |
| 3   | C     | 230 | MET  |
| 3   | C     | 236 | VAL  |
| 3   | C     | 283 | PHE  |
| 3   | C     | 295 | THR  |
| 4   | D     | 60  | TYR  |
| 4   | D     | 77  | GLU  |
| 4   | D     | 81  | ARG  |
| 4   | D     | 82  | ILE  |
| 4   | D     | 105 | SER  |
| 4   | D     | 150 | SER  |
| 4   | D     | 152 | MET  |
| 4   | D     | 172 | ILE  |
| 4   | D     | 176 | GLU  |
| 4   | D     | 190 | LEU  |
| 4   | D     | 240 | LEU  |
| 4   | D     | 270 | ILE  |
| 4   | D     | 292 | LEU  |
| 4   | D     | 304 | ASN  |
| 4   | D     | 352 | MET  |
| 4   | D     | 355 | SER  |
| 4   | D     | 374 | ASP  |
| 5   | E     | 65  | THR  |
| 5   | E     | 98  | VAL  |
| 5   | E     | 102 | MET  |
| 5   | E     | 130 | VAL  |
| 5   | E     | 149 | ILE  |
| 5   | E     | 161 | ARG  |
| 5   | E     | 162 | VAL  |
| 5   | E     | 217 | GLU  |
| 5   | E     | 236 | ASP  |
| 5   | E     | 247 | THR  |
| 5   | E     | 254 | GLN  |
| 5   | E     | 267 | PHE  |
| 5   | E     | 309 | ARG  |
| 5   | E     | 333 | LYS  |
| 5   | E     | 363 | VAL  |
| 5   | E     | 374 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6   | G     | 75  | ASN  |
| 6   | G     | 109 | ILE  |
| 6   | G     | 131 | MET  |
| 6   | G     | 202 | LEU  |
| 7   | H     | 117 | MET  |
| 7   | H     | 126 | VAL  |
| 8   | I     | 7   | SER  |
| 8   | I     | 50  | ARG  |
| 8   | I     | 168 | SER  |
| 8   | I     | 177 | GLN  |
| 8   | I     | 188 | SER  |
| 8   | I     | 209 | GLU  |
| 9   | J     | 26  | VAL  |
| 9   | J     | 167 | SER  |
| 10  | K     | 47  | CYS  |
| 10  | K     | 159 | SER  |
| 10  | K     | 180 | SER  |
| 11  | L     | 39  | LYS  |
| 11  | L     | 83  | LEU  |
| 11  | L     | 121 | GLN  |
| 11  | L     | 146 | GLN  |
| 11  | L     | 156 | CYS  |
| 11  | L     | 222 | THR  |
| 12  | M     | 24  | GLU  |
| 12  | M     | 27  | MET  |
| 12  | M     | 45  | VAL  |
| 12  | M     | 75  | MET  |
| 13  | N     | 23  | THR  |
| 13  | N     | 68  | SER  |
| 13  | N     | 70  | GLU  |
| 13  | N     | 87  | MET  |
| 13  | N     | 124 | GLN  |
| 14  | O     | 30  | LYS  |
| 14  | O     | 33  | SER  |
| 14  | O     | 39  | SER  |
| 14  | O     | 66  | LEU  |
| 14  | O     | 195 | LYS  |
| 15  | P     | 121 | CYS  |
| 16  | Q     | 28  | MET  |
| 16  | Q     | 76  | SER  |
| 16  | Q     | 179 | SER  |
| 17  | R     | 14  | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 17  | R     | 45  | THR  |
| 17  | R     | 103 | CYS  |
| 17  | R     | 112 | LEU  |
| 18  | S     | 109 | ILE  |
| 18  | S     | 113 | LEU  |
| 19  | T     | 100 | ARG  |
| 20  | V     | 79  | VAL  |
| 20  | V     | 108 | LEU  |
| 20  | V     | 110 | HIS  |
| 20  | V     | 187 | ILE  |
| 20  | V     | 209 | LYS  |
| 20  | V     | 222 | ASP  |
| 20  | V     | 232 | HIS  |
| 20  | V     | 271 | VAL  |
| 20  | V     | 324 | PHE  |
| 20  | V     | 326 | GLN  |
| 20  | V     | 356 | SER  |
| 20  | V     | 363 | LEU  |
| 20  | V     | 371 | ASN  |
| 20  | V     | 380 | ASP  |
| 20  | V     | 435 | GLU  |
| 20  | V     | 437 | ILE  |
| 20  | V     | 469 | THR  |
| 20  | V     | 471 | GLU  |
| 20  | V     | 486 | ILE  |
| 21  | W     | 16  | MET  |
| 21  | W     | 48  | LEU  |
| 21  | W     | 70  | VAL  |
| 21  | W     | 110 | THR  |
| 21  | W     | 170 | GLN  |
| 21  | W     | 194 | LEU  |
| 21  | W     | 209 | ILE  |
| 21  | W     | 231 | ILE  |
| 21  | W     | 235 | GLN  |
| 21  | W     | 263 | TRP  |
| 21  | W     | 267 | LEU  |
| 21  | W     | 274 | VAL  |
| 21  | W     | 299 | ILE  |
| 21  | W     | 314 | LEU  |
| 21  | W     | 359 | VAL  |
| 21  | W     | 378 | MET  |
| 21  | W     | 383 | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 21  | W     | 406 | VAL  |
| 21  | W     | 409 | LEU  |
| 21  | W     | 446 | ILE  |
| 22  | X     | 130 | GLU  |
| 22  | X     | 295 | LYS  |
| 22  | X     | 312 | GLU  |
| 22  | X     | 313 | LEU  |
| 22  | X     | 321 | THR  |
| 22  | X     | 330 | LEU  |
| 22  | X     | 344 | ARG  |
| 22  | X     | 347 | ILE  |
| 22  | X     | 377 | ILE  |
| 22  | X     | 404 | ILE  |
| 22  | X     | 405 | GLN  |
| 22  | X     | 417 | LYS  |
| 23  | Y     | 28  | LEU  |
| 23  | Y     | 70  | LEU  |
| 23  | Y     | 73  | MET  |
| 23  | Y     | 131 | THR  |
| 23  | Y     | 152 | MET  |
| 23  | Y     | 178 | ASN  |
| 23  | Y     | 206 | SER  |
| 23  | Y     | 207 | THR  |
| 23  | Y     | 218 | THR  |
| 23  | Y     | 231 | LEU  |
| 23  | Y     | 240 | VAL  |
| 23  | Y     | 291 | HIS  |
| 23  | Y     | 315 | THR  |
| 23  | Y     | 348 | ASP  |
| 23  | Y     | 382 | LYS  |
| 23  | Y     | 384 | SER  |
| 24  | Z     | 20  | VAL  |
| 24  | Z     | 43  | TRP  |
| 24  | Z     | 44  | GLN  |
| 24  | Z     | 60  | GLU  |
| 24  | Z     | 77  | ASN  |
| 24  | Z     | 112 | MET  |
| 24  | Z     | 125 | ASP  |
| 24  | Z     | 130 | ASP  |
| 24  | Z     | 159 | THR  |
| 24  | Z     | 169 | GLU  |
| 24  | Z     | 172 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 24  | Z     | 187 | LEU  |
| 24  | Z     | 192 | THR  |
| 24  | Z     | 196 | HIS  |
| 24  | Z     | 210 | SER  |
| 24  | Z     | 214 | LYS  |
| 24  | Z     | 217 | THR  |
| 24  | Z     | 231 | GLN  |
| 24  | Z     | 240 | VAL  |
| 24  | Z     | 274 | ASN  |
| 25  | a     | 8   | LEU  |
| 25  | a     | 33  | LEU  |
| 25  | a     | 72  | ASN  |
| 25  | a     | 75  | SER  |
| 25  | a     | 113 | LEU  |
| 25  | a     | 124 | ASN  |
| 25  | a     | 125 | ILE  |
| 25  | a     | 151 | VAL  |
| 25  | a     | 205 | LEU  |
| 25  | a     | 272 | ILE  |
| 25  | a     | 273 | GLN  |
| 25  | a     | 304 | VAL  |
| 25  | a     | 328 | ASP  |
| 25  | a     | 343 | LEU  |
| 25  | a     | 362 | SER  |
| 25  | a     | 373 | ASP  |
| 26  | b     | 17  | ARG  |
| 26  | b     | 51  | LEU  |
| 26  | b     | 56  | ASN  |
| 26  | b     | 71  | ILE  |
| 26  | b     | 103 | LYS  |
| 26  | b     | 108 | ARG  |
| 26  | b     | 110 | ILE  |
| 26  | b     | 127 | LEU  |
| 26  | b     | 159 | THR  |
| 27  | c     | 66  | THR  |
| 27  | c     | 67  | VAL  |
| 27  | c     | 69  | VAL  |
| 27  | c     | 75  | MET  |
| 27  | c     | 98  | MET  |
| 27  | c     | 101 | GLN  |
| 27  | c     | 157 | ILE  |
| 27  | c     | 166 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 27  | c     | 178 | THR  |
| 27  | c     | 209 | LYS  |
| 27  | c     | 215 | LYS  |
| 27  | c     | 222 | LYS  |
| 27  | c     | 234 | TYR  |
| 27  | c     | 236 | GLU  |
| 27  | c     | 245 | VAL  |
| 27  | c     | 251 | LEU  |
| 27  | c     | 257 | LYS  |
| 27  | c     | 260 | GLU  |
| 27  | c     | 283 | HIS  |
| 27  | c     | 290 | VAL  |
| 28  | d     | 68  | ILE  |
| 28  | d     | 85  | TYR  |
| 28  | d     | 92  | SER  |
| 28  | d     | 106 | LEU  |
| 28  | d     | 122 | LEU  |
| 28  | d     | 151 | VAL  |
| 28  | d     | 158 | ILE  |
| 28  | d     | 163 | TYR  |
| 28  | d     | 181 | CYS  |
| 28  | d     | 197 | ILE  |
| 28  | d     | 198 | LEU  |
| 28  | d     | 222 | TYR  |
| 28  | d     | 246 | VAL  |
| 28  | d     | 252 | GLN  |
| 29  | e     | 46  | ASP  |
| 29  | e     | 47  | ASN  |
| 30  | f     | 75  | LEU  |
| 30  | f     | 236 | CYS  |
| 30  | f     | 294 | MET  |
| 30  | f     | 316 | ASP  |
| 30  | f     | 350 | LYS  |
| 30  | f     | 423 | ASP  |
| 30  | f     | 426 | LEU  |
| 30  | f     | 483 | PHE  |
| 30  | f     | 505 | MET  |
| 30  | f     | 518 | THR  |
| 30  | f     | 558 | LEU  |
| 30  | f     | 596 | ASP  |
| 30  | f     | 613 | LEU  |
| 30  | f     | 634 | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 30  | f     | 882 | LEU  |
| 6   | g     | 39  | SER  |
| 6   | g     | 189 | TRP  |
| 7   | h     | 195 | LYS  |
| 8   | i     | 81  | SER  |
| 8   | i     | 186 | LEU  |
| 8   | i     | 199 | LYS  |
| 8   | i     | 200 | THR  |
| 8   | i     | 209 | GLU  |
| 9   | j     | 71  | MET  |
| 9   | j     | 82  | ILE  |
| 9   | j     | 84  | ILE  |
| 10  | k     | 46  | VAL  |
| 10  | k     | 163 | VAL  |
| 10  | k     | 191 | LEU  |
| 10  | k     | 235 | GLU  |
| 12  | m     | 24  | GLU  |
| 12  | m     | 27  | MET  |
| 12  | m     | 59  | GLU  |
| 12  | m     | 219 | LEU  |
| 13  | n     | 68  | SER  |
| 13  | n     | 124 | GLN  |
| 14  | o     | 18  | ASP  |
| 15  | p     | 164 | GLU  |
| 15  | p     | 182 | MET  |
| 16  | q     | 39  | SER  |
| 17  | r     | 13  | VAL  |
| 17  | r     | 59  | LEU  |
| 17  | r     | 81  | SER  |
| 17  | r     | 117 | SER  |
| 17  | r     | 123 | SER  |
| 17  | r     | 137 | TYR  |
| 18  | s     | 25  | SER  |
| 18  | s     | 81  | LYS  |
| 19  | t     | 108 | ASN  |
| 31  | F     | 97  | LEU  |
| 31  | F     | 121 | CYS  |
| 31  | F     | 145 | LEU  |
| 31  | F     | 146 | LYS  |
| 31  | F     | 151 | VAL  |
| 31  | F     | 179 | GLU  |
| 31  | F     | 186 | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 31  | F     | 196 | GLN  |
| 31  | F     | 209 | LYS  |
| 31  | F     | 217 | ILE  |
| 31  | F     | 257 | VAL  |
| 31  | F     | 281 | SER  |
| 31  | F     | 289 | ASP  |
| 31  | F     | 291 | ILE  |
| 31  | F     | 304 | ARG  |
| 31  | F     | 342 | LEU  |
| 31  | F     | 344 | ARG  |
| 31  | F     | 356 | MET  |
| 31  | F     | 364 | ARG  |
| 31  | F     | 397 | LYS  |
| 31  | F     | 400 | CYS  |
| 31  | F     | 401 | VAL  |
| 31  | F     | 405 | MET  |
| 31  | F     | 431 | LYS  |
| 31  | F     | 435 | LEU  |
| 32  | U     | 10  | SER  |
| 32  | U     | 35  | TRP  |
| 32  | U     | 38  | ILE  |
| 32  | U     | 56  | SER  |
| 32  | U     | 63  | VAL  |
| 32  | U     | 67  | VAL  |
| 32  | U     | 70  | HIS  |
| 32  | U     | 138 | PHE  |
| 32  | U     | 197 | VAL  |
| 32  | U     | 232 | ILE  |
| 32  | U     | 253 | TYR  |
| 32  | U     | 255 | SER  |
| 32  | U     | 267 | ASN  |
| 32  | U     | 349 | ASP  |
| 32  | U     | 352 | ILE  |
| 32  | U     | 367 | THR  |
| 32  | U     | 371 | ILE  |
| 32  | U     | 373 | ASN  |
| 32  | U     | 453 | HIS  |
| 32  | U     | 481 | LEU  |
| 32  | U     | 508 | THR  |
| 32  | U     | 529 | ILE  |
| 32  | U     | 533 | VAL  |
| 32  | U     | 539 | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 32  | U     | 583 | MET  |
| 32  | U     | 659 | CYS  |
| 32  | U     | 689 | ILE  |
| 32  | U     | 706 | VAL  |
| 32  | U     | 723 | ASP  |
| 32  | U     | 802 | TYR  |
| 32  | U     | 879 | ASP  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (114) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 197 | HIS  |
| 1   | A     | 293 | ASN  |
| 1   | A     | 296 | GLN  |
| 1   | A     | 322 | ASN  |
| 2   | B     | 193 | GLN  |
| 2   | B     | 242 | GLN  |
| 2   | B     | 298 | ASN  |
| 2   | B     | 314 | ASN  |
| 2   | B     | 315 | GLN  |
| 3   | C     | 41  | ASN  |
| 3   | C     | 270 | GLN  |
| 3   | C     | 279 | GLN  |
| 3   | C     | 288 | ASN  |
| 3   | C     | 296 | ASN  |
| 4   | D     | 91  | GLN  |
| 4   | D     | 110 | ASN  |
| 4   | D     | 135 | HIS  |
| 4   | D     | 295 | GLN  |
| 6   | G     | 100 | ASN  |
| 6   | G     | 127 | GLN  |
| 6   | G     | 224 | ASN  |
| 7   | H     | 108 | GLN  |
| 8   | I     | 95  | GLN  |
| 8   | I     | 102 | GLN  |
| 8   | I     | 119 | GLN  |
| 8   | I     | 123 | GLN  |
| 10  | K     | 98  | ASN  |
| 10  | K     | 99  | HIS  |
| 12  | M     | 101 | ASN  |
| 12  | M     | 120 | HIS  |
| 12  | M     | 201 | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 13  | N     | 63  | GLN  |
| 13  | N     | 111 | GLN  |
| 13  | N     | 124 | GLN  |
| 14  | O     | 173 | ASN  |
| 15  | P     | 6   | ASN  |
| 15  | P     | 71  | ASN  |
| 16  | Q     | 71  | ASN  |
| 17  | R     | 163 | GLN  |
| 18  | S     | 152 | GLN  |
| 19  | T     | 188 | GLN  |
| 20  | V     | 199 | ASN  |
| 20  | V     | 252 | ASN  |
| 20  | V     | 329 | HIS  |
| 20  | V     | 401 | ASN  |
| 20  | V     | 427 | GLN  |
| 21  | W     | 86  | ASN  |
| 21  | W     | 96  | GLN  |
| 21  | W     | 361 | HIS  |
| 21  | W     | 423 | ASN  |
| 21  | W     | 433 | ASN  |
| 21  | W     | 444 | HIS  |
| 22  | X     | 218 | HIS  |
| 22  | X     | 406 | ASN  |
| 23  | Y     | 48  | ASN  |
| 23  | Y     | 49  | ASN  |
| 23  | Y     | 344 | HIS  |
| 23  | Y     | 367 | GLN  |
| 24  | Z     | 77  | ASN  |
| 24  | Z     | 145 | HIS  |
| 24  | Z     | 157 | HIS  |
| 24  | Z     | 224 | HIS  |
| 24  | Z     | 231 | GLN  |
| 24  | Z     | 256 | GLN  |
| 24  | Z     | 274 | ASN  |
| 25  | a     | 12  | GLN  |
| 25  | a     | 169 | HIS  |
| 25  | a     | 193 | GLN  |
| 25  | a     | 257 | GLN  |
| 25  | a     | 273 | GLN  |
| 25  | a     | 372 | HIS  |
| 26  | b     | 27  | GLN  |
| 26  | b     | 29  | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 26  | b     | 30  | GLN  |
| 26  | b     | 48  | ASN  |
| 26  | b     | 137 | ASN  |
| 27  | c     | 101 | GLN  |
| 27  | c     | 180 | ASN  |
| 27  | c     | 221 | HIS  |
| 27  | c     | 237 | HIS  |
| 27  | c     | 241 | ASN  |
| 28  | d     | 96  | HIS  |
| 28  | d     | 141 | GLN  |
| 28  | d     | 245 | GLN  |
| 29  | e     | 55  | GLN  |
| 30  | f     | 245 | ASN  |
| 30  | f     | 378 | ASN  |
| 30  | f     | 457 | ASN  |
| 30  | f     | 610 | GLN  |
| 30  | f     | 747 | GLN  |
| 7   | h     | 122 | GLN  |
| 10  | k     | 98  | ASN  |
| 13  | n     | 124 | GLN  |
| 15  | p     | 168 | GLN  |
| 16  | q     | 63  | ASN  |
| 18  | s     | 151 | ASN  |
| 18  | s     | 152 | GLN  |
| 19  | t     | 108 | ASN  |
| 31  | F     | 76  | ASN  |
| 31  | F     | 194 | GLN  |
| 31  | F     | 307 | GLN  |
| 32  | U     | 115 | ASN  |
| 32  | U     | 192 | GLN  |
| 32  | U     | 218 | GLN  |
| 32  | U     | 247 | GLN  |
| 32  | U     | 373 | ASN  |
| 32  | U     | 384 | GLN  |
| 32  | U     | 463 | ASN  |
| 32  | U     | 647 | HIS  |
| 32  | U     | 685 | GLN  |
| 32  | U     | 777 | HIS  |
| 32  | U     | 801 | GLN  |
| 32  | U     | 880 | ASN  |
| 32  | U     | 901 | GLN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

Of 18 ligands modelled in this entry, 6 are monoatomic - leaving 12 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 |
| 36  | LDZ  | n     | 301 | -    | 33,34,34     | 0.52 | 1 (3%)   | 42,44,44    | 0.77 | 1 (2%)   |
| 33  | ATP  | A     | 501 | 34   | 32,33,33     | 0.59 | 1 (3%)   | 48,52,52    | 0.34 | 0        |
| 36  | LDZ  | O     | 301 | -    | 33,34,34     | 0.54 | 1 (3%)   | 42,44,44    | 0.66 | 1 (2%)   |
| 36  | LDZ  | r     | 301 | -    | 33,34,34     | 0.52 | 1 (3%)   | 42,44,44    | 0.92 | 1 (2%)   |
| 33  | ATP  | D     | 501 | -    | 32,33,33     | 0.59 | 0        | 48,52,52    | 0.40 | 0        |
| 36  | LDZ  | o     | 301 | -    | 33,34,34     | 0.50 | 1 (3%)   | 42,44,44    | 0.71 | 1 (2%)   |
| 36  | LDZ  | N     | 301 | -    | 33,34,34     | 0.55 | 1 (3%)   | 42,44,44    | 0.80 | 1 (2%)   |
| 36  | LDZ  | R     | 301 | -    | 33,34,34     | 0.50 | 1 (3%)   | 42,44,44    | 0.74 | 1 (2%)   |
| 33  | ATP  | E     | 402 | 34   | 32,33,33     | 0.45 | 0        | 48,52,52    | 0.39 | 0        |
| 35  | ADP  | C     | 501 | -    | 28,29,29     | 1.36 | 5 (17%)  | 43,45,45    | 1.84 | 9 (20%)  |
| 33  | ATP  | B     | 501 | 34   | 32,33,33     | 0.36 | 0        | 48,52,52    | 0.40 | 0        |
| 35  | ADP  | F     | 501 | -    | 28,29,29     | 1.36 | 5 (17%)  | 43,45,45    | 1.81 | 9 (20%)  |

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   |
|-----|------|-------|-----|------|---------|-------------|---------|
| 36  | LDZ  | n     | 301 | -    | -       | 13/38/39/39 | 0/1/1/1 |
| 33  | ATP  | A     | 501 | 34   | -       | 3/22/38/38  | 0/3/3/3 |
| 36  | LDZ  | O     | 301 | -    | -       | 13/38/39/39 | 0/1/1/1 |
| 36  | LDZ  | r     | 301 | -    | -       | 13/38/39/39 | 0/1/1/1 |
| 33  | ATP  | D     | 501 | -    | -       | 0/22/38/38  | 0/3/3/3 |
| 36  | LDZ  | o     | 301 | -    | -       | 5/38/39/39  | 0/1/1/1 |
| 36  | LDZ  | N     | 301 | -    | -       | 11/38/39/39 | 0/1/1/1 |
| 36  | LDZ  | R     | 301 | -    | -       | 4/38/39/39  | 0/1/1/1 |
| 33  | ATP  | E     | 402 | 34   | -       | 7/22/38/38  | 0/3/3/3 |
| 35  | ADP  | C     | 501 | -    | -       | 3/16/32/32  | 0/3/3/3 |
| 33  | ATP  | B     | 501 | 34   | -       | 3/22/38/38  | 0/3/3/3 |
| 35  | ADP  | F     | 501 | -    | -       | 2/16/32/32  | 0/3/3/3 |

All (17) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 35  | C     | 501 | ADP  | C5-C4   | 4.42  | 1.47        | 1.39     |
| 35  | F     | 501 | ADP  | C5-C4   | 4.36  | 1.46        | 1.39     |
| 35  | F     | 501 | ADP  | C5-N7   | -2.56 | 1.34        | 1.39     |
| 35  | C     | 501 | ADP  | C5-C6   | 2.54  | 1.48        | 1.41     |
| 35  | C     | 501 | ADP  | C5-N7   | -2.51 | 1.34        | 1.39     |
| 35  | F     | 501 | ADP  | C5-C6   | 2.38  | 1.47        | 1.41     |
| 36  | O     | 301 | LDZ  | C17-N16 | -2.29 | 1.43        | 1.46     |
| 36  | N     | 301 | LDZ  | C17-N16 | -2.27 | 1.43        | 1.46     |
| 35  | C     | 501 | ADP  | C8-N7   | 2.23  | 1.36        | 1.31     |
| 35  | F     | 501 | ADP  | C8-N7   | 2.19  | 1.35        | 1.31     |
| 35  | F     | 501 | ADP  | C4-N9   | -2.14 | 1.33        | 1.37     |
| 35  | C     | 501 | ADP  | C4-N9   | -2.09 | 1.33        | 1.37     |
| 36  | o     | 301 | LDZ  | C17-N16 | -2.06 | 1.43        | 1.46     |
| 36  | r     | 301 | LDZ  | C17-N16 | -2.05 | 1.43        | 1.46     |
| 33  | A     | 501 | ATP  | PB-O3B  | -2.04 | 1.57        | 1.59     |
| 36  | R     | 301 | LDZ  | C17-N16 | -2.03 | 1.43        | 1.46     |
| 36  | n     | 301 | LDZ  | C17-N16 | -2.01 | 1.43        | 1.46     |

All (24) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 35  | C     | 501 | ADP  | C5-C4-N3 | -5.85 | 118.66      | 126.72   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 35  | F     | 501 | ADP  | C5-C4-N3    | -5.70 | 118.87      | 126.72   |
| 35  | C     | 501 | ADP  | N3-C4-N9    | 4.51  | 134.84      | 127.17   |
| 35  | F     | 501 | ADP  | N3-C4-N9    | 4.50  | 134.82      | 127.17   |
| 36  | r     | 301 | LDZ  | C14-N13-C12 | 3.87  | 129.96      | 121.65   |
| 35  | C     | 501 | ADP  | C2-N3-C4    | 3.70  | 120.87      | 111.83   |
| 35  | F     | 501 | ADP  | C2-N3-C4    | 3.57  | 120.55      | 111.83   |
| 35  | C     | 501 | ADP  | C4-C5-N7    | -3.49 | 106.59      | 110.58   |
| 35  | F     | 501 | ADP  | C4-C5-N7    | -3.36 | 106.74      | 110.58   |
| 35  | C     | 501 | ADP  | N3-C2-N1    | -3.29 | 123.60      | 128.58   |
| 35  | F     | 501 | ADP  | N3-C2-N1    | -3.19 | 123.75      | 128.58   |
| 36  | N     | 301 | LDZ  | C15-C14-N13 | -2.97 | 103.08      | 111.11   |
| 35  | F     | 501 | ADP  | C4-N9-C8    | 2.70  | 108.57      | 105.74   |
| 36  | n     | 301 | LDZ  | C15-C14-N13 | -2.69 | 103.84      | 111.11   |
| 35  | C     | 501 | ADP  | C4-N9-C8    | 2.50  | 108.36      | 105.74   |
| 35  | F     | 501 | ADP  | C5-N7-C8    | 2.49  | 107.36      | 103.45   |
| 35  | C     | 501 | ADP  | C3'-C2'-C1' | 2.48  | 106.16      | 101.46   |
| 35  | C     | 501 | ADP  | C5-N7-C8    | 2.48  | 107.35      | 103.45   |
| 36  | O     | 301 | LDZ  | C15-C14-N13 | -2.32 | 104.84      | 111.11   |
| 36  | o     | 301 | LDZ  | C15-C14-N13 | -2.29 | 104.91      | 111.11   |
| 36  | R     | 301 | LDZ  | C15-C14-N13 | -2.25 | 105.02      | 111.11   |
| 35  | F     | 501 | ADP  | C3'-C2'-C1' | 2.12  | 105.47      | 101.46   |
| 35  | F     | 501 | ADP  | N9-C8-N7    | -2.06 | 111.02      | 113.94   |
| 35  | C     | 501 | ADP  | C6-C5-N7    | 2.01  | 135.96      | 132.09   |

There are no chirality outliers.

All (77) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 33  | A     | 501 | ATP  | PB-O3B-PG-O3G   |
| 33  | B     | 501 | ATP  | C4'-C5'-O5'-PA  |
| 33  | E     | 402 | ATP  | C5'-O5'-PA-O2A  |
| 33  | E     | 402 | ATP  | C5'-O5'-PA-O3A  |
| 35  | C     | 501 | ADP  | C5'-O5'-PA-O1A  |
| 35  | F     | 501 | ADP  | C5'-O5'-PA-O3A  |
| 36  | N     | 301 | LDZ  | C22-C17-C18-C19 |
| 36  | O     | 301 | LDZ  | O31-C9-O8-C7    |
| 36  | O     | 301 | LDZ  | N10-C9-O8-C7    |
| 36  | O     | 301 | LDZ  | O8-C9-N10-C11   |
| 36  | R     | 301 | LDZ  | O31-C9-O8-C7    |
| 36  | R     | 301 | LDZ  | N10-C9-O8-C7    |
| 36  | R     | 301 | LDZ  | C22-C17-C18-C19 |
| 36  | n     | 301 | LDZ  | O31-C9-O8-C7    |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 36  | n     | 301 | LDZ  | N10-C9-O8-C7    |
| 36  | n     | 301 | LDZ  | O31-C9-N10-C11  |
| 36  | r     | 301 | LDZ  | O31-C9-O8-C7    |
| 36  | r     | 301 | LDZ  | N10-C9-O8-C7    |
| 36  | O     | 301 | LDZ  | O31-C9-N10-C11  |
| 36  | r     | 301 | LDZ  | C12-C11-C30-C31 |
| 36  | n     | 301 | LDZ  | O8-C9-N10-C11   |
| 36  | n     | 301 | LDZ  | C15-C14-C24-C25 |
| 36  | O     | 301 | LDZ  | C15-C14-C24-C25 |
| 33  | A     | 501 | ATP  | O4'-C4'-C5'-O5' |
| 33  | A     | 501 | ATP  | C3'-C4'-C5'-O5' |
| 35  | C     | 501 | ADP  | O4'-C4'-C5'-O5' |
| 36  | R     | 301 | LDZ  | N16-C17-C18-C19 |
| 36  | N     | 301 | LDZ  | C30-C11-C12-N13 |
| 36  | N     | 301 | LDZ  | C30-C11-C12-O32 |
| 36  | n     | 301 | LDZ  | C11-C30-C31-C33 |
| 36  | n     | 301 | LDZ  | N13-C14-C24-C25 |
| 36  | r     | 301 | LDZ  | C30-C11-N10-C9  |
| 33  | E     | 402 | ATP  | O4'-C4'-C5'-O5' |
| 35  | C     | 501 | ADP  | C3'-C4'-C5'-O5' |
| 36  | O     | 301 | LDZ  | N13-C14-C24-C25 |
| 36  | n     | 301 | LDZ  | C11-C30-C31-C32 |
| 36  | r     | 301 | LDZ  | C11-C12-N13-C14 |
| 36  | r     | 301 | LDZ  | O32-C12-N13-C14 |
| 36  | n     | 301 | LDZ  | C17-C18-C19-C21 |
| 36  | n     | 301 | LDZ  | C17-C18-C19-C20 |
| 36  | O     | 301 | LDZ  | N16-C17-C18-C19 |
| 36  | r     | 301 | LDZ  | O8-C9-N10-C11   |
| 36  | O     | 301 | LDZ  | C14-C24-C25-C27 |
| 36  | r     | 301 | LDZ  | O31-C9-N10-C11  |
| 36  | O     | 301 | LDZ  | C14-C24-C25-C26 |
| 36  | o     | 301 | LDZ  | C3-C7-O8-C9     |
| 33  | B     | 501 | ATP  | O4'-C4'-C5'-O5' |
| 36  | o     | 301 | LDZ  | C11-C30-C31-C32 |
| 36  | r     | 301 | LDZ  | N13-C14-C24-C25 |
| 33  | E     | 402 | ATP  | C3'-C4'-C5'-O5' |
| 36  | o     | 301 | LDZ  | C11-C30-C31-C33 |
| 36  | N     | 301 | LDZ  | C18-C17-N16-C15 |
| 36  | n     | 301 | LDZ  | C18-C17-N16-C15 |
| 36  | N     | 301 | LDZ  | N10-C11-C12-O32 |
| 36  | r     | 301 | LDZ  | C11-C30-C31-C32 |
| 33  | E     | 402 | ATP  | C5'-O5'-PA-O1A  |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 35  | F     | 501 | ADP  | C5'-O5'-PA-O1A  |
| 36  | N     | 301 | LDZ  | N10-C11-C12-N13 |
| 36  | N     | 301 | LDZ  | C14-C24-C25-C26 |
| 36  | N     | 301 | LDZ  | N13-C14-C15-O34 |
| 36  | r     | 301 | LDZ  | N10-C11-C30-C31 |
| 36  | r     | 301 | LDZ  | C11-C30-C31-C33 |
| 36  | O     | 301 | LDZ  | C11-C30-C31-C32 |
| 36  | N     | 301 | LDZ  | N13-C14-C15-N16 |
| 36  | n     | 301 | LDZ  | C3-C7-O8-C9     |
| 36  | O     | 301 | LDZ  | C11-C30-C31-C33 |
| 36  | o     | 301 | LDZ  | N13-C14-C24-C25 |
| 36  | O     | 301 | LDZ  | C22-C17-N16-C15 |
| 36  | n     | 301 | LDZ  | C22-C17-N16-C15 |
| 36  | N     | 301 | LDZ  | O8-C9-N10-C11   |
| 36  | N     | 301 | LDZ  | O31-C9-N10-C11  |
| 33  | E     | 402 | ATP  | C2'-C1'-N9-C8   |
| 36  | O     | 301 | LDZ  | C18-C17-N16-C15 |
| 36  | r     | 301 | LDZ  | C18-C17-N16-C15 |
| 33  | B     | 501 | ATP  | C3'-C4'-C5'-O5' |
| 33  | E     | 402 | ATP  | C2'-C1'-N9-C4   |
| 36  | o     | 301 | LDZ  | N16-C17-C18-C19 |

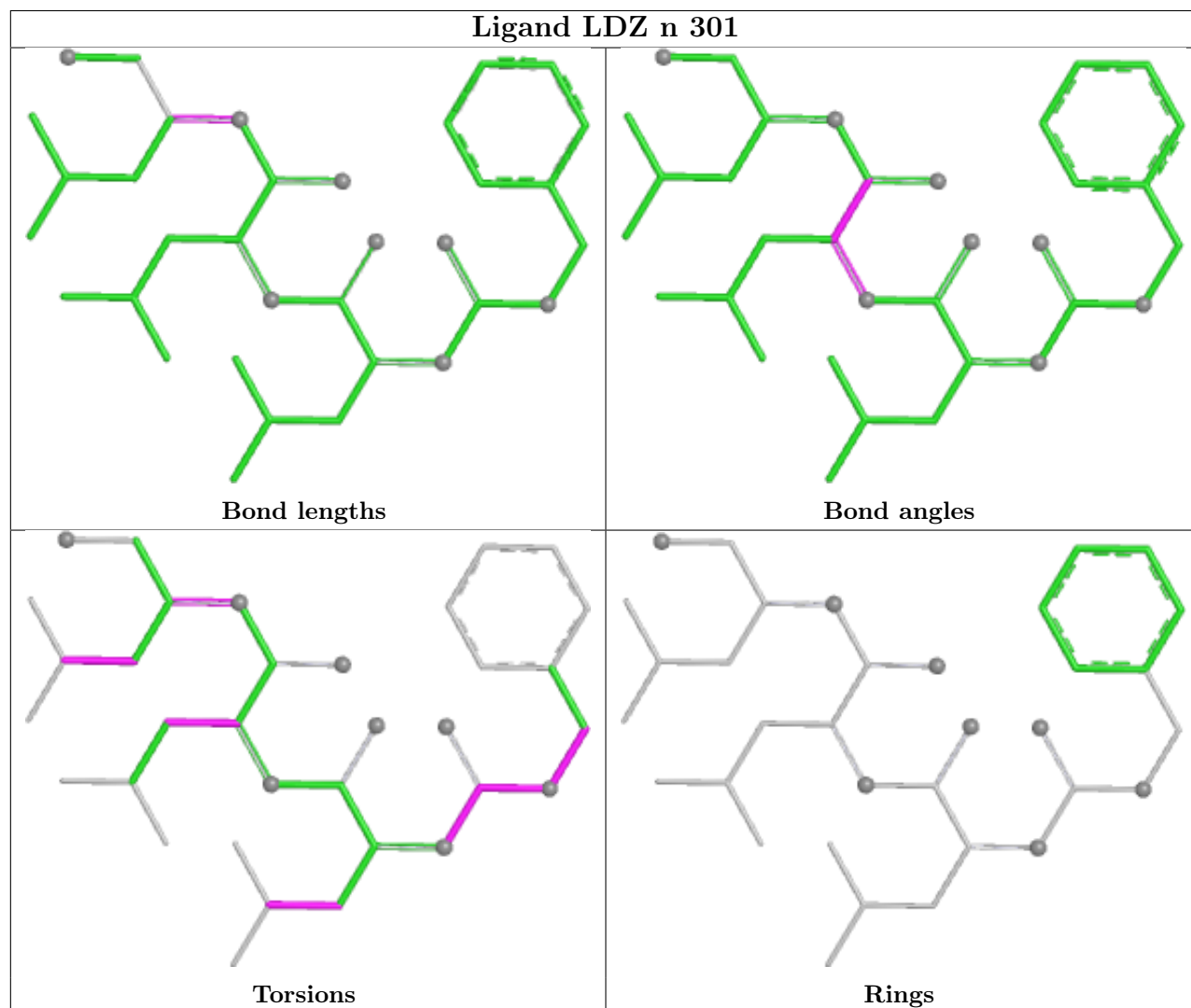
There are no ring outliers.

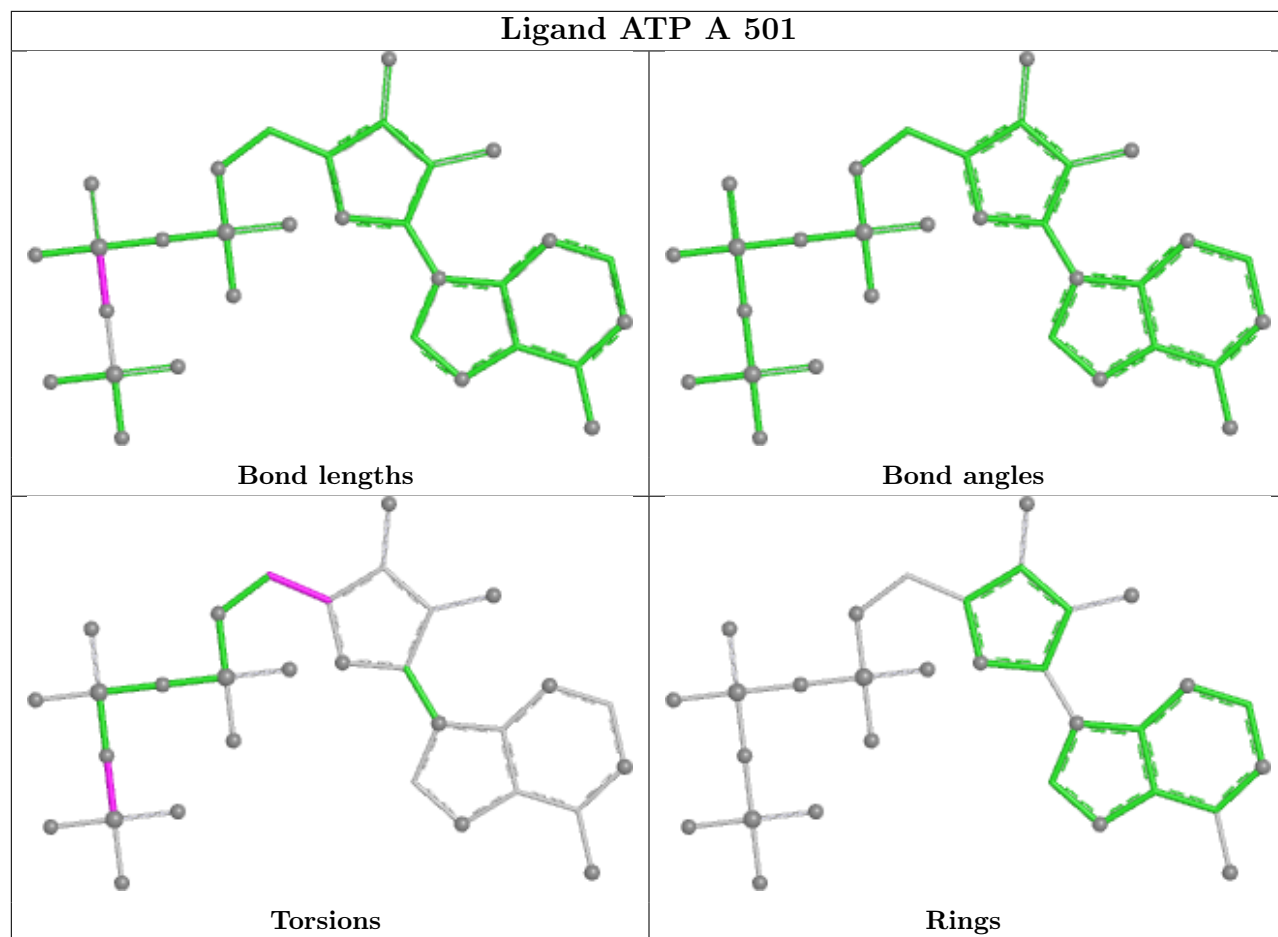
10 monomers are involved in 40 short contacts:

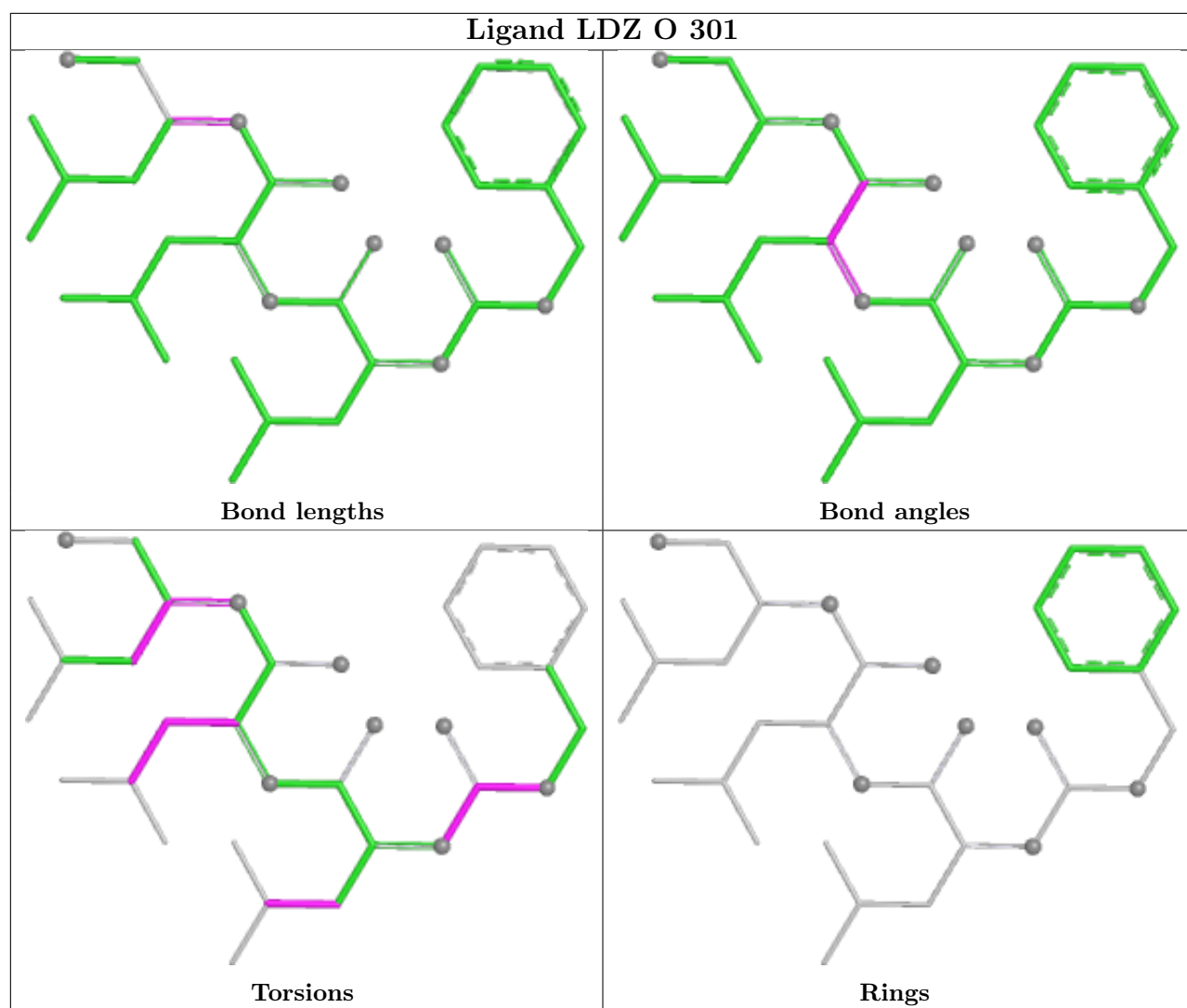
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 36  | n     | 301 | LDZ  | 3       | 0            |
| 33  | A     | 501 | ATP  | 4       | 0            |
| 33  | D     | 501 | ATP  | 8       | 0            |
| 36  | o     | 301 | LDZ  | 1       | 0            |
| 36  | N     | 301 | LDZ  | 1       | 0            |
| 36  | R     | 301 | LDZ  | 7       | 0            |
| 33  | E     | 402 | ATP  | 7       | 0            |
| 35  | C     | 501 | ADP  | 4       | 0            |
| 33  | B     | 501 | ATP  | 3       | 0            |
| 35  | F     | 501 | ADP  | 2       | 0            |

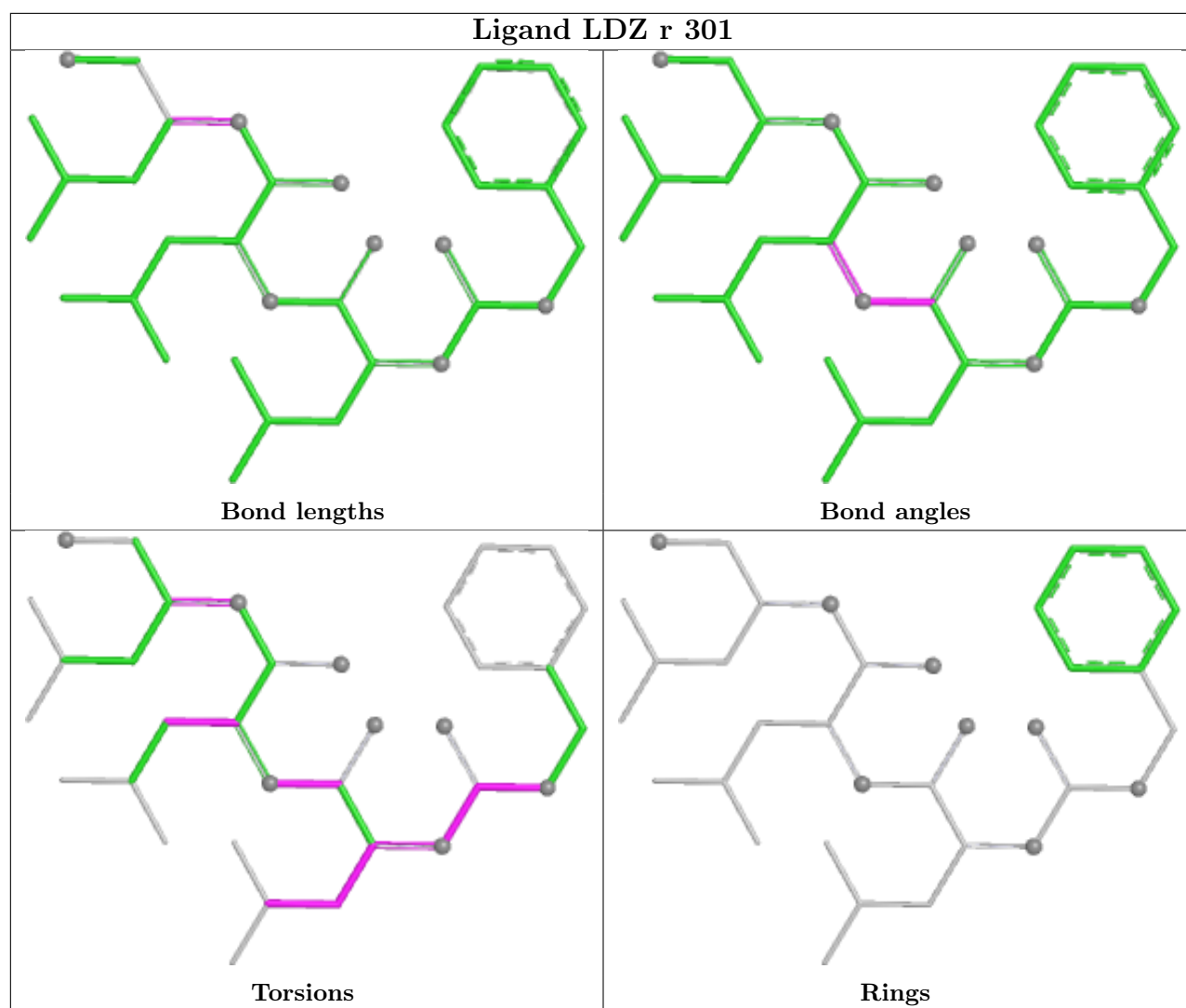
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

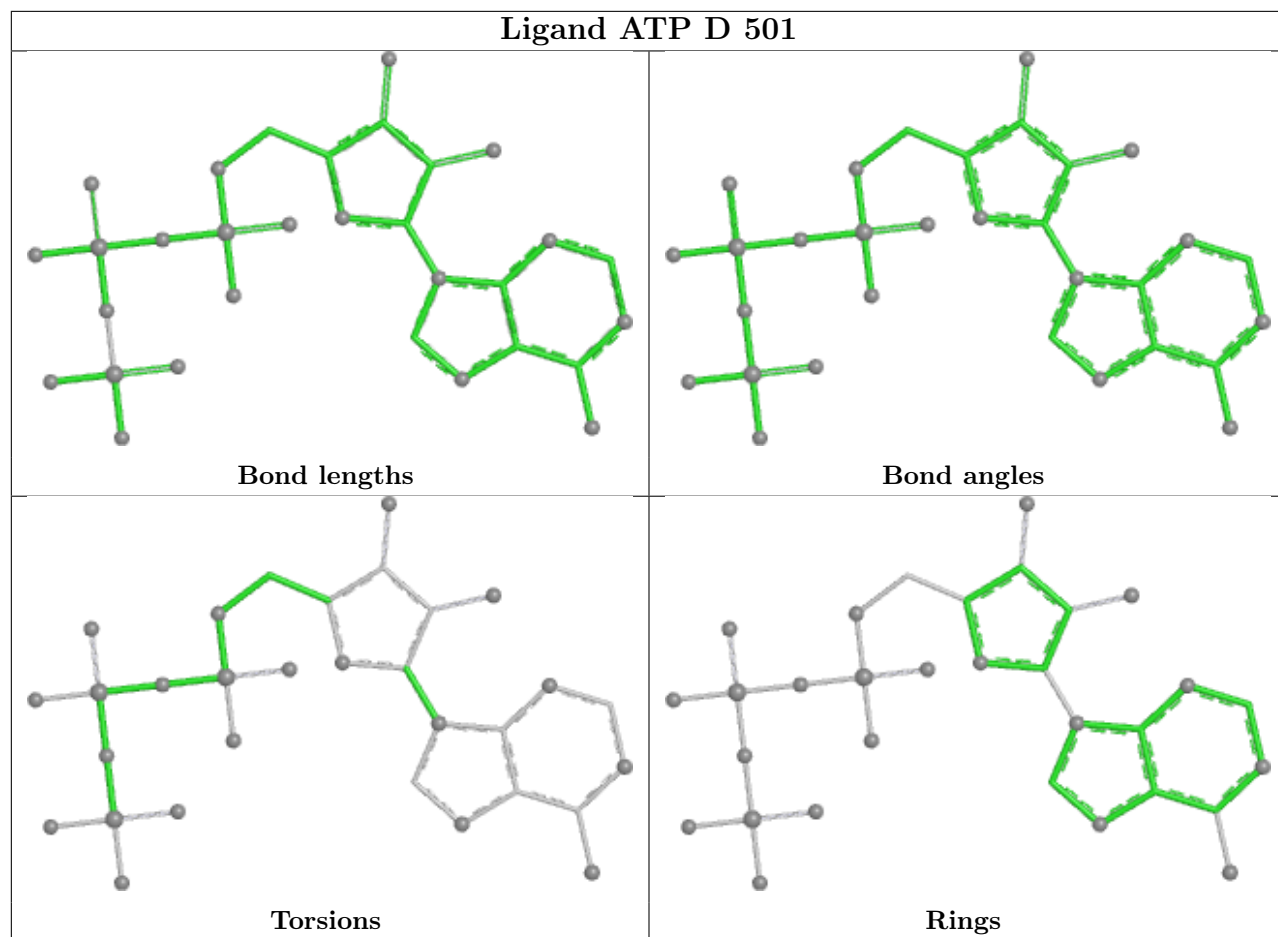
Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD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

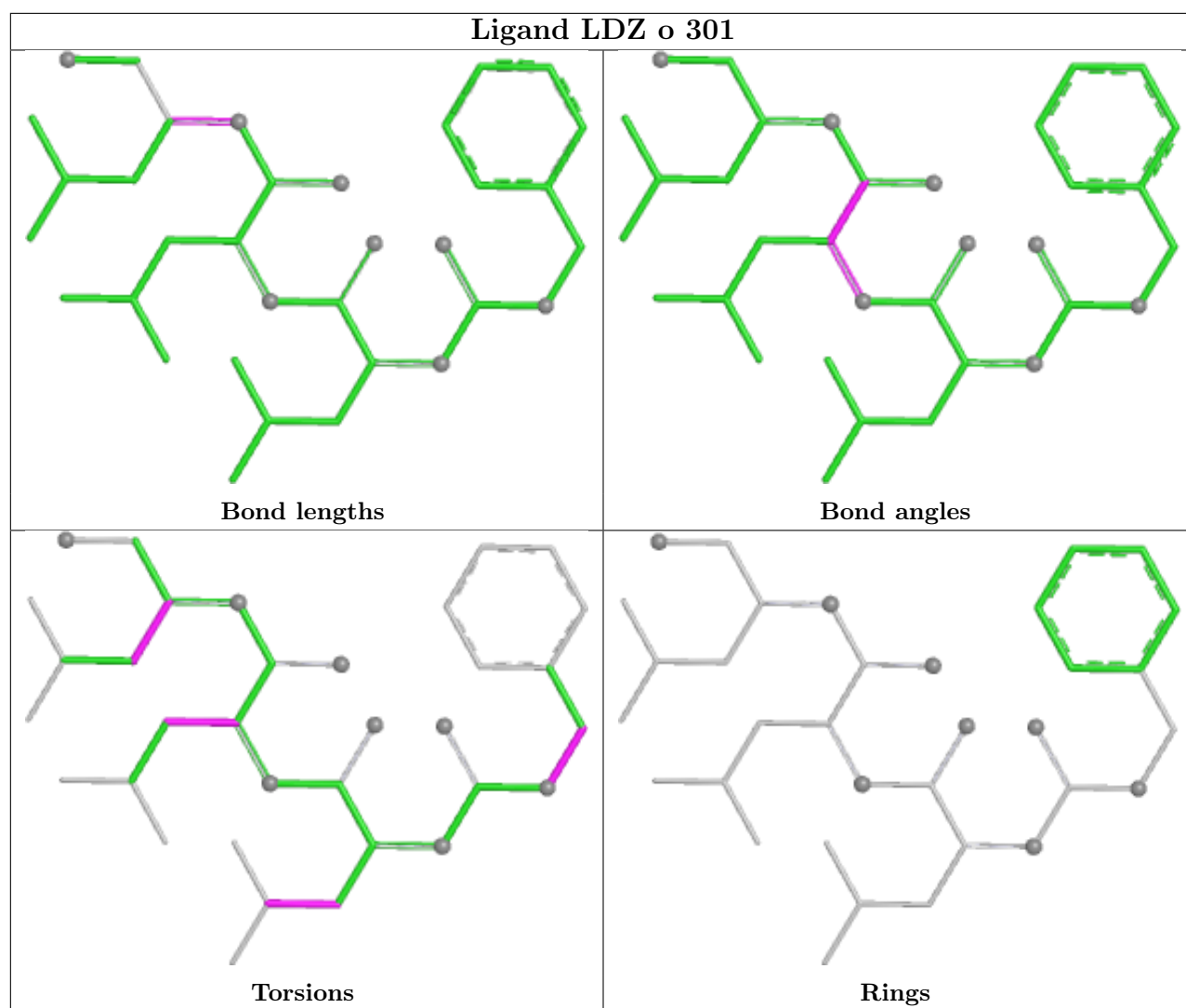


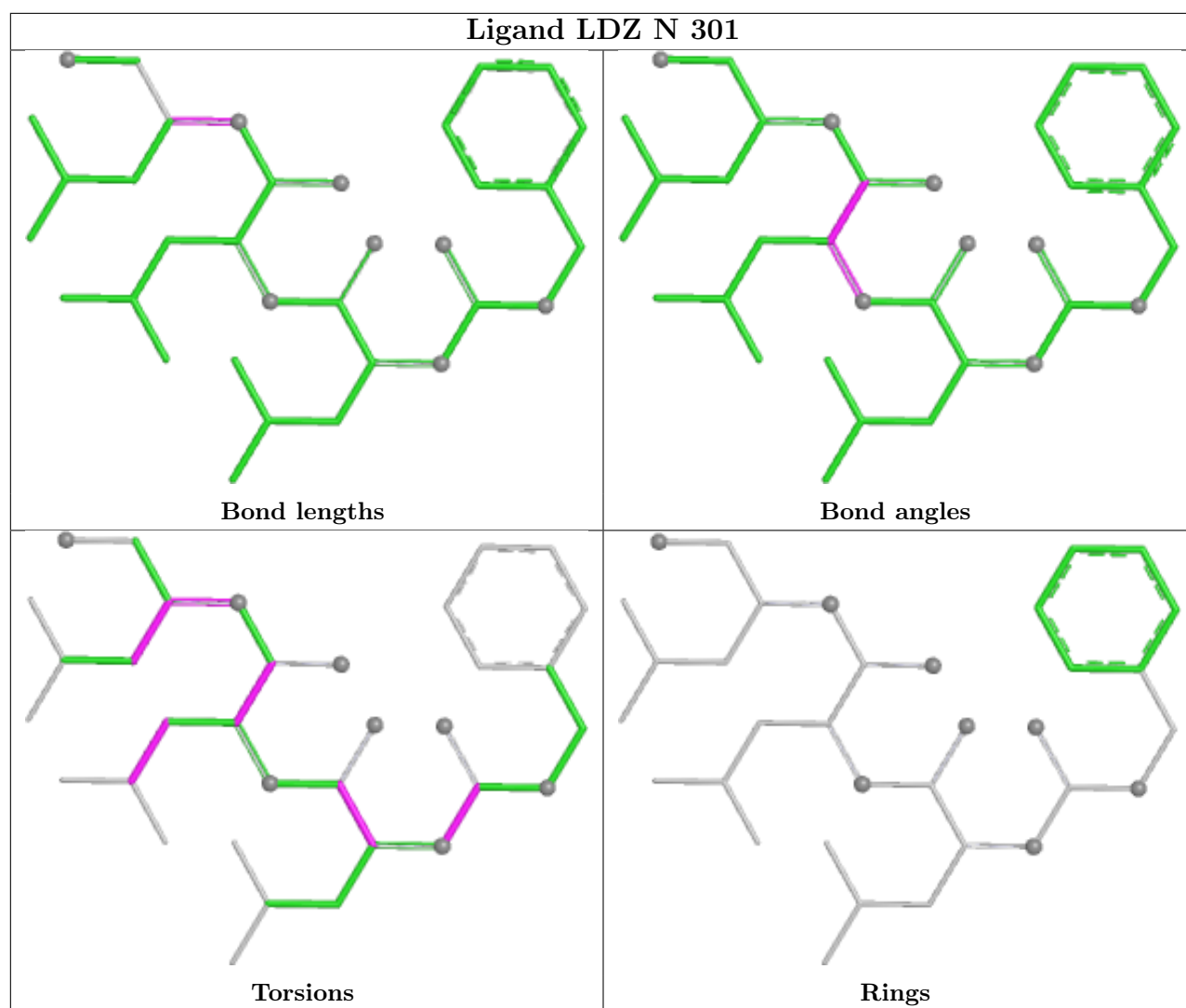


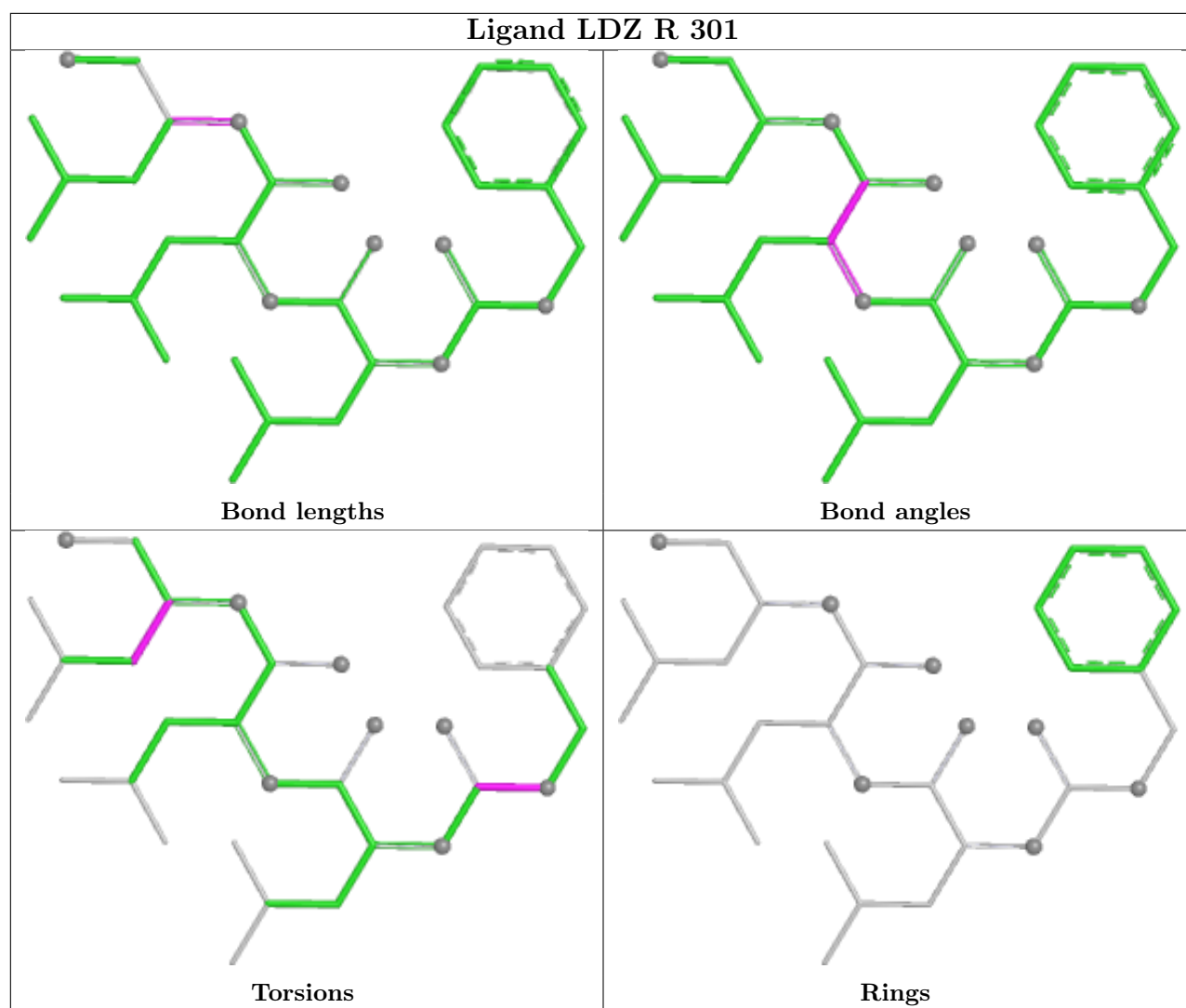




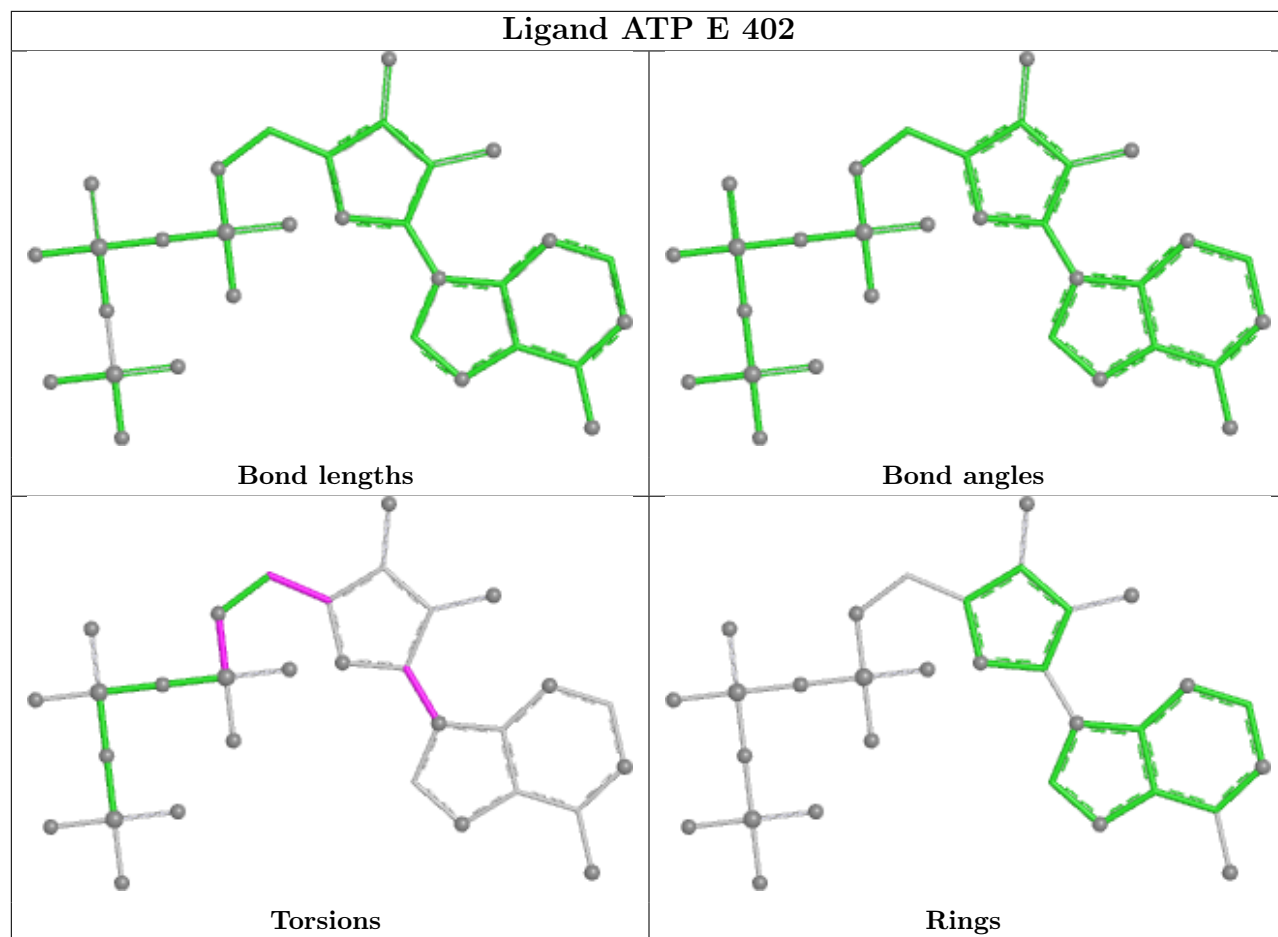




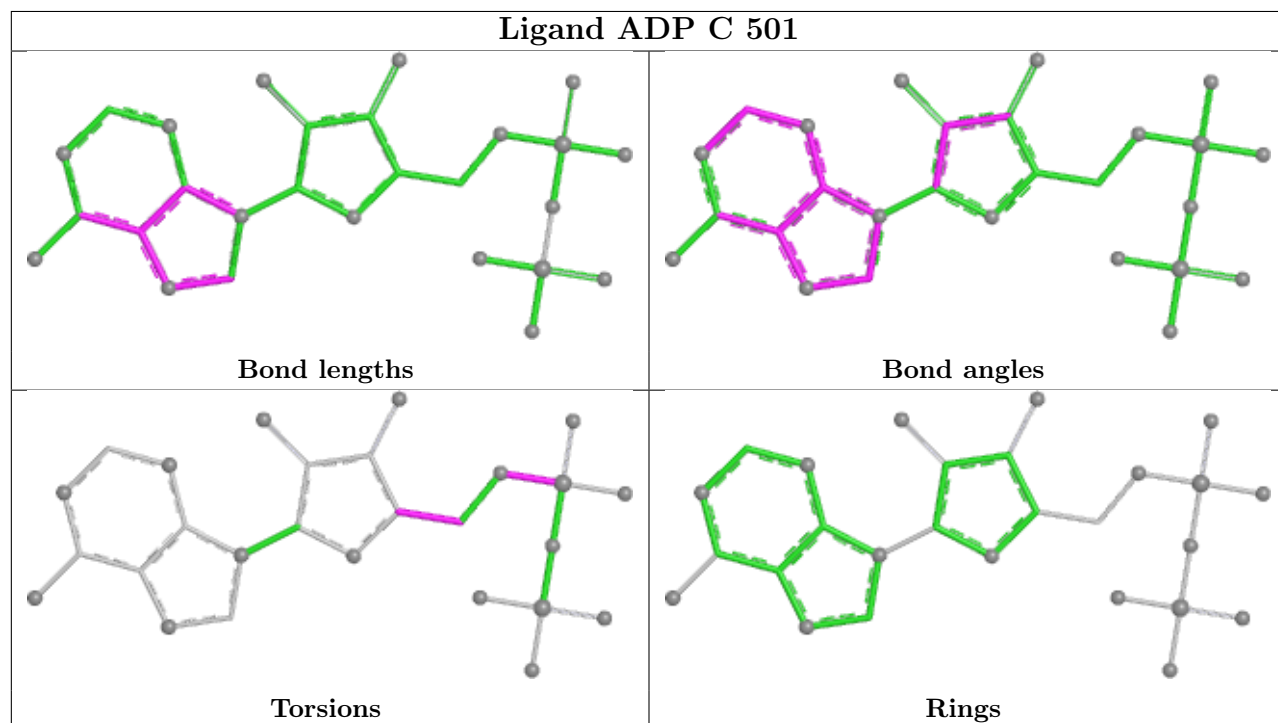




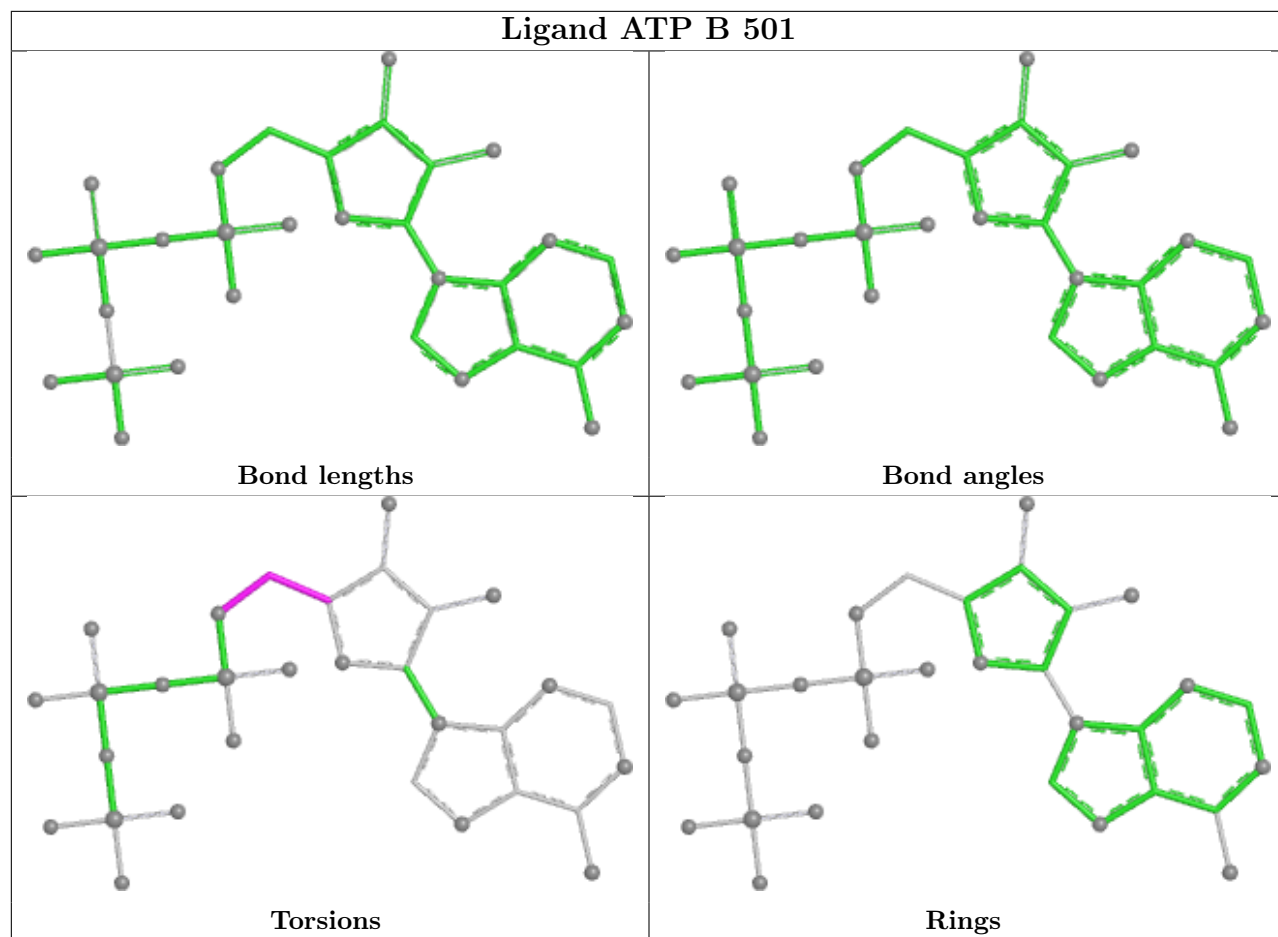
## Ligand ATP E 402



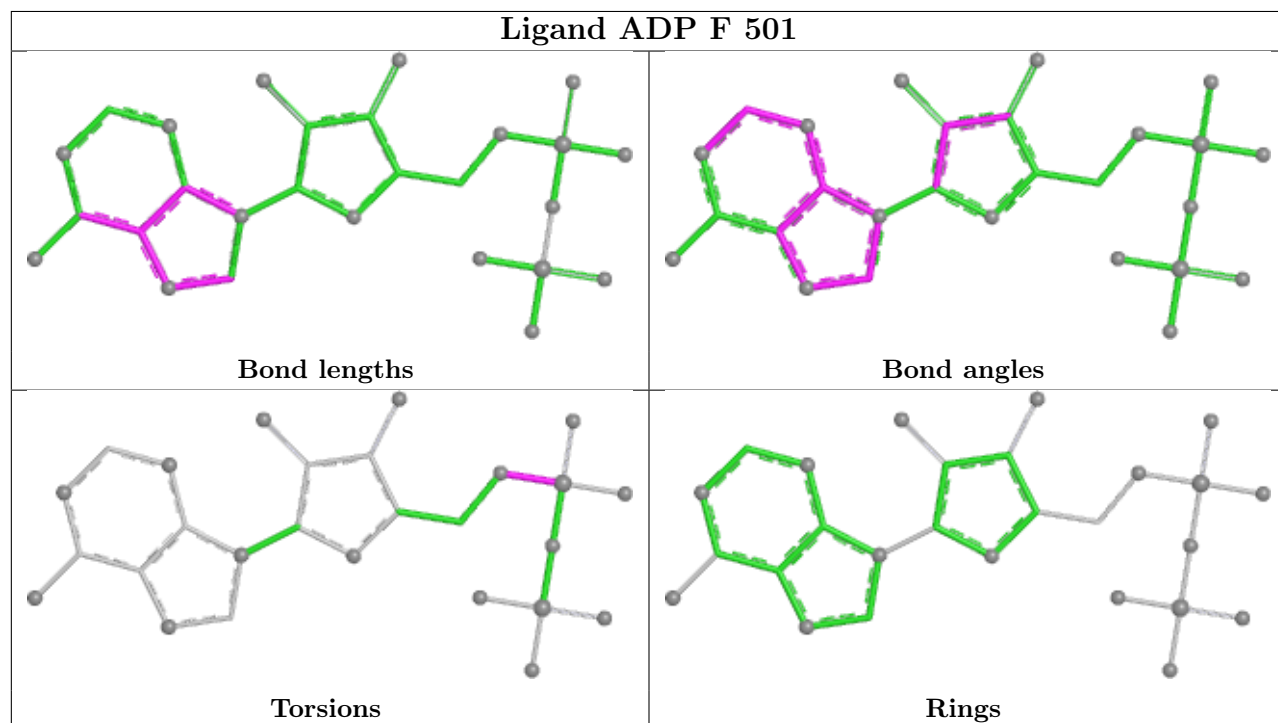
## Ligand ADP C 501



## Ligand ATP B 501



## Ligand ADP F 501



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-49507. These allow visual inspection of the internal detail of the map and identification of artifacts.

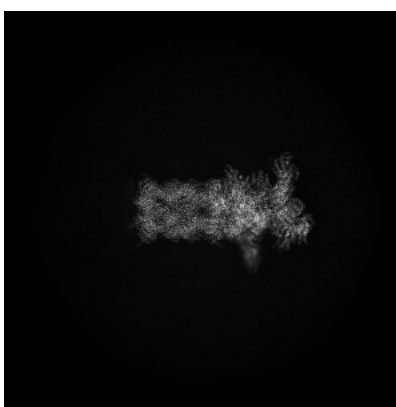
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

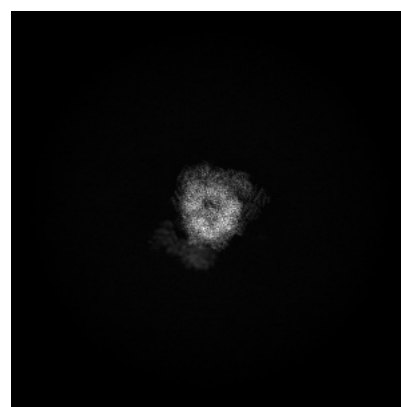
#### 6.1.1 Primary map



X



Y



Z

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

### 6.2 Central slices [i](#)

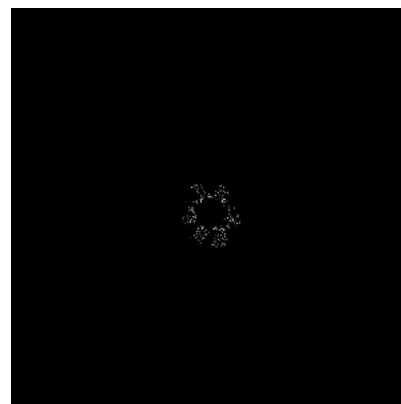
#### 6.2.1 Primary map



X Index: 322



Y Index: 321

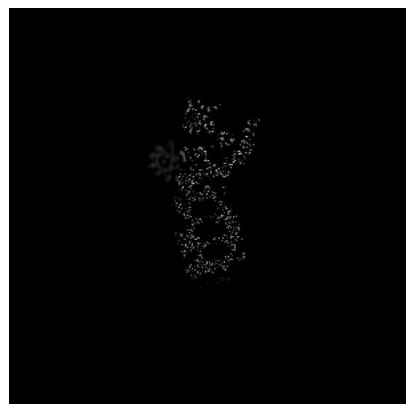


Z Index: 322

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: 309



Y Index: 300



Z Index: 454

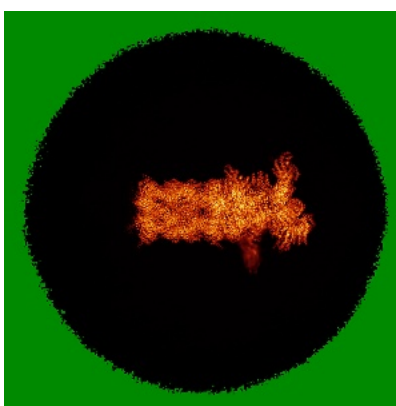
The images above show the largest variance slices of the map in three orthogonal directions.

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

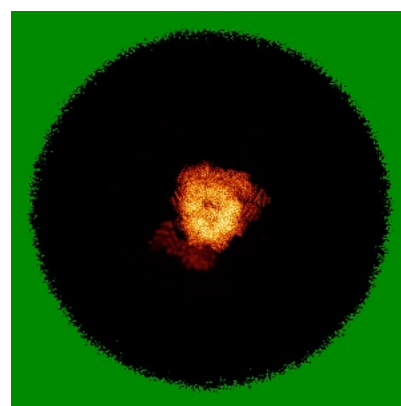
### 6.4.1 Primary map



X



Y



Z

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

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

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.165. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

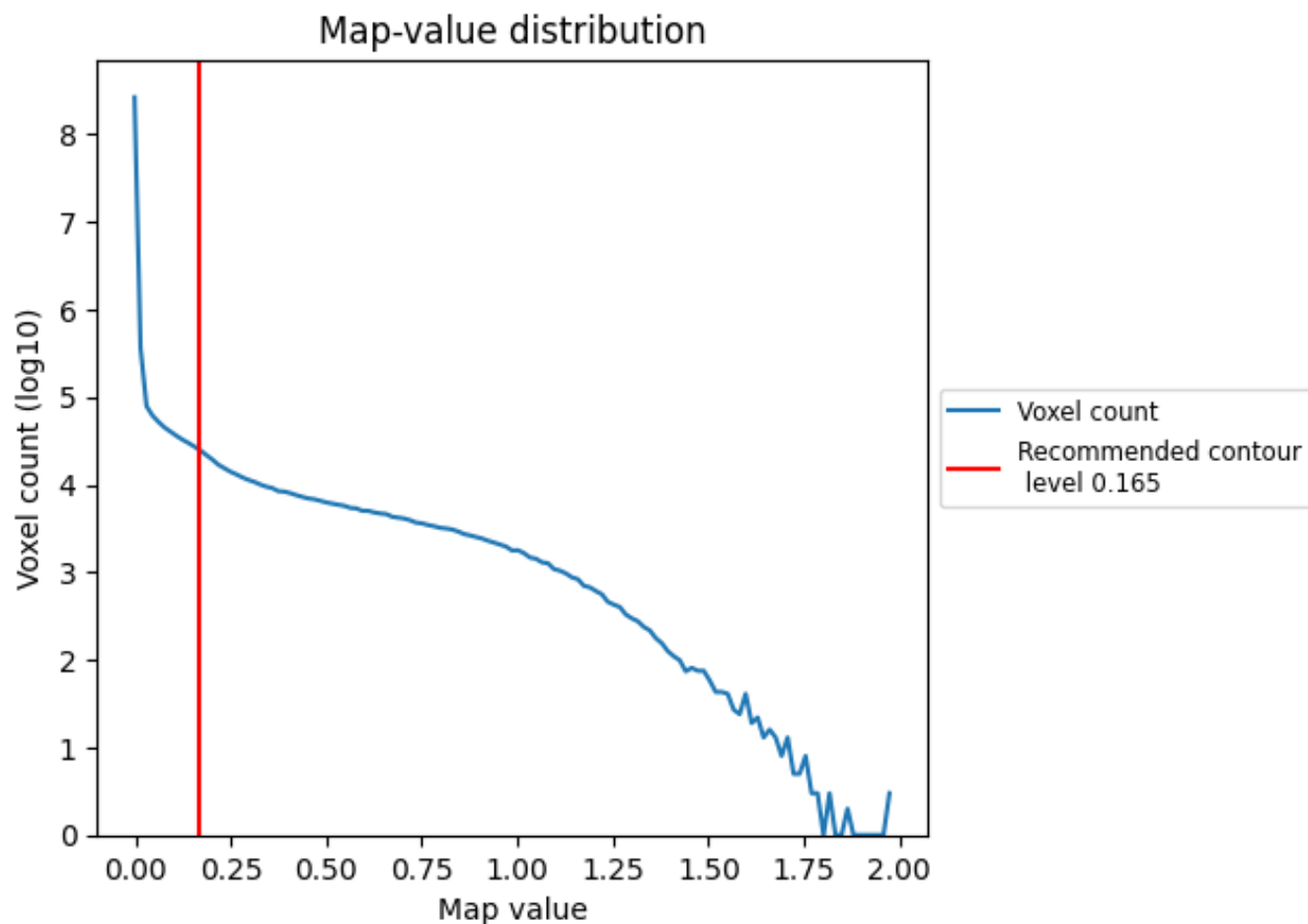
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

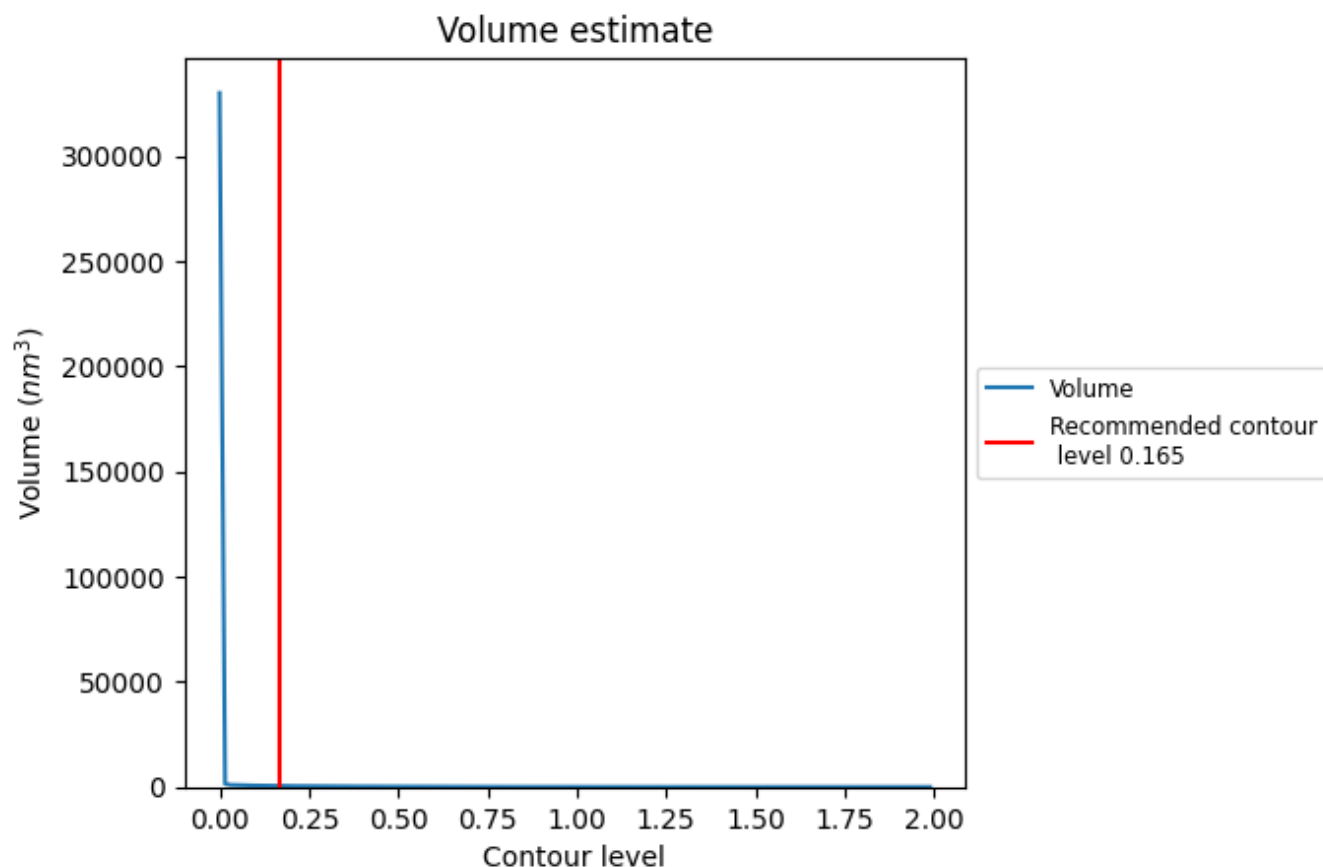
This section contains the results of statistical analysis of the map.

### 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 497 nm<sup>3</sup>; this corresponds to an approximate mass of 449 kDa.

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

## 7.3 Rotationally averaged power spectrum [i](#)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

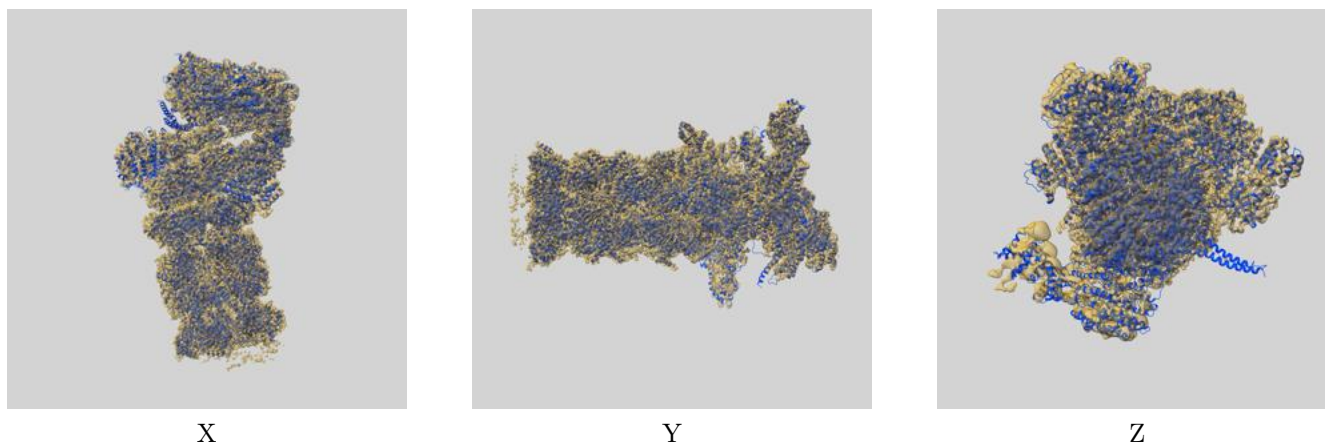
## 8 Fourier-Shell correlation

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

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

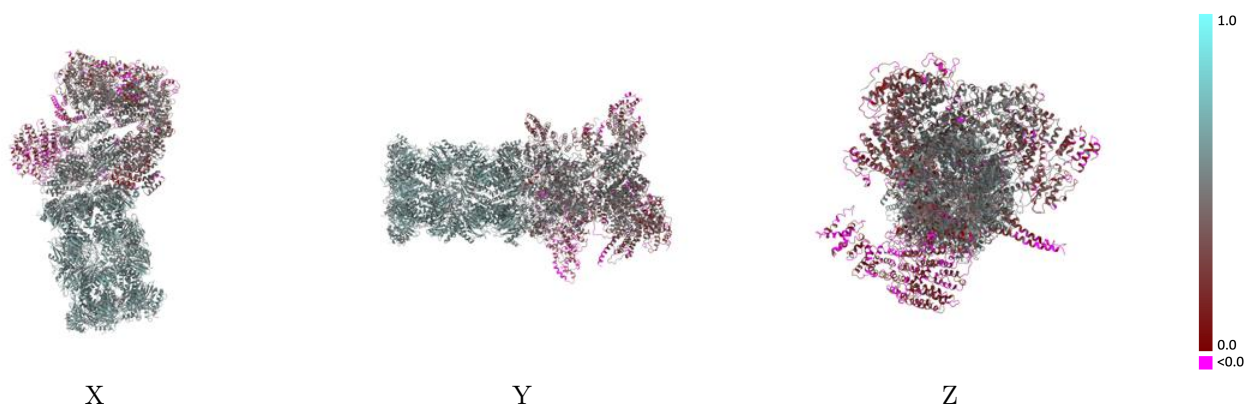
This section contains information regarding the fit between EMDB map EMD-49507 and PDB model 9NKF. Per-residue inclusion information can be found in section 3 on page 13.

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



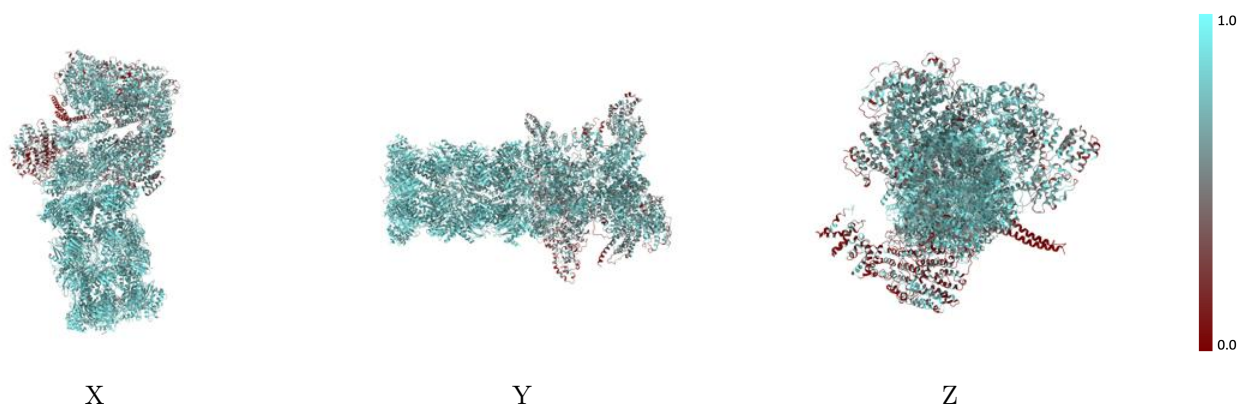
The images above show the 3D surface view of the map at the recommended contour level 0.165 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



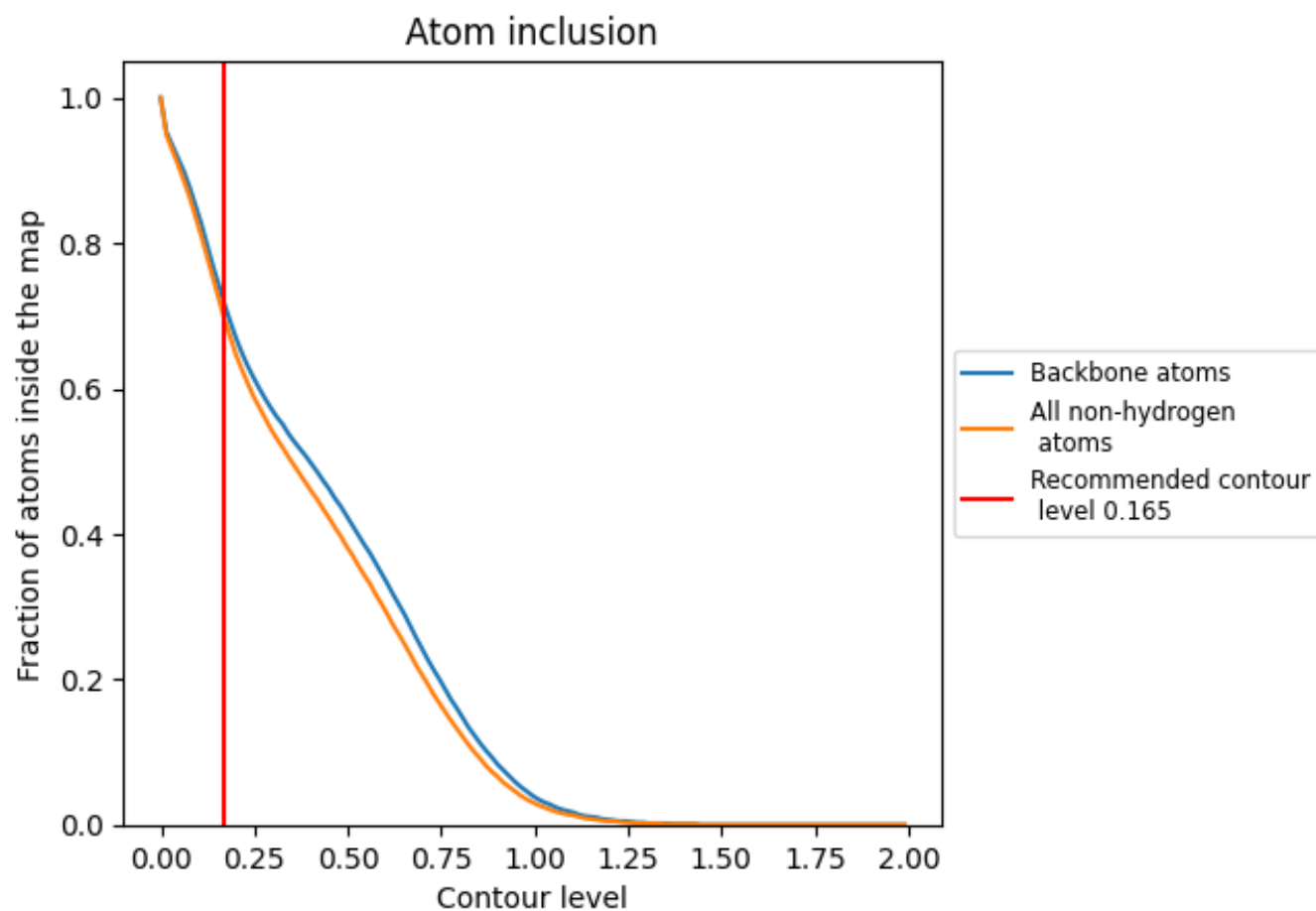
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.165).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 72% of all backbone atoms, 70% 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 (0.165) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| All   |  0.7030   |  0.4450   |
| A     |  0.7920   |  0.4600   |
| B     |  0.6900   |  0.3920   |
| C     |  0.7200   |  0.4500   |
| D     |  0.7410   |  0.4630   |
| E     |  0.7280   |  0.4590   |
| F     |  0.7060   |  0.4510   |
| G     |  0.8350   |  0.5330   |
| H     |  0.8500   |  0.5530   |
| I     |  0.8230   |  0.5480   |
| J     |  0.8520   |  0.5590   |
| K     |  0.8200   |  0.5460   |
| L     |  0.8480   |  0.5620   |
| M     |  0.8290   |  0.5430   |
| N     |  0.8060  |  0.5640  |
| O     |  0.7820 |  0.5670 |
| P     |  0.7960 |  0.5650 |
| Q     |  0.8280 |  0.5750 |
| R     |  0.8200 |  0.5730 |
| S     |  0.8060 |  0.5710 |
| T     |  0.8260 |  0.5700 |
| U     |  0.6610 |  0.3550 |
| V     |  0.5890 |  0.3150 |
| W     |  0.6160 |  0.3330 |
| X     |  0.6240 |  0.3900 |
| Y     |  0.6510 |  0.3810 |
| Z     |  0.7060 |  0.4050 |
| a     |  0.6230 |  0.3350 |
| b     |  0.5920 |  0.3200 |
| c     |  0.7140 |  0.4250 |
| d     |  0.5510 |  0.2510 |
| e     |  0.4560 |  0.2660 |
| f     |  0.3110 |  0.0940 |
| g     |  0.7900 |  0.5540 |
| h     |  0.8220 |  0.5660 |



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| Chain | Atom inclusion                                                                           | Q-score                                                                                  |
|-------|------------------------------------------------------------------------------------------|------------------------------------------------------------------------------------------|
| i     |  0.8200 |  0.5610 |
| j     |  0.8260 |  0.5590 |
| k     |  0.7850 |  0.5530 |
| l     |  0.8140 |  0.5700 |
| m     |  0.7960 |  0.5570 |
| n     |  0.8120 |  0.5720 |
| o     |  0.8120 |  0.5680 |
| p     |  0.8250 |  0.5740 |
| q     |  0.8260 |  0.5820 |
| r     |  0.8130 |  0.5650 |
| s     |  0.8150 |  0.5730 |
| t     |  0.8400 |  0.5750 |