



## Full wwPDB EM Validation Report ⓘ

Mar 24, 2026 – 02:58 AM UTC

PDB ID : 9E8J / pdb\_00009e8j  
EMDB ID : EMD-47722  
Title : Nub1/Fat10-processing human 26S proteasome bound to Txnl1 with Rpt1 at top of spiral staircase  
Authors : Arkinson, C.; Gee, C.L.; Martin, A.  
Deposited on : 2024-11-05  
Resolution : 3.47 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

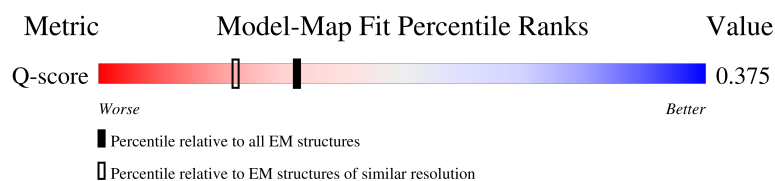
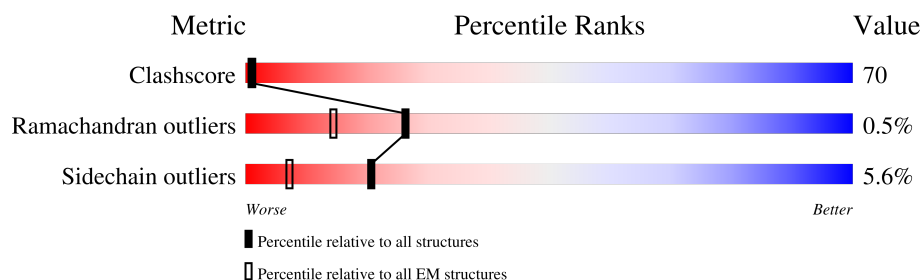
EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

# 1 Overall quality at a glance

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

The reported resolution of this entry is 3.47 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.



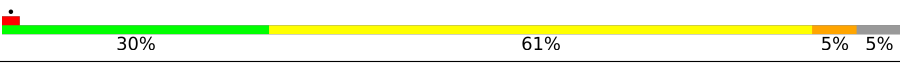
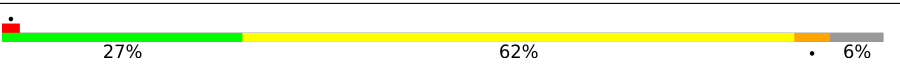
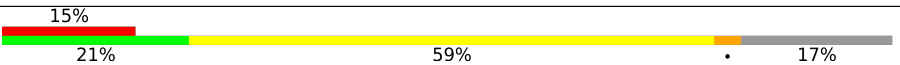
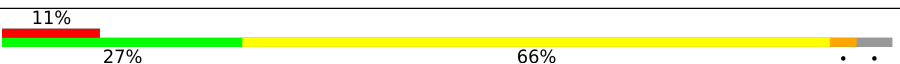
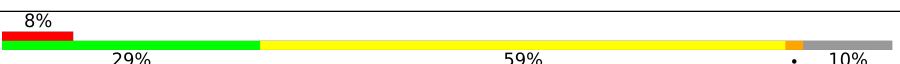
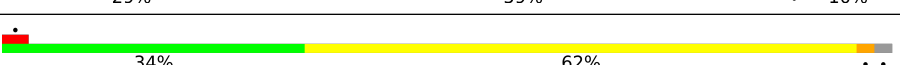
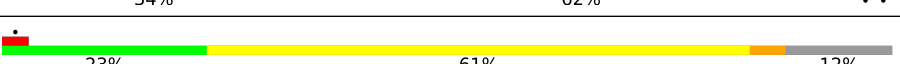
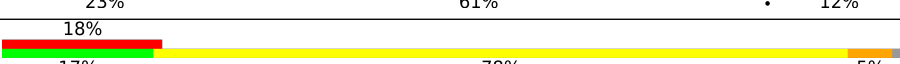
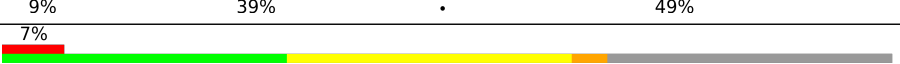
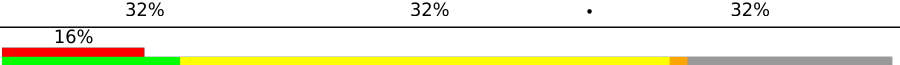
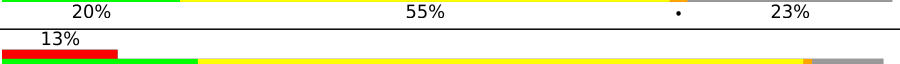
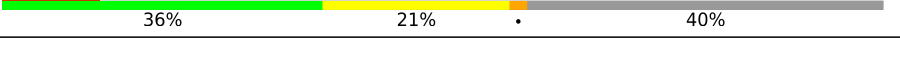
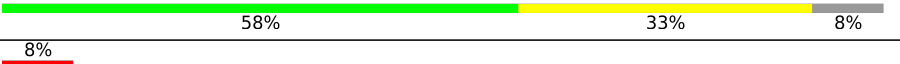
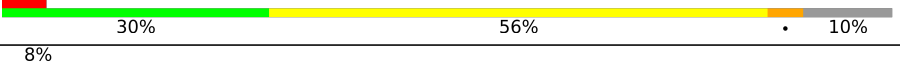
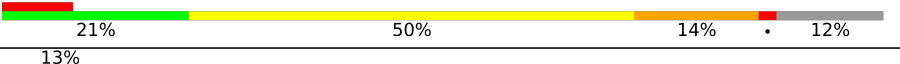
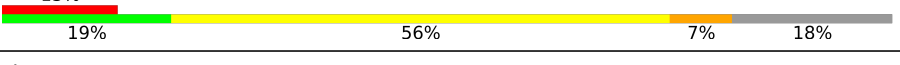
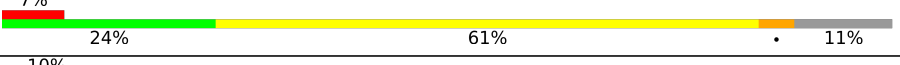
| Metric                | Whole archive<br>(#Entries) | EM structures<br>(#Entries) | Similar EM resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-----------------------------|----------------------------------------------------------|
| Clashscore            | 229148                      | 23984                       | -                                                        |
| Ramachandran outliers | 224038                      | 23583                       | -                                                        |
| Sidechain outliers    | 223484                      | 23102                       | -                                                        |
| Q-score               | -                           | 25397                       | 13733 ( 2.97 - 3.97 )                                    |

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   | C     | 406    |                  |
| 2   | D     | 418    |                  |
| 3   | G     | 246    |                  |
| 4   | H     | 234    |                  |

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| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 5   | I     | 261    |    |
| 6   | J     | 248    |    |
| 7   | L     | 263    |    |
| 8   | M     | 255    |    |
| 9   | V     | 534    |    |
| 10  | W     | 456    |    |
| 11  | X     | 422    |    |
| 12  | Y     | 389    |    |
| 13  | Z     | 324    |    |
| 14  | a     | 376    |    |
| 15  | b     | 377    |    |
| 16  | c     | 424    |    |
| 17  | d     | 350    |   |
| 18  | f     | 908    |  |
| 19  | g     | 601    |  |
| 20  | u     | 289    |  |
| 21  | v     | 12     |  |
| 22  | A     | 433    |  |
| 23  | B     | 440    |  |
| 24  | E     | 389    |  |
| 25  | F     | 439    |  |
| 26  | K     | 241    |  |
| 27  | U     | 953    |  |
| 28  | e     | 70     |  |

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 29  | ATP  | F     | 501 | -         | -        | X       | -                |

## 2 Entry composition

There are 32 unique types of molecules in this entry. The entry contains 70858 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 26S protease regulatory subunit 8.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 1   | C     | 386      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3051  | 1919 | 547 | 567 | 18 |         |       |

- Molecule 2 is a protein called 26S proteasome regulatory subunit 6B.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 2   | D     | 380      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3040  | 1923 | 524 | 580 | 13 |         |       |

- Molecule 3 is a protein called Proteasome subunit alpha type-6.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 3   | G     | 239      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1820  | 1157 | 304 | 346 | 13 |         |       |

- Molecule 4 is a protein called Proteasome subunit alpha type-2.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 4   | H     | 232      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1813  | 1158 | 307 | 342 | 6 |         |       |

- Molecule 5 is a protein called Proteasome subunit alpha type-4.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 5   | I     | 248      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1895  | 1195 | 324 | 368 | 8 |         |       |

- Molecule 6 is a protein called Proteasome subunit alpha type-7.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 6   | J     | 239      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1733  | 1076 | 315 | 337 | 5 |         |       |

- Molecule 7 is a protein called Proteasome subunit alpha type-1.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 7   | L     | 238      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1850  | 1159 | 334 | 346 | 11 |         |       |

- Molecule 8 is a protein called Proteasome subunit alpha type-3.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 8   | M     | 240      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1856  | 1178 | 314 | 353 | 11 |         |       |

- Molecule 9 is a protein called 26S proteasome non-ATPase regulatory subunit 3.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 9   | V     | 443      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3608  | 2299 | 644 | 652 | 13 |         |       |

- Molecule 10 is a protein called 26S proteasome non-ATPase regulatory subunit 12.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 10  | W     | 438      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3570  | 2261 | 609 | 677 | 23 |         |       |

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

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 11  | X     | 378      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2994  | 1909 | 507 | 566 | 12 |         |       |

- Molecule 12 is a protein called 26S proteasome non-ATPase regulatory subunit 6.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 12  | Y     | 380      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3127  | 1995 | 535 | 580 | 17 |         |       |

- Molecule 13 is a protein called 26S proteasome non-ATPase regulatory subunit 7.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 13  | Z     | 286      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2281  | 1457 | 392 | 427 | 5 |         |       |

- Molecule 14 is a protein called 26S proteasome non-ATPase regulatory subunit 13.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 14  | a     | 373      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2995  | 1911 | 510 | 559 | 15 |         |       |

- Molecule 15 is a protein called 26S proteasome non-ATPase regulatory subunit 4.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 15  | b     | 191      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1458  | 910 | 261 | 279 | 8 |         |       |

- Molecule 16 is a protein called 26S proteasome non-ATPase regulatory subunit 14.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 16  | c     | 289      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2269  | 1436 | 391 | 423 | 19 |         |       |

There are 114 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| c     | 311     | LEU      | -      | expression tag | UNP O00487 |
| c     | 312     | ILE      | -      | expression tag | UNP O00487 |
| c     | 313     | ASN      | -      | expression tag | UNP O00487 |
| c     | 314     | HIS      | -      | expression tag | UNP O00487 |
| c     | 315     | HIS      | -      | expression tag | UNP O00487 |
| c     | 316     | HIS      | -      | expression tag | UNP O00487 |
| c     | 317     | HIS      | -      | expression tag | UNP O00487 |
| c     | 318     | HIS      | -      | expression tag | UNP O00487 |
| c     | 319     | HIS      | -      | expression tag | UNP O00487 |
| c     | 320     | ASP      | -      | expression tag | UNP O00487 |
| c     | 321     | TYR      | -      | expression tag | UNP O00487 |
| c     | 322     | ASP      | -      | expression tag | UNP O00487 |
| c     | 323     | ILE      | -      | expression tag | UNP O00487 |
| c     | 324     | PRO      | -      | expression tag | UNP O00487 |
| c     | 325     | THR      | -      | expression tag | UNP O00487 |
| c     | 326     | THR      | -      | expression tag | UNP O00487 |
| c     | 327     | ALA      | -      | expression tag | UNP O00487 |
| c     | 328     | SER      | -      | expression tag | UNP O00487 |
| c     | 329     | GLU      | -      | expression tag | UNP O00487 |
| c     | 330     | ASN      | -      | expression tag | UNP O00487 |
| c     | 331     | LEU      | -      | expression tag | UNP O00487 |
| c     | 332     | TYR      | -      | expression tag | UNP O00487 |
| c     | 333     | PHE      | -      | expression tag | UNP O00487 |
| c     | 334     | GLN      | -      | expression tag | UNP O00487 |
| c     | 335     | GLY      | -      | expression tag | UNP O00487 |

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| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| c     | 336     | GLU      | -      | expression tag | UNP O00487 |
| c     | 337     | LEU      | -      | expression tag | UNP O00487 |
| c     | 338     | GLY      | -      | expression tag | UNP O00487 |
| c     | 339     | MET      | -      | expression tag | UNP O00487 |
| c     | 340     | ARG      | -      | expression tag | UNP O00487 |
| c     | 341     | GLY      | -      | expression tag | UNP O00487 |
| c     | 342     | SER      | -      | expression tag | UNP O00487 |
| c     | 343     | ALA      | -      | expression tag | UNP O00487 |
| c     | 344     | GLY      | -      | expression tag | UNP O00487 |
| c     | 345     | LYS      | -      | expression tag | UNP O00487 |
| c     | 346     | ALA      | -      | expression tag | UNP O00487 |
| c     | 347     | GLY      | -      | expression tag | UNP O00487 |
| c     | 348     | GLU      | -      | expression tag | UNP O00487 |
| c     | 349     | GLY      | -      | expression tag | UNP O00487 |
| c     | 350     | GLU      | -      | expression tag | UNP O00487 |
| c     | 351     | ILE      | -      | expression tag | UNP O00487 |
| c     | 352     | PRO      | -      | expression tag | UNP O00487 |
| c     | 353     | ALA      | -      | expression tag | UNP O00487 |
| c     | 354     | PRO      | -      | expression tag | UNP O00487 |
| c     | 355     | LEU      | -      | expression tag | UNP O00487 |
| c     | 356     | ALA      | -      | expression tag | UNP O00487 |
| c     | 357     | GLY      | -      | expression tag | UNP O00487 |
| c     | 358     | THR      | -      | expression tag | UNP O00487 |
| c     | 359     | VAL      | -      | expression tag | UNP O00487 |
| c     | 360     | SER      | -      | expression tag | UNP O00487 |
| c     | 361     | LYS      | -      | expression tag | UNP O00487 |
| c     | 362     | ILE      | -      | expression tag | UNP O00487 |
| c     | 363     | LEU      | -      | expression tag | UNP O00487 |
| c     | 364     | VAL      | -      | expression tag | UNP O00487 |
| c     | 365     | LYS      | -      | expression tag | UNP O00487 |
| c     | 366     | GLU      | -      | expression tag | UNP O00487 |
| c     | 367     | GLY      | -      | expression tag | UNP O00487 |
| c     | 368     | ASP      | -      | expression tag | UNP O00487 |
| c     | 369     | THR      | -      | expression tag | UNP O00487 |
| c     | 370     | VAL      | -      | expression tag | UNP O00487 |
| c     | 371     | LYS      | -      | expression tag | UNP O00487 |
| c     | 372     | ALA      | -      | expression tag | UNP O00487 |
| c     | 373     | GLY      | -      | expression tag | UNP O00487 |
| c     | 374     | GLN      | -      | expression tag | UNP O00487 |
| c     | 375     | THR      | -      | expression tag | UNP O00487 |
| c     | 376     | VAL      | -      | expression tag | UNP O00487 |
| c     | 377     | LEU      | -      | expression tag | UNP O00487 |

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| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| c     | 378     | VAL      | -      | expression tag | UNP O00487 |
| c     | 379     | LEU      | -      | expression tag | UNP O00487 |
| c     | 380     | GLU      | -      | expression tag | UNP O00487 |
| c     | 381     | ALA      | -      | expression tag | UNP O00487 |
| c     | 382     | MET      | -      | expression tag | UNP O00487 |
| c     | 383     | LYS      | -      | expression tag | UNP O00487 |
| c     | 384     | MET      | -      | expression tag | UNP O00487 |
| c     | 385     | GLU      | -      | expression tag | UNP O00487 |
| c     | 386     | THR      | -      | expression tag | UNP O00487 |
| c     | 387     | GLU      | -      | expression tag | UNP O00487 |
| c     | 388     | ILE      | -      | expression tag | UNP O00487 |
| c     | 389     | ASN      | -      | expression tag | UNP O00487 |
| c     | 390     | ALA      | -      | expression tag | UNP O00487 |
| c     | 391     | PRO      | -      | expression tag | UNP O00487 |
| c     | 392     | THR      | -      | expression tag | UNP O00487 |
| c     | 393     | ASP      | -      | expression tag | UNP O00487 |
| c     | 394     | GLY      | -      | expression tag | UNP O00487 |
| c     | 395     | LYS      | -      | expression tag | UNP O00487 |
| c     | 396     | VAL      | -      | expression tag | UNP O00487 |
| c     | 397     | GLU      | -      | expression tag | UNP O00487 |
| c     | 398     | LYS      | -      | expression tag | UNP O00487 |
| c     | 399     | VAL      | -      | expression tag | UNP O00487 |
| c     | 400     | LEU      | -      | expression tag | UNP O00487 |
| c     | 401     | VAL      | -      | expression tag | UNP O00487 |
| c     | 402     | LYS      | -      | expression tag | UNP O00487 |
| c     | 403     | GLU      | -      | expression tag | UNP O00487 |
| c     | 404     | ARG      | -      | expression tag | UNP O00487 |
| c     | 405     | ASP      | -      | expression tag | UNP O00487 |
| c     | 406     | ALA      | -      | expression tag | UNP O00487 |
| c     | 407     | VAL      | -      | expression tag | UNP O00487 |
| c     | 408     | GLN      | -      | expression tag | UNP O00487 |
| c     | 409     | GLY      | -      | expression tag | UNP O00487 |
| c     | 410     | GLY      | -      | expression tag | UNP O00487 |
| c     | 411     | GLN      | -      | expression tag | UNP O00487 |
| c     | 412     | GLY      | -      | expression tag | UNP O00487 |
| c     | 413     | LEU      | -      | expression tag | UNP O00487 |
| c     | 414     | ILE      | -      | expression tag | UNP O00487 |
| c     | 415     | LYS      | -      | expression tag | UNP O00487 |
| c     | 416     | ILE      | -      | expression tag | UNP O00487 |
| c     | 417     | GLY      | -      | expression tag | UNP O00487 |
| c     | 418     | VAL      | -      | expression tag | UNP O00487 |
| c     | 419     | HIS      | -      | expression tag | UNP O00487 |

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| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| c     | 420     | HIS      | -      | expression tag | UNP O00487 |
| c     | 421     | HIS      | -      | expression tag | UNP O00487 |
| c     | 422     | HIS      | -      | expression tag | UNP O00487 |
| c     | 423     | HIS      | -      | expression tag | UNP O00487 |
| c     | 424     | HIS      | -      | expression tag | UNP O00487 |

- Molecule 17 is a protein called 26S proteasome non-ATPase regulatory subunit 8.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 17  | d     | 269      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2188  | 1414 | 359 | 406 | 9 |         |       |

- Molecule 18 is a protein called 26S proteasome non-ATPase regulatory subunit 2.

| Mol | Chain | Residues | Atoms |      |      |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
| 18  | f     | 832      | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 6442  | 4076 | 1090 | 1231 | 45 |         |       |

- Molecule 19 is a protein called Isoform 2 of NEDD8 ultimate buster 1.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 19  | g     | 95       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 771   | 487 | 139 | 144 | 1 |         |       |

- Molecule 20 is a protein called Thioredoxin-like protein 1.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 20  | u     | 172      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1376  | 865 | 226 | 276 | 9 |         |       |

- Molecule 21 is a protein called substrate peptide.

| Mol | Chain | Residues | Atoms |    |    |    | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---------|-------|
| 21  | v     | 11       | Total | C  | N  | O  | 0       | 0     |
|     |       |          | 55    | 33 | 11 | 11 |         |       |

- Molecule 22 is a protein called 26S proteasome regulatory subunit 7.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 22  | A     | 407      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3199  | 2015 | 561 | 605 | 18 |         |       |

- Molecule 23 is a protein called 26S proteasome regulatory subunit 4.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 23  | B     | 396      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3107  | 1957 | 529 | 606 | 15 |         |       |

- Molecule 24 is a protein called 26S protease regulatory subunit 10B.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 24  | E     | 343      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2701  | 1699 | 477 | 509 | 16 |         |       |

- Molecule 25 is a protein called 26S proteasome regulatory subunit 6A.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 25  | F     | 359      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2801  | 1768 | 485 | 532 | 16 |         |       |

- Molecule 26 is a protein called Proteasome subunit alpha type-5.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 26  | K     | 228      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1737  | 1092 | 286 | 349 | 10 |         |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| K     | 83      | LYS      | ALA    | conflict | UNP P28066 |

- Molecule 27 is a protein called 26S proteasome non-ATPase regulatory subunit 1.

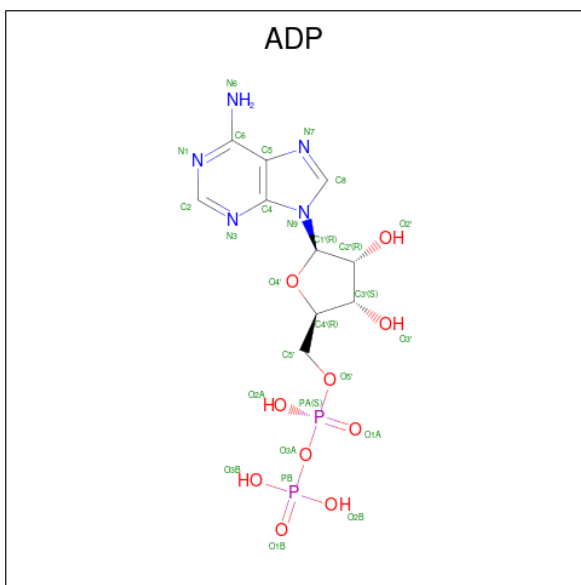
| Mol | Chain | Residues | Atoms |      |      |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
| 27  | U     | 844      | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 6584  | 4178 | 1119 | 1243 | 44 |         |       |

- Molecule 28 is a protein called 26S proteasome complex subunit SEM1.

| Mol | Chain | Residues | Atoms |     |    |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 28  | e     | 41       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 353   | 217 | 55 | 81 |         |       |

- Molecule 29 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>13</sub>P<sub>3</sub>) (labeled as "Ligand of Interest" by depositor).





| Mol | Chain | Residues | Atoms       |         |        |         |        | AltConf |
|-----|-------|----------|-------------|---------|--------|---------|--------|---------|
| 31  | D     | 1        | Total<br>27 | C<br>10 | N<br>5 | O<br>10 | P<br>2 | 0       |
| 31  | E     | 1        | Total<br>27 | C<br>10 | N<br>5 | O<br>10 | P<br>2 | 0       |

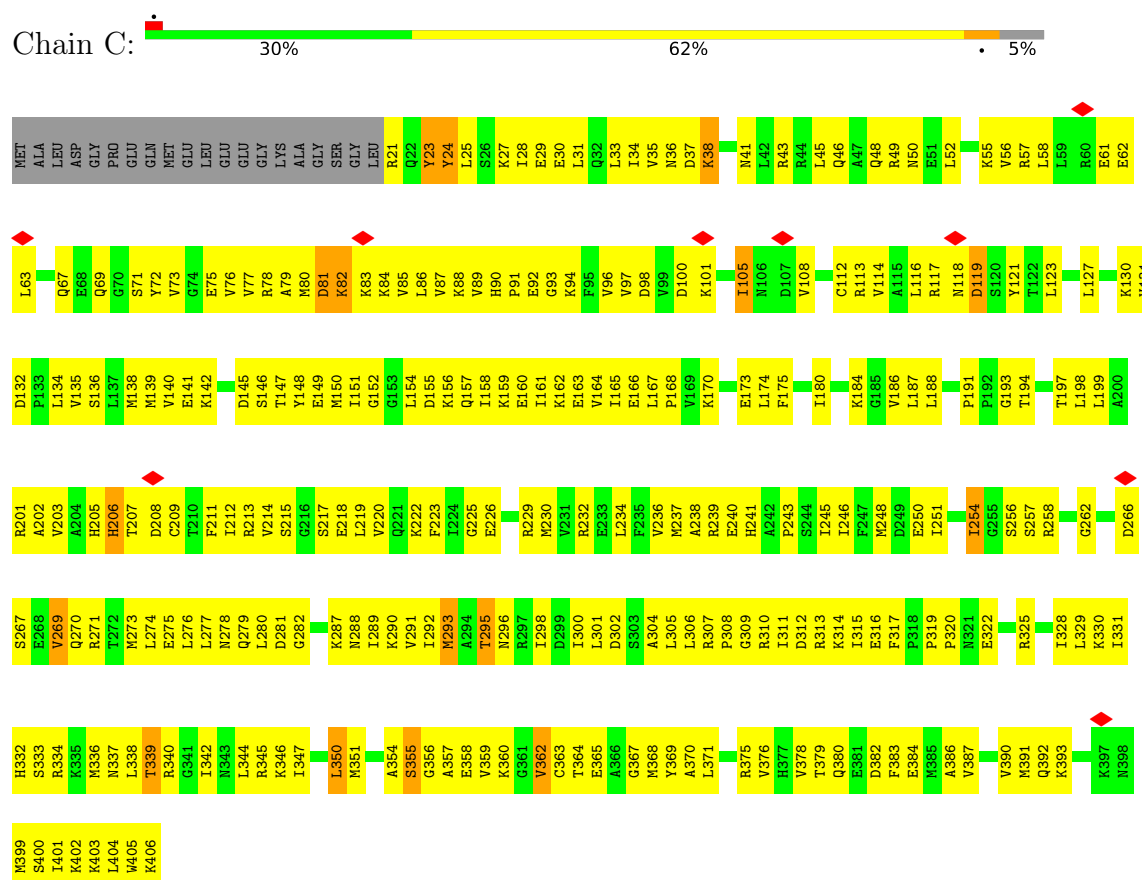
- Molecule 32 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

| Mol | Chain | Residues | Atoms           | AltConf |
|-----|-------|----------|-----------------|---------|
| 32  | c     | 1        | Total Zn<br>1 1 | 0       |

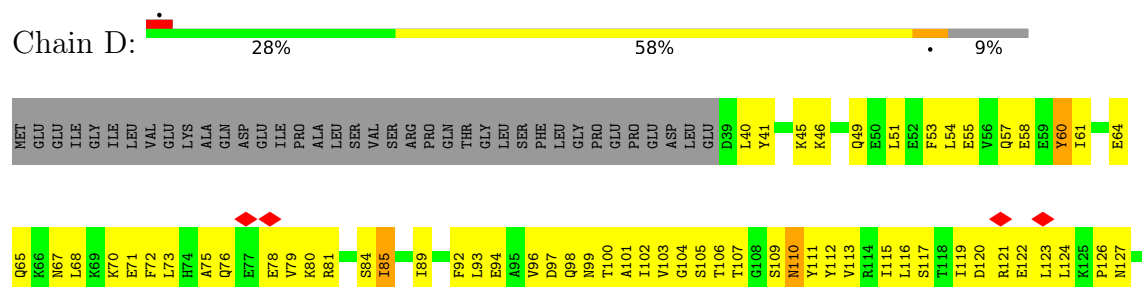
### 3 Residue-property plots

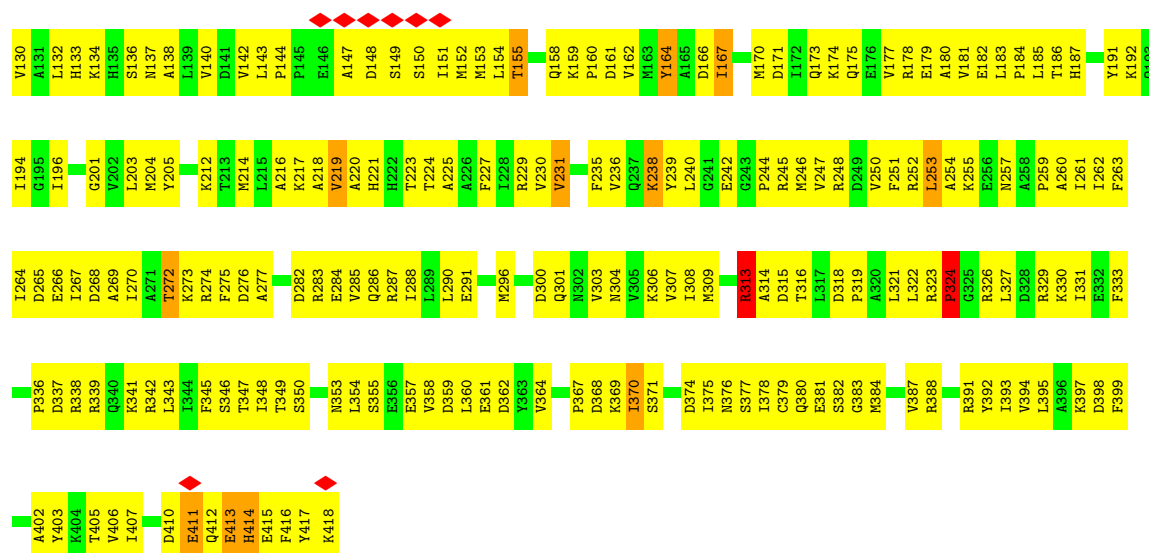
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

#### • Molecule 1: 26S protease regulatory subunit 8

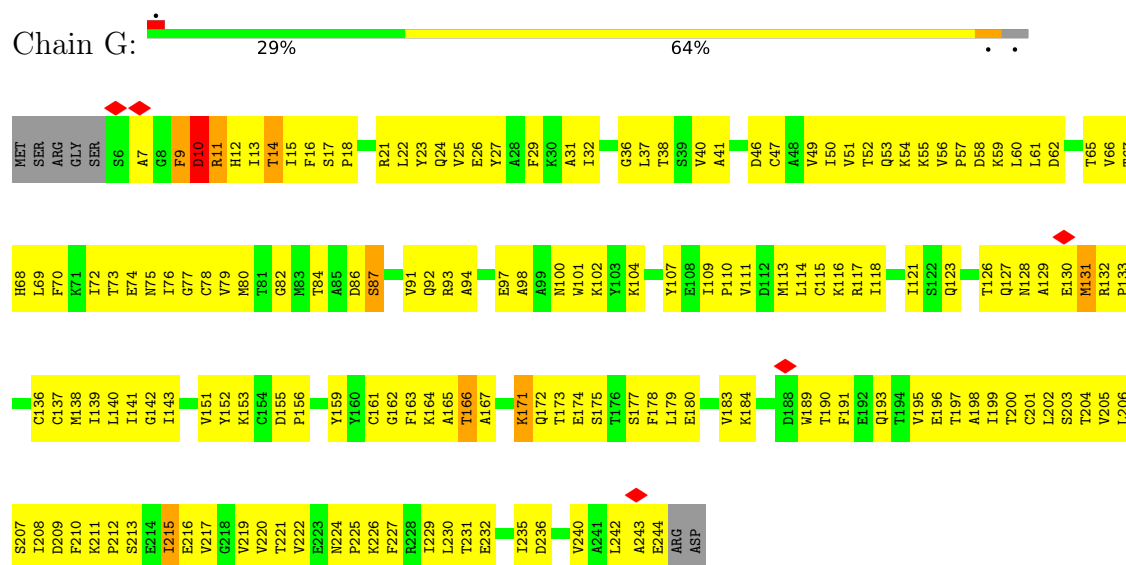


#### • Molecule 2: 26S proteasome regulatory subunit 6B





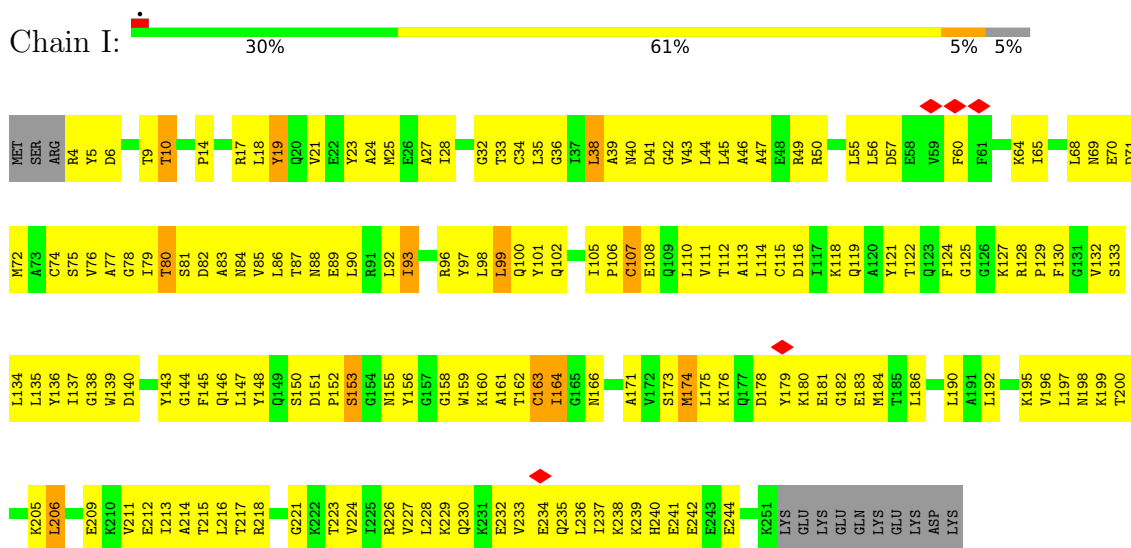
### • Molecule 3: Proteasome subunit alpha type-6



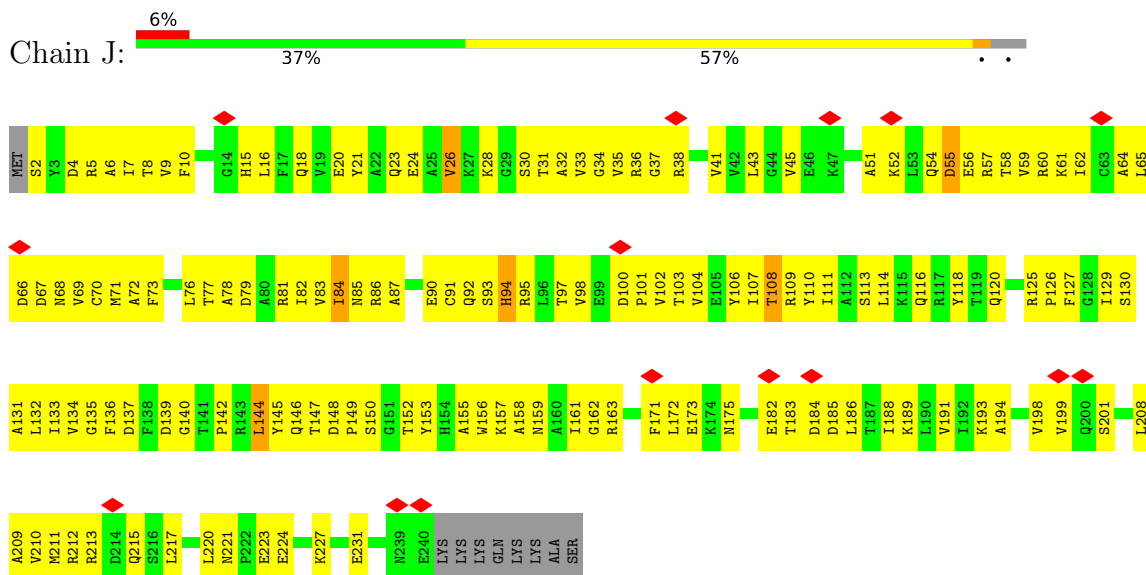
### • Molecule 4: Proteasome subunit alpha type-2



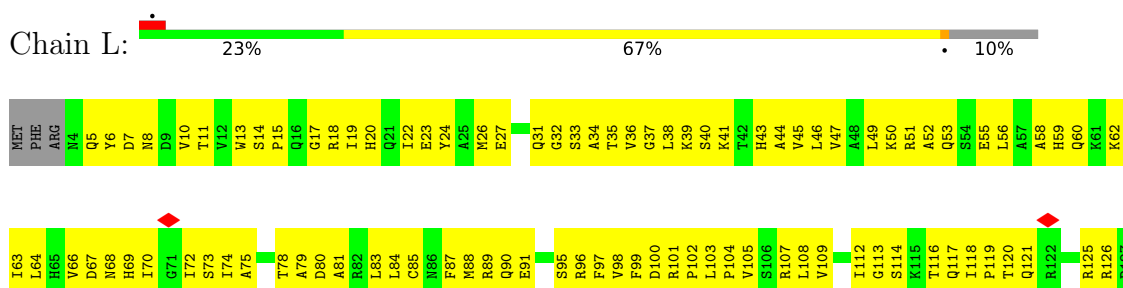
- Molecule 5: Proteasome subunit alpha type-4



- Molecule 6: Proteasome subunit alpha type-7

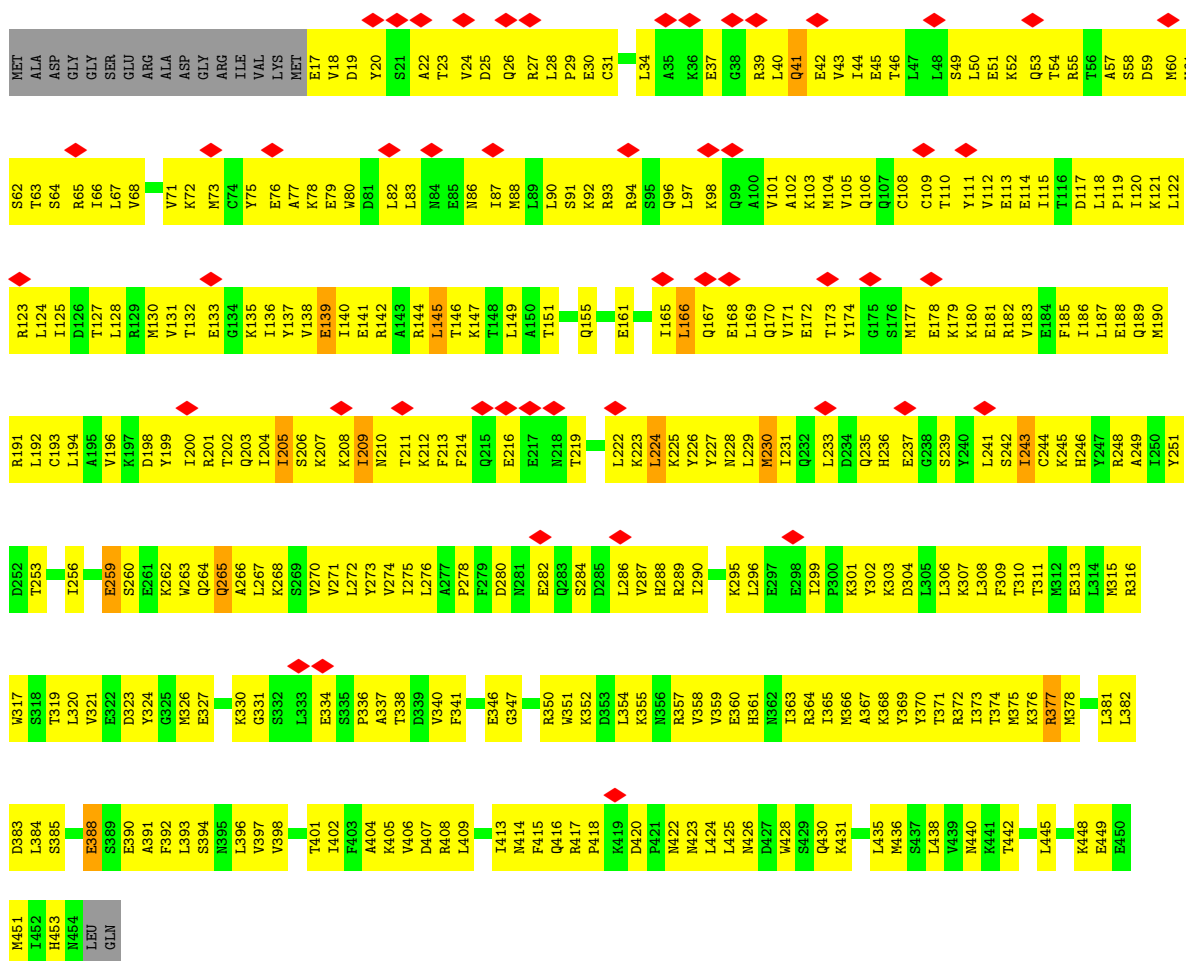


- Molecule 7: Proteasome subunit alpha type-1



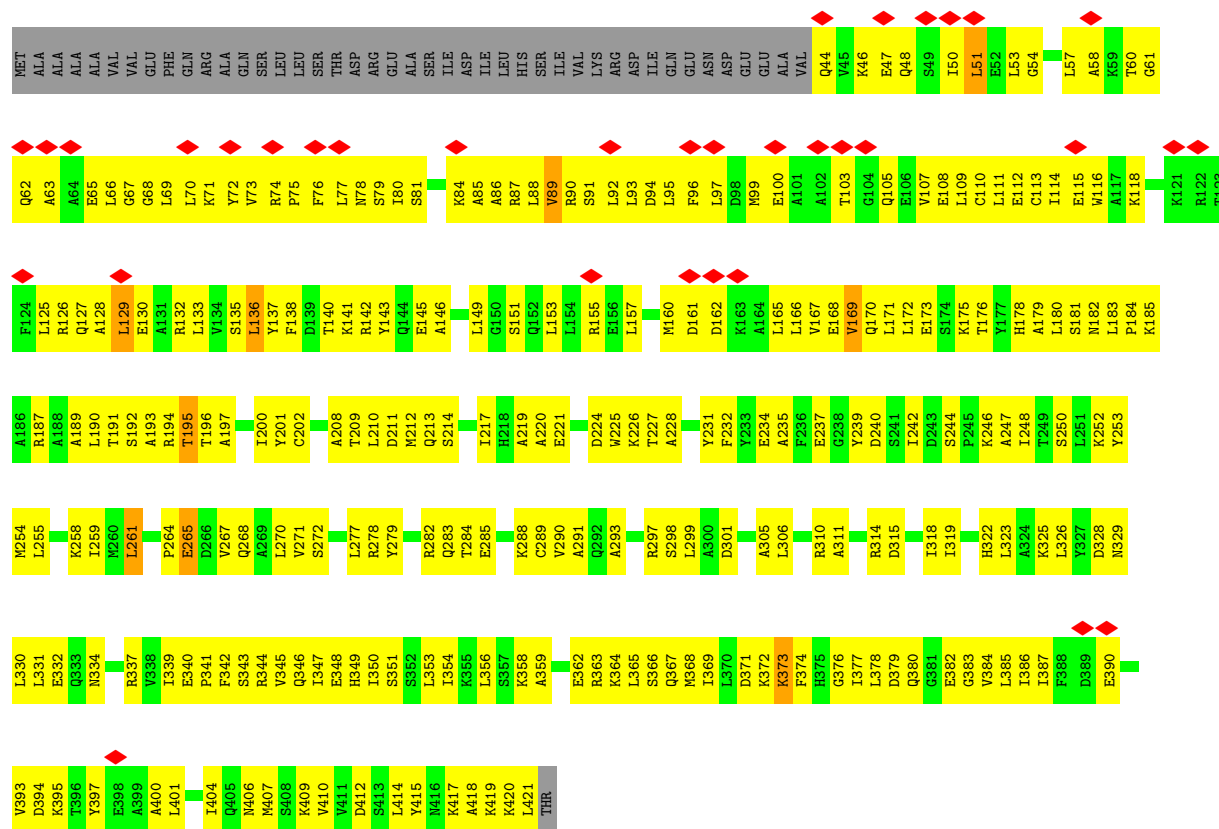


- Molecule 10: 26S proteasome non-ATPase regulatory subunit 12



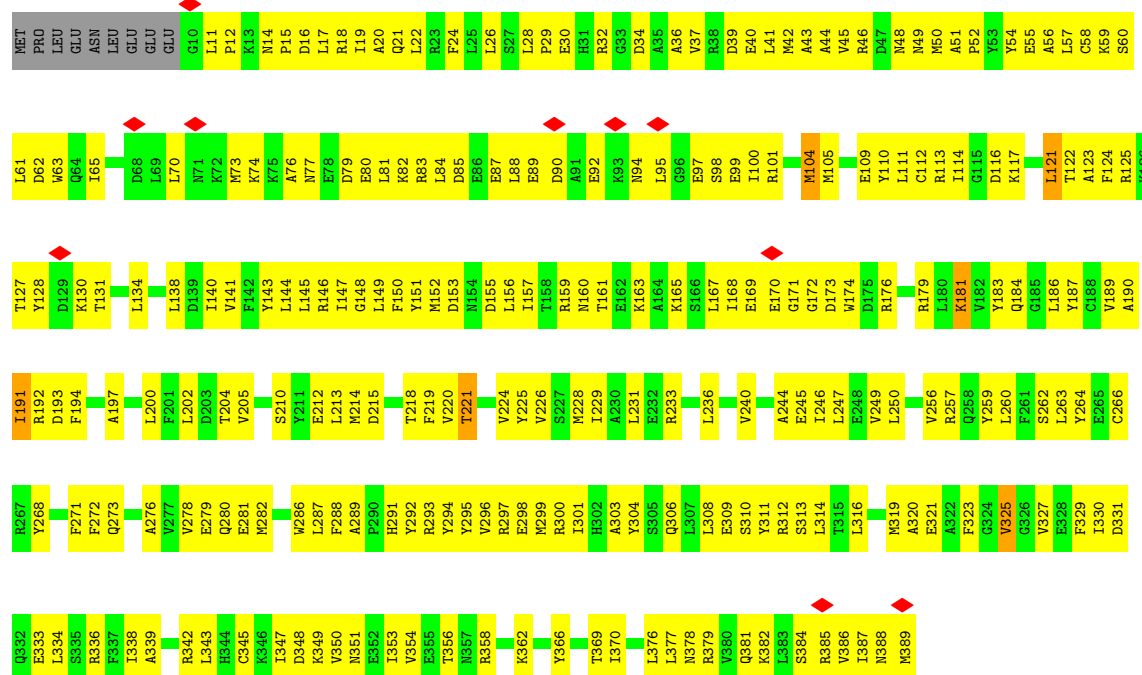
- Molecule 11: 26S proteasome non-ATPase regulatory subunit 11



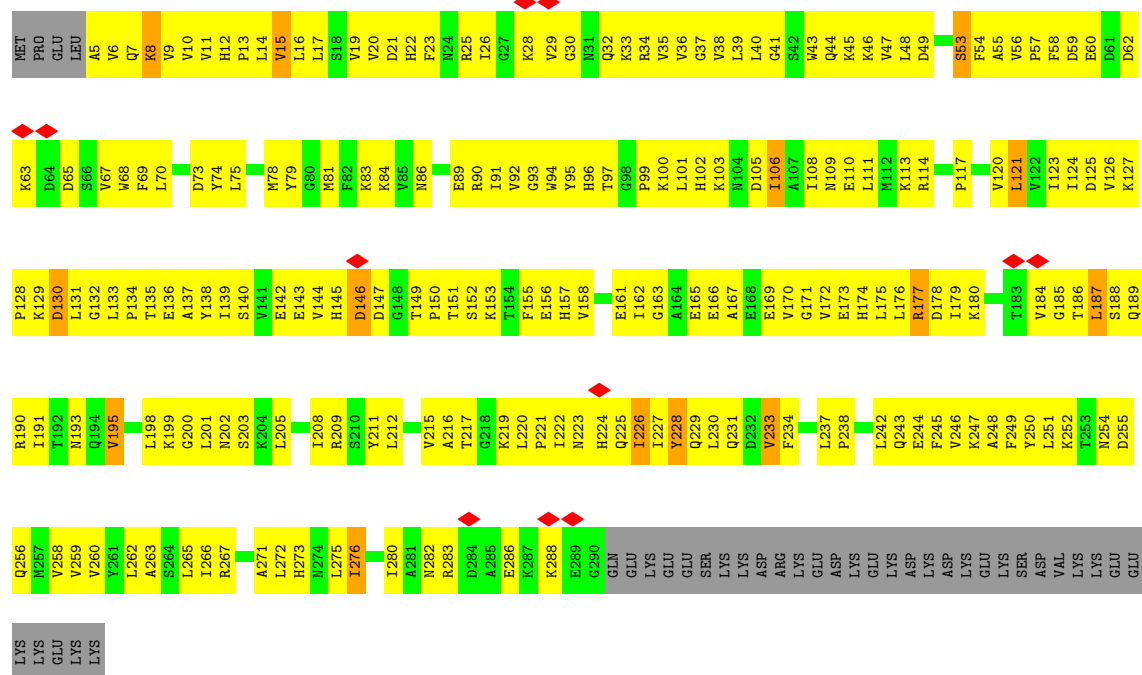


- Molecule 12: 26S proteasome non-ATPase regulatory subunit 6

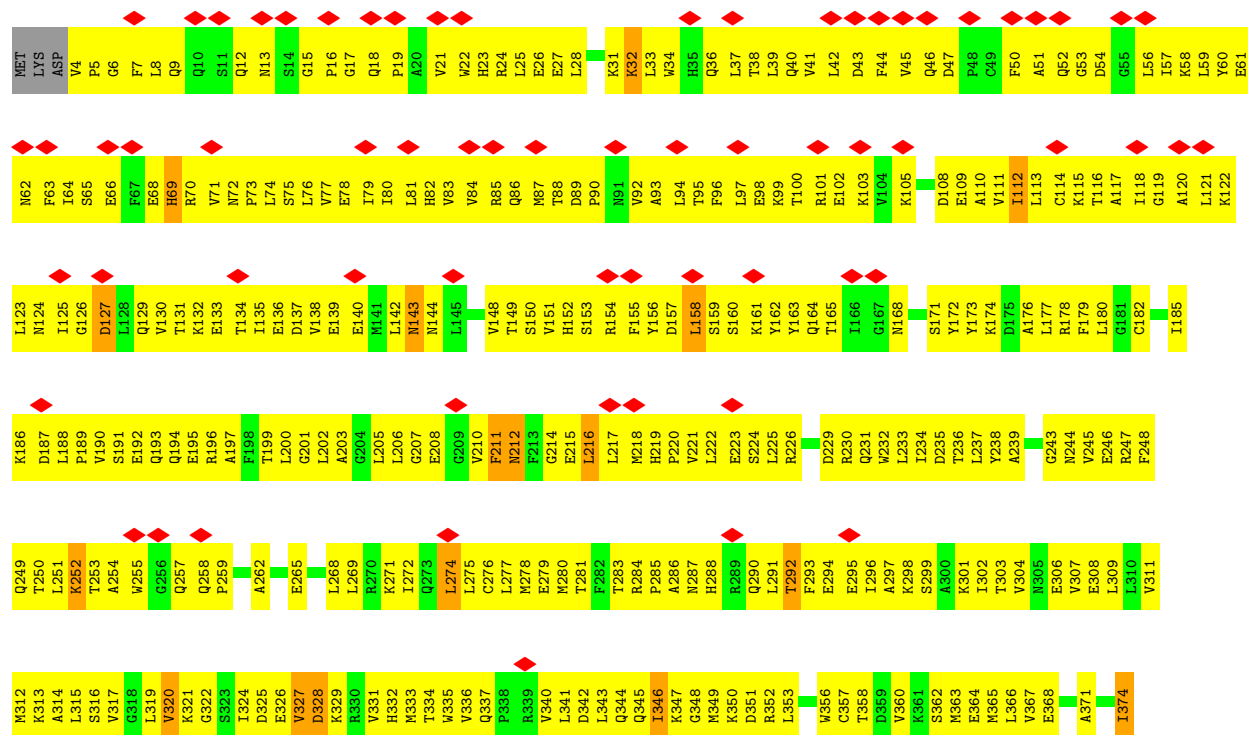
Chain Y: 34% 62%



- Molecule 13: 26S proteasome non-ATPase regulatory subunit 7



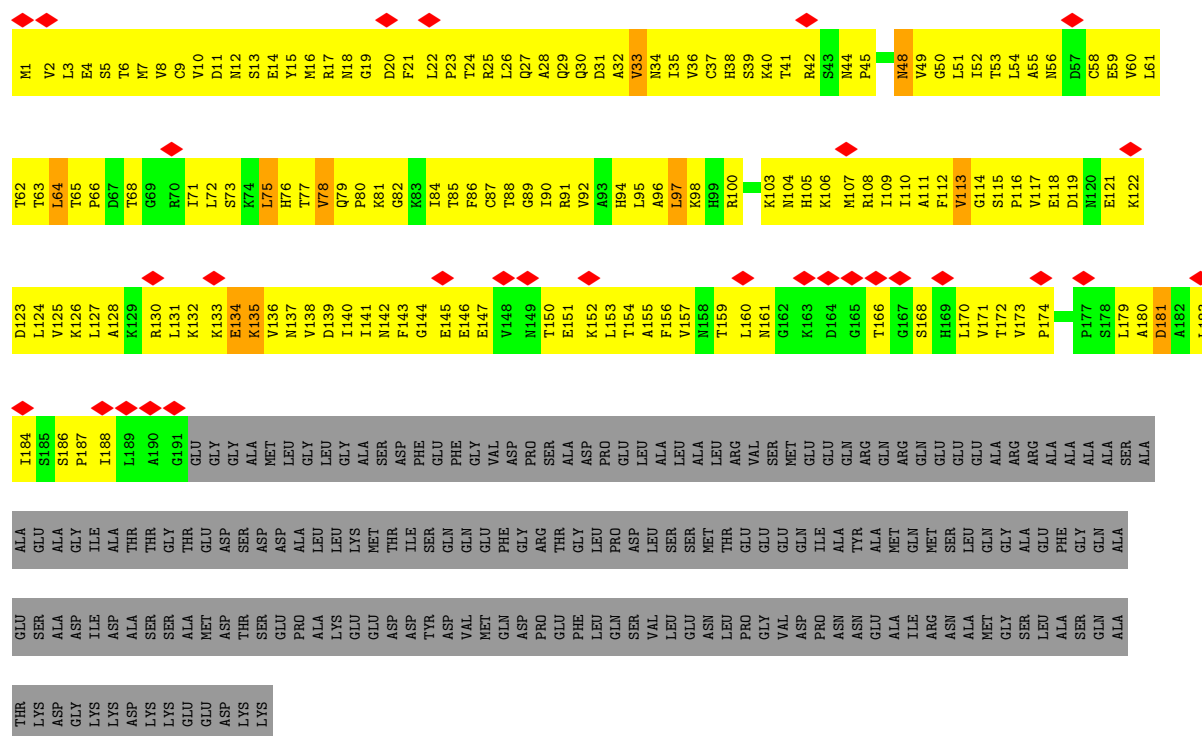
Chain a: 



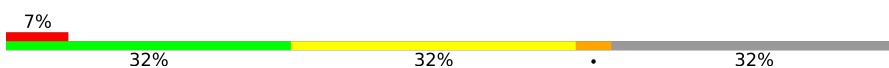
L375  
T376

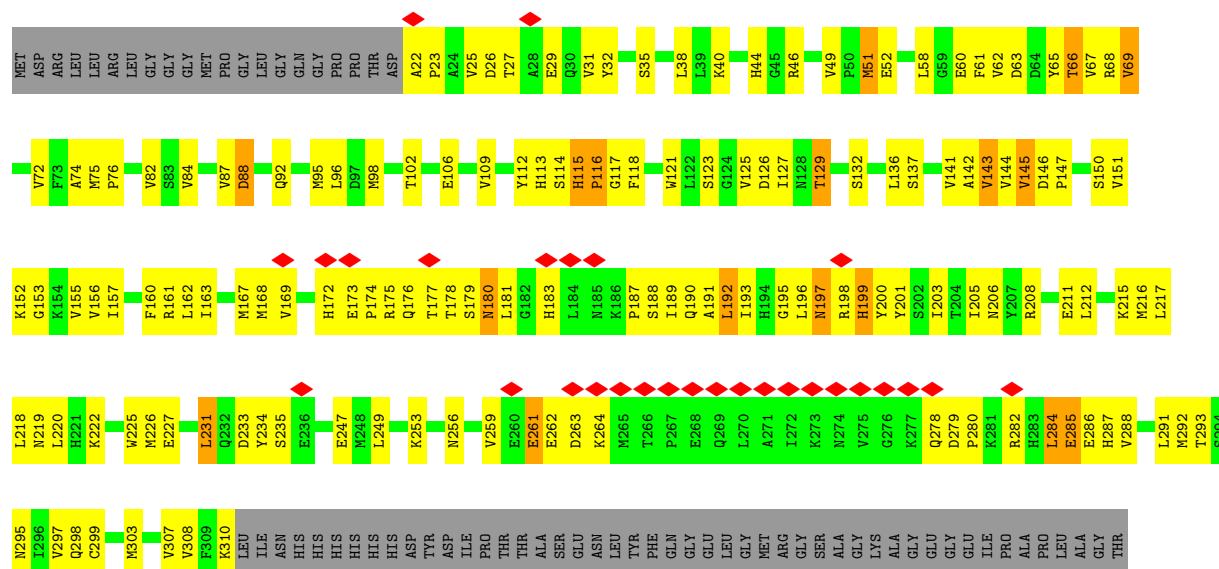
- Molecule 15: 26S proteasome non-ATPase regulatory subunit 4

Chain b: 



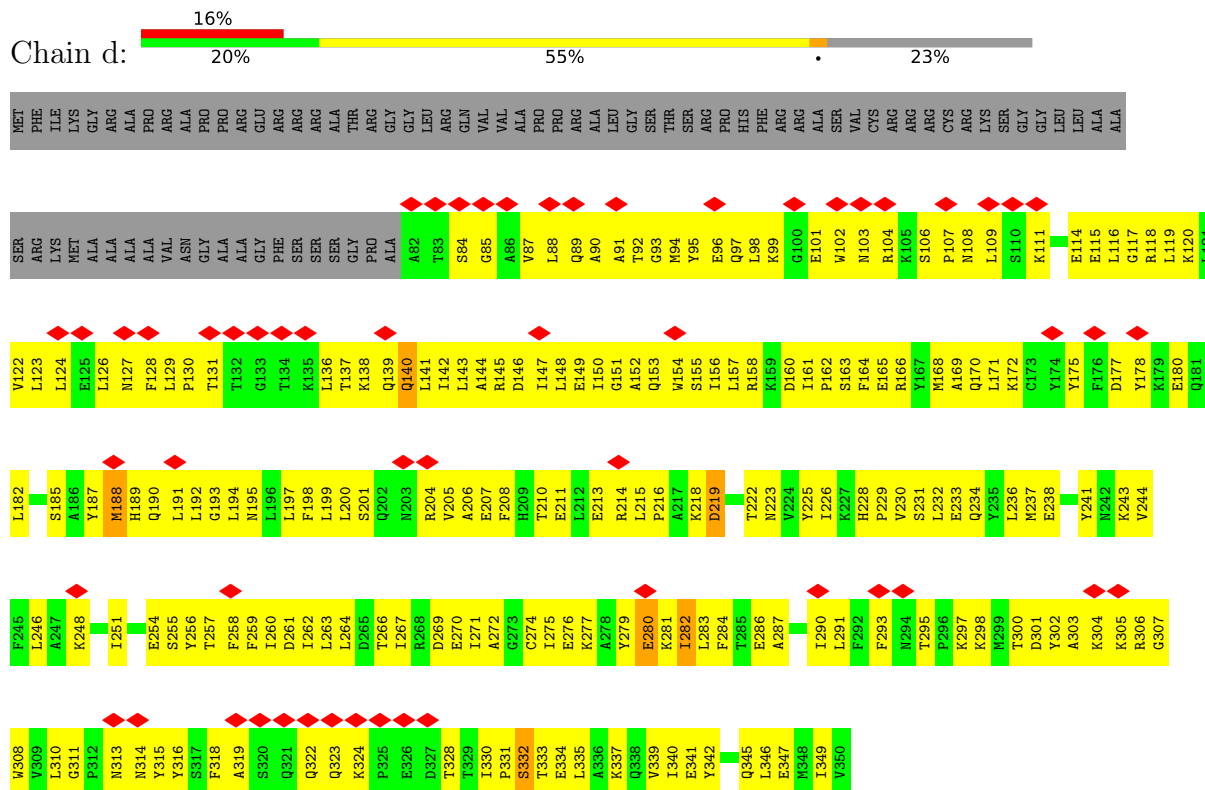
- Molecule 16: 26S proteasome non-ATPase regulatory subunit 14

Chain c: 

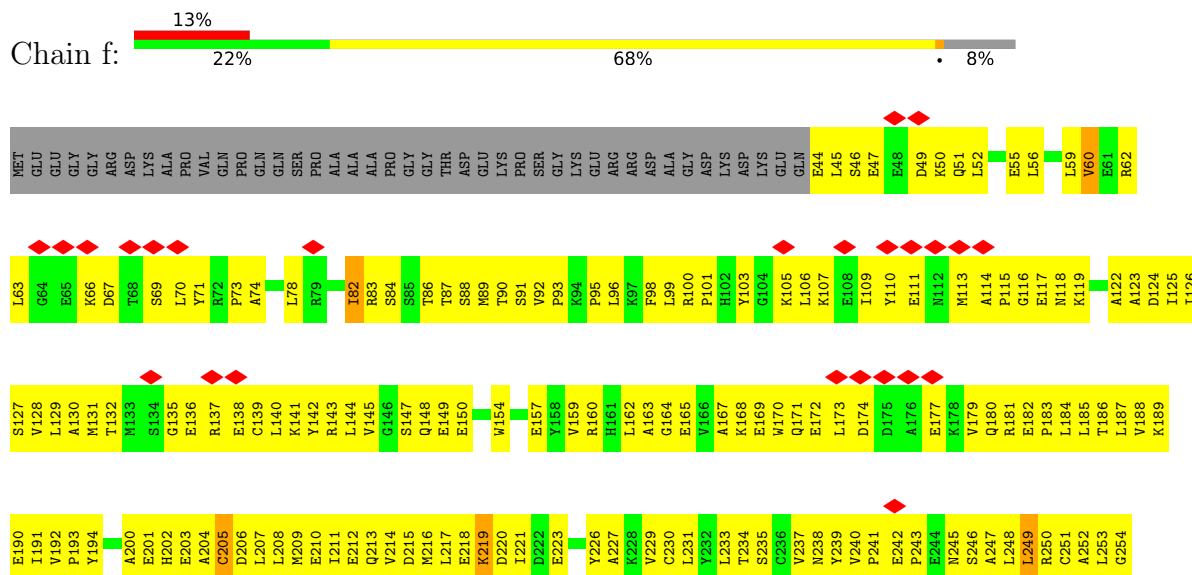


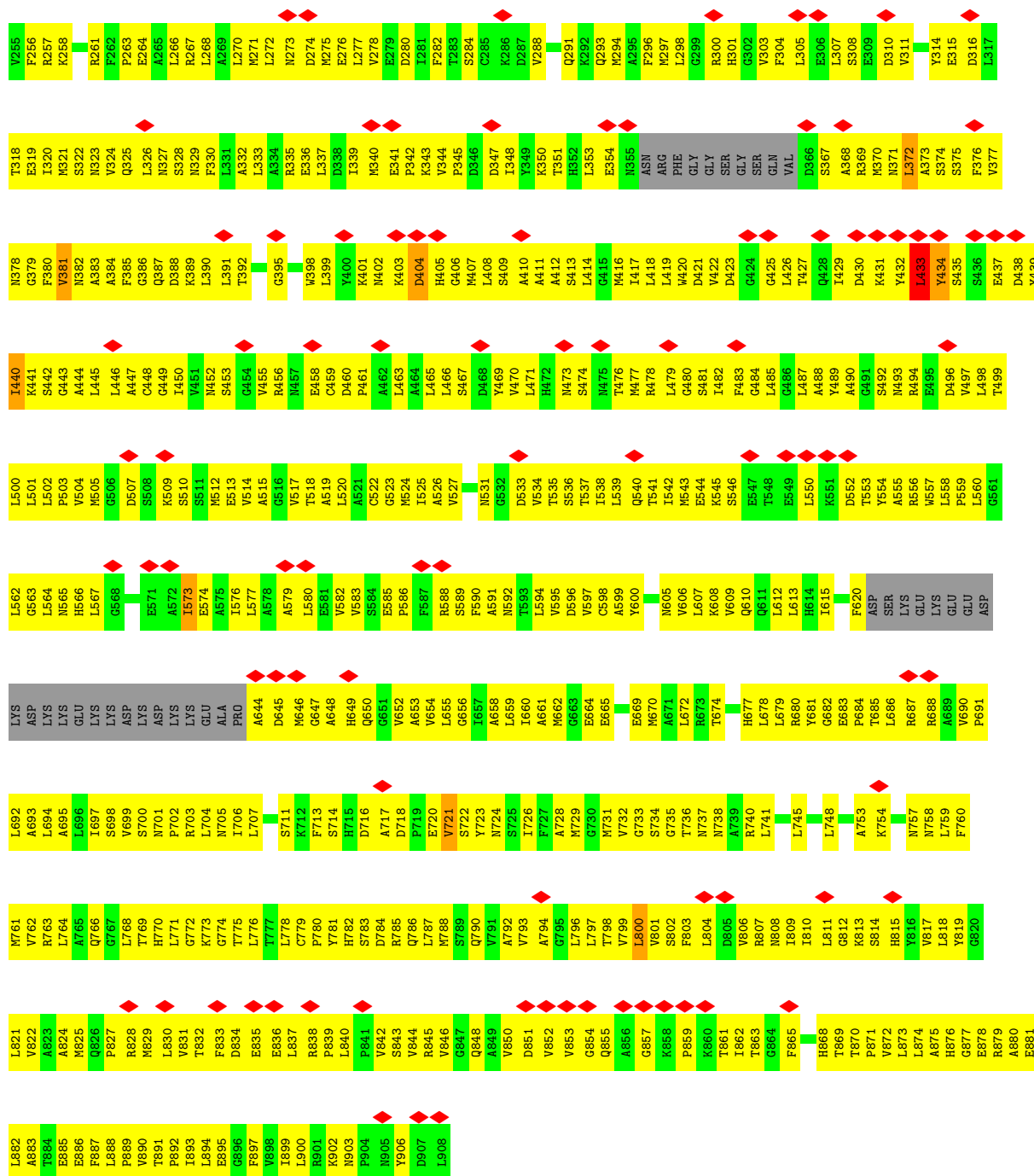
|     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| VAL | SER | GLY | ILE | VAL | LYS | GLY | GLY | THR | VAL | LYS | ALA | GLY | GLN | THR | THR | LEU | VAL | LEU | GLY | GLY | ALA | MET | LYS | GLN | GLY | THR | THR | LEU | VAL | LEU | GLY | GLY | ILE | LYS | GLY | VAL |
| HIS | HIS | HIS | HIS | HIS | HIS | HIS | HIS | HIS | HIS | HIS | HIS | HIS | HIS | HIS | HIS | HIS | HIS | HIS | HIS | HIS | HIS | HIS | HIS | HIS | HIS | HIS | HIS | HIS | HIS | HIS | HIS | HIS | HIS | HIS | HIS | HIS |

• Molecule 17: 26S proteasome non-ATPase regulatory subunit 8



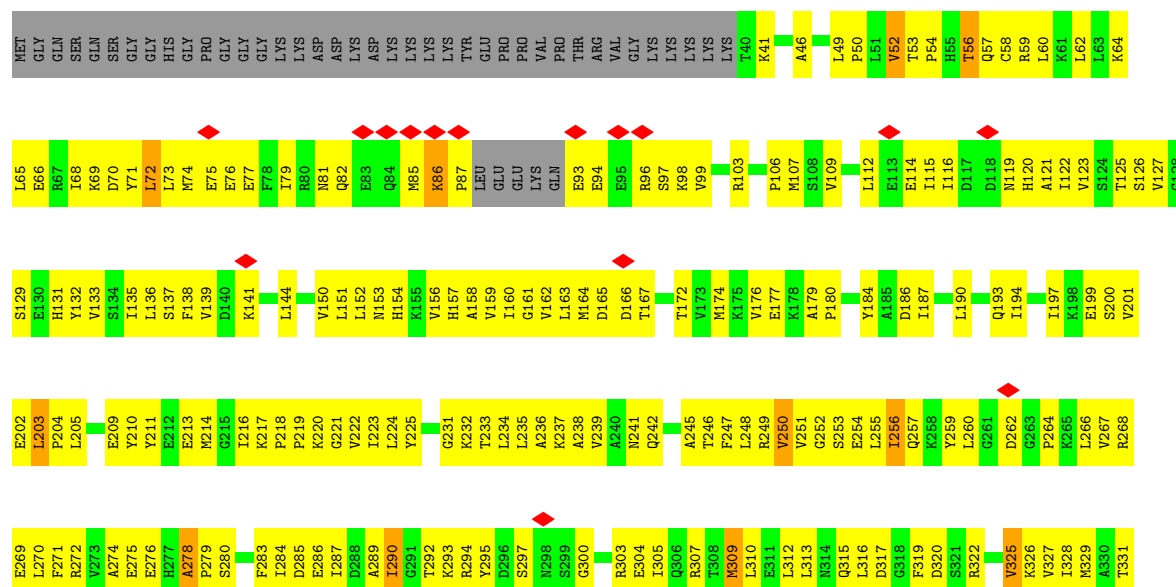
• Molecule 18: 26S proteasome non-ATPase regulatory subunit 2

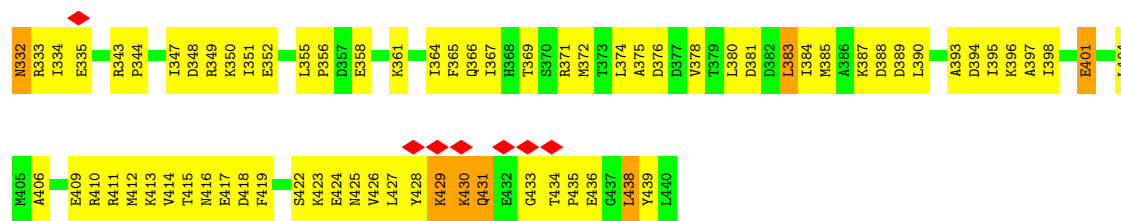




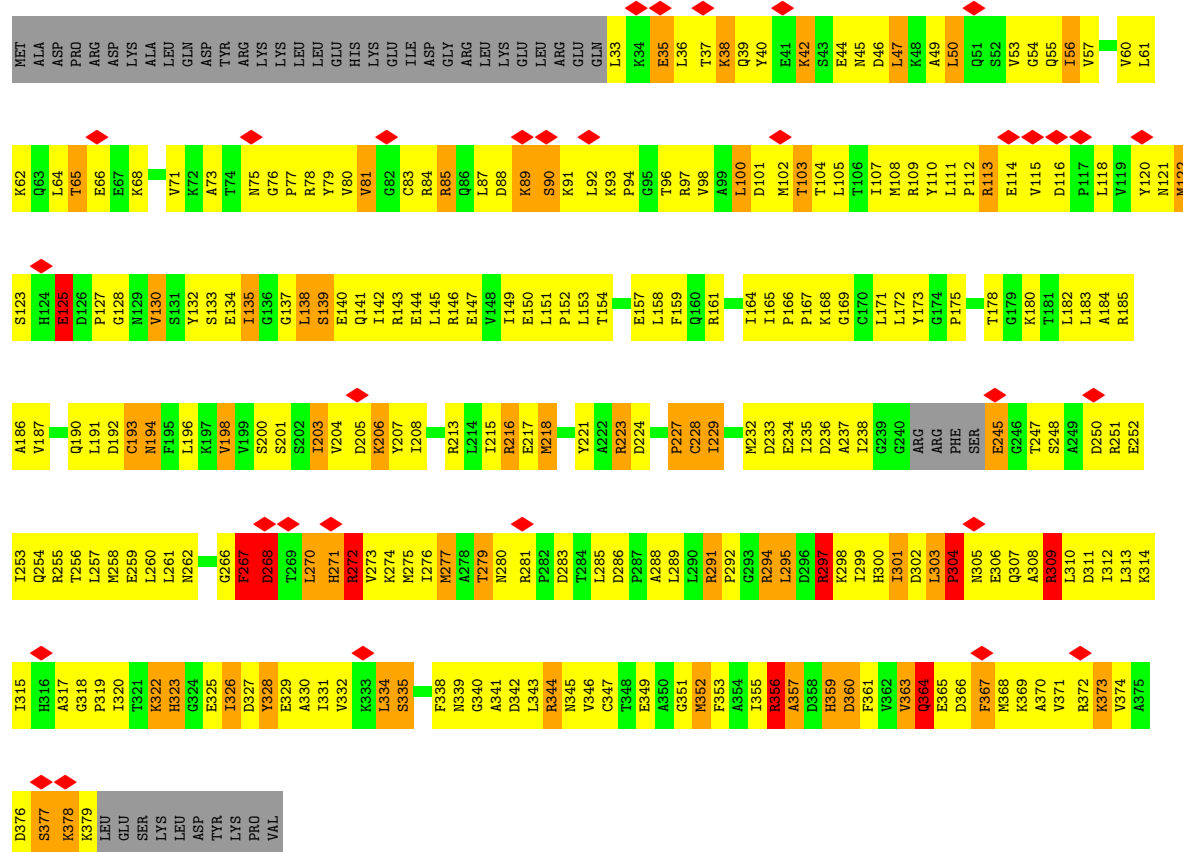
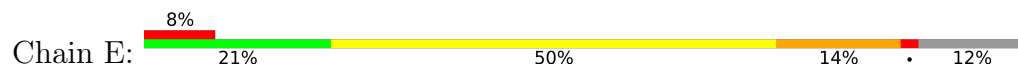


Chain A:  8% 31% 60% 6%

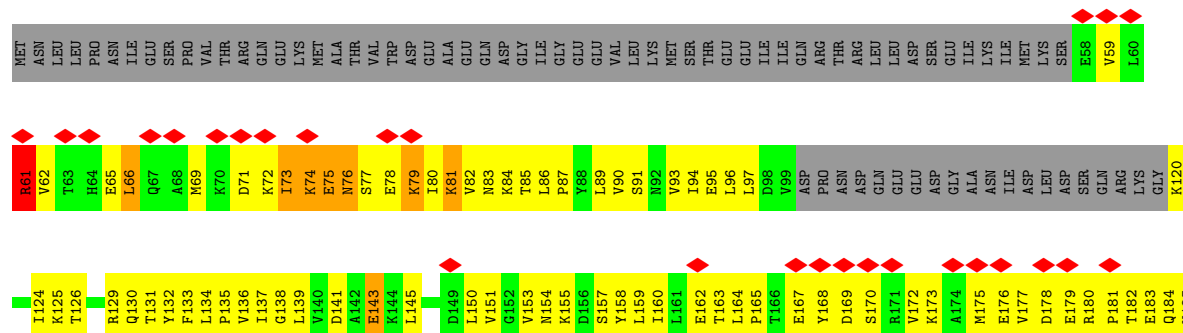


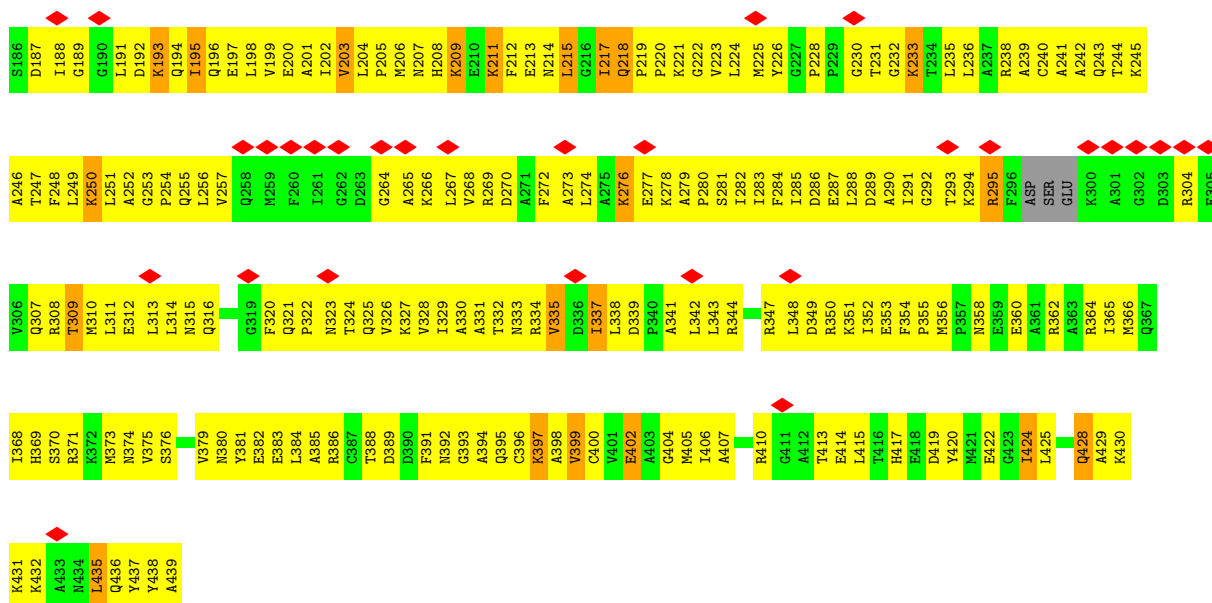


• Molecule 24: 26S protease regulatory subunit 10B



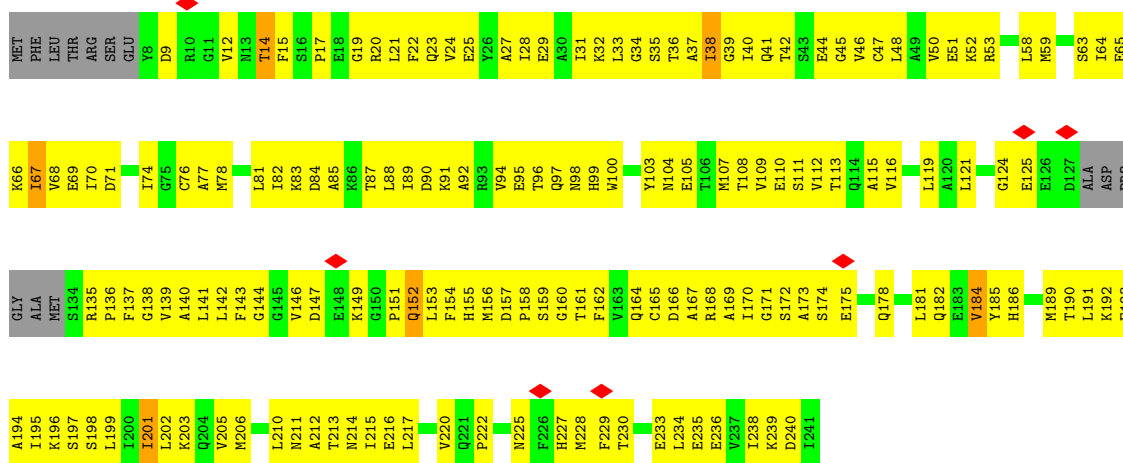
• Molecule 25: 26S proteasome regulatory subunit 6A





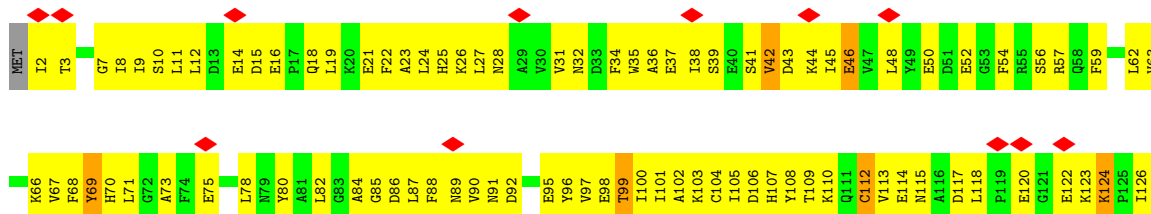
• Molecule 26: Proteasome subunit alpha type-5

Chain K: 26% 66% 5%

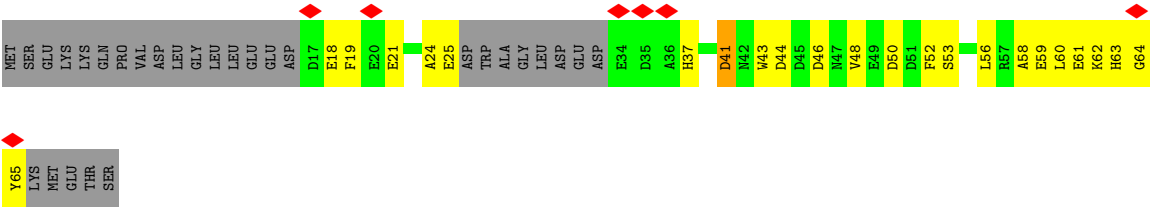


• Molecule 27: 26S proteasome non-ATPase regulatory subunit 1

Chain U: 7% 24% 61% 11%







## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|-----------------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, Not provided                     |           |
| Number of particles used             | 19309                                   | 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)                 | 500                                     | Depositor |
| Maximum defocus (nm)                 | 1700                                    | Depositor |
| Magnification                        | Not provided                            |           |
| Image detector                       | GATAN K3 (6k x 4k)                      | Depositor |
| Maximum map value                    | 0.618                                   | Depositor |
| Minimum map value                    | -0.230                                  | Depositor |
| Average map value                    | 0.004                                   | Depositor |
| Map value standard deviation         | 0.034                                   | Depositor |
| Recommended contour level            | 0.15                                    | Depositor |
| Map size ( $\text{\AA}$ )            | 356.32, 356.32, 356.32                  | wwPDB     |
| Map dimensions                       | 340, 340, 340                           | wwPDB     |
| Map angles ( $^\circ$ )              | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing ( $\text{\AA}$ )       | 1.048, 1.048, 1.048                     | Depositor |

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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   | C     | 0.29         | 0/3092         | 0.45        | 0/4154          |
| 2   | D     | 0.44         | 0/3090         | 0.65        | 0/4168          |
| 3   | G     | 0.28         | 0/1853         | 0.45        | 2/2515 (0.1%)   |
| 4   | H     | 0.29         | 0/1852         | 0.52        | 1/2507 (0.0%)   |
| 5   | I     | 0.23         | 0/1925         | 0.39        | 0/2606          |
| 6   | J     | 0.22         | 0/1758         | 0.37        | 0/2394          |
| 7   | L     | 0.24         | 0/1885         | 0.36        | 0/2552          |
| 8   | M     | 0.25         | 0/1891         | 0.40        | 0/2552          |
| 9   | V     | 0.20         | 0/3678         | 0.40        | 0/4965          |
| 10  | W     | 0.19         | 0/3618         | 0.32        | 0/4868          |
| 11  | X     | 0.24         | 0/3038         | 0.38        | 0/4095          |
| 12  | Y     | 0.24         | 0/3185         | 0.31        | 0/4290          |
| 13  | Z     | 0.28         | 0/2324         | 0.40        | 0/3150          |
| 14  | a     | 0.20         | 0/3053         | 0.43        | 0/4133          |
| 15  | b     | 0.21         | 0/1478         | 0.42        | 0/2001          |
| 16  | c     | 0.38         | 0/2311         | 0.60        | 2/3124 (0.1%)   |
| 17  | d     | 0.16         | 0/2234         | 0.34        | 0/3018          |
| 18  | f     | 0.19         | 0/6550         | 0.34        | 0/8865          |
| 19  | g     | 0.31         | 0/778          | 0.93        | 4/1041 (0.4%)   |
| 20  | u     | 0.20         | 0/1403         | 0.36        | 0/1892          |
| 21  | v     | 0.80         | 0/4            | 1.05        | 0/4             |
| 22  | A     | 0.26         | 0/3250         | 0.45        | 0/4386          |
| 23  | B     | 0.32         | 0/3153         | 0.49        | 0/4255          |
| 24  | E     | 0.77         | 1/2742 (0.0%)  | 1.23        | 21/3696 (0.6%)  |
| 25  | F     | 0.37         | 0/2838         | 0.63        | 1/3825 (0.0%)   |
| 26  | K     | 0.26         | 0/1763         | 0.43        | 0/2383          |
| 27  | U     | 0.23         | 0/6696         | 0.38        | 2/9052 (0.0%)   |
| 28  | e     | 0.20         | 0/362          | 0.32        | 0/490           |
| All | All   | 0.30         | 1/71804 (0.0%) | 0.49        | 33/96981 (0.0%) |

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 2   | D     | 0                   | 2                   |
| 4   | H     | 0                   | 1                   |
| 23  | B     | 0                   | 1                   |
| 24  | E     | 0                   | 16                  |
| 25  | F     | 0                   | 1                   |
| 27  | U     | 0                   | 1                   |
| All | All   | 0                   | 22                  |

All (1) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 24  | E     | 89  | LYS  | CA-C  | 5.07 | 1.59        | 1.52     |

All (33) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|--------|-------------|----------|
| 19  | g     | 166 | ARG  | N-CA-C   | -14.71 | 95.40       | 113.20   |
| 24  | E     | 90  | SER  | N-CA-C   | 9.07   | 122.09      | 111.02   |
| 19  | g     | 171 | LEU  | N-CA-C   | -8.62  | 100.90      | 111.33   |
| 19  | g     | 165 | ALA  | N-CA-C   | -8.33  | 101.11      | 113.61   |
| 27  | U     | 644 | TYR  | CA-C-N   | -8.05  | 109.27      | 121.83   |
| 27  | U     | 644 | TYR  | C-N-CA   | -8.05  | 109.27      | 121.83   |
| 24  | E     | 334 | LEU  | N-CA-C   | -7.93  | 102.86      | 112.54   |
| 24  | E     | 271 | HIS  | CA-CB-CG | 7.81   | 121.61      | 113.80   |
| 25  | F     | 73  | ILE  | N-CA-C   | -7.78  | 102.86      | 110.72   |
| 24  | E     | 128 | GLY  | N-CA-C   | -7.69  | 103.67      | 112.29   |
| 19  | g     | 167 | LYS  | N-CA-C   | -7.63  | 103.93      | 113.55   |
| 24  | E     | 127 | PRO  | N-CA-C   | -7.02  | 103.77      | 113.53   |
| 16  | c     | 23  | PRO  | N-CA-CB  | 6.97   | 110.57      | 103.25   |
| 24  | E     | 341 | ALA  | N-CA-C   | -6.61  | 104.07      | 111.28   |
| 24  | E     | 128 | GLY  | CA-C-O   | -6.32  | 117.87      | 122.23   |
| 24  | E     | 128 | GLY  | CA-C-N   | -6.22  | 114.14      | 122.42   |
| 24  | E     | 128 | GLY  | C-N-CA   | -6.22  | 114.14      | 122.42   |
| 24  | E     | 118 | LEU  | N-CA-C   | -6.16  | 105.41      | 113.17   |
| 24  | E     | 217 | GLU  | N-CA-C   | -5.96  | 104.86      | 111.36   |
| 24  | E     | 267 | PHE  | N-CA-CB  | -5.94  | 100.45      | 110.49   |
| 3   | G     | 9   | PHE  | N-CA-C   | -5.91  | 104.83      | 111.28   |
| 24  | E     | 89  | LYS  | CB-CA-C  | 5.75   | 120.07      | 110.92   |
| 24  | E     | 227 | PRO  | CA-C-N   | -5.69  | 114.98      | 123.00   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 24  | E     | 227 | PRO  | C-N-CA  | -5.69 | 114.98      | 123.00   |
| 24  | E     | 270 | LEU  | CA-C-O  | -5.66 | 114.55      | 120.55   |
| 24  | E     | 364 | GLN  | N-CA-C  | -5.66 | 105.88      | 112.89   |
| 4   | H     | 8   | PHE  | N-CA-C  | 5.61  | 117.25      | 111.03   |
| 24  | E     | 369 | LYS  | N-CA-C  | 5.51  | 117.99      | 111.33   |
| 24  | E     | 50  | LEU  | N-CA-C  | -5.37 | 105.43      | 111.28   |
| 24  | E     | 192 | ASP  | N-CA-CB | -5.34 | 103.79      | 111.91   |
| 3   | G     | 10  | ASP  | CB-CA-C | -5.29 | 99.89       | 110.42   |
| 24  | E     | 367 | PHE  | N-CA-C  | -5.04 | 105.86      | 111.36   |
| 16  | c     | 197 | ASN  | N-CA-C  | -5.03 | 106.24      | 112.47   |

There are no chirality outliers.

All (22) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 23  | B     | 53  | THR  | Peptide   |
| 2   | D     | 313 | ARG  | Sidechain |
| 2   | D     | 85  | ILE  | Peptide   |
| 24  | E     | 113 | ARG  | Sidechain |
| 24  | E     | 185 | ARG  | Sidechain |
| 24  | E     | 213 | ARG  | Sidechain |
| 24  | E     | 216 | ARG  | Sidechain |
| 24  | E     | 223 | ARG  | Sidechain |
| 24  | E     | 228 | CYS  | Mainchain |
| 24  | E     | 272 | ARG  | Sidechain |
| 24  | E     | 291 | ARG  | Sidechain |
| 24  | E     | 294 | ARG  | Sidechain |
| 24  | E     | 297 | ARG  | Sidechain |
| 24  | E     | 309 | ARG  | Sidechain |
| 24  | E     | 344 | ARG  | Sidechain |
| 24  | E     | 356 | ARG  | Sidechain |
| 24  | E     | 372 | ARG  | Sidechain |
| 24  | E     | 84  | ARG  | Sidechain |
| 24  | E     | 85  | ARG  | Sidechain |
| 25  | F     | 61  | ARG  | Sidechain |
| 4   | H     | 4   | ARG  | Sidechain |
| 27  | U     | 873 | PRO  | Peptide   |

## 5.2 Too-close contacts ⓘ

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | C     | 3051  | 0        | 3165     | 449     | 0            |
| 2   | D     | 3040  | 0        | 3075     | 400     | 0            |
| 3   | G     | 1820  | 0        | 1789     | 275     | 0            |
| 4   | H     | 1813  | 0        | 1802     | 246     | 0            |
| 5   | I     | 1895  | 0        | 1833     | 271     | 0            |
| 6   | J     | 1733  | 0        | 1570     | 205     | 0            |
| 7   | L     | 1850  | 0        | 1822     | 306     | 0            |
| 8   | M     | 1856  | 0        | 1814     | 281     | 0            |
| 9   | V     | 3608  | 0        | 3677     | 642     | 0            |
| 10  | W     | 3570  | 0        | 3685     | 526     | 0            |
| 11  | X     | 2994  | 0        | 3097     | 412     | 0            |
| 12  | Y     | 3127  | 0        | 3133     | 330     | 0            |
| 13  | Z     | 2281  | 0        | 2312     | 375     | 0            |
| 14  | a     | 2995  | 0        | 3012     | 752     | 0            |
| 15  | b     | 1458  | 0        | 1505     | 334     | 0            |
| 16  | c     | 2269  | 0        | 2282     | 190     | 0            |
| 17  | d     | 2188  | 0        | 2216     | 354     | 0            |
| 18  | f     | 6442  | 0        | 6463     | 1089    | 0            |
| 19  | g     | 771   | 0        | 815      | 380     | 0            |
| 20  | u     | 1376  | 0        | 1324     | 64      | 0            |
| 21  | v     | 55    | 0        | 17       | 3       | 0            |
| 22  | A     | 3199  | 0        | 3258     | 409     | 0            |
| 23  | B     | 3107  | 0        | 3169     | 408     | 0            |
| 24  | E     | 2701  | 0        | 2758     | 391     | 0            |
| 25  | F     | 2801  | 0        | 2877     | 494     | 0            |
| 26  | K     | 1737  | 0        | 1699     | 277     | 0            |
| 27  | U     | 6584  | 0        | 6626     | 1014    | 0            |
| 28  | e     | 353   | 0        | 276      | 34      | 0            |
| 29  | A     | 31    | 0        | 12       | 2       | 0            |
| 29  | B     | 31    | 0        | 12       | 5       | 0            |
| 29  | C     | 31    | 0        | 12       | 2       | 0            |
| 29  | F     | 31    | 0        | 12       | 9       | 0            |
| 30  | A     | 1     | 0        | 0        | 0       | 0            |
| 30  | B     | 1     | 0        | 0        | 0       | 0            |
| 30  | C     | 1     | 0        | 0        | 0       | 0            |
| 30  | D     | 1     | 0        | 0        | 0       | 0            |
| 30  | F     | 1     | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 31  | D     | 27    | 0        | 12       | 1       | 0            |
| 31  | E     | 27    | 0        | 12       | 0       | 0            |
| 32  | c     | 1     | 0        | 0        | 0       | 0            |
| All | All   | 70858 | 0        | 71143    | 9936    | 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 70.

All (9936) 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) |
|-------------------|-------------------|--------------------------|-------------------|
| 24:E:352:MET:SD   | 24:E:355:ILE:HD12 | 1.44                     | 1.58              |
| 24:E:235:ILE:CD1  | 24:E:277:MET:HB3  | 1.29                     | 1.55              |
| 24:E:235:ILE:CD1  | 24:E:277:MET:CB   | 1.80                     | 1.55              |
| 24:E:277:MET:CE   | 24:E:295:LEU:HD13 | 1.37                     | 1.54              |
| 24:E:235:ILE:HD11 | 24:E:277:MET:CB   | 1.36                     | 1.43              |
| 24:E:277:MET:CE   | 24:E:295:LEU:CD1  | 2.07                     | 1.33              |
| 24:E:122:MET:HE1  | 25:F:344:ARG:CD   | 1.65                     | 1.26              |
| 24:E:122:MET:HE1  | 25:F:344:ARG:NE   | 1.50                     | 1.23              |
| 24:E:137:GLY:O    | 24:E:305:ASN:ND2  | 1.69                     | 1.23              |
| 24:E:352:MET:SD   | 24:E:355:ILE:CD1  | 2.26                     | 1.22              |
| 3:G:208:ILE:HD11  | 24:E:306:GLU:OE2  | 1.40                     | 1.18              |
| 2:D:369:LYS:HA    | 2:D:369:LYS:HE3   | 1.21                     | 1.17              |
| 19:g:170:GLN:HG2  | 19:g:173:GLU:HG3  | 1.20                     | 1.16              |
| 19:g:107:ILE:HD12 | 19:g:111:GLU:HB3  | 1.25                     | 1.16              |
| 19:g:129:ILE:HD12 | 19:g:155:VAL:HG22 | 1.18                     | 1.15              |
| 24:E:277:MET:SD   | 24:E:295:LEU:HD11 | 1.87                     | 1.14              |
| 27:U:536:ALA:HB1  | 27:U:578:LEU:HD21 | 1.23                     | 1.14              |
| 10:W:409:LEU:HD22 | 11:X:384:VAL:HG11 | 1.28                     | 1.13              |
| 12:Y:22:LEU:HD22  | 12:Y:37:VAL:HG13  | 1.22                     | 1.13              |
| 24:E:235:ILE:CD1  | 24:E:277:MET:HB2  | 1.70                     | 1.13              |
| 4:H:111:VAL:HG22  | 4:H:136:ILE:HD12  | 1.27                     | 1.13              |
| 24:E:149:ILE:HD13 | 24:E:276:ILE:HD11 | 1.28                     | 1.13              |
| 3:G:171:LYS:HA    | 3:G:171:LYS:HE3   | 1.30                     | 1.13              |
| 18:f:474:SER:HB3  | 18:f:477:MET:HG2  | 1.29                     | 1.13              |
| 18:f:831:VAL:HG22 | 18:f:871:PRO:HB3  | 1.28                     | 1.12              |
| 18:f:831:VAL:HG13 | 18:f:871:PRO:HG3  | 1.20                     | 1.12              |
| 24:E:277:MET:HE2  | 24:E:295:LEU:CD1  | 1.71                     | 1.12              |
| 23:B:86:LYS:HD2   | 23:B:87:PRO:HD2   | 1.31                     | 1.12              |
| 11:X:344:ARG:HG2  | 11:X:386:ILE:HD12 | 1.28                     | 1.11              |
| 14:a:112:ILE:HG21 | 14:a:151:VAL:HG12 | 1.15                     | 1.11              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 27:U:810:THR:HG21 | 27:U:873:PRO:HG2  | 1.21                     | 1.11              |
| 5:I:161:ALA:HB1   | 5:I:175:LEU:HD23  | 1.30                     | 1.11              |
| 14:a:81:LEU:HA    | 14:a:84:VAL:HG12  | 1.30                     | 1.11              |
| 10:W:202:THR:HG22 | 10:W:233:LEU:HD22 | 1.33                     | 1.10              |
| 12:Y:49:ASN:HA    | 12:Y:73:MET:HE2   | 1.28                     | 1.10              |
| 27:U:803:LYS:HG3  | 27:U:893:THR:HB   | 1.26                     | 1.10              |
| 24:E:87:LEU:HD21  | 24:E:92:LEU:HD11  | 1.25                     | 1.09              |
| 6:J:158:ALA:HB3   | 26:K:58:LEU:HD22  | 1.35                     | 1.09              |
| 3:G:118:ILE:HD13  | 3:G:138:MET:HE1   | 1.29                     | 1.09              |
| 9:V:333:ILE:HD12  | 9:V:357:LEU:HD22  | 1.34                     | 1.09              |
| 18:f:450:ILE:HD11 | 18:f:822:VAL:HG21 | 1.25                     | 1.09              |
| 14:a:293:PHE:HB3  | 14:a:329:LYS:HG3  | 1.26                     | 1.08              |
| 25:F:231:THR:HG21 | 25:F:354:PHE:HB3  | 1.34                     | 1.08              |
| 15:b:107:MET:HA   | 15:b:107:MET:HE3  | 1.32                     | 1.08              |
| 24:E:112:PRO:HD2  | 25:F:97:LEU:HD13  | 1.35                     | 1.08              |
| 14:a:94:LEU:HD21  | 14:a:118:ILE:HA   | 1.32                     | 1.08              |
| 22:A:92:PRO:HD3   | 23:B:156:VAL:HG13 | 1.33                     | 1.08              |
| 24:E:235:ILE:HD13 | 24:E:277:MET:CB   | 1.78                     | 1.08              |
| 27:U:28:ASN:HB2   | 27:U:63:VAL:HG22  | 1.30                     | 1.08              |
| 27:U:509:GLY:HA3  | 27:U:544:ILE:HG13 | 1.36                     | 1.08              |
| 23:B:251:VAL:HG12 | 23:B:254:GLU:HG3  | 1.37                     | 1.07              |
| 1:C:24:TYR:HB2    | 2:D:40:LEU:HD21   | 1.31                     | 1.07              |
| 5:I:90:LEU:HG     | 5:I:114:LEU:HD22  | 1.35                     | 1.07              |
| 7:L:26:MET:HE1    | 7:L:148:CYS:HB2   | 1.29                     | 1.07              |
| 23:B:197:ILE:HG21 | 23:B:235:LEU:HD21 | 1.13                     | 1.07              |
| 22:A:393:GLY:HA3  | 23:B:216:ILE:HD11 | 1.36                     | 1.07              |
| 27:U:876:GLN:HB3  | 27:U:878:LEU:HD21 | 1.16                     | 1.07              |
| 24:E:87:LEU:CD2   | 24:E:92:LEU:HD11  | 1.85                     | 1.06              |
| 3:G:208:ILE:CD1   | 24:E:306:GLU:OE2  | 2.03                     | 1.06              |
| 27:U:324:LYS:HE3  | 27:U:794:ASP:HB2  | 1.32                     | 1.06              |
| 18:f:439:TYR:HA   | 18:f:477:MET:HE1  | 1.34                     | 1.06              |
| 4:H:135:LEU:HD12  | 4:H:163:MET:HE2   | 1.09                     | 1.06              |
| 12:Y:181:LYS:HG2  | 12:Y:200:LEU:HD13 | 1.37                     | 1.06              |
| 25:F:226:TYR:HB3  | 25:F:335:VAL:HG11 | 1.37                     | 1.06              |
| 17:d:261:ASP:HA   | 17:d:264:LEU:HD12 | 1.37                     | 1.06              |
| 3:G:13:ILE:HD11   | 3:G:126:THR:HA    | 1.38                     | 1.05              |
| 24:E:275:MET:HG3  | 24:E:295:LEU:HD21 | 1.08                     | 1.05              |
| 8:M:186:CYS:HA    | 8:M:189:ILE:HB    | 1.39                     | 1.05              |
| 27:U:903:PHE:HB2  | 27:U:915:LYS:HB2  | 1.37                     | 1.05              |
| 2:D:154:LEU:HD12  | 2:D:227:PHE:HB3   | 1.34                     | 1.05              |
| 10:W:31:CYS:HB3   | 10:W:43:VAL:HG13  | 1.37                     | 1.05              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 15:b:171:VAL:HG21 | 15:b:187:PRO:HG3  | 1.39                     | 1.05              |
| 18:f:221:ILE:HD13 | 18:f:229:VAL:HG11 | 1.39                     | 1.04              |
| 27:U:879:ASP:HB3  | 27:U:881:PRO:HD2  | 1.33                     | 1.04              |
| 17:d:243:LYS:HD3  | 17:d:246:LEU:HD11 | 1.38                     | 1.04              |
| 19:g:101:LEU:HD21 | 19:g:116:ILE:HG23 | 1.39                     | 1.04              |
| 24:E:275:MET:HG3  | 24:E:295:LEU:CD2  | 1.86                     | 1.04              |
| 27:U:559:ARG:HB3  | 27:U:562:GLU:HB2  | 1.39                     | 1.04              |
| 8:M:108:LEU:HD22  | 8:M:139:SER:HB3   | 1.40                     | 1.03              |
| 10:W:190:MET:HE1  | 10:W:206:SER:HA   | 1.39                     | 1.03              |
| 10:W:203:GLN:HG2  | 10:W:233:LEU:HD21 | 1.36                     | 1.03              |
| 27:U:869:LYS:HA   | 27:U:872:GLU:HB3  | 1.33                     | 1.03              |
| 17:d:149:GLU:HG3  | 17:d:191:LEU:HD11 | 1.39                     | 1.03              |
| 15:b:106:LYS:HE3  | 15:b:107:MET:H    | 1.21                     | 1.03              |
| 24:E:235:ILE:HD11 | 24:E:277:MET:CA   | 1.88                     | 1.03              |
| 1:C:212:ILE:HD13  | 1:C:237:MET:HE3   | 1.36                     | 1.03              |
| 2:D:388:ARG:HH22  | 24:E:147:GLU:HG2  | 1.15                     | 1.03              |
| 8:M:136:MET:HE3   | 8:M:150:MET:HB2   | 1.38                     | 1.03              |
| 26:K:236:GLU:HA   | 26:K:239:LYS:HE3  | 1.40                     | 1.03              |
| 3:G:94:ALA:HB2    | 3:G:118:ILE:HD11  | 1.37                     | 1.03              |
| 11:X:171:LEU:HD22 | 11:X:210:LEU:HD23 | 1.41                     | 1.03              |
| 7:L:60:GLN:HG2    | 25:F:439:ALA:HB1  | 1.39                     | 1.02              |
| 9:V:404:LYS:HD2   | 9:V:446:VAL:HG21  | 1.35                     | 1.02              |
| 9:V:201:ARG:HA    | 9:V:201:ARG:HH11  | 1.22                     | 1.02              |
| 19:g:115:LYS:HA   | 19:g:118:GLU:HG2  | 1.40                     | 1.02              |
| 23:B:387:LYS:HE2  | 23:B:387:LYS:HA   | 1.40                     | 1.02              |
| 27:U:199:ARG:HD2  | 27:U:223:LEU:HD11 | 1.41                     | 1.02              |
| 14:a:112:ILE:HD13 | 14:a:138:VAL:HG21 | 1.40                     | 1.02              |
| 15:b:51:LEU:HD23  | 15:b:71:ILE:HG23  | 1.40                     | 1.02              |
| 27:U:870:GLU:HG3  | 27:U:871:PRO:HD3  | 1.37                     | 1.02              |
| 22:A:375:ARG:HD3  | 26:K:173:ALA:HB2  | 1.42                     | 1.01              |
| 25:F:314:LEU:HD21 | 25:F:342:LEU:HD22 | 1.39                     | 1.01              |
| 2:D:238:LYS:HD2   | 2:D:239:TYR:HD1   | 1.25                     | 1.01              |
| 14:a:78:GLU:O     | 14:a:82:HIS:ND1   | 1.92                     | 1.01              |
| 24:E:277:MET:SD   | 24:E:295:LEU:CD1  | 2.45                     | 1.01              |
| 3:G:143:ILE:HG21  | 3:G:222:VAL:HA    | 1.42                     | 1.01              |
| 9:V:189:ASP:O     | 9:V:193:GLN:N     | 1.92                     | 1.01              |
| 25:F:251:LEU:HD11 | 25:F:256:LEU:HD21 | 1.43                     | 1.01              |
| 3:G:118:ILE:HG21  | 3:G:138:MET:HE1   | 1.43                     | 1.01              |
| 14:a:54:ASP:HA    | 14:a:57:ILE:HG22  | 1.40                     | 1.01              |
| 12:Y:282:MET:HG3  | 12:Y:288:PHE:HB3  | 1.43                     | 1.00              |
| 18:f:586:PRO:HB3  | 18:f:645:ASP:HB3  | 1.42                     | 1.00              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 10:W:18:VAL:HB    | 10:W:57:ALA:HB1   | 1.41                     | 1.00              |
| 27:U:243:LEU:HD23 | 27:U:913:ILE:HD12 | 1.42                     | 1.00              |
| 9:V:190:ASP:HA    | 9:V:193:GLN:HB2   | 1.44                     | 1.00              |
| 14:a:159:SER:HA   | 14:a:162:TYR:HB3  | 1.43                     | 0.99              |
| 10:W:105:VAL:HG11 | 10:W:138:VAL:HG23 | 1.40                     | 0.99              |
| 15:b:146:GLU:OE2  | 15:b:150:THR:OG1  | 1.78                     | 0.99              |
| 19:g:87:VAL:HG11  | 19:g:101:LEU:HB2  | 1.41                     | 0.99              |
| 19:g:123:GLN:HB2  | 19:g:126:TYR:HB2  | 1.44                     | 0.99              |
| 24:E:130:VAL:HG21 | 24:E:182:LEU:HD11 | 1.42                     | 0.99              |
| 18:f:830:LEU:HD22 | 18:f:874:LEU:HD21 | 1.40                     | 0.99              |
| 10:W:230:MET:HE1  | 10:W:233:LEU:HD23 | 1.42                     | 0.99              |
| 5:I:174:MET:HE3   | 5:I:195:LYS:HE3   | 1.45                     | 0.99              |
| 22:A:162:THR:HA   | 22:A:263:MET:HE1  | 1.43                     | 0.99              |
| 15:b:157:VAL:HG21 | 15:b:170:LEU:HB2  | 1.44                     | 0.98              |
| 9:V:184:ALA:O     | 9:V:188:SER:N     | 1.96                     | 0.98              |
| 14:a:84:VAL:HG23  | 14:a:87:MET:HE2   | 1.40                     | 0.98              |
| 17:d:98:LEU:HD21  | 17:d:150:ILE:HG21 | 1.43                     | 0.98              |
| 18:f:417:ILE:HG22 | 18:f:418:LEU:HD23 | 1.45                     | 0.98              |
| 7:L:34:ALA:HA     | 7:L:162:GLY:HA3   | 1.44                     | 0.98              |
| 14:a:158:LEU:O    | 14:a:162:TYR:N    | 1.94                     | 0.98              |
| 14:a:180:LEU:HD13 | 14:a:221:VAL:HG21 | 1.45                     | 0.98              |
| 24:E:122:MET:HE1  | 25:F:344:ARG:CZ   | 1.94                     | 0.98              |
| 8:M:196:ILE:HA    | 8:M:199:ILE:HD12  | 1.46                     | 0.97              |
| 14:a:80:ILE:HA    | 14:a:83:VAL:HB    | 1.44                     | 0.97              |
| 14:a:97:LEU:HD13  | 14:a:114:CYS:HB3  | 1.45                     | 0.97              |
| 26:K:186:HIS:H    | 26:K:189:MET:HE2  | 1.27                     | 0.97              |
| 14:a:112:ILE:O    | 14:a:116:THR:N    | 1.97                     | 0.97              |
| 17:d:156:ILE:HD12 | 17:d:255:SER:HB3  | 1.43                     | 0.97              |
| 19:g:89:LEU:HD12  | 19:g:99:ASN:HB2   | 1.45                     | 0.97              |
| 19:g:112:LEU:HB2  | 19:g:142:LEU:HD11 | 1.45                     | 0.97              |
| 22:A:397:ILE:HD12 | 23:B:210:TYR:HB3  | 1.46                     | 0.97              |
| 14:a:32:LYS:NZ    | 15:b:19:GLY:O     | 1.98                     | 0.97              |
| 9:V:159:LEU:HD22  | 9:V:163:VAL:HG21  | 1.43                     | 0.97              |
| 27:U:247:GLN:HG2  | 27:U:913:ILE:HG12 | 1.44                     | 0.97              |
| 14:a:123:LEU:HD21 | 14:a:161:LYS:HB2  | 1.45                     | 0.97              |
| 17:d:117:GLY:HA2  | 17:d:120:LYS:HE3  | 1.46                     | 0.97              |
| 19:g:140:LYS:HB3  | 19:g:144:GLU:HG3  | 1.46                     | 0.97              |
| 27:U:481:LEU:HD21 | 27:U:493:VAL:HG23 | 1.45                     | 0.96              |
| 14:a:115:LYS:HA   | 14:a:118:ILE:HG22 | 1.43                     | 0.96              |
| 25:F:134:LEU:HD11 | 25:F:159:LEU:HA   | 1.45                     | 0.96              |
| 14:a:80:ILE:O     | 14:a:84:VAL:N     | 1.99                     | 0.96              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:A:213:LEU:HB2  | 22:A:337:LEU:HD13 | 1.47                     | 0.96              |
| 14:a:111:VAL:O    | 14:a:115:LYS:N    | 1.97                     | 0.96              |
| 26:K:210:LEU:HD11 | 26:K:215:ILE:HG12 | 1.46                     | 0.96              |
| 5:I:171:ALA:HB2   | 5:I:200:THR:HG21  | 1.48                     | 0.96              |
| 6:J:30:SER:OG     | 6:J:61:LYS:NZ     | 1.99                     | 0.96              |
| 5:I:45:LEU:HD12   | 5:I:137:ILE:HD13  | 1.45                     | 0.96              |
| 25:F:292:GLY:HA2  | 25:F:310:MET:HE2  | 1.48                     | 0.96              |
| 10:W:54:THR:HG22  | 10:W:59:ASP:HB3   | 1.47                     | 0.95              |
| 25:F:384:LEU:HD11 | 25:F:420:TYR:HB3  | 1.45                     | 0.95              |
| 13:Z:67:VAL:HG21  | 15:b:91:ARG:HD3   | 1.46                     | 0.95              |
| 22:A:384:GLU:HG2  | 23:B:344:PRO:HG2  | 1.47                     | 0.95              |
| 5:I:25:MET:HA     | 5:I:152:PRO:HG2   | 1.48                     | 0.95              |
| 8:M:40:ARG:HA     | 8:M:45:VAL:HA     | 1.48                     | 0.95              |
| 19:g:112:LEU:HD13 | 19:g:142:LEU:HD21 | 1.48                     | 0.95              |
| 25:F:343:LEU:HD23 | 25:F:351:LYS:HD2  | 1.47                     | 0.95              |
| 22:A:161:VAL:HA   | 22:A:164:MET:HE3  | 1.45                     | 0.95              |
| 14:a:172:TYR:OH   | 14:a:199:THR:OG1  | 1.82                     | 0.95              |
| 19:g:163:GLU:HA   | 19:g:166:ARG:HB2  | 1.47                     | 0.95              |
| 10:W:40:LEU:HD23  | 10:W:82:LEU:HD22  | 1.49                     | 0.95              |
| 4:H:10:LEU:HD13   | 4:H:21:GLN:HB3    | 1.47                     | 0.94              |
| 4:H:75:VAL:HG23   | 4:H:135:LEU:HB2   | 1.48                     | 0.94              |
| 5:I:69:ASN:OD1    | 5:I:70:GLU:N      | 1.99                     | 0.94              |
| 17:d:295:THR:HB   | 17:d:298:LYS:HG3  | 1.48                     | 0.94              |
| 5:I:38:LEU:HD23   | 5:I:160:LYS:HB3   | 1.46                     | 0.94              |
| 23:B:294:ARG:HD3  | 23:B:310:LEU:HD11 | 1.48                     | 0.94              |
| 18:f:479:LEU:HD11 | 18:f:513:GLU:HG2  | 1.47                     | 0.94              |
| 19:g:161:SER:H    | 19:g:164:ASP:HB3  | 1.30                     | 0.94              |
| 24:E:235:ILE:HD13 | 24:E:277:MET:HB3  | 1.35                     | 0.94              |
| 17:d:151:GLY:O    | 17:d:155:SER:N    | 2.00                     | 0.94              |
| 14:a:116:THR:O    | 14:a:120:ALA:N    | 1.99                     | 0.94              |
| 15:b:127:LEU:HD23 | 15:b:130:ARG:HH22 | 1.27                     | 0.94              |
| 19:g:132:ASN:N    | 19:g:152:LYS:O    | 2.01                     | 0.94              |
| 24:E:122:MET:SD   | 25:F:344:ARG:NH1  | 2.41                     | 0.94              |
| 26:K:217:LEU:HB2  | 26:K:234:LEU:HD11 | 1.48                     | 0.94              |
| 27:U:177:LEU:HD12 | 27:U:204:ILE:HD13 | 1.49                     | 0.94              |
| 14:a:186:LYS:O    | 14:a:188:LEU:HG   | 1.67                     | 0.94              |
| 18:f:485:LEU:HD23 | 18:f:501:LEU:HD21 | 1.48                     | 0.94              |
| 19:g:131:ILE:HG12 | 19:g:147:VAL:HG13 | 1.46                     | 0.94              |
| 24:E:122:MET:HE1  | 25:F:344:ARG:HD3  | 1.49                     | 0.94              |
| 25:F:279:ALA:HB1  | 25:F:280:PRO:HD2  | 1.47                     | 0.94              |
| 9:V:479:ARG:HH12  | 12:Y:370:ILE:HD13 | 1.32                     | 0.94              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 23:B:383:LEU:HD21 | 23:B:419:PHE:HB3  | 1.47                     | 0.94              |
| 18:f:788:MET:HE2  | 18:f:793:VAL:HG21 | 1.48                     | 0.93              |
| 22:A:246:VAL:HG21 | 23:B:307:ARG:HD2  | 1.48                     | 0.93              |
| 3:G:171:LYS:HE2   | 3:G:174:GLU:OE2   | 1.66                     | 0.93              |
| 7:L:33:SER:OG     | 7:L:51:ARG:NE     | 2.01                     | 0.93              |
| 11:X:212:MET:HE1  | 11:X:250:SER:HA   | 1.48                     | 0.93              |
| 14:a:40:GLN:O     | 14:a:44:PHE:N     | 1.99                     | 0.93              |
| 14:a:114:CYS:HA   | 14:a:117:ALA:HB3  | 1.51                     | 0.93              |
| 3:G:69:LEU:HD12   | 3:G:79:VAL:HG23   | 1.50                     | 0.93              |
| 17:d:137:THR:HB   | 17:d:140:GLN:HB3  | 1.49                     | 0.93              |
| 27:U:401:LYS:NZ   | 27:U:435:SER:OG   | 2.02                     | 0.93              |
| 14:a:186:LYS:HZ3  | 14:a:193:GLN:HB2  | 1.29                     | 0.93              |
| 25:F:292:GLY:HA2  | 25:F:310:MET:CE   | 1.99                     | 0.93              |
| 6:J:155:ALA:HB3   | 26:K:63:SER:HB2   | 1.49                     | 0.93              |
| 14:a:54:ASP:O     | 14:a:58:LYS:N     | 2.00                     | 0.93              |
| 18:f:573:ILE:HG13 | 18:f:599:ALA:HB2  | 1.48                     | 0.93              |
| 18:f:609:VAL:HG12 | 23:B:74:MET:HE1   | 1.50                     | 0.93              |
| 18:f:822:VAL:HG22 | 18:f:825:MET:HE3  | 1.49                     | 0.93              |
| 14:a:53:GLY:O     | 14:a:57:ILE:N     | 2.02                     | 0.92              |
| 14:a:159:SER:O    | 14:a:163:TYR:N    | 2.03                     | 0.92              |
| 18:f:163:ALA:HB2  | 18:f:191:ILE:HD11 | 1.50                     | 0.92              |
| 19:g:132:ASN:HB2  | 19:g:151:VAL:HG13 | 1.48                     | 0.92              |
| 19:g:89:LEU:HD12  | 19:g:99:ASN:HD22  | 1.34                     | 0.92              |
| 3:G:51:VAL:HG12   | 3:G:217:VAL:HG22  | 1.52                     | 0.92              |
| 27:U:78:LEU:HD11  | 27:U:103:LYS:HB3  | 1.50                     | 0.92              |
| 12:Y:22:LEU:HD11  | 12:Y:40:GLU:HB3   | 1.48                     | 0.92              |
| 14:a:113:LEU:O    | 14:a:117:ALA:N    | 2.03                     | 0.92              |
| 10:W:60:MET:HE3   | 10:W:60:MET:H     | 1.32                     | 0.92              |
| 27:U:135:ASN:HA   | 27:U:138:PHE:HB2  | 1.51                     | 0.92              |
| 5:I:68:LEU:HD13   | 5:I:90:LEU:HD13   | 1.51                     | 0.92              |
| 14:a:152:HIS:HB3  | 14:a:156:TYR:CZ   | 2.04                     | 0.92              |
| 14:a:188:LEU:HD13 | 14:a:192:GLU:HB3  | 1.48                     | 0.92              |
| 17:d:283:LEU:O    | 17:d:287:ALA:N    | 2.03                     | 0.92              |
| 22:A:172:VAL:HG21 | 22:A:224:LEU:HD11 | 1.50                     | 0.92              |
| 27:U:364:VAL:HG12 | 27:U:724:VAL:HG11 | 1.52                     | 0.92              |
| 3:G:94:ALA:CB     | 3:G:118:ILE:HD11  | 2.00                     | 0.92              |
| 10:W:331:GLY:HA3  | 10:W:337:ALA:HB2  | 1.49                     | 0.92              |
| 14:a:77:VAL:HA    | 14:a:80:ILE:HG12  | 1.52                     | 0.92              |
| 18:f:597:VAL:HG21 | 18:f:656:GLY:HA2  | 1.51                     | 0.91              |
| 8:M:109:LYS:HA    | 8:M:149:TYR:HE2   | 1.35                     | 0.91              |
| 11:X:71:LYS:HA    | 11:X:74:ARG:HG3   | 1.52                     | 0.91              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 14:a:154:ARG:O    | 14:a:158:LEU:N    | 2.02                     | 0.91              |
| 27:U:368:ALA:HB1  | 27:U:731:ILE:HB   | 1.49                     | 0.91              |
| 23:B:119:ASN:O    | 23:B:120:HIS:ND1  | 2.03                     | 0.91              |
| 27:U:876:GLN:HB3  | 27:U:878:LEU:CD2  | 2.00                     | 0.91              |
| 12:Y:19:ILE:HD11  | 12:Y:44:ALA:HB1   | 1.52                     | 0.91              |
| 27:U:488:THR:HG23 | 27:U:490:ARG:H    | 1.34                     | 0.91              |
| 4:H:29:VAL:HG11   | 4:H:133:SER:HB3   | 1.52                     | 0.91              |
| 17:d:300:THR:HA   | 17:d:303:ALA:HB3  | 1.51                     | 0.91              |
| 1:C:273:MET:HE1   | 1:C:277:LEU:HD12  | 1.51                     | 0.91              |
| 4:H:106:PRO:HG2   | 4:H:109:GLN:HG2   | 1.52                     | 0.91              |
| 5:I:195:LYS:O     | 5:I:195:LYS:HD2   | 1.71                     | 0.91              |
| 8:M:187:ARG:HD2   | 8:M:219:LEU:HD21  | 1.52                     | 0.90              |
| 14:a:57:ILE:O     | 14:a:61:GLU:N     | 2.04                     | 0.90              |
| 19:g:112:LEU:HB3  | 19:g:138:LEU:HD22 | 1.53                     | 0.90              |
| 27:U:401:LYS:HE3  | 27:U:437:TYR:HB2  | 1.51                     | 0.90              |
| 11:X:419:LYS:HA   | 11:X:419:LYS:HE3  | 1.52                     | 0.90              |
| 14:a:58:LYS:O     | 14:a:62:ASN:N     | 2.04                     | 0.90              |
| 22:A:29:ASP:OD2   | 23:B:410:ARG:NE   | 2.03                     | 0.90              |
| 9:V:329:HIS:HB3   | 9:V:357:LEU:HD11  | 1.52                     | 0.90              |
| 10:W:315:MET:HE2  | 10:W:358:VAL:HG22 | 1.52                     | 0.90              |
| 18:f:537:THR:O    | 18:f:541:THR:OG1  | 1.87                     | 0.90              |
| 23:B:381:ASP:HB3  | 23:B:385:MET:HE3  | 1.51                     | 0.90              |
| 1:C:399:MET:HG3   | 4:H:158:TRP:HZ2   | 1.35                     | 0.90              |
| 14:a:94:LEU:HD11  | 14:a:118:ILE:HD12 | 1.54                     | 0.90              |
| 14:a:96:PHE:HD1   | 14:a:99:LYS:HE2   | 1.33                     | 0.90              |
| 19:g:131:ILE:HD12 | 19:g:153:ALA:HB2  | 1.53                     | 0.90              |
| 19:g:131:ILE:HG21 | 19:g:147:VAL:HG22 | 1.54                     | 0.90              |
| 27:U:265:ILE:CG2  | 27:U:326:ILE:HG23 | 2.01                     | 0.90              |
| 3:G:75:ASN:ND2    | 3:G:225:PRO:O     | 2.03                     | 0.90              |
| 3:G:165:ALA:HB1   | 3:G:179:LEU:HD13  | 1.54                     | 0.90              |
| 15:b:23:PRO:HG2   | 15:b:27:GLN:CD    | 1.97                     | 0.90              |
| 15:b:111:ALA:HB3  | 15:b:140:ILE:HD13 | 1.51                     | 0.90              |
| 1:C:232:ARG:NH1   | 1:C:275:GLU:OE2   | 2.05                     | 0.90              |
| 22:A:238:ILE:HG21 | 22:A:260:LEU:HD11 | 1.53                     | 0.90              |
| 18:f:325:GLN:O    | 18:f:329:ASN:ND2  | 2.05                     | 0.89              |
| 27:U:804:SER:HB3  | 27:U:874:ASN:HA   | 1.51                     | 0.89              |
| 19:g:114:SER:HA   | 19:g:124:GLU:HG3  | 1.50                     | 0.89              |
| 1:C:135:VAL:HA    | 1:C:138:MET:HE3   | 1.54                     | 0.89              |
| 11:X:153:LEU:HD13 | 11:X:169:VAL:HG21 | 1.54                     | 0.89              |
| 22:A:375:ARG:CD   | 26:K:173:ALA:HB2  | 2.02                     | 0.89              |
| 27:U:462:LEU:HD12 | 27:U:496:LEU:HD23 | 1.53                     | 0.89              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:H:93:LEU:HD13   | 4:H:113:ARG:HB3   | 1.53                     | 0.89              |
| 4:H:154:ALA:HB2   | 5:I:80:THR:HG21   | 1.55                     | 0.89              |
| 7:L:137:TYR:CE2   | 7:L:217:LYS:HA    | 2.07                     | 0.89              |
| 9:V:122:THR:HA    | 9:V:128:ARG:HD2   | 1.54                     | 0.89              |
| 9:V:358:MET:HE3   | 9:V:359:PRO:HD3   | 1.54                     | 0.89              |
| 14:a:25:LEU:HD13  | 14:a:37:LEU:HD13  | 1.52                     | 0.89              |
| 14:a:214:GLY:HA2  | 14:a:340:VAL:HG11 | 1.51                     | 0.89              |
| 23:B:66:GLU:HG2   | 27:U:834:SER:HB3  | 1.54                     | 0.89              |
| 7:L:125:ARG:HH22  | 26:K:125:GLU:HG3  | 1.36                     | 0.89              |
| 14:a:75:SER:O     | 14:a:79:ILE:N     | 2.06                     | 0.89              |
| 17:d:99:LYS:O     | 17:d:103:ASN:N    | 2.04                     | 0.89              |
| 18:f:845:ARG:HG3  | 18:f:865:PHE:HB2  | 1.55                     | 0.89              |
| 2:D:117:SER:HA    | 2:D:121:ARG:HH22  | 1.37                     | 0.89              |
| 9:V:192:MET:HA    | 9:V:195:ILE:HG13  | 1.52                     | 0.89              |
| 18:f:431:LYS:H    | 19:g:172:GLU:HB2  | 1.38                     | 0.89              |
| 19:g:161:SER:HB3  | 19:g:164:ASP:H    | 1.35                     | 0.89              |
| 25:F:251:LEU:O    | 25:F:285:ILE:HG23 | 1.73                     | 0.89              |
| 14:a:83:VAL:O     | 14:a:87:MET:N     | 2.03                     | 0.89              |
| 17:d:87:VAL:O     | 17:d:91:ALA:N     | 2.06                     | 0.89              |
| 19:g:128:LYS:HB2  | 19:g:162:GLU:HA   | 1.54                     | 0.89              |
| 24:E:122:MET:CE   | 25:F:344:ARG:CD   | 2.51                     | 0.89              |
| 7:L:80:ASP:OD2    | 7:L:126:ARG:NH1   | 2.06                     | 0.89              |
| 10:W:278:PRO:HG3  | 10:W:357:ARG:HH21 | 1.37                     | 0.89              |
| 14:a:335:TRP:HD1  | 14:a:337:GLN:H    | 1.18                     | 0.89              |
| 27:U:419:ALA:HA   | 27:U:422:LEU:HB3  | 1.55                     | 0.89              |
| 27:U:807:LYS:HB2  | 27:U:808:PRO:HD3  | 1.53                     | 0.89              |
| 1:C:94:LYS:HB2    | 23:B:109:VAL:HB   | 1.54                     | 0.89              |
| 2:D:388:ARG:NH2   | 24:E:147:GLU:HG2  | 1.86                     | 0.89              |
| 3:G:211:LYS:HG2   | 3:G:212:PRO:HD2   | 1.55                     | 0.89              |
| 17:d:92:THR:O     | 17:d:96:GLU:N     | 2.06                     | 0.89              |
| 9:V:64:GLN:HG3    | 9:V:109:ASN:HD21  | 1.38                     | 0.89              |
| 25:F:172:VAL:HG22 | 25:F:267:LEU:HD13 | 1.55                     | 0.89              |
| 13:Z:145:HIS:O    | 13:Z:147:ASP:N    | 2.06                     | 0.88              |
| 10:W:86:ASN:O     | 10:W:90:LEU:HG    | 1.73                     | 0.88              |
| 14:a:176:ALA:HB3  | 14:a:200:LEU:HD13 | 1.56                     | 0.88              |
| 18:f:807:ARG:HA   | 18:f:811:LEU:HB2  | 1.55                     | 0.88              |
| 2:D:239:TYR:OH    | 22:A:289:ALA:O    | 1.90                     | 0.88              |
| 11:X:74:ARG:NH2   | 11:X:113:CYS:SG   | 2.46                     | 0.88              |
| 2:D:238:LYS:HD2   | 2:D:239:TYR:CD1   | 2.09                     | 0.88              |
| 15:b:58:CYS:SG    | 15:b:88:THR:OG1   | 2.31                     | 0.88              |
| 24:E:171:LEU:HD11 | 24:E:279:THR:HG22 | 1.55                     | 0.88              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 26:K:71:ASP:OD2   | 26:K:96:THR:OG1   | 1.91                     | 0.88              |
| 9:V:201:ARG:HA    | 9:V:201:ARG:NH1   | 1.88                     | 0.88              |
| 11:X:114:ILE:HD12 | 11:X:130:GLU:HG3  | 1.53                     | 0.88              |
| 14:a:335:TRP:CD1  | 14:a:337:GLN:H    | 1.92                     | 0.88              |
| 18:f:542:ILE:HD12 | 18:f:580:LEU:HD21 | 1.55                     | 0.88              |
| 18:f:832:THR:OG1  | 18:f:870:THR:OG1  | 1.77                     | 0.88              |
| 2:D:296:MET:HE1   | 2:D:309:MET:HE2   | 1.53                     | 0.88              |
| 9:V:440:LYS:HE3   | 9:V:443:ARG:HH21  | 1.38                     | 0.88              |
| 14:a:115:LYS:O    | 14:a:119:GLY:N    | 2.07                     | 0.88              |
| 15:b:130:ARG:HE   | 15:b:131:LEU:HD22 | 1.39                     | 0.88              |
| 18:f:342:PRO:HD3  | 18:f:387:GLN:HE21 | 1.39                     | 0.88              |
| 9:V:294:ARG:NH2   | 9:V:390:GLY:O     | 2.07                     | 0.87              |
| 11:X:412:ASP:OD1  | 12:Y:379:ARG:NH2  | 2.07                     | 0.87              |
| 13:Z:188:SER:HA   | 14:a:374:ILE:HD11 | 1.55                     | 0.87              |
| 17:d:88:LEU:HD22  | 17:d:137:THR:HG21 | 1.56                     | 0.87              |
| 18:f:612:LEU:HA   | 18:f:615:ILE:HD12 | 1.56                     | 0.87              |
| 18:f:764:LEU:HD21 | 18:f:818:LEU:HD21 | 1.56                     | 0.87              |
| 7:L:47:VAL:HG12   | 7:L:195:LEU:HD12  | 1.55                     | 0.87              |
| 18:f:433:LEU:HB3  | 19:g:172:GLU:C    | 1.99                     | 0.87              |
| 24:E:149:ILE:CD1  | 24:E:276:ILE:HD11 | 2.04                     | 0.87              |
| 1:C:86:LEU:HD21   | 1:C:94:LYS:HD3    | 1.56                     | 0.87              |
| 9:V:281:ASN:OD1   | 9:V:283:ASN:N     | 2.07                     | 0.87              |
| 18:f:822:VAL:HA   | 18:f:825:MET:HG3  | 1.55                     | 0.87              |
| 23:B:250:VAL:HG22 | 23:B:284:ILE:HA   | 1.54                     | 0.87              |
| 4:H:10:LEU:HD11   | 4:H:22:ILE:HG13   | 1.55                     | 0.87              |
| 14:a:123:LEU:HD21 | 14:a:161:LYS:CB   | 2.04                     | 0.87              |
| 18:f:726:ILE:HG13 | 18:f:762:VAL:HG22 | 1.56                     | 0.87              |
| 3:G:141:ILE:HG22  | 3:G:151:VAL:HG22  | 1.56                     | 0.87              |
| 7:L:196:ARG:HB3   | 7:L:205:LEU:HD11  | 1.56                     | 0.87              |
| 12:Y:300:ARG:NH1  | 12:Y:333:GLU:OE2  | 2.07                     | 0.87              |
| 10:W:54:THR:CG2   | 10:W:59:ASP:HB3   | 2.04                     | 0.87              |
| 11:X:47:GLU:HA    | 11:X:76:PHE:HZ    | 1.39                     | 0.87              |
| 14:a:79:ILE:O     | 14:a:83:VAL:N     | 2.07                     | 0.87              |
| 17:d:145:ARG:O    | 17:d:149:GLU:N    | 2.08                     | 0.87              |
| 24:E:147:GLU:HA   | 24:E:151:LEU:HD13 | 1.54                     | 0.87              |
| 7:L:47:VAL:HG11   | 7:L:192:LEU:HD23  | 1.57                     | 0.87              |
| 26:K:201:ILE:O    | 26:K:205:VAL:HG12 | 1.74                     | 0.87              |
| 10:W:424:LEU:HD11 | 13:Z:244:GLU:OE2  | 1.75                     | 0.87              |
| 12:Y:387:ILE:HG12 | 13:Z:276:ILE:HG12 | 1.57                     | 0.87              |
| 19:g:89:LEU:CD1   | 19:g:99:ASN:HB2   | 2.04                     | 0.87              |
| 19:g:156:LEU:HB3  | 19:g:158:LEU:HD11 | 1.57                     | 0.87              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 26:K:181:LEU:HD13 | 26:K:201:ILE:HD12 | 1.57                     | 0.87              |
| 8:M:136:MET:HE1   | 8:M:163:CYS:HB3   | 1.57                     | 0.87              |
| 22:A:393:GLY:CA   | 23:B:216:ILE:HD11 | 2.05                     | 0.87              |
| 2:D:250:VAL:HG12  | 2:D:262:ILE:HD13  | 1.57                     | 0.86              |
| 9:V:439:ALA:O     | 9:V:443:ARG:N     | 2.08                     | 0.86              |
| 17:d:95:TYR:O     | 17:d:99:LYS:N     | 2.08                     | 0.86              |
| 27:U:209:GLU:HG2  | 27:U:210:LYS:HG2  | 1.56                     | 0.86              |
| 9:V:358:MET:HE1   | 9:V:382:PHE:HE2   | 1.38                     | 0.86              |
| 11:X:244:SER:OG   | 11:X:246:LYS:NZ   | 2.08                     | 0.86              |
| 14:a:43:ASP:O     | 14:a:47:ASP:N     | 2.08                     | 0.86              |
| 18:f:543:MET:HE1  | 18:f:583:VAL:HB   | 1.57                     | 0.86              |
| 27:U:680:VAL:HB   | 27:U:683:VAL:HG12 | 1.56                     | 0.86              |
| 25:F:125:LYS:HG3  | 25:F:131:THR:HG22 | 1.56                     | 0.86              |
| 27:U:748:LEU:HD23 | 27:U:760:VAL:HG22 | 1.56                     | 0.86              |
| 9:V:62:HIS:HA     | 9:V:65:ARG:HD3    | 1.57                     | 0.86              |
| 14:a:70:ARG:HH12  | 15:b:17:ARG:HD2   | 1.40                     | 0.86              |
| 27:U:804:SER:N    | 27:U:874:ASN:O    | 2.07                     | 0.86              |
| 10:W:194:LEU:HD21 | 10:W:202:THR:HG21 | 1.58                     | 0.86              |
| 19:g:131:ILE:HG13 | 19:g:151:VAL:HG12 | 1.58                     | 0.86              |
| 27:U:137:MET:HE1  | 27:U:140:ARG:HD3  | 1.57                     | 0.86              |
| 27:U:791:LEU:O    | 27:U:913:ILE:HA   | 1.75                     | 0.86              |
| 6:J:91:CYS:SG     | 6:J:92:GLN:NE2    | 2.49                     | 0.86              |
| 14:a:276:CYS:O    | 14:a:280:MET:HG2  | 1.75                     | 0.86              |
| 14:a:342:ASP:OD1  | 14:a:343:LEU:N    | 2.08                     | 0.86              |
| 15:b:25:ARG:CZ    | 15:b:144:GLY:HA3  | 2.06                     | 0.86              |
| 18:f:386:GLY:HA2  | 18:f:418:LEU:CD1  | 2.04                     | 0.86              |
| 27:U:792:ASN:HB3  | 27:U:914:LEU:HB3  | 1.57                     | 0.86              |
| 1:C:88:LYS:HE2    | 1:C:94:LYS:NZ     | 1.90                     | 0.86              |
| 1:C:367:GLY:HA3   | 2:D:196:ILE:HG21  | 1.58                     | 0.86              |
| 14:a:84:VAL:HG22  | 14:a:121:LEU:HD21 | 1.57                     | 0.86              |
| 15:b:12:ASN:OD1   | 15:b:55:ALA:HB3   | 1.75                     | 0.86              |
| 5:I:190:LEU:HD12  | 5:I:236:LEU:HD21  | 1.56                     | 0.86              |
| 12:Y:49:ASN:CA    | 12:Y:73:MET:HE2   | 2.05                     | 0.86              |
| 22:A:212:VAL:HG22 | 22:A:318:LEU:HD23 | 1.57                     | 0.86              |
| 27:U:163:PHE:HE2  | 27:U:197:VAL:HG13 | 1.39                     | 0.86              |
| 27:U:261:LEU:O    | 27:U:265:ILE:HG13 | 1.75                     | 0.86              |
| 27:U:870:GLU:CG   | 27:U:871:PRO:HD3  | 2.05                     | 0.86              |
| 18:f:45:LEU:HG    | 18:f:49:ASP:HB3   | 1.58                     | 0.86              |
| 11:X:414:LEU:HD11 | 13:Z:273:HIS:HB2  | 1.56                     | 0.85              |
| 12:Y:181:LYS:O    | 12:Y:200:LEU:HD12 | 1.75                     | 0.85              |
| 13:Z:227:ILE:HD11 | 14:a:346:ILE:HG13 | 1.58                     | 0.85              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 14:a:156:TYR:O    | 14:a:160:SER:N    | 2.09                     | 0.85              |
| 6:J:171:PHE:O     | 6:J:175:ASN:ND2   | 2.09                     | 0.85              |
| 7:L:184:LEU:HD11  | 7:L:214:ILE:HG21  | 1.56                     | 0.85              |
| 14:a:28:LEU:HD12  | 14:a:33:LEU:HD21  | 1.58                     | 0.85              |
| 14:a:274:LEU:HD21 | 14:a:319:LEU:CD2  | 2.06                     | 0.85              |
| 18:f:583:VAL:O    | 18:f:588:ARG:NE   | 2.08                     | 0.85              |
| 19:g:101:LEU:CD2  | 19:g:116:ILE:HG23 | 2.06                     | 0.85              |
| 23:B:234:LEU:HD22 | 29:B:501:ATP:H2'  | 1.57                     | 0.85              |
| 6:J:10:PHE:HE1    | 6:J:16:LEU:HG     | 1.41                     | 0.85              |
| 24:E:346:VAL:HA   | 24:E:374:VAL:HG21 | 1.58                     | 0.85              |
| 9:V:337:LEU:HD22  | 9:V:367:VAL:HG21  | 1.58                     | 0.85              |
| 13:Z:34:ARG:HD2   | 13:Z:102:HIS:CE1  | 2.10                     | 0.85              |
| 19:g:88:PHE:O     | 19:g:155:VAL:N    | 2.08                     | 0.85              |
| 27:U:206:MET:HE2  | 27:U:206:MET:HA   | 1.59                     | 0.85              |
| 4:H:133:SER:OG    | 4:H:163:MET:SD    | 2.34                     | 0.85              |
| 7:L:74:ILE:HG21   | 7:L:81:ALA:HB1    | 1.55                     | 0.85              |
| 10:W:63:THR:O     | 10:W:67:LEU:N     | 2.09                     | 0.85              |
| 19:g:129:ILE:CD1  | 19:g:155:VAL:HG22 | 2.04                     | 0.85              |
| 22:A:219:GLY:HA3  | 23:B:343:ARG:HD2  | 1.58                     | 0.85              |
| 27:U:660:CYS:O    | 27:U:694:ILE:HG22 | 1.75                     | 0.85              |
| 9:V:309:MET:HE2   | 9:V:328:VAL:HG13  | 1.59                     | 0.85              |
| 17:d:98:LEU:O     | 17:d:102:TRP:N    | 2.10                     | 0.85              |
| 17:d:149:GLU:HG3  | 17:d:191:LEU:CD1  | 2.07                     | 0.85              |
| 25:F:362:ARG:NH2  | 25:F:389:ASP:OD1  | 2.09                     | 0.85              |
| 26:K:88:LEU:HD22  | 26:K:116:VAL:HG13 | 1.55                     | 0.85              |
| 7:L:196:ARG:HB3   | 7:L:205:LEU:CD1   | 2.07                     | 0.85              |
| 14:a:205:LEU:HD21 | 14:a:237:LEU:HD13 | 1.58                     | 0.85              |
| 18:f:594:LEU:HD12 | 18:f:652:VAL:HG11 | 1.58                     | 0.85              |
| 18:f:702:PRO:HD3  | 18:f:736:THR:HG21 | 1.56                     | 0.85              |
| 18:f:213:GLN:NE2  | 18:f:216:MET:SD   | 2.50                     | 0.85              |
| 18:f:701:ASN:HD21 | 18:f:703:ARG:HH12 | 1.24                     | 0.85              |
| 14:a:157:ASP:O    | 14:a:161:LYS:N    | 2.08                     | 0.85              |
| 15:b:112:PHE:CE1  | 15:b:141:ILE:HD11 | 2.11                     | 0.85              |
| 18:f:83:ARG:O     | 18:f:87:THR:OG1   | 1.93                     | 0.85              |
| 18:f:325:GLN:NE2  | 18:f:328:SER:OG   | 2.10                     | 0.85              |
| 26:K:151:PRO:O    | 26:K:152:GLN:HG2  | 1.77                     | 0.85              |
| 27:U:443:LEU:HD23 | 27:U:477:GLY:HA2  | 1.56                     | 0.85              |
| 27:U:641:SER:HB2  | 27:U:675:MET:HE1  | 1.59                     | 0.85              |
| 6:J:116:GLN:NE2   | 26:K:87:THR:OG1   | 2.08                     | 0.85              |
| 22:A:153:LEU:HD23 | 23:B:122:ILE:HD11 | 1.59                     | 0.85              |
| 3:G:126:THR:HG22  | 4:H:128:ARG:HH12  | 1.40                     | 0.84              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 10:W:270:VAL:HG13 | 10:W:290:ILE:HD11 | 1.59                     | 0.84              |
| 10:W:309:PHE:CE1  | 10:W:315:MET:HE1  | 2.12                     | 0.84              |
| 15:b:100:ARG:NH2  | 20:u:136:GLU:OE1  | 2.10                     | 0.84              |
| 8:M:167:LYS:NZ    | 8:M:206:ASP:OD2   | 2.10                     | 0.84              |
| 9:V:345:ARG:O     | 9:V:345:ARG:HD3   | 1.76                     | 0.84              |
| 10:W:183:VAL:HG12 | 10:W:222:LEU:HD13 | 1.58                     | 0.84              |
| 18:f:543:MET:HE2  | 18:f:543:MET:HA   | 1.59                     | 0.84              |
| 27:U:389:ASN:OD1  | 27:U:392:TRP:HB3  | 1.78                     | 0.84              |
| 4:H:111:VAL:HG22  | 4:H:136:ILE:CD1   | 2.07                     | 0.84              |
| 9:V:192:MET:O     | 9:V:196:SER:N     | 2.10                     | 0.84              |
| 14:a:42:LEU:O     | 14:a:46:GLN:N     | 2.09                     | 0.84              |
| 18:f:62:ARG:HB3   | 18:f:70:LEU:HD22  | 1.57                     | 0.84              |
| 23:B:365:PHE:O    | 23:B:369:THR:HG22 | 1.77                     | 0.84              |
| 9:V:438:VAL:HG12  | 9:V:451:ILE:HD11  | 1.58                     | 0.84              |
| 11:X:190:LEU:HD21 | 11:X:214:SER:HB2  | 1.59                     | 0.84              |
| 13:Z:149:THR:HG23 | 13:Z:150:PRO:HD2  | 1.58                     | 0.84              |
| 17:d:127:ASN:HD22 | 17:d:136:LEU:HD11 | 1.40                     | 0.84              |
| 1:C:214:VAL:HG11  | 1:C:219:LEU:HD21  | 1.60                     | 0.84              |
| 2:D:309:MET:HE3   | 2:D:327:LEU:HD11  | 1.60                     | 0.84              |
| 5:I:47:ALA:HB1    | 5:I:64:LYS:HD3    | 1.59                     | 0.84              |
| 9:V:190:ASP:O     | 9:V:194:LYS:N     | 2.09                     | 0.84              |
| 18:f:478:ARG:NH1  | 18:f:510:SER:OG   | 2.08                     | 0.84              |
| 5:I:138:GLY:HA2   | 5:I:216:LEU:HD13  | 1.60                     | 0.84              |
| 10:W:108:CYS:HB3  | 10:W:128:LEU:HD11 | 1.58                     | 0.84              |
| 10:W:268:LYS:HE3  | 10:W:299:ILE:HG22 | 1.58                     | 0.84              |
| 11:X:140:THR:HG22 | 11:X:142:ARG:HG3  | 1.59                     | 0.84              |
| 18:f:367:SER:O    | 18:f:371:ASN:ND2  | 2.11                     | 0.84              |
| 18:f:680:ARG:NH1  | 22:A:66:LYS:HG3   | 1.92                     | 0.84              |
| 23:B:436:GLU:OE1  | 23:B:436:GLU:N    | 2.11                     | 0.84              |
| 5:I:218:ARG:NH1   | 5:I:223:THR:OG1   | 2.10                     | 0.84              |
| 10:W:62:SER:O     | 10:W:66:ILE:N     | 2.11                     | 0.84              |
| 10:W:186:ILE:HG21 | 10:W:209:ILE:HB   | 1.59                     | 0.84              |
| 15:b:35:ILE:HG13  | 15:b:188:ILE:HD13 | 1.59                     | 0.84              |
| 26:K:157:ASP:HB2  | 26:K:158:PRO:HD2  | 1.57                     | 0.84              |
| 2:D:384:MET:HE1   | 24:E:159:PHE:HE1  | 1.42                     | 0.84              |
| 9:V:184:ALA:HA    | 9:V:187:ILE:HB    | 1.60                     | 0.84              |
| 11:X:407:MET:HE2  | 11:X:407:MET:HA   | 1.59                     | 0.84              |
| 14:a:293:PHE:CB   | 14:a:329:LYS:HG3  | 2.07                     | 0.84              |
| 25:F:254:PRO:HD3  | 25:F:287:GLU:HB2  | 1.59                     | 0.84              |
| 1:C:399:MET:HG3   | 4:H:158:TRP:CZ2   | 2.13                     | 0.83              |
| 11:X:299:LEU:HD12 | 11:X:299:LEU:H    | 1.42                     | 0.83              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 14:a:28:LEU:HB3   | 14:a:33:LEU:HD11  | 1.58                     | 0.83              |
| 25:F:188:ILE:HD12 | 25:F:239:ALA:HB2  | 1.60                     | 0.83              |
| 6:J:79:ASP:OD2    | 6:J:125:ARG:NH1   | 2.10                     | 0.83              |
| 18:f:466:LEU:HD12 | 18:f:481:SER:HA   | 1.59                     | 0.83              |
| 22:A:195:LEU:HD21 | 22:A:316:LYS:HD3  | 1.59                     | 0.83              |
| 27:U:465:LEU:HD22 | 27:U:496:LEU:HD21 | 1.59                     | 0.83              |
| 27:U:469:SER:OG   | 27:U:471:ASP:OD2  | 1.95                     | 0.83              |
| 1:C:88:LYS:HE2    | 1:C:94:LYS:HZ3    | 1.41                     | 0.83              |
| 3:G:118:ILE:HG21  | 3:G:138:MET:CE    | 2.07                     | 0.83              |
| 5:I:82:ASP:OD2    | 5:I:128:ARG:NH1   | 2.10                     | 0.83              |
| 14:a:149:THR:HB   | 14:a:182:CYS:HB3  | 1.59                     | 0.83              |
| 25:F:130:GLN:OE1  | 25:F:132:TYR:OH   | 1.96                     | 0.83              |
| 15:b:18:ASN:OD1   | 15:b:25:ARG:NH1   | 2.11                     | 0.83              |
| 18:f:109:ILE:O    | 18:f:113:MET:N    | 2.11                     | 0.83              |
| 18:f:830:LEU:N    | 18:f:872:VAL:O    | 2.11                     | 0.83              |
| 27:U:324:LYS:O    | 27:U:328:ILE:HG12 | 1.78                     | 0.83              |
| 27:U:900:TYR:HB3  | 27:U:914:LEU:HD21 | 1.59                     | 0.83              |
| 7:L:137:TYR:HE2   | 7:L:217:LYS:HA    | 1.43                     | 0.83              |
| 8:M:27:MET:HG2    | 8:M:153:PRO:HD2   | 1.60                     | 0.83              |
| 10:W:144:ARG:NH2  | 10:W:181:GLU:OE2  | 2.11                     | 0.83              |
| 11:X:365:LEU:O    | 11:X:369:ILE:HG13 | 1.77                     | 0.83              |
| 17:d:102:TRP:CE3  | 17:d:150:ILE:HG12 | 2.13                     | 0.83              |
| 18:f:257:ARG:HA   | 18:f:257:ARG:CZ   | 2.08                     | 0.83              |
| 19:g:140:LYS:HB2  | 19:g:145:GLN:HB3  | 1.57                     | 0.83              |
| 24:E:50:LEU:HD21  | 25:F:139:LEU:HD11 | 1.60                     | 0.83              |
| 13:Z:45:LYS:H     | 13:Z:45:LYS:HD2   | 1.41                     | 0.83              |
| 1:C:132:ASP:HB2   | 1:C:135:VAL:HG12  | 1.60                     | 0.83              |
| 3:G:208:ILE:CD1   | 24:E:306:GLU:CD   | 2.50                     | 0.83              |
| 4:H:130:PHE:O     | 4:H:151:PRO:HB3   | 1.79                     | 0.83              |
| 18:f:425:GLY:O    | 18:f:429:ILE:HG12 | 1.77                     | 0.83              |
| 22:A:113:ILE:HD12 | 22:A:142:VAL:HG11 | 1.59                     | 0.83              |
| 22:A:120:LYS:HB2  | 25:F:90:VAL:CG1   | 2.08                     | 0.83              |
| 2:D:153:MET:SD    | 2:D:257:ASN:ND2   | 2.51                     | 0.83              |
| 2:D:388:ARG:HH21  | 24:E:297:ARG:NH1  | 1.76                     | 0.83              |
| 5:I:174:MET:SD    | 5:I:196:VAL:HA    | 2.19                     | 0.83              |
| 9:V:174:PHE:O     | 9:V:178:SER:N     | 2.11                     | 0.83              |
| 13:Z:243:GLN:HE21 | 13:Z:247:LYS:HE3  | 1.44                     | 0.83              |
| 14:a:115:LYS:HA   | 14:a:118:ILE:CG2  | 2.09                     | 0.83              |
| 14:a:231:GLN:O    | 14:a:234:ILE:HG22 | 1.78                     | 0.83              |
| 17:d:119:LEU:HD13 | 17:d:147:ILE:HG12 | 1.59                     | 0.83              |
| 23:B:322:ARG:HD2  | 23:B:325:VAL:HG13 | 1.60                     | 0.83              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:I:108:GLU:OE1   | 6:J:57:ARG:NH1    | 2.12                     | 0.83              |
| 2:D:167:ILE:HG22  | 2:D:214:MET:HG2   | 1.61                     | 0.82              |
| 4:H:65:VAL:HG22   | 4:H:75:VAL:CG1    | 2.08                     | 0.82              |
| 7:L:133:LEU:HD21  | 7:L:161:ILE:HG12  | 1.60                     | 0.82              |
| 9:V:482:PHE:HZ    | 12:Y:381:GLN:HB2  | 1.44                     | 0.82              |
| 13:Z:125:ASP:HB2  | 13:Z:128:PRO:HG2  | 1.60                     | 0.82              |
| 14:a:61:GLU:O     | 14:a:65:SER:N     | 2.12                     | 0.82              |
| 19:g:128:LYS:HA   | 19:g:162:GLU:HB3  | 1.59                     | 0.82              |
| 19:g:140:LYS:O    | 19:g:145:GLN:NE2  | 2.12                     | 0.82              |
| 10:W:113:GLU:OE2  | 10:W:113:GLU:N    | 2.12                     | 0.82              |
| 15:b:35:ILE:HG21  | 15:b:184:ILE:HG22 | 1.59                     | 0.82              |
| 22:A:187:LEU:HD21 | 22:A:229:VAL:HG21 | 1.61                     | 0.82              |
| 6:J:148:ASP:OD1   | 6:J:149:PRO:HD2   | 1.80                     | 0.82              |
| 10:W:316:ARG:NH2  | 10:W:383:ASP:OD1  | 2.09                     | 0.82              |
| 17:d:190:GLN:O    | 17:d:194:LEU:HD12 | 1.79                     | 0.82              |
| 18:f:703:ARG:HB3  | 18:f:706:ILE:HG22 | 1.60                     | 0.82              |
| 9:V:463:MET:SD    | 9:V:464:ILE:N     | 2.51                     | 0.82              |
| 14:a:114:CYS:O    | 14:a:118:ILE:N    | 2.11                     | 0.82              |
| 15:b:97:LEU:HD21  | 15:b:109:ILE:HD11 | 1.58                     | 0.82              |
| 1:C:184:LYS:N     | 1:C:312:ASP:OD2   | 2.13                     | 0.82              |
| 2:D:80:LYS:HA     | 2:D:80:LYS:HE2    | 1.59                     | 0.82              |
| 3:G:80:MET:SD     | 3:G:138:MET:HG3   | 2.19                     | 0.82              |
| 5:I:86:LEU:HD21   | 5:I:118:LYS:NZ    | 1.94                     | 0.82              |
| 9:V:457:TYR:HE1   | 9:V:459:GLN:HB2   | 1.43                     | 0.82              |
| 10:W:267:LEU:HA   | 10:W:270:VAL:HG12 | 1.60                     | 0.82              |
| 17:d:85:GLY:HA2   | 17:d:88:LEU:HB3   | 1.59                     | 0.82              |
| 24:E:122:MET:CE   | 25:F:344:ARG:HD3  | 2.10                     | 0.82              |
| 25:F:124:ILE:HG13 | 25:F:160:ILE:HD11 | 1.61                     | 0.82              |
| 26:K:107:MET:HG2  | 26:K:111:SER:OG   | 1.80                     | 0.82              |
| 27:U:483:LEU:HD13 | 27:U:778:PHE:HE1  | 1.45                     | 0.82              |
| 18:f:784:ASP:N    | 18:f:895:GLU:OE2  | 2.10                     | 0.82              |
| 19:g:128:LYS:HD3  | 19:g:162:GLU:HB2  | 1.62                     | 0.82              |
| 24:E:47:LEU:HD22  | 25:F:76:ASN:HD22  | 1.44                     | 0.82              |
| 2:D:349:THR:HG21  | 2:D:360:LEU:HD11  | 1.61                     | 0.82              |
| 3:G:202:LEU:HG    | 3:G:210:PHE:HZ    | 1.45                     | 0.82              |
| 6:J:68:ASN:HA     | 6:J:211:MET:HE1   | 1.62                     | 0.82              |
| 9:V:169:LEU:O     | 9:V:173:ILE:N     | 2.10                     | 0.82              |
| 12:Y:114:ILE:HD11 | 12:Y:116:ASP:HB2  | 1.62                     | 0.82              |
| 18:f:226:TYR:CE2  | 18:f:261:ARG:HG3  | 2.15                     | 0.82              |
| 18:f:772:GLY:O    | 18:f:775:THR:OG1  | 1.96                     | 0.82              |
| 19:g:113:ARG:HG2  | 19:g:124:GLU:HG2  | 1.61                     | 0.82              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 23:B:295:TYR:HE1  | 23:B:297:SER:HB2  | 1.42                     | 0.82              |
| 27:U:810:THR:CG2  | 27:U:873:PRO:HG2  | 2.08                     | 0.82              |
| 11:X:363:ARG:NH2  | 12:Y:266:CYS:O    | 2.13                     | 0.82              |
| 11:X:407:MET:HA   | 11:X:410:VAL:HG12 | 1.61                     | 0.82              |
| 14:a:162:TYR:O    | 14:a:165:THR:OG1  | 1.98                     | 0.82              |
| 9:V:313:LEU:HD21  | 9:V:329:HIS:NE2   | 1.95                     | 0.82              |
| 14:a:97:LEU:HD22  | 14:a:117:ALA:CB   | 2.10                     | 0.82              |
| 15:b:97:LEU:CD2   | 15:b:109:ILE:HD11 | 2.08                     | 0.82              |
| 1:C:212:ILE:HD13  | 1:C:237:MET:CE    | 2.09                     | 0.82              |
| 7:L:202:GLU:OE1   | 7:L:202:GLU:N     | 2.12                     | 0.82              |
| 9:V:358:MET:HE1   | 9:V:382:PHE:CE2   | 2.14                     | 0.82              |
| 10:W:51:GLU:OE1   | 10:W:93:ARG:NH1   | 2.13                     | 0.82              |
| 14:a:313:LYS:O    | 14:a:316:SER:N    | 2.11                     | 0.82              |
| 23:B:82:GLN:O     | 23:B:86:LYS:HB2   | 1.80                     | 0.82              |
| 9:V:282:ASN:HD21  | 12:Y:385:ARG:HB2  | 1.44                     | 0.81              |
| 12:Y:218:THR:O    | 12:Y:221:THR:HG22 | 1.80                     | 0.81              |
| 14:a:112:ILE:CG2  | 14:a:151:VAL:HG12 | 2.07                     | 0.81              |
| 14:a:211:PHE:HB2  | 14:a:275:LEU:HD21 | 1.61                     | 0.81              |
| 17:d:129:LEU:HB3  | 17:d:130:PRO:HD2  | 1.60                     | 0.81              |
| 18:f:267:ARG:CZ   | 18:f:297:MET:HE3  | 2.09                     | 0.81              |
| 27:U:244:MET:HG2  | 27:U:903:PHE:HE2  | 1.43                     | 0.81              |
| 14:a:216:LEU:HD21 | 14:a:238:TYR:HA   | 1.62                     | 0.81              |
| 2:D:89:ILE:O      | 2:D:106:THR:OG1   | 1.98                     | 0.81              |
| 4:H:35:SER:HB2    | 4:H:163:MET:HE3   | 1.61                     | 0.81              |
| 7:L:166:GLN:OE1   | 7:L:169:ARG:NH1   | 2.12                     | 0.81              |
| 12:Y:279:GLU:HG3  | 12:Y:296:VAL:HG21 | 1.63                     | 0.81              |
| 15:b:33:VAL:HA    | 15:b:36:VAL:HG22  | 1.62                     | 0.81              |
| 17:d:223:ASN:HB3  | 17:d:226:ILE:HD12 | 1.61                     | 0.81              |
| 18:f:332:ALA:HA   | 18:f:335:ARG:HE   | 1.45                     | 0.81              |
| 19:g:130:VAL:HG22 | 19:g:154:MET:O    | 1.79                     | 0.81              |
| 19:g:132:ASN:O    | 19:g:134:LYS:NZ   | 2.12                     | 0.81              |
| 27:U:259:GLN:NE2  | 27:U:487:GLY:O    | 2.10                     | 0.81              |
| 9:V:358:MET:HE3   | 9:V:359:PRO:CD    | 2.09                     | 0.81              |
| 14:a:118:ILE:O    | 14:a:122:LYS:HB3  | 1.80                     | 0.81              |
| 14:a:280:MET:SD   | 14:a:296:ILE:HG12 | 2.20                     | 0.81              |
| 9:V:167:LEU:O     | 9:V:171:VAL:HG23  | 1.80                     | 0.81              |
| 10:W:106:GLN:HA   | 10:W:109:CYS:SG   | 2.20                     | 0.81              |
| 18:f:683:GLU:HB2  | 18:f:684:PRO:HD2  | 1.62                     | 0.81              |
| 22:A:426:THR:HG22 | 22:A:430:MET:HE3  | 1.63                     | 0.81              |
| 23:B:259:TYR:HB2  | 23:B:262:ASP:HB2  | 1.63                     | 0.81              |
| 27:U:103:LYS:O    | 27:U:107:HIS:N    | 2.11                     | 0.81              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:I:90:LEU:HD11   | 5:I:136:TYR:HE2   | 1.42                     | 0.81              |
| 7:L:125:ARG:NH1   | 26:K:125:GLU:HA   | 1.96                     | 0.81              |
| 9:V:196:SER:HA    | 9:V:234:ARG:HH12  | 1.44                     | 0.81              |
| 14:a:34:TRP:CE3   | 14:a:70:ARG:HG3   | 2.16                     | 0.81              |
| 14:a:177:LEU:HD23 | 14:a:200:LEU:HD21 | 1.62                     | 0.81              |
| 23:B:257:GLN:HB2  | 23:B:262:ASP:HB3  | 1.63                     | 0.81              |
| 2:D:275:PHE:HZ    | 24:E:251:ARG:HH12 | 1.29                     | 0.81              |
| 9:V:67:LEU:HA     | 9:V:70:VAL:HG12   | 1.63                     | 0.81              |
| 9:V:330:LYS:NZ    | 9:V:389:ASP:OD2   | 2.13                     | 0.81              |
| 11:X:54:GLY:HA2   | 11:X:66:LEU:HD11  | 1.62                     | 0.81              |
| 25:F:225:MET:HA   | 25:F:352:ILE:HG22 | 1.61                     | 0.81              |
| 27:U:567:ILE:HD13 | 27:U:586:VAL:HG22 | 1.63                     | 0.81              |
| 1:C:35:VAL:HG12   | 2:D:51:LEU:HB2    | 1.62                     | 0.81              |
| 1:C:161:ILE:HD11  | 1:C:292:ILE:HD12  | 1.63                     | 0.81              |
| 3:G:118:ILE:CD1   | 3:G:138:MET:HE1   | 2.08                     | 0.81              |
| 4:H:135:LEU:CD1   | 4:H:163:MET:HE2   | 2.03                     | 0.81              |
| 9:V:175:MET:CB    | 9:V:184:ALA:HB2   | 2.11                     | 0.81              |
| 9:V:212:TYR:O     | 9:V:216:ARG:N     | 2.12                     | 0.81              |
| 14:a:18:GLN:HB2   | 14:a:19:PRO:HD3   | 1.60                     | 0.81              |
| 18:f:788:MET:CE   | 18:f:793:VAL:HG21 | 2.11                     | 0.81              |
| 2:D:309:MET:HE3   | 2:D:327:LEU:HD21  | 1.63                     | 0.81              |
| 5:I:40:ASN:ND2    | 5:I:182:GLY:O     | 2.14                     | 0.81              |
| 6:J:64:ALA:HB2    | 6:J:217:LEU:HD22  | 1.62                     | 0.81              |
| 17:d:172:LYS:NZ   | 17:d:211:GLU:OE2  | 2.13                     | 0.81              |
| 19:g:112:LEU:CB   | 19:g:142:LEU:HD11 | 2.11                     | 0.81              |
| 24:E:33:LEU:HD11  | 25:F:65:GLU:HB2   | 1.63                     | 0.81              |
| 9:V:463:MET:HA    | 9:V:463:MET:HE2   | 1.63                     | 0.81              |
| 10:W:105:VAL:HG21 | 10:W:138:VAL:HG21 | 1.59                     | 0.81              |
| 17:d:94:MET:HB2   | 17:d:119:LEU:HD21 | 1.63                     | 0.81              |
| 17:d:276:GLU:OE2  | 17:d:308:TRP:NE1  | 2.14                     | 0.81              |
| 25:F:424:ILE:O    | 25:F:428:GLN:NE2  | 2.13                     | 0.81              |
| 3:G:80:MET:HE2    | 3:G:91:VAL:HG23   | 1.62                     | 0.80              |
| 10:W:346:GLU:HB2  | 10:W:350:ARG:NH2  | 1.96                     | 0.80              |
| 18:f:670:MET:CE   | 23:B:68:ILE:HG23  | 2.10                     | 0.80              |
| 23:B:278:ALA:HB1  | 23:B:279:PRO:CD   | 2.11                     | 0.80              |
| 24:E:142:ILE:O    | 24:E:146:ARG:HG2  | 1.82                     | 0.80              |
| 25:F:226:TYR:HB3  | 25:F:335:VAL:CG1  | 2.10                     | 0.80              |
| 1:C:93:GLY:HA3    | 23:B:126:SER:HB3  | 1.63                     | 0.80              |
| 10:W:55:ARG:NH1   | 10:W:93:ARG:HB3   | 1.96                     | 0.80              |
| 18:f:564:LEU:HA   | 18:f:567:LEU:HD21 | 1.63                     | 0.80              |
| 18:f:679:LEU:HG   | 18:f:690:VAL:HG11 | 1.61                     | 0.80              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:A:88:GLN:NE2   | 22:A:88:GLN:O     | 2.15                     | 0.80              |
| 2:D:361:GLU:HA    | 2:D:364:VAL:HG22  | 1.63                     | 0.80              |
| 6:J:171:PHE:HE2   | 6:J:194:ALA:HA    | 1.45                     | 0.80              |
| 9:V:182:LYS:HA    | 9:V:185:GLN:HB2   | 1.64                     | 0.80              |
| 10:W:34:LEU:HB3   | 10:W:39:ARG:HD3   | 1.62                     | 0.80              |
| 14:a:123:LEU:HD22 | 14:a:158:LEU:HD13 | 1.61                     | 0.80              |
| 18:f:433:LEU:HB2  | 18:f:444:ALA:CB   | 2.11                     | 0.80              |
| 5:I:72:MET:SD     | 5:I:138:GLY:HA3   | 2.21                     | 0.80              |
| 6:J:61:LYS:HE2    | 6:J:73:PHE:O      | 1.80                     | 0.80              |
| 10:W:211:THR:HA   | 10:W:214:PHE:HE2  | 1.44                     | 0.80              |
| 13:Z:67:VAL:CG2   | 15:b:91:ARG:HD3   | 2.12                     | 0.80              |
| 14:a:58:LYS:NZ    | 14:a:83:VAL:HG13  | 1.97                     | 0.80              |
| 18:f:433:LEU:HD13 | 18:f:441:LYS:HA   | 1.64                     | 0.80              |
| 25:F:172:VAL:HG12 | 25:F:274:LEU:CD2  | 2.12                     | 0.80              |
| 26:K:91:LYS:O     | 26:K:91:LYS:NZ    | 2.15                     | 0.80              |
| 8:M:77:VAL:HG11   | 8:M:84:ALA:HB1    | 1.62                     | 0.80              |
| 9:V:212:TYR:HD1   | 9:V:253:LEU:HD11  | 1.44                     | 0.80              |
| 19:g:87:VAL:HG23  | 19:g:153:ALA:HB3  | 1.62                     | 0.80              |
| 25:F:188:ILE:HD13 | 25:F:236:LEU:HA   | 1.61                     | 0.80              |
| 27:U:137:MET:SD   | 27:U:140:ARG:NH1  | 2.54                     | 0.80              |
| 27:U:810:THR:HG21 | 27:U:873:PRO:CG   | 2.10                     | 0.80              |
| 1:C:33:LEU:HD12   | 9:V:201:ARG:HG2   | 1.62                     | 0.80              |
| 4:H:49:GLU:HA     | 4:H:208:ILE:HD13  | 1.63                     | 0.80              |
| 9:V:469:THR:HG22  | 9:V:470:ARG:H     | 1.47                     | 0.80              |
| 10:W:102:ALA:O    | 10:W:105:VAL:HG12 | 1.82                     | 0.80              |
| 10:W:109:CYS:HA   | 10:W:112:VAL:CG2  | 2.11                     | 0.80              |
| 12:Y:268:TYR:OH   | 12:Y:306:GLN:HG2  | 1.80                     | 0.80              |
| 14:a:61:GLU:HA    | 14:a:64:ILE:HG22  | 1.64                     | 0.80              |
| 18:f:208:LEU:CD1  | 18:f:217:LEU:HD13 | 2.11                     | 0.80              |
| 26:K:74:ILE:HD11  | 26:K:109:VAL:HG23 | 1.63                     | 0.80              |
| 26:K:84:ASP:OD2   | 26:K:135:ARG:NH1  | 2.12                     | 0.80              |
| 9:V:411:SER:OG    | 9:V:447:ILE:HD12  | 1.82                     | 0.80              |
| 11:X:89:VAL:O     | 11:X:93:LEU:N     | 2.12                     | 0.80              |
| 14:a:342:ASP:HB3  | 14:a:345:GLN:HG3  | 1.64                     | 0.80              |
| 15:b:106:LYS:HE3  | 15:b:107:MET:N    | 1.96                     | 0.80              |
| 24:E:277:MET:HE1  | 24:E:295:LEU:CD1  | 2.11                     | 0.80              |
| 27:U:243:LEU:CD2  | 27:U:913:ILE:HD12 | 2.10                     | 0.80              |
| 7:L:45:VAL:HG21   | 7:L:188:VAL:HG23  | 1.62                     | 0.80              |
| 9:V:72:LEU:HD12   | 9:V:120:PHE:HE1   | 1.46                     | 0.80              |
| 13:Z:227:ILE:HD11 | 14:a:346:ILE:CG1  | 2.12                     | 0.80              |
| 14:a:160:SER:HA   | 14:a:163:TYR:HB3  | 1.61                     | 0.80              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 17:d:123:LEU:HD22 | 17:d:144:ALA:HB2  | 1.62                     | 0.80              |
| 18:f:726:ILE:HD11 | 18:f:748:LEU:HD13 | 1.61                     | 0.80              |
| 23:B:295:TYR:CE1  | 23:B:297:SER:HB2  | 2.17                     | 0.80              |
| 23:B:434:THR:HB   | 23:B:435:PRO:HD2  | 1.64                     | 0.80              |
| 24:E:165:ILE:HG23 | 24:E:166:PRO:HD2  | 1.63                     | 0.80              |
| 27:U:69:TYR:CE1   | 27:U:99:THR:HG21  | 2.17                     | 0.80              |
| 27:U:347:ASN:HB3  | 27:U:813:TYR:CE2  | 2.15                     | 0.80              |
| 3:G:118:ILE:HD13  | 3:G:138:MET:CE    | 2.11                     | 0.80              |
| 9:V:75:ILE:O      | 9:V:79:VAL:HG23   | 1.80                     | 0.80              |
| 9:V:108:LEU:HD11  | 9:V:177:ASN:HD22  | 1.46                     | 0.80              |
| 9:V:446:VAL:O     | 9:V:447:ILE:HD13  | 1.82                     | 0.80              |
| 19:g:167:LYS:O    | 19:g:171:LEU:HG   | 1.82                     | 0.80              |
| 27:U:649:ARG:HD2  | 27:U:678:ASP:OD2  | 1.81                     | 0.80              |
| 10:W:409:LEU:CD2  | 11:X:384:VAL:HG11 | 2.09                     | 0.80              |
| 12:Y:146:ARG:NH1  | 12:Y:183:TYR:OH   | 2.15                     | 0.80              |
| 14:a:156:TYR:HD2  | 14:a:179:PHE:HB2  | 1.47                     | 0.80              |
| 19:g:165:ALA:HA   | 19:g:168:ASN:H    | 1.45                     | 0.80              |
| 22:A:114:ASN:OD1  | 22:A:120:LYS:HG2  | 1.82                     | 0.80              |
| 27:U:658:ILE:HD11 | 27:U:767:THR:HG21 | 1.64                     | 0.80              |
| 11:X:344:ARG:HG2  | 11:X:386:ILE:CD1  | 2.11                     | 0.79              |
| 18:f:562:LEU:HD21 | 18:f:576:ILE:HG21 | 1.64                     | 0.79              |
| 22:A:153:LEU:CD2  | 23:B:122:ILE:HD11 | 2.12                     | 0.79              |
| 25:F:94:ILE:HG13  | 25:F:125:LYS:HB2  | 1.64                     | 0.79              |
| 1:C:45:LEU:HB3    | 2:D:61:ILE:HG12   | 1.64                     | 0.79              |
| 4:H:39:LYS:HZ3    | 4:H:144:PRO:HG2   | 1.48                     | 0.79              |
| 6:J:83:VAL:HG11   | 6:J:129:ILE:CD1   | 2.13                     | 0.79              |
| 19:g:158:LEU:HD23 | 19:g:165:ALA:CB   | 2.12                     | 0.79              |
| 27:U:532:MET:HB3  | 27:U:552:ILE:HG22 | 1.64                     | 0.79              |
| 5:I:138:GLY:HA2   | 5:I:216:LEU:CD1   | 2.12                     | 0.79              |
| 14:a:192:GLU:OE2  | 14:a:196:ARG:NH1  | 2.15                     | 0.79              |
| 23:B:414:VAL:HG23 | 23:B:418:ASP:HB2  | 1.64                     | 0.79              |
| 25:F:224:LEU:HD23 | 25:F:343:LEU:HD21 | 1.63                     | 0.79              |
| 27:U:241:ASN:HD21 | 27:U:244:MET:HB2  | 1.47                     | 0.79              |
| 2:D:85:ILE:HD11   | 24:E:68:LYS:HE2   | 1.62                     | 0.79              |
| 3:G:162:GLY:O     | 4:H:58:ASP:N      | 2.14                     | 0.79              |
| 4:H:139:TRP:HZ3   | 4:H:144:PRO:HD3   | 1.46                     | 0.79              |
| 16:c:284:LEU:O    | 16:c:286:GLU:N    | 2.15                     | 0.79              |
| 18:f:458:GLU:O    | 19:g:133:LYS:NZ   | 2.14                     | 0.79              |
| 24:E:235:ILE:HD11 | 24:E:277:MET:HB3  | 0.80                     | 0.79              |
| 27:U:537:GLN:OE1  | 27:U:537:GLN:N    | 2.13                     | 0.79              |
| 9:V:288:TYR:O     | 9:V:292:THR:HG22  | 1.82                     | 0.79              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 13:Z:145:HIS:CE1  | 13:Z:151:THR:HA   | 2.18                     | 0.79              |
| 27:U:872:GLU:HG3  | 27:U:873:PRO:O    | 1.81                     | 0.79              |
| 9:V:224:LEU:HD21  | 9:V:257:ASN:HA    | 1.64                     | 0.79              |
| 9:V:472:PRO:HB2   | 13:Z:254:ASN:OD1  | 1.82                     | 0.79              |
| 14:a:155:PHE:O    | 14:a:159:SER:N    | 2.12                     | 0.79              |
| 18:f:91:SER:HA    | 23:B:410:ARG:O    | 1.81                     | 0.79              |
| 18:f:114:ALA:HB3  | 18:f:118:ASN:HB2  | 1.65                     | 0.79              |
| 18:f:831:VAL:HG13 | 18:f:871:PRO:CG   | 2.10                     | 0.79              |
| 25:F:85:THR:HG22  | 25:F:86:LEU:H     | 1.48                     | 0.79              |
| 27:U:97:VAL:O     | 27:U:101:ILE:HG23 | 1.83                     | 0.79              |
| 2:D:179:GLU:O     | 2:D:191:TYR:OH    | 2.00                     | 0.79              |
| 14:a:100:THR:O    | 14:a:103:LYS:HG2  | 1.83                     | 0.79              |
| 17:d:128:PHE:O    | 17:d:129:LEU:HD23 | 1.81                     | 0.79              |
| 18:f:271:MET:HE2  | 18:f:786:GLN:HB3  | 1.65                     | 0.79              |
| 4:H:204:THR:HG22  | 4:H:205:GLU:OE2   | 1.83                     | 0.79              |
| 5:I:100:GLN:HG2   | 5:I:101:TYR:CE1   | 2.17                     | 0.79              |
| 10:W:373:ILE:HA   | 14:a:326:GLU:HB2  | 1.64                     | 0.79              |
| 24:E:252:GLU:OE1  | 24:E:255:ARG:NH1  | 2.16                     | 0.79              |
| 1:C:403:LYS:HD2   | 4:H:156:PHE:HD1   | 1.48                     | 0.79              |
| 2:D:45:LYS:HB3    | 27:U:187:LEU:HD13 | 1.65                     | 0.79              |
| 8:M:98:PHE:CG     | 8:M:106:ILE:HB    | 2.17                     | 0.79              |
| 18:f:56:LEU:HD12  | 18:f:99:LEU:HD21  | 1.63                     | 0.79              |
| 19:g:138:LEU:HD12 | 19:g:162:GLU:HG3  | 1.63                     | 0.79              |
| 7:L:117:GLN:O     | 7:L:120:THR:HG22  | 1.82                     | 0.79              |
| 15:b:79:GLN:OE1   | 15:b:81:LYS:HE3   | 1.83                     | 0.79              |
| 15:b:141:ILE:HD12 | 15:b:183:LEU:HD23 | 1.64                     | 0.79              |
| 9:V:259:LEU:HG    | 9:V:264:TYR:HE1   | 1.47                     | 0.78              |
| 12:Y:77:ASN:HA    | 12:Y:110:TYR:OH   | 1.83                     | 0.78              |
| 22:A:334:PRO:HG3  | 25:F:395:GLN:HA   | 1.65                     | 0.78              |
| 24:E:235:ILE:HD12 | 24:E:277:MET:CB   | 2.10                     | 0.78              |
| 24:E:255:ARG:HA   | 24:E:258:MET:HE3  | 1.64                     | 0.78              |
| 3:G:211:LYS:HG2   | 3:G:212:PRO:CD    | 2.13                     | 0.78              |
| 4:H:205:GLU:OE2   | 4:H:205:GLU:N     | 2.15                     | 0.78              |
| 12:Y:245:GLU:OE1  | 12:Y:245:GLU:N    | 2.16                     | 0.78              |
| 12:Y:316:LEU:CD2  | 12:Y:327:VAL:HG13 | 2.14                     | 0.78              |
| 18:f:840:LEU:HG   | 18:f:842:VAL:HG23 | 1.64                     | 0.78              |
| 19:g:108:THR:HA   | 19:g:141:THR:HA   | 1.65                     | 0.78              |
| 24:E:361:PHE:CE1  | 24:E:366:ASP:HB3  | 2.17                     | 0.78              |
| 26:K:31:ILE:CD1   | 26:K:140:ALA:HB3  | 2.13                     | 0.78              |
| 2:D:274:ARG:NE    | 2:D:318:ASP:OD2   | 2.17                     | 0.78              |
| 6:J:36:ARG:HD3    | 6:J:157:LYS:HA    | 1.64                     | 0.78              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 9:V:61:GLU:HA     | 9:V:64:GLN:HB3    | 1.64                     | 0.78              |
| 9:V:69:THR:O      | 9:V:73:GLU:N      | 2.15                     | 0.78              |
| 13:Z:21:ASP:O     | 13:Z:25:ARG:HG3   | 1.84                     | 0.78              |
| 18:f:573:ILE:HG13 | 18:f:599:ALA:CB   | 2.11                     | 0.78              |
| 18:f:733:GLY:HA3  | 18:f:741:LEU:HD23 | 1.65                     | 0.78              |
| 22:A:279:ALA:O    | 23:B:307:ARG:NH1  | 2.15                     | 0.78              |
| 2:D:130:VAL:HG12  | 2:D:142:VAL:HA    | 1.64                     | 0.78              |
| 2:D:368:ASP:OD2   | 2:D:407:ILE:HD13  | 1.82                     | 0.78              |
| 6:J:56:GLU:OE1    | 6:J:56:GLU:N      | 2.15                     | 0.78              |
| 6:J:71:MET:HE3    | 6:J:131:ALA:CB    | 2.12                     | 0.78              |
| 6:J:145:TYR:CE1   | 6:J:155:ALA:HB2   | 2.18                     | 0.78              |
| 9:V:72:LEU:O      | 9:V:76:LYS:N      | 2.11                     | 0.78              |
| 18:f:373:ALA:HB2  | 18:f:760:PHE:HD1  | 1.47                     | 0.78              |
| 18:f:429:ILE:C    | 19:g:172:GLU:HB3  | 2.07                     | 0.78              |
| 18:f:535:THR:OG1  | 18:f:565:ASN:OD1  | 2.01                     | 0.78              |
| 18:f:597:VAL:CG2  | 18:f:656:GLY:HA2  | 2.12                     | 0.78              |
| 9:V:495:ARG:HA    | 9:V:495:ARG:NE    | 1.96                     | 0.78              |
| 10:W:235:GLN:HA   | 10:W:243:ILE:HD11 | 1.64                     | 0.78              |
| 12:Y:181:LYS:HD2  | 12:Y:204:THR:HG23 | 1.66                     | 0.78              |
| 14:a:59:LEU:O     | 14:a:63:PHE:N     | 2.11                     | 0.78              |
| 17:d:283:LEU:HD13 | 17:d:315:TYR:HE1  | 1.47                     | 0.78              |
| 2:D:267:ILE:HG12  | 2:D:309:MET:SD    | 2.23                     | 0.78              |
| 4:H:86:LEU:HD21   | 4:H:118:MET:SD    | 2.24                     | 0.78              |
| 10:W:435:LEU:HG   | 13:Z:233:VAL:HG22 | 1.66                     | 0.78              |
| 12:Y:112:CYS:SG   | 12:Y:147:ILE:HD11 | 2.23                     | 0.78              |
| 14:a:73:PRO:HA    | 14:a:76:LEU:HB3   | 1.65                     | 0.78              |
| 18:f:718:ASP:HB3  | 18:f:721:VAL:HG12 | 1.66                     | 0.78              |
| 19:g:160:GLN:OE1  | 19:g:168:ASN:ND2  | 2.16                     | 0.78              |
| 22:A:364:VAL:CG2  | 22:A:368:ILE:HG13 | 2.14                     | 0.78              |
| 24:E:310:LEU:O    | 24:E:314:LYS:HG2  | 1.84                     | 0.78              |
| 25:F:270:ASP:O    | 25:F:274:LEU:N    | 2.15                     | 0.78              |
| 1:C:113:ARG:HD3   | 1:C:130:LYS:HB2   | 1.66                     | 0.78              |
| 3:G:211:LYS:NZ    | 3:G:213:SER:OG    | 2.14                     | 0.78              |
| 9:V:213:TYR:O     | 9:V:217:VAL:N     | 2.15                     | 0.78              |
| 14:a:25:LEU:HD22  | 14:a:37:LEU:HD12  | 1.64                     | 0.78              |
| 15:b:131:LEU:HD12 | 15:b:136:VAL:HB   | 1.64                     | 0.78              |
| 16:c:106:GLU:N    | 16:c:106:GLU:OE2  | 2.17                     | 0.78              |
| 17:d:139:GLN:O    | 17:d:143:LEU:HG   | 1.83                     | 0.78              |
| 18:f:231:LEU:HG   | 18:f:853:VAL:HG22 | 1.63                     | 0.78              |
| 18:f:266:LEU:HD22 | 18:f:294:MET:HB2  | 1.63                     | 0.78              |
| 18:f:456:ARG:NH2  | 18:f:492:SER:HA   | 1.98                     | 0.78              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 18:f:703:ARG:HG2  | 18:f:705:ASN:OD1  | 1.83                     | 0.78              |
| 19:g:90:PRO:HB2   | 19:g:157:GLU:OE2  | 1.83                     | 0.78              |
| 3:G:14:THR:OG1    | 3:G:129:ALA:HB2   | 1.84                     | 0.78              |
| 5:I:137:ILE:HG22  | 5:I:147:LEU:CD1   | 2.13                     | 0.78              |
| 7:L:26:MET:HA     | 7:L:26:MET:HE2    | 1.66                     | 0.78              |
| 10:W:31:CYS:CB    | 10:W:43:VAL:HG13  | 2.13                     | 0.78              |
| 10:W:210:ASN:HD21 | 10:W:212:LYS:HB3  | 1.48                     | 0.78              |
| 12:Y:336:ARG:HH12 | 28:e:44:ASP:HB3   | 1.47                     | 0.78              |
| 7:L:66:VAL:HG21   | 7:L:72:ILE:HG23   | 1.65                     | 0.78              |
| 19:g:98:LYS:HG2   | 19:g:98:LYS:O     | 1.82                     | 0.78              |
| 19:g:109:GLY:HA3  | 19:g:138:LEU:HA   | 1.64                     | 0.78              |
| 24:E:289:LEU:HD22 | 24:E:295:LEU:HD12 | 1.66                     | 0.78              |
| 27:U:421:GLN:O    | 27:U:425:THR:HG23 | 1.84                     | 0.78              |
| 27:U:481:LEU:HD23 | 27:U:497:LEU:HD21 | 1.65                     | 0.78              |
| 5:I:137:ILE:HG22  | 5:I:147:LEU:HD13  | 1.64                     | 0.78              |
| 8:M:40:ARG:CB     | 8:M:45:VAL:HG22   | 2.14                     | 0.78              |
| 11:X:44:GLN:NE2   | 11:X:48:GLN:OE1   | 2.16                     | 0.78              |
| 12:Y:51:ALA:HB2   | 12:Y:73:MET:HG2   | 1.65                     | 0.78              |
| 13:Z:142:GLU:OE1  | 13:Z:153:LYS:HA   | 1.84                     | 0.78              |
| 14:a:12:GLN:HG2   | 14:a:18:GLN:HB3   | 1.65                     | 0.78              |
| 14:a:81:LEU:CA    | 14:a:84:VAL:HG12  | 2.12                     | 0.78              |
| 14:a:94:LEU:HD11  | 14:a:118:ILE:HB   | 1.64                     | 0.78              |
| 18:f:430:ASP:CB   | 19:g:169:PHE:HA   | 2.14                     | 0.78              |
| 27:U:587:ALA:HB2  | 27:U:621:SER:OG   | 1.83                     | 0.78              |
| 4:H:139:TRP:CD1   | 4:H:215:GLU:HA    | 2.18                     | 0.77              |
| 9:V:159:LEU:HD22  | 9:V:163:VAL:CG2   | 2.14                     | 0.77              |
| 9:V:452:ASN:HA    | 17:d:280:GLU:OE1  | 1.83                     | 0.77              |
| 11:X:319:ILE:O    | 11:X:323:LEU:HB2  | 1.83                     | 0.77              |
| 15:b:18:ASN:O     | 15:b:25:ARG:HD2   | 1.84                     | 0.77              |
| 19:g:89:LEU:HD12  | 19:g:99:ASN:ND2   | 1.97                     | 0.77              |
| 19:g:156:LEU:HB3  | 19:g:158:LEU:CD1  | 2.14                     | 0.77              |
| 22:A:195:LEU:HD11 | 22:A:316:LYS:HG3  | 1.66                     | 0.77              |
| 23:B:223:ILE:HB   | 23:B:347:ILE:HG21 | 1.65                     | 0.77              |
| 25:F:202:ILE:HD12 | 25:F:327:LYS:HB3  | 1.66                     | 0.77              |
| 26:K:76:CYS:SG    | 26:K:89:ILE:HD11  | 2.23                     | 0.77              |
| 1:C:350:LEU:HD23  | 1:C:387:VAL:HG11  | 1.65                     | 0.77              |
| 4:H:36:VAL:HG11   | 4:H:194:THR:HG22  | 1.66                     | 0.77              |
| 4:H:203:MET:O     | 4:H:230:LEU:HD13  | 1.84                     | 0.77              |
| 6:J:23:GLN:HE22   | 6:J:150:SER:HB3   | 1.48                     | 0.77              |
| 9:V:457:TYR:CE1   | 9:V:459:GLN:HB2   | 2.19                     | 0.77              |
| 14:a:51:ALA:HB3   | 14:a:86:GLN:HG2   | 1.65                     | 0.77              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 14:a:363:MET:HE3  | 16:c:307:VAL:HG11 | 1.66                     | 0.77              |
| 23:B:103:ARG:HA   | 23:B:160:ILE:HD13 | 1.66                     | 0.77              |
| 23:B:121:ALA:HB3  | 23:B:135:ILE:HD11 | 1.65                     | 0.77              |
| 24:E:149:ILE:HD13 | 24:E:276:ILE:CD1  | 2.11                     | 0.77              |
| 25:F:223:VAL:CG2  | 25:F:329:ILE:HG12 | 2.14                     | 0.77              |
| 2:D:383:GLY:HA3   | 24:E:164:ILE:HD12 | 1.67                     | 0.77              |
| 18:f:430:ASP:HB3  | 19:g:169:PHE:HA   | 1.66                     | 0.77              |
| 19:g:158:LEU:HD23 | 19:g:165:ALA:HB3  | 1.66                     | 0.77              |
| 2:D:391:ARG:NH1   | 2:D:395:LEU:HD12  | 2.00                     | 0.77              |
| 6:J:95:ARG:NH1    | 6:J:101:PRO:HB3   | 1.99                     | 0.77              |
| 14:a:4:VAL:HB     | 14:a:5:PRO:HD3    | 1.67                     | 0.77              |
| 14:a:180:LEU:CD1  | 14:a:221:VAL:HG21 | 2.12                     | 0.77              |
| 24:E:122:MET:CE   | 25:F:344:ARG:CZ   | 2.61                     | 0.77              |
| 2:D:45:LYS:HG2    | 27:U:187:LEU:HB3  | 1.67                     | 0.77              |
| 6:J:70:CYS:HB3    | 6:J:217:LEU:HD21  | 1.67                     | 0.77              |
| 7:L:32:GLY:O      | 7:L:163:ALA:N     | 2.16                     | 0.77              |
| 9:V:298:ILE:HA    | 9:V:397:ARG:HH22  | 1.49                     | 0.77              |
| 10:W:393:LEU:O    | 10:W:397:VAL:HG23 | 1.84                     | 0.77              |
| 11:X:160:MET:HG2  | 11:X:161:ASP:H    | 1.48                     | 0.77              |
| 15:b:25:ARG:NH2   | 15:b:114:GLY:O    | 2.16                     | 0.77              |
| 16:c:181:LEU:HD21 | 27:U:725:MET:HE2  | 1.66                     | 0.77              |
| 19:g:92:ARG:HB3   | 19:g:157:GLU:CD   | 2.09                     | 0.77              |
| 23:B:313:LEU:HD23 | 23:B:313:LEU:O    | 1.84                     | 0.77              |
| 24:E:235:ILE:HD12 | 24:E:277:MET:HB2  | 1.65                     | 0.77              |
| 27:U:203:LYS:O    | 27:U:207:ASN:ND2  | 2.17                     | 0.77              |
| 3:G:80:MET:HE1    | 3:G:138:MET:HG3   | 1.66                     | 0.77              |
| 9:V:276:PHE:HD1   | 9:V:277:PRO:HD2   | 1.48                     | 0.77              |
| 13:Z:143:GLU:HG3  | 13:Z:145:HIS:H    | 1.50                     | 0.77              |
| 13:Z:256:GLN:O    | 13:Z:259:VAL:HG12 | 1.85                     | 0.77              |
| 19:g:115:LYS:NZ   | 19:g:142:LEU:HD13 | 1.99                     | 0.77              |
| 25:F:322:PRO:O    | 25:F:323:ASN:HB3  | 1.85                     | 0.77              |
| 1:C:292:ILE:O     | 1:C:292:ILE:HG22  | 1.84                     | 0.77              |
| 4:H:65:VAL:N      | 4:H:209:GLU:OE1   | 2.13                     | 0.77              |
| 5:I:174:MET:CE    | 5:I:195:LYS:HE3   | 2.14                     | 0.77              |
| 9:V:224:LEU:O     | 9:V:257:ASN:ND2   | 2.17                     | 0.77              |
| 15:b:107:MET:HA   | 15:b:107:MET:CE   | 2.12                     | 0.77              |
| 15:b:113:VAL:O    | 15:b:142:ASN:HA   | 1.84                     | 0.77              |
| 17:d:120:LYS:O    | 17:d:124:LEU:N    | 2.17                     | 0.77              |
| 17:d:145:ARG:NH2  | 17:d:185:SER:OG   | 2.18                     | 0.77              |
| 23:B:372:MET:HE2  | 23:B:414:VAL:HG11 | 1.65                     | 0.77              |
| 3:G:163:PHE:CD2   | 3:G:166:THR:HB    | 2.20                     | 0.77              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 9:V:64:GLN:O      | 9:V:68:ASP:N      | 2.16                     | 0.77              |
| 10:W:451:MET:HE1  | 13:Z:99:PRO:O     | 1.84                     | 0.77              |
| 17:d:342:TYR:O    | 17:d:346:LEU:HD12 | 1.83                     | 0.77              |
| 24:E:145:LEU:HG   | 24:E:149:ILE:HD12 | 1.67                     | 0.77              |
| 26:K:100:TRP:O    | 26:K:104:ASN:N    | 2.18                     | 0.77              |
| 26:K:186:HIS:N    | 26:K:189:MET:HE2  | 1.98                     | 0.77              |
| 1:C:406:LYS:OXT   | 5:I:64:LYS:NZ     | 2.18                     | 0.77              |
| 2:D:231:VAL:HG11  | 24:E:262:ASN:ND2  | 2.00                     | 0.77              |
| 2:D:296:MET:HE1   | 2:D:309:MET:CE    | 2.15                     | 0.77              |
| 7:L:196:ARG:NH1   | 7:L:239:ARG:HG3   | 1.98                     | 0.77              |
| 8:M:65:ARG:HH22   | 8:M:78:ALA:HA     | 1.49                     | 0.77              |
| 8:M:173:LYS:O     | 8:M:177:GLU:HG3   | 1.85                     | 0.77              |
| 9:V:172:VAL:O     | 9:V:176:MET:HG3   | 1.85                     | 0.77              |
| 13:Z:126:VAL:HA   | 16:c:216:MET:HE1  | 1.64                     | 0.77              |
| 14:a:189:PRO:HG2  | 14:a:192:GLU:HB2  | 1.64                     | 0.77              |
| 14:a:216:LEU:HD13 | 14:a:237:LEU:HG   | 1.67                     | 0.77              |
| 24:E:352:MET:HE1  | 24:E:355:ILE:HD13 | 1.67                     | 0.77              |
| 27:U:554:LEU:HD23 | 27:U:588:MET:HG3  | 1.65                     | 0.77              |
| 1:C:258:ARG:HD3   | 1:C:273:MET:CE    | 2.14                     | 0.77              |
| 9:V:219:GLU:OE2   | 9:V:256:ARG:NE    | 2.18                     | 0.77              |
| 10:W:82:LEU:O     | 10:W:86:ASN:ND2   | 2.14                     | 0.77              |
| 14:a:64:ILE:O     | 14:a:68:GLU:HB3   | 1.84                     | 0.77              |
| 18:f:520:LEU:HD11 | 18:f:798:THR:HB   | 1.65                     | 0.77              |
| 18:f:814:SER:O    | 18:f:817:VAL:HG12 | 1.85                     | 0.77              |
| 22:A:161:VAL:HG13 | 22:A:260:LEU:HD12 | 1.67                     | 0.77              |
| 1:C:21:ARG:HA     | 1:C:24:TYR:CD2    | 2.20                     | 0.76              |
| 9:V:120:PHE:CE2   | 9:V:149:PRO:HG2   | 2.20                     | 0.76              |
| 10:W:17:GLU:N     | 10:W:58:SER:O     | 2.18                     | 0.76              |
| 14:a:81:LEU:HA    | 14:a:84:VAL:CG1   | 2.13                     | 0.76              |
| 17:d:226:ILE:O    | 17:d:230:VAL:HG12 | 1.85                     | 0.76              |
| 19:g:170:GLN:HA   | 19:g:173:GLU:HB3  | 1.66                     | 0.76              |
| 25:F:248:PHE:HD1  | 25:F:282:ILE:HD11 | 1.50                     | 0.76              |
| 27:U:873:PRO:HB2  | 27:U:876:GLN:NE2  | 2.00                     | 0.76              |
| 1:C:193:GLY:HA3   | 2:D:323:ARG:HD2   | 1.66                     | 0.76              |
| 6:J:91:CYS:HA     | 6:J:102:VAL:HG21  | 1.67                     | 0.76              |
| 6:J:133:ILE:HD13  | 6:J:147:THR:HG23  | 1.66                     | 0.76              |
| 14:a:74:LEU:O     | 14:a:78:GLU:N     | 2.14                     | 0.76              |
| 14:a:97:LEU:HD22  | 14:a:117:ALA:HB1  | 1.68                     | 0.76              |
| 14:a:123:LEU:HD22 | 14:a:158:LEU:CD1  | 2.15                     | 0.76              |
| 17:d:138:LYS:O    | 17:d:142:ILE:HG12 | 1.85                     | 0.76              |
| 18:f:245:ASN:O    | 18:f:249:LEU:HG   | 1.85                     | 0.76              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 24:E:47:LEU:HA    | 24:E:50:LEU:HD12  | 1.67                     | 0.76              |
| 26:K:28:ILE:HG13  | 26:K:158:PRO:HG2  | 1.65                     | 0.76              |
| 2:D:391:ARG:HH12  | 2:D:397:LYS:HD2   | 1.50                     | 0.76              |
| 10:W:23:THR:HA    | 10:W:26:GLN:HG2   | 1.67                     | 0.76              |
| 14:a:321:LYS:HD2  | 14:a:336:VAL:HG11 | 1.65                     | 0.76              |
| 15:b:36:VAL:O     | 15:b:40:LYS:HG2   | 1.86                     | 0.76              |
| 15:b:124:LEU:HD22 | 15:b:152:LYS:HB2  | 1.66                     | 0.76              |
| 17:d:237:MET:O    | 17:d:237:MET:HE3  | 1.86                     | 0.76              |
| 18:f:433:LEU:HB2  | 18:f:444:ALA:HB3  | 1.66                     | 0.76              |
| 27:U:611:ASN:O    | 27:U:614:VAL:HG12 | 1.85                     | 0.76              |
| 1:C:161:ILE:HG21  | 1:C:199:LEU:HD21  | 1.67                     | 0.76              |
| 11:X:211:ASP:HB3  | 11:X:235:ALA:HB2  | 1.66                     | 0.76              |
| 14:a:40:GLN:HG3   | 14:a:44:PHE:CD2   | 2.20                     | 0.76              |
| 18:f:846:VAL:HG22 | 18:f:880:ALA:HA   | 1.67                     | 0.76              |
| 19:g:132:ASN:CB   | 19:g:151:VAL:HG13 | 2.14                     | 0.76              |
| 23:B:425:ASN:HA   | 23:B:428:TYR:OH   | 1.85                     | 0.76              |
| 25:F:406:ILE:HD13 | 25:F:422:GLU:HB3  | 1.66                     | 0.76              |
| 27:U:363:SER:HG   | 27:U:365:CYS:HG   | 0.76                     | 0.76              |
| 1:C:236:VAL:HG22  | 1:C:239:ARG:HH22  | 1.49                     | 0.76              |
| 16:c:123:SER:HB2  | 20:u:289:HIS:HE1  | 1.50                     | 0.76              |
| 19:g:87:VAL:HG22  | 19:g:155:VAL:HG23 | 1.67                     | 0.76              |
| 25:F:369:HIS:CD2  | 25:F:397:LYS:HB2  | 2.20                     | 0.76              |
| 27:U:339:LEU:O    | 27:U:343:ILE:HG12 | 1.85                     | 0.76              |
| 27:U:536:ALA:CB   | 27:U:578:LEU:HD21 | 2.13                     | 0.76              |
| 27:U:583:MET:HE1  | 27:U:605:VAL:HB   | 1.67                     | 0.76              |
| 13:Z:69:PHE:HZ    | 15:b:63:THR:HG23  | 1.50                     | 0.76              |
| 13:Z:217:THR:HG23 | 13:Z:219:LYS:HG3  | 1.68                     | 0.76              |
| 14:a:176:ALA:CB   | 14:a:200:LEU:HD13 | 2.15                     | 0.76              |
| 14:a:293:PHE:HB3  | 14:a:329:LYS:CG   | 2.11                     | 0.76              |
| 18:f:372:LEU:HD22 | 18:f:406:GLY:HA2  | 1.68                     | 0.76              |
| 18:f:563:GLY:O    | 18:f:566:HIS:N    | 2.16                     | 0.76              |
| 1:C:79:ALA:CB     | 22:A:65:ILE:HD13  | 2.15                     | 0.76              |
| 4:H:69:THR:OG1    | 4:H:72:ILE:HD12   | 1.85                     | 0.76              |
| 18:f:460:ASP:HB3  | 19:g:133:LYS:HB3  | 1.66                     | 0.76              |
| 19:g:138:LEU:CD1  | 19:g:162:GLU:HG3  | 2.16                     | 0.76              |
| 27:U:247:GLN:CG   | 27:U:913:ILE:HG12 | 2.14                     | 0.76              |
| 27:U:719:ASP:OD1  | 27:U:720:LYS:N    | 2.19                     | 0.76              |
| 1:C:24:TYR:CD1    | 27:U:153:ILE:HG13 | 2.21                     | 0.76              |
| 3:G:155:ASP:OD1   | 3:G:159:TYR:N     | 2.18                     | 0.76              |
| 5:I:108:GLU:O     | 5:I:112:THR:HG23  | 1.86                     | 0.76              |
| 7:L:13:TRP:HB2    | 8:M:22:GLN:OE1    | 1.85                     | 0.76              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 9:V:72:LEU:HD11   | 9:V:116:ALA:HB2   | 1.68                     | 0.76              |
| 14:a:58:LYS:HZ2   | 14:a:83:VAL:HG13  | 1.50                     | 0.76              |
| 19:g:112:LEU:HD13 | 19:g:142:LEU:HD11 | 1.67                     | 0.76              |
| 22:A:113:ILE:CD1  | 22:A:142:VAL:HG11 | 2.15                     | 0.76              |
| 25:F:90:VAL:HG23  | 25:F:164:LEU:HD12 | 1.67                     | 0.76              |
| 25:F:225:MET:HG2  | 25:F:352:ILE:HG21 | 1.67                     | 0.76              |
| 27:U:138:PHE:HA   | 27:U:141:CYS:SG   | 2.25                     | 0.76              |
| 27:U:204:ILE:HA   | 27:U:207:ASN:HD21 | 1.48                     | 0.76              |
| 3:G:235:ILE:H     | 3:G:235:ILE:HD12  | 1.51                     | 0.76              |
| 10:W:211:THR:HA   | 10:W:214:PHE:CE2  | 2.20                     | 0.76              |
| 17:d:283:LEU:HG   | 17:d:286:GLU:H    | 1.50                     | 0.76              |
| 18:f:99:LEU:C     | 18:f:101:PRO:HD3  | 2.11                     | 0.76              |
| 18:f:398:TRP:O    | 18:f:401:LYS:HG2  | 1.85                     | 0.76              |
| 18:f:701:ASN:HD21 | 18:f:703:ARG:NH1  | 1.82                     | 0.76              |
| 25:F:130:GLN:HB2  | 25:F:132:TYR:HE2  | 1.51                     | 0.76              |
| 25:F:276:LYS:HE3  | 25:F:326:VAL:HG21 | 1.68                     | 0.76              |
| 27:U:399:TRP:CH2  | 27:U:472:ILE:HG23 | 2.21                     | 0.76              |
| 3:G:60:LEU:HD13   | 8:M:162:GLY:O     | 1.85                     | 0.76              |
| 12:Y:48:ASN:HB2   | 12:Y:50:MET:HE2   | 1.68                     | 0.76              |
| 14:a:96:PHE:HA    | 14:a:99:LYS:HD3   | 1.68                     | 0.76              |
| 17:d:142:ILE:O    | 17:d:146:ASP:N    | 2.14                     | 0.76              |
| 18:f:418:LEU:HD12 | 18:f:421:ASP:OD2  | 1.86                     | 0.76              |
| 18:f:499:THR:HA   | 18:f:502:LEU:HG   | 1.68                     | 0.76              |
| 25:F:277:GLU:OE1  | 25:F:278:LYS:NZ   | 2.17                     | 0.76              |
| 26:K:39:GLY:O     | 26:K:167:ALA:HA   | 1.85                     | 0.76              |
| 10:W:105:VAL:HG11 | 10:W:138:VAL:CG2  | 2.16                     | 0.75              |
| 10:W:263:TRP:HZ3  | 10:W:267:LEU:HD12 | 1.50                     | 0.75              |
| 10:W:268:LYS:HE3  | 10:W:299:ILE:CG2  | 2.16                     | 0.75              |
| 13:Z:78:MET:HE2   | 16:c:98:MET:CE    | 2.16                     | 0.75              |
| 15:b:33:VAL:HA    | 15:b:36:VAL:CG2   | 2.16                     | 0.75              |
| 19:g:136:LEU:HD22 | 19:g:147:VAL:HG21 | 1.69                     | 0.75              |
| 24:E:83:CYS:HB2   | 24:E:87:LEU:HD23  | 1.66                     | 0.75              |
| 25:F:284:PHE:HA   | 25:F:329:ILE:O    | 1.86                     | 0.75              |
| 1:C:134:LEU:O     | 1:C:134:LEU:HD23  | 1.86                     | 0.75              |
| 2:D:181:VAL:HG21  | 2:D:308:ILE:HD11  | 1.67                     | 0.75              |
| 3:G:123:GLN:HE22  | 3:G:127:GLN:HE21  | 1.34                     | 0.75              |
| 3:G:141:ILE:HD11  | 3:G:227:PHE:HE1   | 1.52                     | 0.75              |
| 5:I:140:ASP:OD2   | 5:I:146:GLN:NE2   | 2.19                     | 0.75              |
| 12:Y:51:ALA:HB3   | 12:Y:52:PRO:HD3   | 1.69                     | 0.75              |
| 14:a:7:PHE:HE2    | 14:a:60:TYR:HA    | 1.51                     | 0.75              |
| 14:a:231:GLN:O    | 14:a:231:GLN:HG2  | 1.86                     | 0.75              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 18:f:164:GLY:HA3  | 22:A:40:THR:HG21  | 1.66                     | 0.75              |
| 18:f:267:ARG:CZ   | 18:f:893:ILE:HB   | 2.16                     | 0.75              |
| 18:f:413:SER:HA   | 18:f:416:MET:HE2  | 1.68                     | 0.75              |
| 18:f:783:SER:N    | 18:f:895:GLU:OE1  | 2.19                     | 0.75              |
| 19:g:90:PRO:HG3   | 19:g:155:VAL:O    | 1.85                     | 0.75              |
| 19:g:100:LEU:H    | 19:g:100:LEU:HD22 | 1.51                     | 0.75              |
| 19:g:112:LEU:CD1  | 19:g:142:LEU:HD21 | 2.16                     | 0.75              |
| 26:K:50:VAL:HG11  | 26:K:66:LYS:HB3   | 1.68                     | 0.75              |
| 27:U:36:ALA:O     | 27:U:39:SER:OG    | 2.00                     | 0.75              |
| 27:U:599:ILE:HD12 | 27:U:626:LEU:HD11 | 1.68                     | 0.75              |
| 27:U:697:GLN:OE1  | 27:U:786:THR:HG21 | 1.86                     | 0.75              |
| 27:U:717:ILE:CD1  | 27:U:731:ILE:HD11 | 2.15                     | 0.75              |
| 4:H:135:LEU:HD12  | 4:H:163:MET:CE    | 2.04                     | 0.75              |
| 5:I:161:ALA:CB    | 5:I:175:LEU:HD23  | 2.15                     | 0.75              |
| 9:V:115:LYS:O     | 9:V:119:GLY:N     | 2.20                     | 0.75              |
| 12:Y:152:MET:HA   | 12:Y:152:MET:HE2  | 1.65                     | 0.75              |
| 13:Z:69:PHE:CD2   | 15:b:96:ALA:HA    | 2.22                     | 0.75              |
| 14:a:41:VAL:HG12  | 14:a:79:ILE:HD12  | 1.68                     | 0.75              |
| 18:f:391:LEU:HG   | 18:f:414:LEU:HG   | 1.69                     | 0.75              |
| 3:G:143:ILE:HG12  | 3:G:220:VAL:HG22  | 1.67                     | 0.75              |
| 7:L:26:MET:CE     | 7:L:149:PRO:HD2   | 2.15                     | 0.75              |
| 8:M:49:VAL:HG21   | 8:M:65:ARG:HE     | 1.50                     | 0.75              |
| 8:M:196:ILE:HA    | 8:M:199:ILE:CD1   | 2.16                     | 0.75              |
| 10:W:90:LEU:O     | 10:W:93:ARG:HG3   | 1.86                     | 0.75              |
| 10:W:377:ARG:HE   | 10:W:381:LEU:HD21 | 1.50                     | 0.75              |
| 14:a:25:LEU:HA    | 14:a:28:LEU:HD23  | 1.66                     | 0.75              |
| 15:b:33:VAL:HG11  | 15:b:75:LEU:HD11  | 1.68                     | 0.75              |
| 17:d:102:TRP:HA   | 17:d:107:PRO:HB3  | 1.68                     | 0.75              |
| 18:f:96:LEU:CD2   | 18:f:129:LEU:HA   | 2.17                     | 0.75              |
| 19:g:87:VAL:HG11  | 19:g:101:LEU:CB   | 2.15                     | 0.75              |
| 19:g:116:ILE:HD13 | 19:g:129:ILE:HG13 | 1.69                     | 0.75              |
| 24:E:50:LEU:HG    | 25:F:139:LEU:HD21 | 1.67                     | 0.75              |
| 1:C:214:VAL:O     | 1:C:248:MET:HA    | 1.86                     | 0.75              |
| 9:V:62:HIS:HA     | 9:V:65:ARG:CD     | 2.16                     | 0.75              |
| 18:f:426:LEU:HD12 | 19:g:169:PHE:CZ   | 2.21                     | 0.75              |
| 19:g:165:ALA:HA   | 19:g:168:ASN:N    | 2.01                     | 0.75              |
| 22:A:219:GLY:CA   | 23:B:343:ARG:HD2  | 2.16                     | 0.75              |
| 3:G:10:ASP:O      | 3:G:24:GLN:HG2    | 1.87                     | 0.75              |
| 9:V:467:TYR:CE2   | 12:Y:362:LYS:HD2  | 2.22                     | 0.75              |
| 11:X:171:LEU:CD2  | 11:X:210:LEU:HD23 | 2.17                     | 0.75              |
| 18:f:325:GLN:NE2  | 18:f:328:SER:HG   | 1.84                     | 0.75              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 18:f:591:ALA:O    | 18:f:595:VAL:HG22 | 1.86                     | 0.75              |
| 19:g:158:LEU:HB3  | 19:g:165:ALA:CB   | 2.17                     | 0.75              |
| 23:B:66:GLU:CG    | 27:U:834:SER:HB3  | 2.17                     | 0.75              |
| 24:E:87:LEU:HD21  | 24:E:92:LEU:CD1   | 2.13                     | 0.75              |
| 25:F:178:ASP:HA   | 25:F:180:ARG:HH22 | 1.51                     | 0.75              |
| 26:K:81:LEU:HD13  | 26:K:138:GLY:HA3  | 1.69                     | 0.75              |
| 5:I:90:LEU:CG     | 5:I:114:LEU:HD22  | 2.15                     | 0.75              |
| 7:L:74:ILE:HG22   | 7:L:132:LEU:HD21  | 1.67                     | 0.75              |
| 8:M:50:GLU:HB3    | 8:M:197:ILE:HD11  | 1.67                     | 0.75              |
| 10:W:135:LYS:HD3  | 10:W:137:TYR:CE2  | 2.22                     | 0.75              |
| 11:X:334:ASN:OD1  | 11:X:337:ARG:NH2  | 2.18                     | 0.75              |
| 12:Y:70:LEU:HD11  | 12:Y:74:LYS:HE3   | 1.68                     | 0.75              |
| 14:a:80:ILE:HB    | 14:a:96:PHE:HE2   | 1.51                     | 0.75              |
| 15:b:138:VAL:CG1  | 15:b:160:LEU:HD11 | 2.17                     | 0.75              |
| 27:U:797:MET:HG3  | 27:U:880:ASN:OD1  | 1.87                     | 0.75              |
| 5:I:229:LYS:N     | 5:I:232:GLU:OE2   | 2.18                     | 0.75              |
| 9:V:236:ARG:O     | 9:V:240:LEU:HG    | 1.87                     | 0.75              |
| 9:V:417:ILE:HD13  | 9:V:422:ILE:HG13  | 1.69                     | 0.75              |
| 14:a:80:ILE:HB    | 14:a:96:PHE:CE2   | 2.22                     | 0.75              |
| 14:a:195:GLU:O    | 14:a:199:THR:HG23 | 1.87                     | 0.75              |
| 17:d:191:LEU:HA   | 17:d:194:LEU:HD13 | 1.69                     | 0.75              |
| 24:E:351:GLY:O    | 24:E:355:ILE:HG13 | 1.86                     | 0.75              |
| 2:D:323:ARG:HH12  | 2:D:326:ARG:HH12  | 1.35                     | 0.75              |
| 7:L:171:TYR:HD1   | 7:L:172:LEU:HD23  | 1.52                     | 0.75              |
| 9:V:213:TYR:HA    | 9:V:216:ARG:HB3   | 1.68                     | 0.75              |
| 13:Z:246:VAL:HG22 | 17:d:330:ILE:HD11 | 1.68                     | 0.75              |
| 14:a:114:CYS:HA   | 14:a:117:ALA:CB   | 2.17                     | 0.75              |
| 15:b:131:LEU:HA   | 15:b:134:GLU:OE2  | 1.87                     | 0.75              |
| 18:f:567:LEU:HB2  | 18:f:790:GLN:NE2  | 2.02                     | 0.75              |
| 25:F:294:LYS:HA   | 25:F:339:ASP:OD1  | 1.87                     | 0.75              |
| 26:K:91:LYS:HZ3   | 26:K:95:GLU:HG3   | 1.52                     | 0.75              |
| 27:U:516:LEU:HD23 | 27:U:532:MET:HG3  | 1.69                     | 0.75              |
| 1:C:403:LYS:HD2   | 4:H:156:PHE:CD1   | 2.22                     | 0.74              |
| 5:I:32:GLY:CA     | 5:I:50:ARG:HD2    | 2.17                     | 0.74              |
| 11:X:170:GLN:HE22 | 11:X:192:SER:HB3  | 1.52                     | 0.74              |
| 13:Z:10:VAL:HG12  | 13:Z:161:GLU:OE2  | 1.87                     | 0.74              |
| 13:Z:110:GLU:OE2  | 13:Z:153:LYS:NZ   | 2.17                     | 0.74              |
| 14:a:335:TRP:NE1  | 14:a:337:GLN:O    | 2.19                     | 0.74              |
| 15:b:25:ARG:HH12  | 15:b:145:GLU:H    | 1.35                     | 0.74              |
| 15:b:161:ASN:HD21 | 15:b:168:SER:H    | 1.34                     | 0.74              |
| 17:d:259:PHE:HA   | 17:d:262:ILE:HD12 | 1.68                     | 0.74              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 23:B:294:ARG:HD3  | 23:B:310:LEU:CD1  | 2.16                     | 0.74              |
| 26:K:42:THR:OG1   | 26:K:45:GLY:O     | 2.01                     | 0.74              |
| 27:U:187:LEU:O    | 27:U:188:MET:HE2  | 1.87                     | 0.74              |
| 3:G:131:MET:HE3   | 8:M:124:LEU:HD13  | 1.69                     | 0.74              |
| 9:V:78:HIS:O      | 9:V:82:LEU:N      | 2.17                     | 0.74              |
| 10:W:125:ILE:HG22 | 10:W:145:LEU:HD13 | 1.69                     | 0.74              |
| 10:W:445:LEU:HD12 | 13:Z:226:ILE:HG13 | 1.70                     | 0.74              |
| 14:a:131:THR:HG23 | 14:a:132:LYS:HD2  | 1.68                     | 0.74              |
| 16:c:187:PRO:HB2  | 16:c:192:LEU:HD21 | 1.69                     | 0.74              |
| 19:g:129:ILE:HB   | 19:g:136:LEU:CD1  | 2.17                     | 0.74              |
| 24:E:313:LEU:O    | 24:E:317:ALA:N    | 2.19                     | 0.74              |
| 1:C:351:MET:HE1   | 1:C:359:VAL:HG22  | 1.69                     | 0.74              |
| 9:V:333:ILE:HD12  | 9:V:357:LEU:CD2   | 2.17                     | 0.74              |
| 9:V:401:ASN:OD1   | 9:V:404:LYS:NZ    | 2.19                     | 0.74              |
| 14:a:156:TYR:HA   | 14:a:159:SER:OG   | 1.87                     | 0.74              |
| 14:a:220:PRO:O    | 14:a:224:SER:OG   | 2.02                     | 0.74              |
| 15:b:94:HIS:NE2   | 15:b:134:GLU:OE1  | 2.20                     | 0.74              |
| 19:g:104:ARG:O    | 19:g:115:LYS:HE3  | 1.87                     | 0.74              |
| 24:E:101:ASP:OD1  | 24:E:102:MET:N    | 2.21                     | 0.74              |
| 25:F:153:VAL:HG12 | 25:F:160:ILE:HA   | 1.69                     | 0.74              |
| 25:F:197:GLU:HG2  | 25:F:352:ILE:HD11 | 1.69                     | 0.74              |
| 27:U:568:GLU:OE2  | 27:U:601:ARG:NH2  | 2.20                     | 0.74              |
| 1:C:308:PRO:HB3   | 23:B:397:ALA:HB2  | 1.67                     | 0.74              |
| 2:D:355:SER:O     | 2:D:358:VAL:HG12  | 1.86                     | 0.74              |
| 5:I:39:ALA:HA     | 5:I:184:MET:O     | 1.88                     | 0.74              |
| 5:I:68:LEU:HD21   | 5:I:74:CYS:SG     | 2.27                     | 0.74              |
| 10:W:121:LYS:O    | 10:W:125:ILE:HG12 | 1.88                     | 0.74              |
| 10:W:193:CYS:SG   | 10:W:201:ARG:HG2  | 2.27                     | 0.74              |
| 12:Y:11:LEU:HG    | 12:Y:179:ARG:HH11 | 1.52                     | 0.74              |
| 13:Z:19:VAL:HG22  | 13:Z:95:TYR:CE1   | 2.22                     | 0.74              |
| 14:a:153:SER:HB2  | 14:a:179:PHE:CD1  | 2.21                     | 0.74              |
| 16:c:32:TYR:OH    | 27:U:542:GLU:OE2  | 2.04                     | 0.74              |
| 27:U:838:LYS:HA   | 27:U:841:LYS:HD3  | 1.70                     | 0.74              |
| 2:D:355:SER:HB2   | 2:D:393:ILE:CG2   | 2.17                     | 0.74              |
| 9:V:81:GLN:HA     | 9:V:84:LYS:HB3    | 1.68                     | 0.74              |
| 14:a:70:ARG:HH12  | 15:b:17:ARG:CD    | 2.01                     | 0.74              |
| 18:f:45:LEU:HD22  | 18:f:50:LYS:HE2   | 1.68                     | 0.74              |
| 25:F:206:MET:HG3  | 25:F:325:GLN:HE21 | 1.52                     | 0.74              |
| 27:U:588:MET:HE1  | 27:U:760:VAL:CG1  | 2.16                     | 0.74              |
| 1:C:132:ASP:OD2   | 1:C:229:ARG:NH1   | 2.18                     | 0.74              |
| 3:G:208:ILE:HD12  | 24:E:306:GLU:OE1  | 1.87                     | 0.74              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:L:189:LYS:HG2   | 7:L:236:LEU:HD12  | 1.70                     | 0.74              |
| 9:V:139:MET:SD    | 9:V:139:MET:N     | 2.60                     | 0.74              |
| 10:W:331:GLY:CA   | 10:W:337:ALA:HB2  | 2.18                     | 0.74              |
| 13:Z:90:ARG:O     | 13:Z:92:VAL:HG13  | 1.88                     | 0.74              |
| 15:b:8:VAL:O      | 15:b:51:LEU:HA    | 1.87                     | 0.74              |
| 15:b:97:LEU:HD21  | 15:b:107:MET:HE2  | 1.68                     | 0.74              |
| 18:f:115:PRO:O    | 18:f:119:LYS:HD2  | 1.88                     | 0.74              |
| 19:g:115:LYS:HZ1  | 19:g:142:LEU:HD13 | 1.50                     | 0.74              |
| 25:F:280:PRO:HA   | 25:F:325:GLN:HB3  | 1.69                     | 0.74              |
| 5:I:155:ASN:OD1   | 6:J:77:THR:HB     | 1.87                     | 0.74              |
| 9:V:188:SER:O     | 9:V:191:LEU:HB3   | 1.87                     | 0.74              |
| 17:d:345:GLN:OE1  | 17:d:345:GLN:HA   | 1.87                     | 0.74              |
| 18:f:422:VAL:HA   | 18:f:426:LEU:HD23 | 1.70                     | 0.74              |
| 19:g:131:ILE:HA   | 19:g:153:ALA:HB2  | 1.70                     | 0.74              |
| 19:g:161:SER:N    | 19:g:164:ASP:HB3  | 2.01                     | 0.74              |
| 22:A:402:LYS:HE3  | 23:B:213:GLU:OE2  | 1.87                     | 0.74              |
| 5:I:209:GLU:OE1   | 5:I:209:GLU:N     | 2.20                     | 0.74              |
| 10:W:190:MET:HE1  | 10:W:206:SER:CA   | 2.17                     | 0.74              |
| 11:X:373:LYS:HA   | 11:X:373:LYS:HZ3  | 1.51                     | 0.74              |
| 14:a:215:GLU:HB3  | 14:a:219:HIS:HB2  | 1.70                     | 0.74              |
| 18:f:658:ALA:HA   | 18:f:697:ILE:HD11 | 1.70                     | 0.74              |
| 18:f:832:THR:HG23 | 18:f:870:THR:HG21 | 1.69                     | 0.74              |
| 19:g:84:THR:O     | 19:g:150:ASN:HA   | 1.87                     | 0.74              |
| 19:g:161:SER:O    | 19:g:165:ALA:N    | 2.21                     | 0.74              |
| 23:B:233:THR:OG1  | 29:B:501:ATP:O2B  | 2.05                     | 0.74              |
| 25:F:264:GLY:O    | 25:F:268:VAL:HG23 | 1.88                     | 0.74              |
| 27:U:226:PRO:O    | 27:U:229:VAL:HG12 | 1.88                     | 0.74              |
| 28:e:58:ALA:O     | 28:e:62:LYS:HG3   | 1.86                     | 0.74              |
| 4:H:139:TRP:CE2   | 4:H:215:GLU:HG2   | 2.23                     | 0.74              |
| 9:V:106:ARG:NH1   | 28:e:18:GLU:OE2   | 2.21                     | 0.74              |
| 9:V:482:PHE:CZ    | 12:Y:381:GLN:HB2  | 2.22                     | 0.74              |
| 10:W:244:CYS:HB2  | 10:W:273:TYR:HB3  | 1.68                     | 0.74              |
| 11:X:109:LEU:O    | 11:X:112:GLU:HG2  | 1.87                     | 0.74              |
| 18:f:395:GLY:O    | 18:f:399:LEU:HG   | 1.88                     | 0.74              |
| 18:f:612:LEU:HD22 | 18:f:660:ILE:HD12 | 1.68                     | 0.74              |
| 19:g:164:ASP:O    | 19:g:168:ASN:N    | 2.20                     | 0.74              |
| 24:E:33:LEU:HD21  | 25:F:66:LEU:CA    | 2.17                     | 0.74              |
| 25:F:233:LYS:HA   | 25:F:354:PHE:CE2  | 2.22                     | 0.74              |
| 27:U:602:LEU:HD21 | 27:U:618:ALA:HA   | 1.70                     | 0.74              |
| 7:L:125:ARG:HH11  | 7:L:125:ARG:HG3   | 1.53                     | 0.74              |
| 9:V:64:GLN:NE2    | 9:V:109:ASN:OD1   | 2.21                     | 0.74              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 11:X:73:VAL:O     | 11:X:77:LEU:HG    | 1.88                     | 0.74              |
| 11:X:114:ILE:CD1  | 11:X:130:GLU:HG3  | 2.17                     | 0.74              |
| 11:X:166:LEU:O    | 11:X:170:GLN:HB2  | 1.88                     | 0.74              |
| 11:X:255:LEU:O    | 11:X:259:ILE:HG12 | 1.88                     | 0.74              |
| 12:Y:22:LEU:CD1   | 12:Y:40:GLU:HB3   | 2.17                     | 0.74              |
| 14:a:112:ILE:O    | 14:a:116:THR:HG23 | 1.88                     | 0.74              |
| 18:f:62:ARG:HH12  | 18:f:74:ALA:HB2   | 1.52                     | 0.74              |
| 18:f:411:ALA:HB3  | 18:f:443:GLY:HA3  | 1.70                     | 0.74              |
| 18:f:848:GLN:HA   | 18:f:878:GLU:OE1  | 1.88                     | 0.74              |
| 22:A:213:LEU:HD11 | 22:A:321:THR:CG2  | 2.18                     | 0.74              |
| 1:C:314:LYS:NZ    | 23:B:429:LYS:HB3  | 2.02                     | 0.73              |
| 5:I:21:VAL:CG1    | 23:B:438:LEU:HD21 | 2.17                     | 0.73              |
| 6:J:83:VAL:HG11   | 6:J:129:ILE:HD13  | 1.70                     | 0.73              |
| 9:V:67:LEU:HD12   | 9:V:107:ARG:HH11  | 1.53                     | 0.73              |
| 14:a:115:LYS:CA   | 14:a:118:ILE:HG22 | 2.17                     | 0.73              |
| 18:f:267:ARG:HH21 | 18:f:891:THR:HG21 | 1.52                     | 0.73              |
| 19:g:112:LEU:HB2  | 19:g:142:LEU:CD1  | 2.17                     | 0.73              |
| 3:G:72:ILE:HD12   | 3:G:78:CYS:HB3    | 1.69                     | 0.73              |
| 14:a:81:LEU:O     | 14:a:85:ARG:N     | 2.15                     | 0.73              |
| 14:a:159:SER:HB2  | 14:a:168:ASN:HD21 | 1.53                     | 0.73              |
| 14:a:320:VAL:HG11 | 14:a:333:MET:HE1  | 1.69                     | 0.73              |
| 17:d:282:ILE:HB   | 17:d:318:PHE:HE2  | 1.54                     | 0.73              |
| 18:f:520:LEU:HD12 | 18:f:560:LEU:HD13 | 1.68                     | 0.73              |
| 18:f:882:LEU:HD23 | 18:f:882:LEU:H    | 1.53                     | 0.73              |
| 4:H:74:LEU:HD22   | 4:H:136:ILE:HG12  | 1.70                     | 0.73              |
| 6:J:94:HIS:ND1    | 6:J:102:VAL:HG22  | 2.03                     | 0.73              |
| 8:M:40:ARG:HB2    | 8:M:45:VAL:HG22   | 1.70                     | 0.73              |
| 8:M:42:LYS:HE2    | 8:M:183:GLU:O     | 1.89                     | 0.73              |
| 8:M:50:GLU:CB     | 8:M:197:ILE:HD11  | 2.17                     | 0.73              |
| 11:X:118:LYS:HD2  | 11:X:126:ARG:HG3  | 1.69                     | 0.73              |
| 12:Y:314:LEU:HD12 | 12:Y:314:LEU:O    | 1.88                     | 0.73              |
| 14:a:124:ASN:O    | 14:a:125:ILE:HD13 | 1.87                     | 0.73              |
| 14:a:307:VAL:O    | 14:a:311:VAL:HG12 | 1.88                     | 0.73              |
| 18:f:466:LEU:CD1  | 18:f:481:SER:HA   | 2.18                     | 0.73              |
| 27:U:188:MET:HE2  | 27:U:188:MET:HA   | 1.68                     | 0.73              |
| 5:I:230:GLN:O     | 5:I:234:GLU:HG2   | 1.88                     | 0.73              |
| 14:a:45:VAL:HG21  | 14:a:79:ILE:HG13  | 1.70                     | 0.73              |
| 14:a:94:LEU:HD11  | 14:a:118:ILE:CD1  | 2.16                     | 0.73              |
| 14:a:226:ARG:NH2  | 14:a:230:ARG:O    | 2.20                     | 0.73              |
| 18:f:432:TYR:H    | 19:g:172:GLU:HB2  | 1.53                     | 0.73              |
| 22:A:241:ILE:HD12 | 22:A:244:GLU:HG3  | 1.67                     | 0.73              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 27:U:804:SER:H    | 27:U:874:ASN:C    | 1.97                     | 0.73              |
| 1:C:399:MET:CE    | 1:C:402:LYS:HD2   | 2.18                     | 0.73              |
| 3:G:38:THR:HG23   | 3:G:202:LEU:HD11  | 1.70                     | 0.73              |
| 10:W:210:ASN:OD1  | 10:W:212:LYS:N    | 2.15                     | 0.73              |
| 14:a:21:VAL:HA    | 14:a:44:PHE:CZ    | 2.23                     | 0.73              |
| 14:a:92:VAL:O     | 14:a:96:PHE:N     | 2.17                     | 0.73              |
| 18:f:267:ARG:NE   | 18:f:893:ILE:HD13 | 2.03                     | 0.73              |
| 18:f:892:PRO:HG2  | 18:f:893:ILE:HD12 | 1.69                     | 0.73              |
| 26:K:121:LEU:CD2  | 26:K:160:GLY:HA3  | 2.18                     | 0.73              |
| 26:K:206:MET:HE1  | 26:K:215:ILE:HG21 | 1.70                     | 0.73              |
| 27:U:115:ASN:HB3  | 27:U:123:LYS:HD3  | 1.70                     | 0.73              |
| 27:U:127:ASP:OD2  | 27:U:130:LEU:N    | 2.18                     | 0.73              |
| 1:C:207:THR:HG23  | 1:C:209:CYS:H     | 1.54                     | 0.73              |
| 2:D:359:ASP:HB3   | 2:D:362:ASP:OD2   | 1.87                     | 0.73              |
| 9:V:79:VAL:HG21   | 9:V:120:PHE:CE2   | 2.23                     | 0.73              |
| 11:X:90:ARG:O     | 11:X:94:ASP:N     | 2.14                     | 0.73              |
| 14:a:84:VAL:HA    | 14:a:87:MET:HG3   | 1.68                     | 0.73              |
| 22:A:157:ILE:HD11 | 23:B:114:GLU:OE2  | 1.87                     | 0.73              |
| 24:E:277:MET:HE2  | 24:E:295:LEU:HD13 | 0.75                     | 0.73              |
| 25:F:254:PRO:CD   | 25:F:287:GLU:HB2  | 2.18                     | 0.73              |
| 27:U:798:PRO:O    | 27:U:880:ASN:ND2  | 2.21                     | 0.73              |
| 3:G:240:VAL:HA    | 10:W:94:ARG:HD3   | 1.70                     | 0.73              |
| 7:L:125:ARG:NH1   | 26:K:124:GLY:O    | 2.22                     | 0.73              |
| 9:V:71:THR:O      | 9:V:75:ILE:N      | 2.17                     | 0.73              |
| 9:V:75:ILE:O      | 9:V:79:VAL:N      | 2.17                     | 0.73              |
| 11:X:282:ARG:O    | 11:X:285:GLU:HG2  | 1.88                     | 0.73              |
| 15:b:16:MET:C     | 15:b:25:ARG:HD3   | 2.13                     | 0.73              |
| 15:b:97:LEU:CD2   | 15:b:107:MET:HE2  | 2.19                     | 0.73              |
| 18:f:485:LEU:CD2  | 18:f:501:LEU:HD21 | 2.18                     | 0.73              |
| 19:g:89:LEU:HD12  | 19:g:99:ASN:CB    | 2.18                     | 0.73              |
| 23:B:278:ALA:HB1  | 23:B:279:PRO:HD2  | 1.68                     | 0.73              |
| 2:D:354:LEU:HB3   | 2:D:358:VAL:HG11  | 1.70                     | 0.73              |
| 4:H:196:LYS:HA    | 4:H:203:MET:HE1   | 1.69                     | 0.73              |
| 6:J:7:ILE:HG12    | 6:J:18:GLN:HG2    | 1.69                     | 0.73              |
| 10:W:341:PHE:CZ   | 10:W:354:LEU:HD22 | 2.24                     | 0.73              |
| 13:Z:20:VAL:HG22  | 13:Z:126:VAL:CG2  | 2.17                     | 0.73              |
| 14:a:77:VAL:HA    | 14:a:80:ILE:CG1   | 2.19                     | 0.73              |
| 14:a:94:LEU:CD2   | 14:a:118:ILE:HA   | 2.16                     | 0.73              |
| 18:f:527:VAL:HA   | 18:f:564:LEU:O    | 1.88                     | 0.73              |
| 19:g:131:ILE:CG1  | 19:g:151:VAL:HG12 | 2.18                     | 0.73              |
| 27:U:587:ALA:HB1  | 27:U:624:PHE:HD2  | 1.52                     | 0.73              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:288:ASN:C     | 1:C:289:ILE:HD13  | 2.13                     | 0.73              |
| 1:C:338:LEU:HD22  | 1:C:342:ILE:HG21  | 1.70                     | 0.73              |
| 2:D:384:MET:HE3   | 24:E:167:PRO:HG3  | 1.71                     | 0.73              |
| 10:W:171:VAL:HG11 | 10:W:185:PHE:HB3  | 1.71                     | 0.73              |
| 17:d:143:LEU:O    | 17:d:147:ILE:N    | 2.14                     | 0.73              |
| 18:f:275:MET:HE2  | 18:f:275:MET:HA   | 1.71                     | 0.73              |
| 22:A:125:LEU:HD22 | 22:A:149:ILE:HB   | 1.70                     | 0.73              |
| 23:B:388:ASP:OD2  | 23:B:427:LEU:HD21 | 1.88                     | 0.73              |
| 24:E:46:ASP:HB3   | 25:F:139:LEU:HD22 | 1.71                     | 0.73              |
| 24:E:276:ILE:O    | 24:E:276:ILE:HG22 | 1.88                     | 0.73              |
| 27:U:141:CYS:HB2  | 27:U:150:ALA:HB2  | 1.71                     | 0.73              |
| 27:U:470:ASN:OD1  | 27:U:474:ARG:NH1  | 2.21                     | 0.73              |
| 4:H:83:TYR:HE1    | 4:H:134:LEU:HD21  | 1.54                     | 0.73              |
| 5:I:90:LEU:HD22   | 5:I:110:LEU:HD11  | 1.69                     | 0.73              |
| 5:I:135:LEU:HD21  | 5:I:162:THR:HG23  | 1.71                     | 0.73              |
| 9:V:375:PHE:CE2   | 9:V:398:LEU:HD23  | 2.24                     | 0.73              |
| 10:W:96:GLN:OE1   | 10:W:97:LEU:N     | 2.21                     | 0.73              |
| 17:d:88:LEU:CD1   | 17:d:143:LEU:HD11 | 2.19                     | 0.73              |
| 17:d:260:ILE:O    | 17:d:264:LEU:HG   | 1.88                     | 0.73              |
| 18:f:562:LEU:HD21 | 18:f:576:ILE:CG2  | 2.19                     | 0.73              |
| 19:g:129:ILE:HB   | 19:g:136:LEU:CG   | 2.19                     | 0.73              |
| 22:A:238:ILE:CG2  | 22:A:260:LEU:HD11 | 2.19                     | 0.73              |
| 27:U:465:LEU:HD21 | 27:U:500:ASN:HD21 | 1.54                     | 0.73              |
| 27:U:549:ALA:HA   | 27:U:581:SER:HB2  | 1.71                     | 0.73              |
| 1:C:406:LYS:HG2   | 5:I:64:LYS:HZ2    | 1.54                     | 0.72              |
| 3:G:80:MET:CE     | 3:G:138:MET:HG3   | 2.19                     | 0.72              |
| 4:H:106:PRO:HG2   | 4:H:109:GLN:CG    | 2.18                     | 0.72              |
| 9:V:70:VAL:O      | 9:V:74:ASP:N      | 2.18                     | 0.72              |
| 9:V:333:ILE:CD1   | 9:V:357:LEU:HD22  | 2.18                     | 0.72              |
| 9:V:438:VAL:CG1   | 9:V:451:ILE:HD11  | 2.19                     | 0.72              |
| 10:W:275:ILE:HG23 | 10:W:309:PHE:CE2  | 2.24                     | 0.72              |
| 11:X:331:LEU:CD2  | 11:X:364:LYS:HG2  | 2.19                     | 0.72              |
| 13:Z:101:LEU:CD2  | 13:Z:123:ILE:HD11 | 2.18                     | 0.72              |
| 14:a:177:LEU:CD2  | 14:a:200:LEU:HD21 | 2.17                     | 0.72              |
| 15:b:104:ASN:HB3  | 20:u:133:ALA:O    | 1.89                     | 0.72              |
| 15:b:121:GLU:HA   | 15:b:124:LEU:CD2  | 2.19                     | 0.72              |
| 17:d:141:LEU:HD12 | 17:d:182:LEU:HD11 | 1.71                     | 0.72              |
| 18:f:500:LEU:O    | 18:f:503:PRO:HD2  | 1.89                     | 0.72              |
| 23:B:251:VAL:CG1  | 23:B:254:GLU:HG3  | 2.16                     | 0.72              |
| 26:K:27:ALA:HB2   | 26:K:136:PRO:HG2  | 1.70                     | 0.72              |
| 26:K:186:HIS:CD2  | 26:K:189:MET:HE1  | 2.23                     | 0.72              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:226:GLU:OE2   | 1:C:229:ARG:NE    | 2.22                     | 0.72              |
| 9:V:276:PHE:CD1   | 9:V:277:PRO:HD2   | 2.23                     | 0.72              |
| 14:a:243:GLY:HA2  | 14:a:272:ILE:CD1  | 2.19                     | 0.72              |
| 18:f:386:GLY:HA2  | 18:f:418:LEU:HD13 | 1.71                     | 0.72              |
| 18:f:430:ASP:HB2  | 19:g:168:ASN:C    | 2.13                     | 0.72              |
| 18:f:692:LEU:HB3  | 18:f:800:LEU:HD12 | 1.69                     | 0.72              |
| 24:E:345:ASN:OD1  | 24:E:378:LYS:NZ   | 2.21                     | 0.72              |
| 25:F:314:LEU:HD21 | 25:F:342:LEU:CD2  | 2.19                     | 0.72              |
| 27:U:886:PRO:O    | 27:U:889:LEU:HD22 | 1.89                     | 0.72              |
| 1:C:229:ARG:HG2   | 1:C:229:ARG:HH11  | 1.54                     | 0.72              |
| 3:G:208:ILE:HD11  | 24:E:306:GLU:CD   | 2.13                     | 0.72              |
| 9:V:318:GLN:O     | 9:V:325:LYS:NZ    | 2.21                     | 0.72              |
| 12:Y:97:GLU:HA    | 12:Y:100:ILE:HG12 | 1.70                     | 0.72              |
| 14:a:222:LEU:HD21 | 14:a:237:LEU:HD23 | 1.71                     | 0.72              |
| 19:g:86:GLU:OE1   | 19:g:152:LYS:HG2  | 1.89                     | 0.72              |
| 19:g:166:ARG:C    | 19:g:170:GLN:HB2  | 2.14                     | 0.72              |
| 24:E:235:ILE:HD13 | 24:E:277:MET:HB2  | 1.55                     | 0.72              |
| 27:U:748:LEU:H    | 27:U:748:LEU:HD12 | 1.54                     | 0.72              |
| 1:C:24:TYR:HB2    | 2:D:40:LEU:CD2    | 2.15                     | 0.72              |
| 1:C:79:ALA:HB3    | 22:A:65:ILE:HD13  | 1.71                     | 0.72              |
| 1:C:314:LYS:HZ1   | 23:B:429:LYS:HB3  | 1.52                     | 0.72              |
| 1:C:338:LEU:CD2   | 1:C:342:ILE:HG12  | 2.18                     | 0.72              |
| 4:H:40:ALA:HB2    | 4:H:187:ALA:HB2   | 1.71                     | 0.72              |
| 14:a:37:LEU:O     | 14:a:41:VAL:HG23  | 1.88                     | 0.72              |
| 14:a:180:LEU:HD12 | 14:a:219:HIS:NE2  | 2.04                     | 0.72              |
| 14:a:296:ILE:HG21 | 14:a:307:VAL:HG23 | 1.72                     | 0.72              |
| 15:b:11:ASP:OD1   | 15:b:12:ASN:N     | 2.23                     | 0.72              |
| 17:d:244:VAL:HG11 | 17:d:267:ILE:CD1  | 2.19                     | 0.72              |
| 19:g:93:LEU:N     | 19:g:157:GLU:OE1  | 2.22                     | 0.72              |
| 19:g:129:ILE:HB   | 19:g:136:LEU:HG   | 1.71                     | 0.72              |
| 19:g:158:LEU:CD2  | 19:g:165:ALA:HB3  | 2.19                     | 0.72              |
| 23:B:364:ILE:HG22 | 23:B:395:ILE:HG21 | 1.71                     | 0.72              |
| 23:B:387:LYS:HE2  | 23:B:387:LYS:CA   | 2.13                     | 0.72              |
| 24:E:40:TYR:HE2   | 25:F:72:LYS:HE2   | 1.55                     | 0.72              |
| 27:U:545:LEU:HB3  | 27:U:577:ILE:HG21 | 1.71                     | 0.72              |
| 3:G:200:THR:O     | 3:G:204:THR:HG23  | 1.89                     | 0.72              |
| 4:H:10:LEU:CD1    | 4:H:21:GLN:HB3    | 2.18                     | 0.72              |
| 4:H:214:ASN:OD1   | 4:H:216:ALA:N     | 2.19                     | 0.72              |
| 5:I:38:LEU:O      | 5:I:180:LYS:NZ    | 2.23                     | 0.72              |
| 7:L:125:ARG:HH12  | 26:K:125:GLU:HA   | 1.52                     | 0.72              |
| 10:W:122:LEU:HA   | 10:W:125:ILE:HD11 | 1.71                     | 0.72              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 11:X:62:GLN:HB3   | 11:X:65:GLU:HB2   | 1.71                     | 0.72              |
| 11:X:345:VAL:CG1  | 11:X:350:ILE:HD11 | 2.19                     | 0.72              |
| 14:a:51:ALA:CB    | 14:a:86:GLN:HG2   | 2.19                     | 0.72              |
| 16:c:129:THR:O    | 16:c:132:SER:OG   | 2.06                     | 0.72              |
| 17:d:114:GLU:O    | 17:d:118:ARG:NH1  | 2.22                     | 0.72              |
| 18:f:423:ASP:HA   | 19:g:156:LEU:CD1  | 2.19                     | 0.72              |
| 22:A:366:ARG:O    | 22:A:367:ASP:HB3  | 1.89                     | 0.72              |
| 23:B:388:ASP:OD2  | 23:B:390:LEU:HD13 | 1.89                     | 0.72              |
| 24:E:172:LEU:HB3  | 24:E:301:ILE:HD11 | 1.72                     | 0.72              |
| 24:E:351:GLY:HA3  | 25:F:217:ILE:HD11 | 1.71                     | 0.72              |
| 25:F:384:LEU:HD11 | 25:F:420:TYR:CB   | 2.19                     | 0.72              |
| 27:U:443:LEU:HD23 | 27:U:477:GLY:CA   | 2.20                     | 0.72              |
| 1:C:127:LEU:HD11  | 2:D:96:VAL:HG21   | 1.70                     | 0.72              |
| 3:G:80:MET:HE2    | 3:G:91:VAL:CG2    | 2.18                     | 0.72              |
| 3:G:190:THR:OG1   | 3:G:193:GLN:OE1   | 2.02                     | 0.72              |
| 10:W:313:GLU:OE2  | 14:a:313:LYS:HD3  | 1.90                     | 0.72              |
| 14:a:112:ILE:CD1  | 14:a:138:VAL:HG21 | 2.16                     | 0.72              |
| 19:g:125:ASN:HA   | 19:g:161:SER:OG   | 1.89                     | 0.72              |
| 23:B:121:ALA:CB   | 23:B:135:ILE:HD11 | 2.20                     | 0.72              |
| 27:U:448:LEU:HD22 | 27:U:483:LEU:HD23 | 1.71                     | 0.72              |
| 8:M:33:SER:HB2    | 8:M:79:GLY:HA2    | 1.70                     | 0.72              |
| 9:V:363:LEU:HD21  | 9:V:395:ILE:HD12  | 1.71                     | 0.72              |
| 10:W:26:GLN:O     | 10:W:29:PRO:HD2   | 1.89                     | 0.72              |
| 15:b:16:MET:O     | 15:b:16:MET:HE3   | 1.90                     | 0.72              |
| 18:f:187:LEU:O    | 18:f:191:ILE:HG22 | 1.89                     | 0.72              |
| 18:f:402:ASN:HB3  | 18:f:406:GLY:HA3  | 1.70                     | 0.72              |
| 19:g:88:PHE:N     | 19:g:153:ALA:O    | 2.21                     | 0.72              |
| 19:g:114:SER:CA   | 19:g:124:GLU:HG3  | 2.20                     | 0.72              |
| 22:A:72:LEU:HD22  | 23:B:96:ARG:HH21  | 1.53                     | 0.72              |
| 23:B:257:GLN:CB   | 23:B:262:ASP:HB3  | 2.19                     | 0.72              |
| 27:U:101:ILE:HG13 | 27:U:102:ALA:N    | 2.04                     | 0.72              |
| 27:U:137:MET:CE   | 27:U:140:ARG:HD3  | 2.20                     | 0.72              |
| 1:C:113:ARG:CD    | 1:C:130:LYS:HB2   | 2.18                     | 0.72              |
| 2:D:178:ARG:HG2   | 2:D:182:GLU:OE1   | 1.88                     | 0.72              |
| 2:D:203:LEU:HD23  | 2:D:330:LYS:HG2   | 1.71                     | 0.72              |
| 4:H:73:GLY:C      | 4:H:74:LEU:HD23   | 2.14                     | 0.72              |
| 5:I:71:ASP:CB     | 5:I:223:THR:HG21  | 2.20                     | 0.72              |
| 8:M:65:ARG:NH2    | 8:M:78:ALA:HA     | 2.03                     | 0.72              |
| 9:V:86:VAL:HG13   | 9:V:200:ARG:HH12  | 1.53                     | 0.72              |
| 9:V:131:LEU:CD1   | 9:V:171:VAL:HG21  | 2.19                     | 0.72              |
| 10:W:394:SER:O    | 10:W:398:VAL:HG23 | 1.90                     | 0.72              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 11:X:57:LEU:HD22  | 11:X:66:LEU:HD13  | 1.72                     | 0.72              |
| 11:X:225:TRP:O    | 11:X:228:ALA:N    | 2.22                     | 0.72              |
| 15:b:186:SER:HB3  | 15:b:187:PRO:HD3  | 1.72                     | 0.72              |
| 19:g:88:PHE:HB2   | 19:g:154:MET:HA   | 1.71                     | 0.72              |
| 22:A:356:LYS:O    | 22:A:360:ARG:HG3  | 1.90                     | 0.72              |
| 23:B:197:ILE:HG13 | 23:B:197:ILE:O    | 1.88                     | 0.72              |
| 24:E:73:ALA:HB3   | 24:E:76:GLY:HA3   | 1.72                     | 0.72              |
| 25:F:177:VAL:CG1  | 25:F:179:GLU:HG3  | 2.19                     | 0.72              |
| 2:D:355:SER:HB2   | 2:D:393:ILE:HG21  | 1.71                     | 0.72              |
| 5:I:45:LEU:HD11   | 5:I:137:ILE:HG23  | 1.72                     | 0.72              |
| 11:X:194:ARG:NH2  | 11:X:210:LEU:O    | 2.23                     | 0.72              |
| 14:a:159:SER:O    | 14:a:168:ASN:ND2  | 2.23                     | 0.72              |
| 17:d:90:ALA:O     | 17:d:94:MET:N     | 2.20                     | 0.72              |
| 17:d:200:LEU:HD23 | 17:d:263:LEU:HD21 | 1.72                     | 0.72              |
| 19:g:117:ALA:HB1  | 19:g:122:LEU:O    | 1.89                     | 0.72              |
| 19:g:170:GLN:HG2  | 19:g:173:GLU:CG   | 2.11                     | 0.72              |
| 22:A:213:LEU:HD11 | 22:A:321:THR:HG21 | 1.72                     | 0.72              |
| 25:F:362:ARG:NE   | 25:F:388:THR:O    | 2.22                     | 0.72              |
| 3:G:38:THR:CG2    | 3:G:202:LEU:HD11  | 2.19                     | 0.72              |
| 3:G:72:ILE:HG21   | 3:G:114:LEU:HD21  | 1.70                     | 0.72              |
| 3:G:171:LYS:HA    | 3:G:171:LYS:CE    | 2.12                     | 0.72              |
| 9:V:228:ARG:O     | 9:V:232:HIS:HB2   | 1.90                     | 0.72              |
| 9:V:311:ASN:OD1   | 9:V:314:ARG:NH2   | 2.22                     | 0.72              |
| 13:Z:73:ASP:OD2   | 15:b:63:THR:HB    | 1.89                     | 0.72              |
| 22:A:60:ASN:O     | 22:A:64:GLY:N     | 2.23                     | 0.72              |
| 22:A:121:PHE:CE2  | 25:F:89:LEU:HD13  | 2.25                     | 0.72              |
| 25:F:247:THR:HB   | 25:F:281:SER:CB   | 2.20                     | 0.72              |
| 27:U:427:LEU:HD12 | 27:U:438:GLN:CG   | 2.20                     | 0.72              |
| 27:U:474:ARG:NH2  | 27:U:500:ASN:OD1  | 2.21                     | 0.72              |
| 27:U:588:MET:HE1  | 27:U:760:VAL:HG12 | 1.71                     | 0.72              |
| 1:C:159:LYS:HD3   | 22:A:22:ILE:O     | 1.89                     | 0.71              |
| 1:C:232:ARG:HH12  | 1:C:275:GLU:CD    | 1.98                     | 0.71              |
| 1:C:258:ARG:HD3   | 1:C:273:MET:HE2   | 1.70                     | 0.71              |
| 1:C:336:MET:HE3   | 1:C:378:VAL:HG21  | 1.72                     | 0.71              |
| 7:L:49:LEU:HD21   | 7:L:199:LEU:HD21  | 1.72                     | 0.71              |
| 7:L:60:GLN:HG2    | 25:F:439:ALA:CB   | 2.20                     | 0.71              |
| 12:Y:49:ASN:HA    | 12:Y:73:MET:CE    | 2.15                     | 0.71              |
| 14:a:101:ARG:HD2  | 14:a:111:VAL:HG23 | 1.71                     | 0.71              |
| 14:a:148:VAL:HG13 | 14:a:151:VAL:HG22 | 1.70                     | 0.71              |
| 18:f:109:ILE:HG12 | 18:f:113:MET:HB2  | 1.72                     | 0.71              |
| 18:f:270:LEU:HD13 | 18:f:787:LEU:HD11 | 1.72                     | 0.71              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 18:f:567:LEU:HA   | 18:f:598:CYS:O    | 1.89                     | 0.71              |
| 23:B:151:LEU:N    | 23:B:161:GLY:O    | 2.16                     | 0.71              |
| 23:B:358:GLU:OE1  | 23:B:387:LYS:NZ   | 2.23                     | 0.71              |
| 1:C:135:VAL:HA    | 1:C:138:MET:CE    | 2.19                     | 0.71              |
| 13:Z:147:ASP:HB3  | 14:a:215:GLU:OE1  | 1.89                     | 0.71              |
| 14:a:45:VAL:HG21  | 14:a:79:ILE:CD1   | 2.19                     | 0.71              |
| 17:d:123:LEU:HA   | 17:d:126:LEU:HB2  | 1.72                     | 0.71              |
| 4:H:39:LYS:NZ     | 4:H:144:PRO:HG2   | 2.04                     | 0.71              |
| 10:W:98:LYS:HD2   | 10:W:137:TYR:CD1  | 2.24                     | 0.71              |
| 11:X:267:VAL:HG11 | 11:X:291:ALA:CB   | 2.20                     | 0.71              |
| 14:a:22:TRP:O     | 14:a:25:LEU:HG    | 1.90                     | 0.71              |
| 18:f:505:MET:HB3  | 18:f:541:THR:HG21 | 1.72                     | 0.71              |
| 19:g:89:LEU:HD23  | 19:g:155:VAL:HB   | 1.72                     | 0.71              |
| 24:E:180:LYS:HG2  | 24:E:301:ILE:HG13 | 1.72                     | 0.71              |
| 25:F:268:VAL:HG11 | 25:F:313:LEU:CB   | 2.19                     | 0.71              |
| 26:K:40:ILE:HB    | 26:K:47:CYS:SG    | 2.30                     | 0.71              |
| 26:K:137:PHE:O    | 26:K:158:PRO:HB3  | 1.89                     | 0.71              |
| 27:U:12:LEU:HD22  | 27:U:45:ILE:CD1   | 2.21                     | 0.71              |
| 27:U:521:LEU:HD12 | 27:U:522:GLY:N    | 2.05                     | 0.71              |
| 27:U:634:PRO:O    | 27:U:638:SER:OG   | 2.09                     | 0.71              |
| 5:I:32:GLY:N      | 5:I:50:ARG:HD2    | 2.04                     | 0.71              |
| 7:L:109:VAL:HG22  | 7:L:134:ILE:HD12  | 1.71                     | 0.71              |
| 8:M:69:VAL:HG11   | 8:M:111:LEU:HD21  | 1.72                     | 0.71              |
| 14:a:97:LEU:CD1   | 14:a:114:CYS:HB3  | 2.20                     | 0.71              |
| 15:b:17:ARG:HD3   | 15:b:81:LYS:NZ    | 2.05                     | 0.71              |
| 18:f:103:TYR:HD2  | 18:f:107:LYS:HB2  | 1.55                     | 0.71              |
| 22:A:135:GLU:N    | 22:A:138:MET:SD   | 2.64                     | 0.71              |
| 23:B:374:LEU:HG   | 23:B:378:VAL:HG11 | 1.71                     | 0.71              |
| 25:F:172:VAL:HG12 | 25:F:274:LEU:HD22 | 1.72                     | 0.71              |
| 27:U:422:LEU:HG   | 27:U:426:TYR:CE2  | 2.24                     | 0.71              |
| 27:U:489:ALA:HA   | 27:U:520:MET:CE   | 2.19                     | 0.71              |
| 1:C:220:VAL:HG22  | 1:C:269:VAL:HG23  | 1.71                     | 0.71              |
| 4:H:71:HIS:NE2    | 4:H:72:ILE:HD11   | 2.06                     | 0.71              |
| 4:H:135:LEU:HD22  | 4:H:146:LEU:HD21  | 1.70                     | 0.71              |
| 14:a:149:THR:HA   | 14:a:152:HIS:ND1  | 2.05                     | 0.71              |
| 17:d:88:LEU:HD13  | 17:d:143:LEU:HD11 | 1.73                     | 0.71              |
| 18:f:221:ILE:CD1  | 18:f:229:VAL:HG11 | 2.20                     | 0.71              |
| 18:f:553:THR:O    | 18:f:556:ARG:HB3  | 1.91                     | 0.71              |
| 19:g:111:GLU:OE1  | 19:g:111:GLU:N    | 2.23                     | 0.71              |
| 19:g:128:LYS:CD   | 19:g:162:GLU:HB2  | 2.21                     | 0.71              |
| 24:E:167:PRO:O    | 24:E:274:LYS:HE3  | 1.89                     | 0.71              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:362:VAL:HG23  | 1:C:390:VAL:HG11  | 1.72                     | 0.71              |
| 8:M:187:ARG:NH1   | 8:M:187:ARG:O     | 2.24                     | 0.71              |
| 9:V:349:ARG:NH2   | 28:e:37:HIS:O     | 2.23                     | 0.71              |
| 10:W:214:PHE:HB3  | 10:W:223:LYS:HB2  | 1.71                     | 0.71              |
| 10:W:359:VAL:HG13 | 10:W:382:LEU:HD22 | 1.71                     | 0.71              |
| 18:f:343:LYS:HD3  | 18:f:773:LYS:HE2  | 1.72                     | 0.71              |
| 19:g:130:VAL:HG12 | 19:g:135:GLN:HG2  | 1.72                     | 0.71              |
| 19:g:165:ALA:HB1  | 19:g:169:PHE:H    | 1.53                     | 0.71              |
| 22:A:191:VAL:HG11 | 22:A:229:VAL:HG11 | 1.72                     | 0.71              |
| 25:F:247:THR:HB   | 25:F:281:SER:HB2  | 1.72                     | 0.71              |
| 27:U:11:LEU:HD22  | 27:U:19:LEU:HD11  | 1.72                     | 0.71              |
| 27:U:606:ALA:HB1  | 27:U:619:VAL:HG23 | 1.72                     | 0.71              |
| 27:U:638:SER:HA   | 27:U:671:LEU:HD11 | 1.70                     | 0.71              |
| 2:D:259:PRO:HB3   | 2:D:304:ASN:HB3   | 1.72                     | 0.71              |
| 5:I:153:SER:OG    | 5:I:155:ASN:ND2   | 2.23                     | 0.71              |
| 9:V:77:GLU:O      | 9:V:81:GLN:HG2    | 1.91                     | 0.71              |
| 10:W:445:LEU:HB3  | 13:Z:226:ILE:HG21 | 1.73                     | 0.71              |
| 12:Y:181:LYS:HG2  | 12:Y:200:LEU:CD1  | 2.19                     | 0.71              |
| 14:a:57:ILE:HA    | 14:a:60:TYR:HB3   | 1.72                     | 0.71              |
| 14:a:122:LYS:NZ   | 14:a:126:GLY:O    | 2.17                     | 0.71              |
| 14:a:148:VAL:O    | 14:a:149:THR:OG1  | 2.06                     | 0.71              |
| 17:d:85:GLY:O     | 17:d:89:GLN:N     | 2.20                     | 0.71              |
| 18:f:217:LEU:O    | 18:f:221:ILE:HG13 | 1.90                     | 0.71              |
| 18:f:351:THR:HA   | 18:f:354:GLU:OE1  | 1.91                     | 0.71              |
| 18:f:377:VAL:O    | 18:f:381:VAL:HB   | 1.91                     | 0.71              |
| 18:f:431:LYS:HA   | 19:g:171:LEU:HB3  | 1.71                     | 0.71              |
| 18:f:831:VAL:HA   | 18:f:871:PRO:HA   | 1.72                     | 0.71              |
| 19:g:112:LEU:HD13 | 19:g:142:LEU:CD2  | 2.21                     | 0.71              |
| 24:E:172:LEU:HD23 | 24:E:299:ILE:HB   | 1.71                     | 0.71              |
| 27:U:462:LEU:CD1  | 27:U:496:LEU:HD23 | 2.20                     | 0.71              |
| 27:U:707:ASN:O    | 27:U:711:GLN:NE2  | 2.23                     | 0.71              |
| 5:I:92:LEU:HD21   | 5:I:96:ARG:HH11   | 1.55                     | 0.71              |
| 9:V:111:TYR:CZ    | 9:V:115:LYS:HG3   | 2.26                     | 0.71              |
| 12:Y:362:LYS:NZ   | 13:Z:255:ASP:OD2  | 2.22                     | 0.71              |
| 14:a:62:ASN:O     | 14:a:66:GLU:N     | 2.23                     | 0.71              |
| 14:a:73:PRO:O     | 14:a:77:VAL:HG12  | 1.91                     | 0.71              |
| 15:b:63:THR:O     | 15:b:65:THR:HG23  | 1.91                     | 0.71              |
| 17:d:116:LEU:HD21 | 17:d:150:ILE:HG22 | 1.72                     | 0.71              |
| 18:f:446:LEU:HD21 | 18:f:480:GLY:HA2  | 1.73                     | 0.71              |
| 18:f:594:LEU:O    | 18:f:597:VAL:HG12 | 1.90                     | 0.71              |
| 27:U:250:PHE:HZ   | 27:U:333:MET:HG2  | 1.56                     | 0.71              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:400:SER:HB3   | 4:H:26:LEU:HD22   | 1.72                     | 0.71              |
| 5:I:135:LEU:HG    | 5:I:164:ILE:CD1   | 2.20                     | 0.71              |
| 6:J:132:LEU:CD2   | 6:J:146:GLN:HB2   | 2.21                     | 0.71              |
| 6:J:171:PHE:CE2   | 6:J:194:ALA:HA    | 2.25                     | 0.71              |
| 7:L:36:VAL:HG21   | 7:L:194:ALA:HB3   | 1.73                     | 0.71              |
| 10:W:267:LEU:O    | 10:W:271:VAL:HG12 | 1.91                     | 0.71              |
| 12:Y:56:ALA:HA    | 12:Y:59:LYS:HD3   | 1.73                     | 0.71              |
| 12:Y:134:LEU:HD12 | 12:Y:134:LEU:O    | 1.90                     | 0.71              |
| 14:a:249:GLN:O    | 14:a:253:THR:HG22 | 1.90                     | 0.71              |
| 17:d:156:ILE:HD12 | 17:d:255:SER:CB   | 2.20                     | 0.71              |
| 18:f:447:ALA:HA   | 18:f:450:ILE:HG22 | 1.71                     | 0.71              |
| 18:f:878:GLU:OE1  | 18:f:878:GLU:HA   | 1.90                     | 0.71              |
| 22:A:52:ILE:HD11  | 23:B:69:LYS:HA    | 1.73                     | 0.71              |
| 25:F:198:LEU:HD22 | 25:F:240:CYS:SG   | 2.30                     | 0.71              |
| 25:F:268:VAL:HG11 | 25:F:313:LEU:HB2  | 1.73                     | 0.71              |
| 27:U:101:ILE:O    | 27:U:105:ILE:HG12 | 1.91                     | 0.71              |
| 27:U:195:ASN:O    | 27:U:199:ARG:HG2  | 1.89                     | 0.71              |
| 27:U:900:TYR:CB   | 27:U:914:LEU:HD21 | 2.21                     | 0.71              |
| 1:C:277:LEU:O     | 1:C:310:ARG:NE    | 2.24                     | 0.71              |
| 2:D:369:LYS:HE3   | 2:D:369:LYS:CA    | 2.06                     | 0.71              |
| 5:I:195:LYS:HD2   | 5:I:195:LYS:C     | 2.16                     | 0.71              |
| 9:V:76:LYS:O      | 9:V:80:LYS:HB3    | 1.91                     | 0.71              |
| 9:V:493:ALA:C     | 9:V:495:ARG:H     | 1.97                     | 0.71              |
| 10:W:17:GLU:HG2   | 10:W:58:SER:HB2   | 1.72                     | 0.71              |
| 11:X:368:MET:HE2  | 11:X:374:PHE:HD1  | 1.56                     | 0.71              |
| 11:X:409:LYS:HD2  | 16:c:256:ASN:HD21 | 1.55                     | 0.71              |
| 12:Y:41:LEU:O     | 12:Y:45:VAL:HG23  | 1.89                     | 0.71              |
| 12:Y:97:GLU:HA    | 12:Y:100:ILE:CG1  | 2.21                     | 0.71              |
| 12:Y:348:ASP:HB3  | 12:Y:353:ILE:O    | 1.91                     | 0.71              |
| 27:U:199:ARG:HD2  | 27:U:223:LEU:CD1  | 2.20                     | 0.71              |
| 8:M:75:MET:HE1    | 8:M:88:ALA:HA     | 1.73                     | 0.70              |
| 10:W:127:THR:O    | 10:W:131:VAL:HG22 | 1.91                     | 0.70              |
| 13:Z:139:ILE:HG22 | 13:Z:140:SER:H    | 1.56                     | 0.70              |
| 14:a:109:GLU:OE1  | 14:a:112:ILE:HG22 | 1.90                     | 0.70              |
| 15:b:104:ASN:OD1  | 15:b:105:HIS:ND1  | 2.23                     | 0.70              |
| 17:d:178:TYR:HB3  | 17:d:182:LEU:HG   | 1.73                     | 0.70              |
| 22:A:369:ARG:NH2  | 26:K:206:MET:O    | 2.23                     | 0.70              |
| 26:K:235:GLU:N    | 26:K:235:GLU:OE1  | 2.21                     | 0.70              |
| 27:U:341:PHE:CE2  | 27:U:787:CYS:HB3  | 2.26                     | 0.70              |
| 2:D:154:LEU:HD11  | 24:E:267:PHE:CE1  | 2.26                     | 0.70              |
| 2:D:410:ASP:HB2   | 2:D:413:GLU:CG    | 2.21                     | 0.70              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 9:V:169:LEU:HA    | 9:V:172:VAL:HB    | 1.73                     | 0.70              |
| 14:a:78:GLU:HA    | 14:a:81:LEU:CD2   | 2.21                     | 0.70              |
| 18:f:71:TYR:CD2   | 18:f:113:MET:HG3  | 2.27                     | 0.70              |
| 18:f:433:LEU:H    | 19:g:172:GLU:HG3  | 1.54                     | 0.70              |
| 18:f:527:VAL:HG11 | 18:f:794:ALA:CB   | 2.21                     | 0.70              |
| 26:K:140:ALA:HB1  | 26:K:156:MET:O    | 1.90                     | 0.70              |
| 27:U:27:LEU:O     | 27:U:31:VAL:N     | 2.24                     | 0.70              |
| 27:U:115:ASN:HD22 | 27:U:123:LYS:HG2  | 1.54                     | 0.70              |
| 7:L:158:ALA:O     | 8:M:57:LEU:HD22   | 1.91                     | 0.70              |
| 9:V:322:VAL:O     | 9:V:326:GLN:HG3   | 1.91                     | 0.70              |
| 11:X:187:ARG:HD3  | 11:X:221:GLU:OE2  | 1.91                     | 0.70              |
| 17:d:146:ASP:O    | 17:d:150:ILE:N    | 2.22                     | 0.70              |
| 17:d:177:ASP:OD1  | 27:U:2:ILE:N      | 2.24                     | 0.70              |
| 18:f:606:VAL:HG12 | 27:U:835:ILE:HD11 | 1.72                     | 0.70              |
| 3:G:208:ILE:HD12  | 24:E:306:GLU:CD   | 2.15                     | 0.70              |
| 11:X:173:GLU:HA   | 11:X:176:THR:HG22 | 1.74                     | 0.70              |
| 14:a:94:LEU:HD11  | 14:a:118:ILE:CB   | 2.21                     | 0.70              |
| 14:a:94:LEU:HD11  | 14:a:118:ILE:CG1  | 2.20                     | 0.70              |
| 15:b:30:GLN:HG3   | 15:b:75:LEU:HD13  | 1.73                     | 0.70              |
| 15:b:132:LYS:HD2  | 15:b:159:THR:O    | 1.92                     | 0.70              |
| 15:b:184:ILE:O    | 15:b:188:ILE:HG22 | 1.91                     | 0.70              |
| 18:f:542:ILE:O    | 18:f:545:LYS:HG2  | 1.90                     | 0.70              |
| 27:U:78:LEU:HD21  | 27:U:103:LYS:HB2  | 1.72                     | 0.70              |
| 27:U:347:ASN:HB3  | 27:U:813:TYR:HE2  | 1.56                     | 0.70              |
| 2:D:383:GLY:HA3   | 24:E:164:ILE:CD1  | 2.22                     | 0.70              |
| 3:G:132:ARG:NH1   | 8:M:20:VAL:HG21   | 2.06                     | 0.70              |
| 7:L:70:ILE:HG12   | 7:L:105:VAL:HG22  | 1.73                     | 0.70              |
| 9:V:79:VAL:HG13   | 9:V:163:VAL:CG1   | 2.22                     | 0.70              |
| 14:a:94:LEU:CD1   | 14:a:118:ILE:HD12 | 2.22                     | 0.70              |
| 15:b:32:ALA:O     | 15:b:35:ILE:HG22  | 1.91                     | 0.70              |
| 15:b:117:VAL:O    | 15:b:152:LYS:NZ   | 2.21                     | 0.70              |
| 16:c:177:THR:HB   | 27:U:774:PRO:HD3  | 1.72                     | 0.70              |
| 17:d:194:LEU:HD12 | 17:d:194:LEU:H    | 1.54                     | 0.70              |
| 18:f:431:LYS:N    | 19:g:172:GLU:HB2  | 2.06                     | 0.70              |
| 18:f:539:LEU:HA   | 18:f:542:ILE:CD1  | 2.21                     | 0.70              |
| 18:f:606:VAL:CG1  | 27:U:835:ILE:HD11 | 2.22                     | 0.70              |
| 27:U:108:TYR:CD2  | 27:U:134:VAL:HG11 | 2.25                     | 0.70              |
| 27:U:680:VAL:HB   | 27:U:683:VAL:CG1  | 2.22                     | 0.70              |
| 3:G:79:VAL:CG1    | 3:G:139:ILE:HD12  | 2.21                     | 0.70              |
| 5:I:86:LEU:HG     | 5:I:114:LEU:HD21  | 1.72                     | 0.70              |
| 9:V:173:ILE:HG12  | 9:V:213:TYR:CE2   | 2.27                     | 0.70              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 9:V:437:ILE:HD13  | 17:d:238:GLU:O    | 1.91                     | 0.70              |
| 10:W:259:GLU:HG3  | 10:W:262:LYS:HB2  | 1.73                     | 0.70              |
| 12:Y:309:GLU:HA   | 12:Y:309:GLU:OE2  | 1.90                     | 0.70              |
| 17:d:151:GLY:HA2  | 17:d:154:TRP:HB3  | 1.74                     | 0.70              |
| 18:f:326:LEU:HD21 | 18:f:420:TRP:CE3  | 2.27                     | 0.70              |
| 22:A:230:ALA:HA   | 22:A:233:THR:HG23 | 1.74                     | 0.70              |
| 24:E:203:ILE:HD11 | 24:E:238:ILE:HG12 | 1.72                     | 0.70              |
| 1:C:154:LEU:O     | 1:C:158:ILE:HD12  | 1.92                     | 0.70              |
| 5:I:45:LEU:CD1    | 5:I:137:ILE:HD13  | 2.21                     | 0.70              |
| 14:a:275:LEU:O    | 14:a:279:GLU:HG2  | 1.91                     | 0.70              |
| 15:b:147:GLU:CG   | 15:b:150:THR:HG23 | 2.21                     | 0.70              |
| 4:H:80:GLY:O      | 4:H:83:TYR:N      | 2.20                     | 0.70              |
| 14:a:215:GLU:N    | 14:a:215:GLU:OE2  | 2.24                     | 0.70              |
| 18:f:86:THR:HG22  | 18:f:154:TRP:O    | 1.91                     | 0.70              |
| 18:f:282:PHE:CD2  | 18:f:294:MET:HE2  | 2.26                     | 0.70              |
| 18:f:513:GLU:HB2  | 18:f:554:TYR:CE2  | 2.26                     | 0.70              |
| 25:F:341:ALA:O    | 25:F:347:ARG:HD2  | 1.92                     | 0.70              |
| 27:U:372:ALA:HB2  | 27:U:731:ILE:HG22 | 1.74                     | 0.70              |
| 27:U:501:LEU:HD12 | 27:U:544:ILE:HD11 | 1.74                     | 0.70              |
| 27:U:509:GLY:CA   | 27:U:544:ILE:HG13 | 2.19                     | 0.70              |
| 27:U:641:SER:OG   | 27:U:642:GLU:OE1  | 2.10                     | 0.70              |
| 1:C:161:ILE:HD11  | 1:C:292:ILE:CD1   | 2.21                     | 0.70              |
| 8:M:87:LEU:HD13   | 8:M:131:PHE:CE2   | 2.27                     | 0.70              |
| 10:W:383:ASP:O    | 10:W:384:LEU:HD23 | 1.92                     | 0.70              |
| 12:Y:280:GLN:NE2  | 28:e:53:SER:OG    | 2.24                     | 0.70              |
| 14:a:90:PRO:HA    | 14:a:121:LEU:HD22 | 1.72                     | 0.70              |
| 14:a:173:TYR:O    | 14:a:177:LEU:HG   | 1.91                     | 0.70              |
| 14:a:173:TYR:CE1  | 14:a:177:LEU:HD11 | 2.27                     | 0.70              |
| 18:f:63:LEU:HD13  | 18:f:106:LEU:HD11 | 1.72                     | 0.70              |
| 18:f:245:ASN:OD1  | 18:f:246:SER:N    | 2.24                     | 0.70              |
| 19:g:145:GLN:HG3  | 19:g:147:VAL:HG23 | 1.73                     | 0.70              |
| 22:A:120:LYS:HB2  | 25:F:90:VAL:HG12  | 1.74                     | 0.70              |
| 26:K:206:MET:CE   | 26:K:215:ILE:HG21 | 2.21                     | 0.70              |
| 27:U:532:MET:HB3  | 27:U:552:ILE:CG2  | 2.21                     | 0.70              |
| 3:G:36:GLY:C      | 3:G:37:LEU:HD23   | 2.16                     | 0.70              |
| 7:L:40:SER:HB2    | 7:L:182:CYS:HB2   | 1.73                     | 0.70              |
| 10:W:307:LYS:O    | 10:W:311:THR:HG23 | 1.91                     | 0.70              |
| 15:b:53:THR:CG2   | 15:b:59:GLU:HB2   | 2.22                     | 0.70              |
| 17:d:311:GLY:HA3  | 17:d:315:TYR:O    | 1.92                     | 0.70              |
| 18:f:845:ARG:HB3  | 18:f:881:GLU:OE2  | 1.92                     | 0.70              |
| 23:B:119:ASN:C    | 23:B:120:HIS:HD1  | 1.98                     | 0.70              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 23:B:394:ASP:O    | 23:B:398:ILE:HG22 | 1.92                     | 0.70              |
| 24:E:149:ILE:HD11 | 24:E:276:ILE:HG12 | 1.74                     | 0.70              |
| 2:D:264:ILE:HG21  | 2:D:267:ILE:HD13  | 1.73                     | 0.69              |
| 3:G:196:GLU:O     | 3:G:199:ILE:HG22  | 1.92                     | 0.69              |
| 3:G:232:GLU:HA    | 3:G:235:ILE:HD13  | 1.74                     | 0.69              |
| 6:J:76:LEU:HD23   | 6:J:76:LEU:H      | 1.56                     | 0.69              |
| 9:V:438:VAL:HG11  | 9:V:458:VAL:HG21  | 1.74                     | 0.69              |
| 10:W:210:ASN:OD1  | 10:W:211:THR:N    | 2.25                     | 0.69              |
| 10:W:230:MET:HE1  | 10:W:233:LEU:CD2  | 2.20                     | 0.69              |
| 10:W:375:MET:HE1  | 10:W:390:GLU:HG2  | 1.74                     | 0.69              |
| 17:d:126:LEU:HB3  | 17:d:140:GLN:HE21 | 1.57                     | 0.69              |
| 18:f:769:THR:HG23 | 18:f:770:HIS:ND1  | 2.07                     | 0.69              |
| 18:f:806:VAL:O    | 18:f:810:ILE:N    | 2.24                     | 0.69              |
| 22:A:364:VAL:HG21 | 22:A:368:ILE:HG13 | 1.72                     | 0.69              |
| 23:B:223:ILE:CG2  | 23:B:350:LYS:HG2  | 2.22                     | 0.69              |
| 23:B:414:VAL:HG23 | 23:B:418:ASP:CB   | 2.21                     | 0.69              |
| 24:E:33:LEU:HD21  | 25:F:66:LEU:HA    | 1.74                     | 0.69              |
| 27:U:169:GLU:O    | 27:U:171:ASN:ND2  | 2.20                     | 0.69              |
| 27:U:198:LEU:HB3  | 27:U:223:LEU:HG   | 1.72                     | 0.69              |
| 27:U:472:ILE:H    | 27:U:472:ILE:HD12 | 1.55                     | 0.69              |
| 27:U:689:ILE:HD11 | 27:U:729:GLY:HA2  | 1.74                     | 0.69              |
| 1:C:77:VAL:HB     | 1:C:86:LEU:HD22   | 1.73                     | 0.69              |
| 1:C:313:ARG:NH1   | 23:B:401:GLU:OE2  | 2.25                     | 0.69              |
| 1:C:351:MET:CE    | 1:C:359:VAL:HG22  | 2.23                     | 0.69              |
| 7:L:15:PRO:HA     | 8:M:25:TYR:CE2    | 2.26                     | 0.69              |
| 7:L:58:ALA:HB3    | 26:K:164:GLN:HG3  | 1.74                     | 0.69              |
| 8:M:227:VAL:O     | 8:M:232:ARG:NH2   | 2.22                     | 0.69              |
| 12:Y:228:MET:HE1  | 12:Y:259:TYR:CZ   | 2.26                     | 0.69              |
| 18:f:541:THR:O    | 18:f:544:GLU:HG3  | 1.92                     | 0.69              |
| 18:f:648:ALA:O    | 18:f:652:VAL:HG22 | 1.92                     | 0.69              |
| 19:g:131:ILE:HD12 | 19:g:153:ALA:CB   | 2.21                     | 0.69              |
| 19:g:162:GLU:OE1  | 19:g:162:GLU:N    | 2.20                     | 0.69              |
| 24:E:151:LEU:HB3  | 24:E:159:PHE:CE2  | 2.27                     | 0.69              |
| 25:F:231:THR:CG2  | 25:F:354:PHE:HB3  | 2.15                     | 0.69              |
| 26:K:67:ILE:HD13  | 26:K:77:ALA:HA    | 1.74                     | 0.69              |
| 27:U:465:LEU:HD21 | 27:U:500:ASN:ND2  | 2.07                     | 0.69              |
| 27:U:641:SER:CB   | 27:U:675:MET:HE1  | 2.21                     | 0.69              |
| 3:G:32:ILE:O      | 3:G:82:GLY:HA2    | 1.92                     | 0.69              |
| 6:J:132:LEU:HG    | 6:J:161:ILE:CD1   | 2.22                     | 0.69              |
| 8:M:228:PRO:HB2   | 8:M:230:ASP:OD1   | 1.91                     | 0.69              |
| 11:X:114:ILE:HD11 | 11:X:130:GLU:N    | 2.07                     | 0.69              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 14:a:152:HIS:HB3  | 14:a:156:TYR:CE2  | 2.27                     | 0.69              |
| 16:c:188:SER:HB2  | 16:c:190:GLN:OE1  | 1.92                     | 0.69              |
| 17:d:153:GLN:HA   | 17:d:156:ILE:HG12 | 1.74                     | 0.69              |
| 18:f:498:LEU:HD13 | 18:f:534:VAL:CG2  | 2.23                     | 0.69              |
| 22:A:125:LEU:HB3  | 22:A:129:VAL:CG1  | 2.22                     | 0.69              |
| 23:B:49:LEU:HD22  | 23:B:50:PRO:HD2   | 1.73                     | 0.69              |
| 26:K:76:CYS:SG    | 26:K:141:LEU:HD22 | 2.33                     | 0.69              |
| 26:K:202:LEU:O    | 26:K:206:MET:HB2  | 1.92                     | 0.69              |
| 27:U:242:LEU:HD21 | 27:U:321:GLN:NE2  | 2.07                     | 0.69              |
| 9:V:84:LYS:O      | 9:V:88:GLY:N      | 2.24                     | 0.69              |
| 10:W:263:TRP:CZ3  | 10:W:295:LYS:HD3  | 2.27                     | 0.69              |
| 12:Y:26:LEU:HD21  | 12:Y:37:VAL:HB    | 1.75                     | 0.69              |
| 14:a:38:THR:O     | 14:a:42:LEU:N     | 2.21                     | 0.69              |
| 14:a:325:ASP:OD1  | 14:a:326:GLU:N    | 2.26                     | 0.69              |
| 15:b:7:MET:CE     | 15:b:64:LEU:HG    | 2.22                     | 0.69              |
| 23:B:297:SER:O    | 23:B:303:ARG:NH2  | 2.26                     | 0.69              |
| 27:U:751:ARG:NE   | 27:U:909:GLY:O    | 2.24                     | 0.69              |
| 27:U:904:LYS:HG3  | 27:U:905:PRO:HD2  | 1.73                     | 0.69              |
| 1:C:337:ASN:HB2   | 1:C:376:VAL:O     | 1.92                     | 0.69              |
| 4:H:118:MET:HE3   | 4:H:151:PRO:HA    | 1.73                     | 0.69              |
| 9:V:68:ASP:CG     | 9:V:112:VAL:HG22  | 2.17                     | 0.69              |
| 14:a:191:SER:HA   | 14:a:194:GLN:NE2  | 2.07                     | 0.69              |
| 14:a:276:CYS:SG   | 14:a:280:MET:HE3  | 2.33                     | 0.69              |
| 15:b:68:THR:O     | 15:b:72:LEU:HG    | 1.92                     | 0.69              |
| 17:d:331:PRO:O    | 17:d:333:THR:N    | 2.25                     | 0.69              |
| 18:f:128:VAL:O    | 18:f:131:MET:HG3  | 1.91                     | 0.69              |
| 18:f:131:MET:HE1  | 22:A:36:TYR:CE1   | 2.26                     | 0.69              |
| 18:f:679:LEU:HD21 | 18:f:690:VAL:HB   | 1.75                     | 0.69              |
| 18:f:771:LEU:HD13 | 18:f:778:LEU:HD21 | 1.74                     | 0.69              |
| 18:f:892:PRO:HG2  | 18:f:893:ILE:CD1  | 2.22                     | 0.69              |
| 19:g:128:LYS:HA   | 19:g:162:GLU:CB   | 2.21                     | 0.69              |
| 22:A:264:ALA:HB1  | 22:A:315:ILE:HD12 | 1.74                     | 0.69              |
| 22:A:284:ARG:HG2  | 22:A:296:GLN:CG   | 2.21                     | 0.69              |
| 25:F:228:PRO:CG   | 25:F:356:MET:HG3  | 2.22                     | 0.69              |
| 26:K:41:GLN:HA    | 26:K:46:VAL:HG22  | 1.74                     | 0.69              |
| 27:U:367:THR:O    | 27:U:371:ILE:HG22 | 1.92                     | 0.69              |
| 2:D:337:ASP:OD1   | 2:D:339:ARG:N     | 2.25                     | 0.69              |
| 4:H:179:ASN:HB3   | 4:H:182:LEU:HD21  | 1.74                     | 0.69              |
| 7:L:228:ASP:O     | 7:L:231:PRO:HD2   | 1.91                     | 0.69              |
| 8:M:74:GLY:O      | 8:M:137:LEU:HA    | 1.93                     | 0.69              |
| 14:a:118:ILE:O    | 14:a:122:LYS:N    | 2.24                     | 0.69              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 14:a:161:LYS:O    | 14:a:164:GLN:HG2  | 1.92                     | 0.69              |
| 14:a:321:LYS:HD2  | 14:a:336:VAL:HG21 | 1.73                     | 0.69              |
| 18:f:239:TYR:OH   | 23:B:64:LYS:HE3   | 1.91                     | 0.69              |
| 18:f:446:LEU:CD2  | 18:f:480:GLY:HA2  | 2.22                     | 0.69              |
| 18:f:702:PRO:CD   | 18:f:736:THR:HG21 | 2.22                     | 0.69              |
| 19:g:129:ILE:HB   | 19:g:136:LEU:HD11 | 1.74                     | 0.69              |
| 26:K:146:VAL:HG12 | 26:K:151:PRO:HA   | 1.74                     | 0.69              |
| 27:U:246:TYR:OH   | 27:U:324:LYS:HG2  | 1.92                     | 0.69              |
| 1:C:212:ILE:CD1   | 1:C:237:MET:HE3   | 2.19                     | 0.69              |
| 9:V:64:GLN:HG3    | 9:V:109:ASN:ND2   | 2.07                     | 0.69              |
| 9:V:68:ASP:O      | 9:V:72:LEU:N      | 2.17                     | 0.69              |
| 9:V:209:LYS:HE3   | 9:V:213:TYR:CE1   | 2.26                     | 0.69              |
| 9:V:289:LEU:HD22  | 9:V:308:THR:HG23  | 1.75                     | 0.69              |
| 10:W:60:MET:HA    | 10:W:97:LEU:HD12  | 1.73                     | 0.69              |
| 12:Y:228:MET:HE1  | 12:Y:259:TYR:CE1  | 2.27                     | 0.69              |
| 14:a:274:LEU:HD21 | 14:a:319:LEU:HD22 | 1.73                     | 0.69              |
| 15:b:33:VAL:CG1   | 15:b:75:LEU:HD11  | 2.22                     | 0.69              |
| 18:f:257:ARG:HA   | 18:f:257:ARG:NH1  | 2.08                     | 0.69              |
| 24:E:112:PRO:CD   | 25:F:97:LEU:HD13  | 2.20                     | 0.69              |
| 27:U:236:LEU:HD23 | 27:U:245:ALA:HB2  | 1.75                     | 0.69              |
| 27:U:552:ILE:O    | 27:U:555:VAL:HG12 | 1.93                     | 0.69              |
| 27:U:869:LYS:CA   | 27:U:872:GLU:HB3  | 2.16                     | 0.69              |
| 1:C:24:TYR:C      | 2:D:40:LEU:HD11   | 2.18                     | 0.69              |
| 2:D:180:ALA:O     | 2:D:306:LYS:NZ    | 2.22                     | 0.69              |
| 3:G:123:GLN:HE22  | 3:G:127:GLN:NE2   | 1.91                     | 0.69              |
| 5:I:21:VAL:HG11   | 23:B:438:LEU:HD21 | 1.75                     | 0.69              |
| 6:J:45:VAL:CG2    | 6:J:61:LYS:HD3    | 2.22                     | 0.69              |
| 7:L:49:LEU:HD21   | 7:L:199:LEU:CD2   | 2.22                     | 0.69              |
| 9:V:122:THR:HA    | 9:V:128:ARG:CD    | 2.21                     | 0.69              |
| 9:V:408:ARG:HA    | 9:V:447:ILE:HD11  | 1.73                     | 0.69              |
| 10:W:171:VAL:HA   | 10:W:174:TYR:CE2  | 2.27                     | 0.69              |
| 13:Z:45:LYS:HD2   | 13:Z:45:LYS:N     | 2.07                     | 0.69              |
| 14:a:222:LEU:HD21 | 14:a:237:LEU:CD2  | 2.23                     | 0.69              |
| 14:a:371:ALA:HB1  | 14:a:374:ILE:HG23 | 1.75                     | 0.69              |
| 15:b:121:GLU:HA   | 15:b:124:LEU:HD21 | 1.75                     | 0.69              |
| 16:c:52:GLU:OE1   | 20:u:289:HIS:CD2  | 2.46                     | 0.69              |
| 17:d:123:LEU:CD2  | 17:d:144:ALA:HB2  | 2.21                     | 0.69              |
| 17:d:168:MET:O    | 17:d:172:LYS:N    | 2.26                     | 0.69              |
| 18:f:174:ASP:O    | 18:f:181:ARG:NH1  | 2.17                     | 0.69              |
| 18:f:379:GLY:HA3  | 18:f:416:MET:HE3  | 1.73                     | 0.69              |
| 18:f:438:ASP:O    | 18:f:441:LYS:HG3  | 1.93                     | 0.69              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 18:f:609:VAL:HG12 | 23:B:74:MET:CE    | 2.20                     | 0.69              |
| 19:g:156:LEU:O    | 19:g:158:LEU:HD12 | 1.93                     | 0.69              |
| 22:A:71:GLY:HA3   | 23:B:162:VAL:HG12 | 1.75                     | 0.69              |
| 22:A:277:ILE:HG23 | 22:A:327:LEU:HD21 | 1.74                     | 0.69              |
| 23:B:356:PRO:HB2  | 23:B:361:LYS:CG   | 2.23                     | 0.69              |
| 25:F:436:GLN:NE2  | 26:K:28:ILE:HD13  | 2.08                     | 0.69              |
| 26:K:68:VAL:HG23  | 26:K:76:CYS:HB3   | 1.75                     | 0.69              |
| 27:U:717:ILE:HD13 | 27:U:731:ILE:HD11 | 1.73                     | 0.69              |
| 3:G:102:LYS:HA    | 3:G:107:TYR:O     | 1.92                     | 0.69              |
| 5:I:147:LEU:HB3   | 5:I:159:TRP:O     | 1.91                     | 0.69              |
| 7:L:43:HIS:CD2    | 7:L:184:LEU:HD13  | 2.28                     | 0.69              |
| 9:V:64:GLN:NE2    | 9:V:68:ASP:OD2    | 2.26                     | 0.69              |
| 14:a:180:LEU:HD12 | 14:a:219:HIS:HE2  | 1.57                     | 0.69              |
| 18:f:163:ALA:HB2  | 18:f:191:ILE:CD1  | 2.23                     | 0.69              |
| 18:f:219:LYS:HA   | 18:f:258:LYS:NZ   | 2.08                     | 0.69              |
| 24:E:352:MET:CE   | 24:E:355:ILE:CD1  | 2.71                     | 0.69              |
| 25:F:93:VAL:HG22  | 25:F:124:ILE:CD1  | 2.23                     | 0.69              |
| 25:F:130:GLN:HB2  | 25:F:132:TYR:CE2  | 2.27                     | 0.69              |
| 25:F:220:PRO:HG2  | 25:F:350:ARG:HD3  | 1.75                     | 0.69              |
| 27:U:344:ARG:HH21 | 27:U:927:PRO:HB2  | 1.58                     | 0.69              |
| 27:U:427:LEU:HD12 | 27:U:438:GLN:HG3  | 1.74                     | 0.69              |
| 1:C:148:TYR:OH    | 1:C:162:LYS:NZ    | 2.26                     | 0.69              |
| 1:C:162:LYS:HG2   | 1:C:166:GLU:HB2   | 1.73                     | 0.69              |
| 3:G:202:LEU:O     | 3:G:206:LEU:HG    | 1.93                     | 0.69              |
| 6:J:132:LEU:HD23  | 6:J:146:GLN:HB2   | 1.75                     | 0.69              |
| 7:L:196:ARG:HH22  | 7:L:239:ARG:HB2   | 1.58                     | 0.69              |
| 8:M:72:HIS:NE2    | 8:M:105:ASN:HB3   | 2.06                     | 0.69              |
| 10:W:132:THR:HB   | 10:W:138:VAL:HG13 | 1.74                     | 0.69              |
| 10:W:186:ILE:HG23 | 10:W:205:ILE:CG2  | 2.22                     | 0.69              |
| 14:a:110:ALA:HA   | 14:a:113:LEU:HD13 | 1.75                     | 0.69              |
| 14:a:274:LEU:CD2  | 14:a:278:MET:HE1  | 2.23                     | 0.69              |
| 17:d:302:TYR:HD1  | 17:d:306:ARG:HG3  | 1.58                     | 0.69              |
| 18:f:479:LEU:HD21 | 18:f:513:GLU:HG3  | 1.75                     | 0.69              |
| 19:g:165:ALA:CA   | 19:g:168:ASN:H    | 2.06                     | 0.69              |
| 22:A:72:LEU:HD22  | 23:B:96:ARG:NH2   | 2.08                     | 0.69              |
| 25:F:201:ALA:C    | 25:F:205:PRO:HG2  | 2.18                     | 0.69              |
| 26:K:25:GLU:O     | 26:K:29:GLU:HG2   | 1.93                     | 0.69              |
| 26:K:48:LEU:O     | 26:K:217:LEU:HD23 | 1.93                     | 0.69              |
| 27:U:876:GLN:O    | 27:U:878:LEU:HG   | 1.93                     | 0.69              |
| 5:I:136:TYR:O     | 5:I:147:LEU:HD12  | 1.93                     | 0.68              |
| 9:V:78:HIS:ND1    | 9:V:166:TYR:OH    | 2.26                     | 0.68              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 11:X:298:SER:CB   | 11:X:301:ASP:HB2  | 2.23                     | 0.68              |
| 12:Y:97:GLU:HA    | 12:Y:100:ILE:CD1  | 2.23                     | 0.68              |
| 13:Z:54:PHE:CD1   | 13:Z:78:MET:HG2   | 2.28                     | 0.68              |
| 16:c:231:LEU:O    | 16:c:298:GLN:NE2  | 2.25                     | 0.68              |
| 18:f:164:GLY:O    | 18:f:168:LYS:HG3  | 1.93                     | 0.68              |
| 18:f:407:MET:HE2  | 18:f:440:ILE:HG21 | 1.75                     | 0.68              |
| 19:g:107:ILE:CD1  | 19:g:111:GLU:HB3  | 2.15                     | 0.68              |
| 19:g:140:LYS:HB3  | 19:g:144:GLU:CG   | 2.20                     | 0.68              |
| 24:E:122:MET:CE   | 25:F:344:ARG:NE   | 2.43                     | 0.68              |
| 24:E:370:ALA:O    | 24:E:374:VAL:HG23 | 1.93                     | 0.68              |
| 25:F:202:ILE:CD1  | 25:F:327:LYS:HB3  | 2.23                     | 0.68              |
| 27:U:135:ASN:O    | 27:U:139:GLN:N    | 2.16                     | 0.68              |
| 27:U:324:LYS:HE3  | 27:U:794:ASP:CB   | 2.19                     | 0.68              |
| 1:C:113:ARG:NH2   | 2:D:102:ILE:HD13  | 2.08                     | 0.68              |
| 2:D:245:ARG:HA    | 2:D:248:ARG:NH1   | 2.08                     | 0.68              |
| 3:G:92:GLN:OE1    | 8:M:117:MET:HG3   | 1.92                     | 0.68              |
| 3:G:126:THR:HG22  | 4:H:128:ARG:NH1   | 2.08                     | 0.68              |
| 9:V:224:LEU:HG    | 9:V:257:ASN:CG    | 2.18                     | 0.68              |
| 15:b:155:ALA:O    | 15:b:159:THR:HG22 | 1.92                     | 0.68              |
| 17:d:171:LEU:HD12 | 17:d:171:LEU:O    | 1.93                     | 0.68              |
| 25:F:220:PRO:HG2  | 25:F:350:ARG:CD   | 2.23                     | 0.68              |
| 27:U:8:ILE:HG23   | 27:U:11:LEU:HD12  | 1.74                     | 0.68              |
| 27:U:42:VAL:HG23  | 27:U:43:ASP:H     | 1.58                     | 0.68              |
| 27:U:244:MET:HG2  | 27:U:903:PHE:CE2  | 2.27                     | 0.68              |
| 27:U:446:LEU:HD21 | 27:U:457:ILE:HD12 | 1.75                     | 0.68              |
| 27:U:748:LEU:HB3  | 27:U:760:VAL:CG2  | 2.23                     | 0.68              |
| 1:C:214:VAL:HG21  | 1:C:234:LEU:HD22  | 1.74                     | 0.68              |
| 2:D:380:GLN:NE2   | 24:E:164:ILE:HG23 | 2.09                     | 0.68              |
| 3:G:101:TRP:CG    | 3:G:109:ILE:HB    | 2.27                     | 0.68              |
| 9:V:68:ASP:OD1    | 9:V:112:VAL:HG22  | 1.94                     | 0.68              |
| 11:X:46:LYS:HG2   | 11:X:76:PHE:CE1   | 2.28                     | 0.68              |
| 14:a:122:LYS:HE3  | 14:a:130:VAL:HG13 | 1.74                     | 0.68              |
| 14:a:290:GLN:OE1  | 14:a:332:HIS:HA   | 1.93                     | 0.68              |
| 14:a:363:MET:HA   | 14:a:363:MET:HE2  | 1.75                     | 0.68              |
| 15:b:7:MET:HB3    | 15:b:109:ILE:HD12 | 1.74                     | 0.68              |
| 15:b:98:LYS:NZ    | 20:u:205:ASP:OD2  | 2.26                     | 0.68              |
| 18:f:169:GLU:OE1  | 18:f:169:GLU:HA   | 1.93                     | 0.68              |
| 22:A:161:VAL:HA   | 22:A:164:MET:CE   | 2.20                     | 0.68              |
| 22:A:348:LEU:HD21 | 22:A:371:GLU:OE2  | 1.92                     | 0.68              |
| 23:B:316:LEU:HD21 | 23:B:327:VAL:HG21 | 1.74                     | 0.68              |
| 25:F:90:VAL:HG23  | 25:F:164:LEU:CD1  | 2.22                     | 0.68              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 25:F:205:PRO:HB3  | 25:F:219:PRO:CB   | 2.23                     | 0.68              |
| 25:F:311:LEU:HD13 | 25:F:314:LEU:HD12 | 1.75                     | 0.68              |
| 25:F:339:ASP:HB2  | 25:F:342:LEU:HD23 | 1.73                     | 0.68              |
| 27:U:554:LEU:HD22 | 27:U:761:VAL:HG22 | 1.74                     | 0.68              |
| 27:U:748:LEU:CD2  | 27:U:760:VAL:HG22 | 2.23                     | 0.68              |
| 1:C:31:LEU:HD12   | 1:C:31:LEU:O      | 1.93                     | 0.68              |
| 1:C:165:ILE:CG1   | 1:C:292:ILE:HD11  | 2.24                     | 0.68              |
| 2:D:102:ILE:O     | 2:D:102:ILE:HG23  | 1.93                     | 0.68              |
| 2:D:418:LYS:HE3   | 4:H:76:TYR:OH     | 1.92                     | 0.68              |
| 3:G:208:ILE:CD1   | 24:E:306:GLU:OE1  | 2.41                     | 0.68              |
| 8:M:211:LEU:HG    | 8:M:213:LEU:HD11  | 1.74                     | 0.68              |
| 10:W:377:ARG:HH21 | 10:W:381:LEU:HD21 | 1.59                     | 0.68              |
| 14:a:112:ILE:HG21 | 14:a:151:VAL:CG1  | 2.08                     | 0.68              |
| 14:a:205:LEU:CD2  | 14:a:237:LEU:HD13 | 2.23                     | 0.68              |
| 15:b:135:LYS:NZ   | 20:u:140:GLU:O    | 2.24                     | 0.68              |
| 18:f:190:GLU:O    | 18:f:193:PRO:HD2  | 1.93                     | 0.68              |
| 18:f:535:THR:O    | 18:f:539:LEU:N    | 2.19                     | 0.68              |
| 19:g:170:GLN:CG   | 19:g:173:GLU:HG3  | 2.13                     | 0.68              |
| 25:F:177:VAL:O    | 25:F:180:ARG:NH2  | 2.27                     | 0.68              |
| 27:U:177:LEU:HD21 | 27:U:205:TYR:OH   | 1.93                     | 0.68              |
| 2:D:181:VAL:HG11  | 2:D:308:ILE:HG12  | 1.75                     | 0.68              |
| 2:D:269:ALA:HB2   | 24:E:258:MET:HE1  | 1.73                     | 0.68              |
| 10:W:30:GLU:O     | 10:W:34:LEU:HG    | 1.93                     | 0.68              |
| 12:Y:76:ALA:HA    | 12:Y:79:ASP:OD2   | 1.93                     | 0.68              |
| 14:a:118:ILE:HG12 | 14:a:122:LYS:HD3  | 1.76                     | 0.68              |
| 15:b:107:MET:HE3  | 15:b:107:MET:CA   | 2.19                     | 0.68              |
| 18:f:274:ASP:HB3  | 18:f:277:LEU:CD1  | 2.24                     | 0.68              |
| 18:f:427:THR:HG23 | 19:g:156:LEU:HD11 | 1.76                     | 0.68              |
| 18:f:527:VAL:HG11 | 18:f:794:ALA:HB2  | 1.75                     | 0.68              |
| 18:f:797:LEU:O    | 18:f:801:VAL:HG22 | 1.93                     | 0.68              |
| 18:f:828:ARG:HD2  | 18:f:874:LEU:H    | 1.58                     | 0.68              |
| 24:E:198:VAL:HG11 | 24:E:218:MET:SD   | 2.32                     | 0.68              |
| 25:F:206:MET:SD   | 25:F:280:PRO:HB2  | 2.34                     | 0.68              |
| 25:F:279:ALA:HB1  | 25:F:280:PRO:CD   | 2.20                     | 0.68              |
| 25:F:438:TYR:OH   | 26:K:19:GLY:O     | 2.12                     | 0.68              |
| 26:K:217:LEU:HB2  | 26:K:234:LEU:CD1  | 2.23                     | 0.68              |
| 27:U:14:GLU:HG3   | 27:U:19:LEU:HD21  | 1.74                     | 0.68              |
| 27:U:213:PHE:HA   | 27:U:216:VAL:HG12 | 1.76                     | 0.68              |
| 8:M:109:LYS:HA    | 8:M:149:TYR:CE2   | 2.24                     | 0.68              |
| 9:V:116:ALA:O     | 9:V:120:PHE:N     | 2.22                     | 0.68              |
| 9:V:329:HIS:CB    | 9:V:357:LEU:HD11  | 2.23                     | 0.68              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 9:V:416:ARG:HB3   | 12:Y:348:ASP:OD1  | 1.94                     | 0.68              |
| 9:V:488:ASN:O     | 9:V:492:LYS:HB3   | 1.94                     | 0.68              |
| 14:a:96:PHE:CD1   | 14:a:99:LYS:HE2   | 2.22                     | 0.68              |
| 18:f:342:PRO:HD3  | 18:f:387:GLN:NE2  | 2.08                     | 0.68              |
| 18:f:384:ALA:HB2  | 18:f:419:LEU:HD13 | 1.75                     | 0.68              |
| 19:g:123:GLN:CB   | 19:g:126:TYR:HB2  | 2.23                     | 0.68              |
| 27:U:128:GLN:O    | 27:U:132:GLY:N    | 2.23                     | 0.68              |
| 1:C:55:LYS:HZ1    | 2:D:72:PHE:HE1    | 1.38                     | 0.68              |
| 2:D:57:GLN:O      | 2:D:61:ILE:HG22   | 1.93                     | 0.68              |
| 4:H:154:ALA:HB2   | 5:I:80:THR:CG2    | 2.24                     | 0.68              |
| 7:L:36:VAL:HG12   | 7:L:195:LEU:HG    | 1.75                     | 0.68              |
| 8:M:186:CYS:O     | 8:M:190:VAL:HG23  | 1.93                     | 0.68              |
| 10:W:268:LYS:HZ3  | 10:W:336:PRO:HD2  | 1.58                     | 0.68              |
| 11:X:414:LEU:HD21 | 13:Z:273:HIS:CD2  | 2.29                     | 0.68              |
| 12:Y:301:ILE:HG23 | 12:Y:343:LEU:CD1  | 2.23                     | 0.68              |
| 12:Y:334:LEU:HB3  | 12:Y:347:ILE:HD11 | 1.76                     | 0.68              |
| 14:a:28:LEU:HB3   | 14:a:33:LEU:CD1   | 2.23                     | 0.68              |
| 14:a:278:MET:SD   | 14:a:319:LEU:HB3  | 2.33                     | 0.68              |
| 16:c:126:ASP:O    | 16:c:129:THR:OG1  | 2.12                     | 0.68              |
| 17:d:160:ASP:OD1  | 17:d:163:SER:N    | 2.18                     | 0.68              |
| 17:d:229:PRO:O    | 17:d:233:GLU:N    | 2.24                     | 0.68              |
| 18:f:862:ILE:HD12 | 18:f:881:GLU:HG3  | 1.76                     | 0.68              |
| 22:A:159:PRO:O    | 22:A:163:MET:HG3  | 1.93                     | 0.68              |
| 22:A:429:TYR:OH   | 26:K:33:LEU:HB3   | 1.93                     | 0.68              |
| 23:B:193:GLN:O    | 23:B:197:ILE:HG22 | 1.94                     | 0.68              |
| 23:B:423:LYS:O    | 23:B:427:LEU:HB2  | 1.94                     | 0.68              |
| 26:K:212:ALA:HB2  | 26:K:235:GLU:HG3  | 1.76                     | 0.68              |
| 27:U:27:LEU:O     | 27:U:31:VAL:HG23  | 1.94                     | 0.68              |
| 27:U:688:LEU:HD22 | 27:U:713:TYR:HE1  | 1.58                     | 0.68              |
| 1:C:134:LEU:HD13  | 1:C:230:MET:HE1   | 1.76                     | 0.68              |
| 3:G:143:ILE:HG23  | 3:G:222:VAL:HG22  | 1.75                     | 0.68              |
| 4:H:74:LEU:HB3    | 4:H:134:LEU:CD2   | 2.24                     | 0.68              |
| 7:L:203:GLN:O     | 7:L:239:ARG:NH2   | 2.24                     | 0.68              |
| 10:W:31:CYS:HB3   | 10:W:43:VAL:CG1   | 2.18                     | 0.68              |
| 10:W:34:LEU:HB2   | 10:W:43:VAL:HG21  | 1.74                     | 0.68              |
| 10:W:34:LEU:HA    | 10:W:37:GLU:CD    | 2.18                     | 0.68              |
| 10:W:96:GLN:HG3   | 10:W:101:VAL:CG2  | 2.23                     | 0.68              |
| 11:X:170:GLN:NE2  | 11:X:192:SER:HB3  | 2.09                     | 0.68              |
| 11:X:297:ARG:HG3  | 11:X:330:LEU:HD11 | 1.74                     | 0.68              |
| 18:f:87:THR:HG23  | 18:f:154:TRP:O    | 1.94                     | 0.68              |
| 18:f:264:GLU:HG3  | 18:f:892:PRO:HG3  | 1.74                     | 0.68              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 19:g:83:ALA:HB1   | 19:g:150:ASN:ND2  | 2.09                     | 0.68              |
| 23:B:107:MET:CE   | 23:B:151:LEU:HD22 | 2.24                     | 0.68              |
| 3:G:117:ARG:O     | 3:G:121:ILE:HG12  | 1.93                     | 0.68              |
| 7:L:126:ARG:NE    | 26:K:21:LEU:HD11  | 2.08                     | 0.68              |
| 10:W:109:CYS:HA   | 10:W:112:VAL:HG23 | 1.73                     | 0.68              |
| 10:W:236:HIS:ND1  | 10:W:237:GLU:OE2  | 2.19                     | 0.68              |
| 11:X:339:ILE:HD11 | 11:X:350:ILE:CD1  | 2.23                     | 0.68              |
| 12:Y:48:ASN:HB2   | 12:Y:50:MET:CE    | 2.24                     | 0.68              |
| 14:a:54:ASP:CA    | 14:a:57:ILE:HG22  | 2.22                     | 0.68              |
| 14:a:278:MET:HG2  | 14:a:335:TRP:CZ2  | 2.29                     | 0.68              |
| 18:f:242:GLU:OE1  | 18:f:243:PRO:HA   | 1.94                     | 0.68              |
| 19:g:166:ARG:HA   | 19:g:170:GLN:HG3  | 1.75                     | 0.68              |
| 20:u:145:GLY:N    | 20:u:148:ASN:OD1  | 2.25                     | 0.68              |
| 22:A:235:ALA:HB1  | 22:A:269:ALA:O    | 1.94                     | 0.68              |
| 24:E:367:PHE:O    | 24:E:371:VAL:N    | 2.25                     | 0.68              |
| 27:U:103:LYS:HA   | 27:U:106:ASP:HB3  | 1.76                     | 0.68              |
| 1:C:50:ASN:HD21   | 27:U:639:LEU:HD11 | 1.58                     | 0.68              |
| 1:C:180:ILE:HD12  | 1:C:180:ILE:O     | 1.94                     | 0.68              |
| 2:D:103:VAL:HG11  | 2:D:132:LEU:CD2   | 2.24                     | 0.68              |
| 2:D:203:LEU:HB2   | 2:D:327:LEU:HD13  | 1.76                     | 0.68              |
| 2:D:378:ILE:O     | 2:D:382:SER:HB2   | 1.94                     | 0.68              |
| 3:G:207:SER:C     | 3:G:208:ILE:HD13  | 2.19                     | 0.68              |
| 4:H:50:LYS:HG2    | 4:H:52:GLN:HE22   | 1.59                     | 0.68              |
| 8:M:233:GLU:O     | 8:M:237:LYS:HG2   | 1.94                     | 0.68              |
| 11:X:213:GLN:O    | 11:X:217:ILE:HG12 | 1.93                     | 0.68              |
| 12:Y:15:PRO:HD2   | 12:Y:146:ARG:HB3  | 1.74                     | 0.68              |
| 13:Z:188:SER:CA   | 14:a:374:ILE:HD11 | 2.24                     | 0.68              |
| 14:a:94:LEU:HD22  | 14:a:97:LEU:HD21  | 1.74                     | 0.68              |
| 18:f:55:GLU:O     | 18:f:59:LEU:HD23  | 1.94                     | 0.68              |
| 22:A:119:ALA:HB3  | 22:A:121:PHE:CZ   | 2.28                     | 0.68              |
| 23:B:213:GLU:HG2  | 23:B:213:GLU:O    | 1.94                     | 0.68              |
| 26:K:74:ILE:HG13  | 26:K:144:GLY:O    | 1.94                     | 0.68              |
| 27:U:669:ILE:HD11 | 27:U:695:MET:HG3  | 1.75                     | 0.68              |
| 1:C:46:GLN:CD     | 27:U:639:LEU:HD22 | 2.19                     | 0.67              |
| 1:C:403:LYS:HB2   | 4:H:156:PHE:HE1   | 1.60                     | 0.67              |
| 8:M:148:LEU:HD22  | 8:M:160:TYR:O     | 1.93                     | 0.67              |
| 9:V:434:ALA:HA    | 9:V:437:ILE:HG22  | 1.74                     | 0.67              |
| 10:W:109:CYS:O    | 10:W:112:VAL:HB   | 1.94                     | 0.67              |
| 10:W:435:LEU:HG   | 13:Z:233:VAL:CG2  | 2.24                     | 0.67              |
| 13:Z:74:TYR:CE1   | 13:Z:78:MET:HE3   | 2.29                     | 0.67              |
| 16:c:307:VAL:HG23 | 17:d:332:SER:HB2  | 1.75                     | 0.67              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 17:d:303:ALA:O    | 17:d:307:GLY:HA2  | 1.94                     | 0.67              |
| 1:C:138:MET:SD    | 1:C:214:VAL:HG22  | 2.34                     | 0.67              |
| 2:D:410:ASP:HB2   | 2:D:413:GLU:HG2   | 1.76                     | 0.67              |
| 4:H:38:ILE:HD13   | 4:H:191:ALA:HB2   | 1.77                     | 0.67              |
| 6:J:15:HIS:ND1    | 6:J:20:GLU:OE2    | 2.26                     | 0.67              |
| 7:L:66:VAL:HG21   | 7:L:72:ILE:CG2    | 2.24                     | 0.67              |
| 8:M:108:LEU:HD22  | 8:M:139:SER:CB    | 2.19                     | 0.67              |
| 9:V:117:VAL:HG11  | 9:V:131:LEU:HD11  | 1.75                     | 0.67              |
| 9:V:434:ALA:O     | 9:V:438:VAL:N     | 2.19                     | 0.67              |
| 10:W:267:LEU:HD23 | 10:W:270:VAL:HG11 | 1.74                     | 0.67              |
| 13:Z:225:GLN:OE1  | 13:Z:226:ILE:HG12 | 1.94                     | 0.67              |
| 14:a:54:ASP:O     | 14:a:58:LYS:HB2   | 1.94                     | 0.67              |
| 18:f:809:ILE:O    | 18:f:814:SER:OG   | 2.07                     | 0.67              |
| 27:U:14:GLU:HB2   | 27:U:19:LEU:HD23  | 1.76                     | 0.67              |
| 27:U:485:ALA:HB1  | 27:U:488:THR:HG21 | 1.77                     | 0.67              |
| 1:C:165:ILE:HG23  | 1:C:245:ILE:HD13  | 1.77                     | 0.67              |
| 2:D:282:ASP:HA    | 2:D:285:VAL:HG12  | 1.76                     | 0.67              |
| 3:G:143:ILE:HG13  | 3:G:221:THR:O     | 1.93                     | 0.67              |
| 3:G:230:LEU:O     | 3:G:235:ILE:HD11  | 1.93                     | 0.67              |
| 5:I:68:LEU:CD1    | 5:I:90:LEU:HD13   | 2.24                     | 0.67              |
| 5:I:233:VAL:O     | 5:I:237:ILE:HG12  | 1.93                     | 0.67              |
| 9:V:117:VAL:CG1   | 9:V:131:LEU:HD11  | 2.25                     | 0.67              |
| 11:X:343:SER:O    | 11:X:344:ARG:HG3  | 1.94                     | 0.67              |
| 14:a:45:VAL:HG21  | 14:a:79:ILE:HD11  | 1.76                     | 0.67              |
| 15:b:24:THR:HG22  | 15:b:26:LEU:H     | 1.59                     | 0.67              |
| 17:d:84:SER:O     | 17:d:88:LEU:N     | 2.23                     | 0.67              |
| 18:f:835:GLU:OE2  | 18:f:902:LYS:N    | 2.24                     | 0.67              |
| 27:U:137:MET:HA   | 27:U:140:ARG:HB2  | 1.75                     | 0.67              |
| 27:U:405:THR:OG1  | 27:U:441:GLY:HA3  | 1.95                     | 0.67              |
| 1:C:392:GLN:O     | 1:C:393:LYS:HD3   | 1.94                     | 0.67              |
| 2:D:361:GLU:HG3   | 2:D:361:GLU:O     | 1.95                     | 0.67              |
| 6:J:220:LEU:HD13  | 6:J:224:GLU:OE1   | 1.94                     | 0.67              |
| 9:V:240:LEU:HD11  | 27:U:69:TYR:HE1   | 1.59                     | 0.67              |
| 13:Z:59:ASP:HB3   | 15:b:95:LEU:HD21  | 1.75                     | 0.67              |
| 14:a:58:LYS:O     | 14:a:62:ASN:HB2   | 1.94                     | 0.67              |
| 16:c:62:VAL:HG13  | 16:c:66:THR:HG23  | 1.76                     | 0.67              |
| 18:f:93:PRO:HB2   | 18:f:96:LEU:HD12  | 1.77                     | 0.67              |
| 18:f:129:LEU:HD23 | 18:f:129:LEU:O    | 1.94                     | 0.67              |
| 18:f:268:LEU:HD13 | 18:f:271:MET:SD   | 2.34                     | 0.67              |
| 18:f:831:VAL:CG2  | 18:f:871:PRO:HB3  | 2.15                     | 0.67              |
| 18:f:852:VAL:HG23 | 18:f:859:PRO:HB2  | 1.77                     | 0.67              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:A:164:MET:HG2  | 22:A:239:ARG:O    | 1.95                     | 0.67              |
| 23:B:250:VAL:CG2  | 23:B:284:ILE:HA   | 2.24                     | 0.67              |
| 1:C:77:VAL:HB     | 1:C:86:LEU:CD2    | 2.25                     | 0.67              |
| 1:C:277:LEU:HD11  | 1:C:304:ALA:HB3   | 1.75                     | 0.67              |
| 1:C:368:MET:HE1   | 1:C:371:LEU:HD22  | 1.76                     | 0.67              |
| 2:D:205:TYR:HB2   | 2:D:314:ALA:HB2   | 1.76                     | 0.67              |
| 6:J:65:LEU:HD11   | 6:J:71:MET:SD     | 2.34                     | 0.67              |
| 9:V:282:ASN:OD1   | 9:V:315:LYS:HD2   | 1.95                     | 0.67              |
| 11:X:298:SER:HB3  | 11:X:301:ASP:HB2  | 1.75                     | 0.67              |
| 14:a:160:SER:O    | 14:a:163:TYR:HB3  | 1.93                     | 0.67              |
| 17:d:87:VAL:HG12  | 17:d:126:LEU:HD11 | 1.77                     | 0.67              |
| 17:d:95:TYR:CD1   | 17:d:99:LYS:HB2   | 2.29                     | 0.67              |
| 18:f:460:ASP:OD1  | 18:f:463:LEU:HB3  | 1.94                     | 0.67              |
| 18:f:735:GLY:HA2  | 18:f:774:GLY:HA2  | 1.77                     | 0.67              |
| 19:g:83:ALA:HB3   | 19:g:149:HIS:CB   | 2.24                     | 0.67              |
| 19:g:136:LEU:HD13 | 19:g:138:LEU:HD21 | 1.77                     | 0.67              |
| 22:A:224:LEU:HB2  | 29:A:501:ATP:H3'  | 1.77                     | 0.67              |
| 22:A:333:ARG:HE   | 22:A:336:ARG:NH1  | 1.93                     | 0.67              |
| 27:U:82:LEU:HD11  | 27:U:130:LEU:N    | 2.09                     | 0.67              |
| 8:M:197:ILE:HD13  | 8:M:211:LEU:CD1   | 2.25                     | 0.67              |
| 10:W:431:LYS:HZ1  | 13:Z:238:PRO:HA   | 1.58                     | 0.67              |
| 11:X:331:LEU:HD23 | 11:X:364:LYS:HG2  | 1.76                     | 0.67              |
| 12:Y:101:ARG:HD2  | 12:Y:131:THR:HA   | 1.76                     | 0.67              |
| 14:a:38:THR:HB    | 14:a:71:VAL:HG13  | 1.75                     | 0.67              |
| 14:a:45:VAL:HG21  | 14:a:79:ILE:CG1   | 2.23                     | 0.67              |
| 18:f:474:SER:HB3  | 18:f:477:MET:CG   | 2.18                     | 0.67              |
| 18:f:478:ARG:HD2  | 18:f:514:VAL:HG11 | 1.76                     | 0.67              |
| 23:B:197:ILE:CG2  | 23:B:235:LEU:HD21 | 2.07                     | 0.67              |
| 25:F:410:ARG:NH2  | 25:F:419:ASP:OD1  | 2.27                     | 0.67              |
| 4:H:173:PHE:O     | 4:H:176:LYS:HB2   | 1.94                     | 0.67              |
| 8:M:192:GLU:HA    | 8:M:195:LYS:HG2   | 1.75                     | 0.67              |
| 9:V:171:VAL:O     | 9:V:175:MET:HG2   | 1.95                     | 0.67              |
| 12:Y:220:VAL:HG11 | 12:Y:249:VAL:CG1  | 2.25                     | 0.67              |
| 13:Z:209:ARG:HB2  | 14:a:353:LEU:HD21 | 1.76                     | 0.67              |
| 14:a:117:ALA:O    | 14:a:121:LEU:HD12 | 1.94                     | 0.67              |
| 18:f:210:GLU:HA   | 18:f:210:GLU:OE1  | 1.93                     | 0.67              |
| 18:f:485:LEU:HD21 | 18:f:497:VAL:HG13 | 1.76                     | 0.67              |
| 19:g:92:ARG:HB3   | 19:g:157:GLU:OE1  | 1.95                     | 0.67              |
| 25:F:178:ASP:HA   | 25:F:180:ARG:NH2  | 2.09                     | 0.67              |
| 27:U:46:GLU:HG3   | 27:U:80:TYR:OH    | 1.93                     | 0.67              |
| 27:U:746:ILE:HA   | 27:U:782:ALA:O    | 1.95                     | 0.67              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 27:U:846:LYS:O    | 27:U:850:GLU:HG2  | 1.94                     | 0.67              |
| 5:I:86:LEU:CD1    | 5:I:114:LEU:HD11  | 2.24                     | 0.67              |
| 5:I:98:LEU:HD12   | 5:I:98:LEU:O      | 1.94                     | 0.67              |
| 6:J:212:ARG:HB2   | 6:J:215:GLN:CD    | 2.19                     | 0.67              |
| 7:L:6:TYR:CD2     | 7:L:15:PRO:HD3    | 2.30                     | 0.67              |
| 12:Y:95:LEU:HB3   | 12:Y:99:GLU:HB2   | 1.77                     | 0.67              |
| 14:a:216:LEU:HD13 | 14:a:237:LEU:HB3  | 1.75                     | 0.67              |
| 14:a:319:LEU:O    | 14:a:320:VAL:HG23 | 1.94                     | 0.67              |
| 24:E:238:ILE:H    | 24:E:238:ILE:HD12 | 1.60                     | 0.67              |
| 24:E:330:ALA:O    | 24:E:334:LEU:HG   | 1.95                     | 0.67              |
| 1:C:406:LYS:HG2   | 5:I:64:LYS:NZ     | 2.10                     | 0.67              |
| 3:G:10:ASP:O      | 3:G:12:HIS:N      | 2.28                     | 0.67              |
| 3:G:50:ILE:HD13   | 3:G:141:ILE:HD13  | 1.75                     | 0.67              |
| 7:L:40:SER:CB     | 7:L:187:LEU:HD22  | 2.25                     | 0.67              |
| 7:L:74:ILE:CG2    | 7:L:81:ALA:HB1    | 2.25                     | 0.67              |
| 12:Y:17:LEU:HD21  | 12:Y:146:ARG:HG2  | 1.76                     | 0.67              |
| 14:a:21:VAL:HG12  | 14:a:44:PHE:CE1   | 2.29                     | 0.67              |
| 14:a:243:GLY:HA2  | 14:a:272:ILE:HD11 | 1.76                     | 0.67              |
| 17:d:323:GLN:O    | 17:d:324:LYS:HG3  | 1.95                     | 0.67              |
| 18:f:231:LEU:CG   | 18:f:853:VAL:HG22 | 2.24                     | 0.67              |
| 20:u:256:GLU:OE1  | 20:u:256:GLU:N    | 2.28                     | 0.67              |
| 22:A:146:LYS:HB2  | 22:A:146:LYS:NZ   | 2.09                     | 0.67              |
| 22:A:269:ALA:HA   | 22:A:314:ASN:OD1  | 1.95                     | 0.67              |
| 22:A:394:MET:HE1  | 23:B:199:GLU:HB3  | 1.77                     | 0.67              |
| 24:E:147:GLU:HA   | 24:E:151:LEU:CD1  | 2.25                     | 0.67              |
| 25:F:238:ARG:HA   | 25:F:241:ALA:HB3  | 1.77                     | 0.67              |
| 26:K:181:LEU:CD1  | 26:K:201:ILE:HD12 | 2.24                     | 0.67              |
| 26:K:203:LYS:HB2  | 26:K:210:LEU:HD23 | 1.77                     | 0.67              |
| 27:U:658:ILE:HD11 | 27:U:767:THR:CG2  | 2.25                     | 0.67              |
| 8:M:211:LEU:HG    | 8:M:213:LEU:CD1   | 2.25                     | 0.67              |
| 9:V:375:PHE:CE1   | 9:V:379:LEU:HD11  | 2.29                     | 0.67              |
| 10:W:413:ILE:HG22 | 10:W:413:ILE:O    | 1.93                     | 0.67              |
| 10:W:431:LYS:NZ   | 13:Z:238:PRO:HA   | 2.09                     | 0.67              |
| 11:X:112:GLU:HA   | 11:X:115:GLU:HG2  | 1.76                     | 0.67              |
| 12:Y:155:ASP:O    | 12:Y:159:ARG:HG3  | 1.95                     | 0.67              |
| 12:Y:202:LEU:HD11 | 12:Y:231:LEU:HD11 | 1.76                     | 0.67              |
| 13:Z:11:VAL:HG13  | 13:Z:15:VAL:HG11  | 1.77                     | 0.67              |
| 13:Z:142:GLU:OE2  | 13:Z:153:LYS:HD2  | 1.95                     | 0.67              |
| 13:Z:242:LEU:O    | 13:Z:246:VAL:HG23 | 1.94                     | 0.67              |
| 14:a:80:ILE:CA    | 14:a:83:VAL:HB    | 2.22                     | 0.67              |
| 18:f:373:ALA:HB2  | 18:f:760:PHE:CD1  | 2.29                     | 0.67              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 18:f:489:TYR:CD2  | 18:f:497:VAL:HG21 | 2.30                     | 0.67              |
| 18:f:646:MET:O    | 18:f:647:GLY:HA2  | 1.95                     | 0.67              |
| 23:B:335:GLU:OE1  | 23:B:335:GLU:N    | 2.21                     | 0.67              |
| 25:F:436:GLN:HE22 | 26:K:28:ILE:HD13  | 1.59                     | 0.67              |
| 1:C:164:VAL:O     | 1:C:290:LYS:HD2   | 1.95                     | 0.66              |
| 1:C:384:GLU:HA    | 1:C:387:VAL:HG12  | 1.75                     | 0.66              |
| 2:D:107:THR:HA    | 24:E:77:PRO:HG3   | 1.76                     | 0.66              |
| 8:M:25:TYR:O      | 8:M:28:LYS:HG2    | 1.94                     | 0.66              |
| 8:M:227:VAL:HB    | 8:M:232:ARG:HH12  | 1.61                     | 0.66              |
| 9:V:66:GLU:HA     | 9:V:69:THR:HG22   | 1.75                     | 0.66              |
| 9:V:86:VAL:O      | 9:V:89:LYS:NZ     | 2.28                     | 0.66              |
| 11:X:99:MET:SD    | 11:X:100:GLU:N    | 2.69                     | 0.66              |
| 15:b:24:THR:O     | 15:b:27:GLN:NE2   | 2.22                     | 0.66              |
| 15:b:35:ILE:HG21  | 15:b:184:ILE:CG2  | 2.25                     | 0.66              |
| 19:g:89:LEU:HD23  | 19:g:155:VAL:CB   | 2.25                     | 0.66              |
| 23:B:201:VAL:HG21 | 23:B:239:VAL:HG21 | 1.77                     | 0.66              |
| 26:K:236:GLU:HA   | 26:K:239:LYS:CE   | 2.21                     | 0.66              |
| 1:C:301:LEU:HD12  | 1:C:306:LEU:HD21  | 1.77                     | 0.66              |
| 2:D:388:ARG:NH2   | 24:E:297:ARG:NH1  | 2.43                     | 0.66              |
| 5:I:100:GLN:HG2   | 5:I:101:TYR:CD1   | 2.30                     | 0.66              |
| 5:I:159:TRP:CD2   | 6:J:54:GLN:HB3    | 2.29                     | 0.66              |
| 9:V:213:TYR:O     | 9:V:217:VAL:HG13  | 1.96                     | 0.66              |
| 9:V:447:ILE:HG22  | 9:V:448:GLU:N     | 2.10                     | 0.66              |
| 10:W:364:ARG:O    | 10:W:368:LYS:HE2  | 1.95                     | 0.66              |
| 10:W:370:TYR:HD2  | 10:W:373:ILE:HB   | 1.60                     | 0.66              |
| 13:Z:37:GLY:HA2   | 13:Z:56:VAL:HG22  | 1.75                     | 0.66              |
| 13:Z:230:LEU:O    | 13:Z:233:VAL:HG12 | 1.95                     | 0.66              |
| 18:f:256:PHE:CE2  | 18:f:264:GLU:HB3  | 2.30                     | 0.66              |
| 18:f:340:MET:O    | 18:f:387:GLN:NE2  | 2.28                     | 0.66              |
| 18:f:433:LEU:HB3  | 19:g:172:GLU:CA   | 2.25                     | 0.66              |
| 18:f:513:GLU:HA   | 18:f:554:TYR:HD2  | 1.59                     | 0.66              |
| 19:g:113:ARG:HB3  | 19:g:138:LEU:HD13 | 1.76                     | 0.66              |
| 23:B:112:LEU:CD1  | 23:B:123:VAL:HG12 | 2.25                     | 0.66              |
| 24:E:60:VAL:HG22  | 24:E:71:VAL:HG22  | 1.77                     | 0.66              |
| 24:E:122:MET:O    | 24:E:125:GLU:N    | 2.28                     | 0.66              |
| 25:F:145:LEU:HD11 | 25:F:151:VAL:HG11 | 1.78                     | 0.66              |
| 25:F:435:LEU:HD12 | 25:F:435:LEU:H    | 1.60                     | 0.66              |
| 27:U:587:ALA:HB1  | 27:U:624:PHE:CD2  | 2.29                     | 0.66              |
| 1:C:52:LEU:O      | 1:C:56:VAL:HG23   | 1.96                     | 0.66              |
| 1:C:232:ARG:CZ    | 1:C:232:ARG:HB2   | 2.26                     | 0.66              |
| 9:V:176:MET:HE1   | 9:V:213:TYR:HA    | 1.78                     | 0.66              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 14:a:54:ASP:HA    | 14:a:57:ILE:CG2   | 2.19                     | 0.66              |
| 14:a:153:SER:HB2  | 14:a:179:PHE:CE1  | 2.30                     | 0.66              |
| 14:a:159:SER:HA   | 14:a:162:TYR:CB   | 2.22                     | 0.66              |
| 15:b:127:LEU:CD2  | 15:b:130:ARG:HH22 | 2.05                     | 0.66              |
| 18:f:261:ARG:HB3  | 18:f:264:GLU:OE1  | 1.94                     | 0.66              |
| 19:g:116:ILE:HG22 | 19:g:127:ILE:CD1  | 2.25                     | 0.66              |
| 23:B:248:LEU:HD22 | 23:B:270:LEU:CD1  | 2.24                     | 0.66              |
| 23:B:372:MET:CE   | 23:B:414:VAL:HG11 | 2.25                     | 0.66              |
| 23:B:383:LEU:HD22 | 23:B:398:ILE:HD11 | 1.75                     | 0.66              |
| 24:E:228:CYS:O    | 24:E:273:VAL:HG23 | 1.95                     | 0.66              |
| 24:E:352:MET:CE   | 24:E:355:ILE:HD13 | 2.26                     | 0.66              |
| 27:U:559:ARG:CB   | 27:U:562:GLU:HB2  | 2.22                     | 0.66              |
| 27:U:799:LYS:HG3  | 27:U:925:VAL:CG2  | 2.26                     | 0.66              |
| 28:e:41:ASP:OD1   | 28:e:41:ASP:N     | 2.28                     | 0.66              |
| 1:C:331:ILE:O     | 1:C:334:ARG:NE    | 2.29                     | 0.66              |
| 2:D:97:ASP:OD1    | 2:D:100:THR:HG22  | 1.96                     | 0.66              |
| 2:D:148:ASP:O     | 2:D:153:MET:HE2   | 1.95                     | 0.66              |
| 2:D:184:PRO:HG2   | 2:D:306:LYS:HZ1   | 1.60                     | 0.66              |
| 3:G:143:ILE:HD11  | 3:G:220:VAL:HG13  | 1.75                     | 0.66              |
| 3:G:196:GLU:HA    | 3:G:242:LEU:HD21  | 1.76                     | 0.66              |
| 6:J:68:ASN:HB2    | 6:J:137:ASP:OD2   | 1.96                     | 0.66              |
| 7:L:117:GLN:HG3   | 8:M:86:SER:OG     | 1.95                     | 0.66              |
| 7:L:176:MET:HA    | 7:L:179:PHE:CD2   | 2.29                     | 0.66              |
| 8:M:75:MET:HE1    | 8:M:88:ALA:CB     | 2.26                     | 0.66              |
| 17:d:261:ASP:HA   | 17:d:264:LEU:CD1  | 2.21                     | 0.66              |
| 17:d:286:GLU:O    | 17:d:290:ILE:HG13 | 1.96                     | 0.66              |
| 22:A:426:THR:HB   | 22:A:427:PRO:HD3  | 1.78                     | 0.66              |
| 25:F:141:ASP:HB3  | 25:F:143:GLU:OE1  | 1.95                     | 0.66              |
| 1:C:240:GLU:HG3   | 1:C:241:HIS:CD2   | 2.29                     | 0.66              |
| 3:G:80:MET:HB3    | 3:G:87:SER:HB2    | 1.75                     | 0.66              |
| 5:I:105:ILE:HD11  | 5:I:110:LEU:HA    | 1.76                     | 0.66              |
| 6:J:64:ALA:HA     | 6:J:70:CYS:HA     | 1.76                     | 0.66              |
| 9:V:131:LEU:HD13  | 9:V:171:VAL:HG21  | 1.76                     | 0.66              |
| 9:V:282:ASN:HD21  | 12:Y:385:ARG:CB   | 2.09                     | 0.66              |
| 9:V:428:LEU:HD11  | 9:V:437:ILE:HG21  | 1.77                     | 0.66              |
| 10:W:341:PHE:CE2  | 10:W:354:LEU:HD22 | 2.31                     | 0.66              |
| 11:X:89:VAL:HG11  | 11:X:125:LEU:HD21 | 1.77                     | 0.66              |
| 11:X:200:ILE:HG13 | 11:X:201:TYR:H    | 1.61                     | 0.66              |
| 11:X:397:TYR:CE1  | 13:Z:258:VAL:HG21 | 2.30                     | 0.66              |
| 13:Z:237:LEU:HD13 | 16:c:310:LYS:HG2  | 1.77                     | 0.66              |
| 14:a:84:VAL:CG2   | 14:a:121:LEU:HD21 | 2.25                     | 0.66              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 15:b:35:ILE:HG23  | 15:b:188:ILE:HD12 | 1.76                     | 0.66              |
| 16:c:151:VAL:HG13 | 16:c:152:LYS:HG2  | 1.78                     | 0.66              |
| 18:f:89:MET:HE3   | 23:B:411:ARG:HD2  | 1.78                     | 0.66              |
| 25:F:184:GLN:O    | 25:F:187:ASP:N    | 2.15                     | 0.66              |
| 1:C:279:GLN:OE1   | 1:C:279:GLN:HA    | 1.95                     | 0.66              |
| 1:C:399:MET:HE2   | 1:C:402:LYS:HD2   | 1.76                     | 0.66              |
| 2:D:120:ASP:HB3   | 2:D:122:GLU:OE1   | 1.95                     | 0.66              |
| 2:D:370:ILE:CG2   | 2:D:407:ILE:HD11  | 2.24                     | 0.66              |
| 3:G:49:VAL:HG21   | 3:G:195:VAL:HG22  | 1.78                     | 0.66              |
| 9:V:204:ASP:HB3   | 9:V:243:ASP:OD2   | 1.95                     | 0.66              |
| 9:V:454:GLU:OE2   | 17:d:281:LYS:HD2  | 1.95                     | 0.66              |
| 9:V:493:ALA:O     | 9:V:495:ARG:N     | 2.27                     | 0.66              |
| 10:W:278:PRO:HA   | 10:W:357:ARG:HE   | 1.60                     | 0.66              |
| 12:Y:14:ASN:HD21  | 12:Y:113:ARG:NH1  | 1.94                     | 0.66              |
| 13:Z:109:ASN:O    | 13:Z:113:LYS:HG3  | 1.95                     | 0.66              |
| 13:Z:198:LEU:HB3  | 14:a:364:GLU:HB2  | 1.77                     | 0.66              |
| 14:a:72:ASN:OD1   | 14:a:73:PRO:HD2   | 1.95                     | 0.66              |
| 15:b:138:VAL:HG13 | 15:b:160:LEU:HD11 | 1.76                     | 0.66              |
| 17:d:153:GLN:HA   | 17:d:156:ILE:CD1  | 2.26                     | 0.66              |
| 18:f:205:CYS:SG   | 18:f:229:VAL:HG23 | 2.35                     | 0.66              |
| 18:f:670:MET:HE1  | 23:B:68:ILE:HG23  | 1.76                     | 0.66              |
| 19:g:127:ILE:O    | 19:g:162:GLU:HB3  | 1.96                     | 0.66              |
| 19:g:141:THR:HG22 | 19:g:144:GLU:OE2  | 1.96                     | 0.66              |
| 22:A:211:GLY:HA2  | 22:A:317:VAL:O    | 1.96                     | 0.66              |
| 25:F:181:PRO:HD2  | 25:F:238:ARG:HD3  | 1.78                     | 0.66              |
| 26:K:78:MET:HE2   | 26:K:85:ALA:HB1   | 1.76                     | 0.66              |
| 2:D:277:ALA:CB    | 2:D:283:ARG:HG2   | 2.25                     | 0.66              |
| 8:M:136:MET:CE    | 8:M:148:LEU:HD21  | 2.26                     | 0.66              |
| 8:M:187:ARG:CD    | 8:M:219:LEU:HD21  | 2.25                     | 0.66              |
| 9:V:497:PRO:HG3   | 13:Z:282:ASN:HB2  | 1.78                     | 0.66              |
| 11:X:340:GLU:HB3  | 11:X:341:PRO:HD3  | 1.75                     | 0.66              |
| 12:Y:20:ALA:HB2   | 12:Y:150:PHE:CD1  | 2.31                     | 0.66              |
| 13:Z:26:ILE:HD11  | 16:c:102:THR:O    | 1.96                     | 0.66              |
| 15:b:22:LEU:HB2   | 15:b:23:PRO:HD3   | 1.77                     | 0.66              |
| 16:c:177:THR:CB   | 27:U:773:PHE:HB2  | 2.26                     | 0.66              |
| 17:d:293:PHE:HD1  | 17:d:298:LYS:HE3  | 1.58                     | 0.66              |
| 23:B:269:GLU:OE1  | 23:B:269:GLU:HA   | 1.95                     | 0.66              |
| 24:E:98:VAL:HG21  | 24:E:107:ILE:HG12 | 1.77                     | 0.66              |
| 24:E:351:GLY:HA3  | 25:F:217:ILE:CD1  | 2.25                     | 0.66              |
| 27:U:250:PHE:CE2  | 27:U:911:ILE:HG21 | 2.31                     | 0.66              |
| 27:U:567:ILE:HD13 | 27:U:586:VAL:CG2  | 2.25                     | 0.66              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:G:32:ILE:HD13   | 3:G:137:CYS:SG    | 2.35                     | 0.66              |
| 5:I:75:SER:O      | 5:I:134:LEU:HB2   | 1.96                     | 0.66              |
| 7:L:40:SER:CB     | 7:L:182:CYS:HB2   | 2.25                     | 0.66              |
| 12:Y:292:TYR:OH   | 12:Y:293:ARG:NH2  | 2.28                     | 0.66              |
| 12:Y:384:SER:O    | 12:Y:388:ASN:ND2  | 2.29                     | 0.66              |
| 13:Z:267:ARG:CZ   | 17:d:346:LEU:HD23 | 2.26                     | 0.66              |
| 14:a:50:PHE:HD2   | 14:a:52:GLN:HB3   | 1.60                     | 0.66              |
| 17:d:190:GLN:NE2  | 17:d:194:LEU:HD11 | 2.11                     | 0.66              |
| 18:f:386:GLY:HA2  | 18:f:418:LEU:HD11 | 1.77                     | 0.66              |
| 22:A:193:THR:HB   | 22:A:194:PRO:HD3  | 1.76                     | 0.66              |
| 2:D:417:TYR:OH    | 3:G:22:LEU:N      | 2.29                     | 0.66              |
| 5:I:93:ILE:HD13   | 5:I:113:ALA:HB1   | 1.77                     | 0.66              |
| 8:M:98:PHE:CE1    | 8:M:106:ILE:HA    | 2.30                     | 0.66              |
| 9:V:169:LEU:HD22  | 9:V:210:CYS:SG    | 2.35                     | 0.66              |
| 9:V:338:LEU:HD23  | 9:V:398:LEU:HD12  | 1.77                     | 0.66              |
| 10:W:18:VAL:HB    | 10:W:57:ALA:CB    | 2.23                     | 0.66              |
| 10:W:61:VAL:O     | 10:W:64:SER:OG    | 2.07                     | 0.66              |
| 10:W:373:ILE:HG22 | 10:W:415:PHE:HE1  | 1.60                     | 0.66              |
| 15:b:151:GLU:HA   | 15:b:154:THR:CG2  | 2.25                     | 0.66              |
| 17:d:188:MET:O    | 17:d:192:LEU:HD23 | 1.94                     | 0.66              |
| 22:A:92:PRO:HD3   | 23:B:156:VAL:CG1  | 2.19                     | 0.66              |
| 23:B:139:VAL:HG21 | 23:B:159:VAL:HG12 | 1.78                     | 0.66              |
| 25:F:181:PRO:HG2  | 25:F:238:ARG:NH1  | 2.11                     | 0.66              |
| 27:U:108:TYR:HD2  | 27:U:134:VAL:HG11 | 1.61                     | 0.66              |
| 27:U:624:PHE:CE1  | 27:U:658:ILE:HG21 | 2.30                     | 0.66              |
| 27:U:803:LYS:CG   | 27:U:893:THR:HB   | 2.17                     | 0.66              |
| 6:J:51:ALA:HB3    | 6:J:54:GLN:HG3    | 1.78                     | 0.66              |
| 7:L:72:ILE:C      | 7:L:72:ILE:HD12   | 2.21                     | 0.66              |
| 8:M:140:TYR:CG    | 8:M:217:GLY:HA2   | 2.31                     | 0.66              |
| 8:M:173:LYS:O     | 8:M:177:GLU:N     | 2.27                     | 0.66              |
| 8:M:185:THR:HG23  | 8:M:187:ARG:HB2   | 1.78                     | 0.66              |
| 14:a:122:LYS:CE   | 14:a:130:VAL:HG13 | 2.26                     | 0.66              |
| 14:a:192:GLU:O    | 14:a:196:ARG:HG3  | 1.96                     | 0.66              |
| 14:a:216:LEU:HD13 | 14:a:237:LEU:CG   | 2.26                     | 0.66              |
| 15:b:130:ARG:HH21 | 15:b:131:LEU:CD2  | 2.09                     | 0.66              |
| 18:f:241:PRO:HB3  | 27:U:835:ILE:HG21 | 1.77                     | 0.66              |
| 18:f:801:VAL:HA   | 18:f:804:LEU:HD12 | 1.78                     | 0.66              |
| 18:f:832:THR:CG2  | 18:f:870:THR:HG21 | 2.26                     | 0.66              |
| 22:A:146:LYS:HB2  | 22:A:146:LYS:HZ3  | 1.61                     | 0.66              |
| 22:A:194:PRO:HG3  | 22:A:201:PHE:CZ   | 2.30                     | 0.66              |
| 25:F:197:GLU:HG2  | 25:F:352:ILE:CD1  | 2.25                     | 0.66              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:345:ARG:HH11  | 1:C:345:ARG:HG3   | 1.61                     | 0.65              |
| 3:G:69:LEU:HD23   | 3:G:229:ILE:HG12  | 1.78                     | 0.65              |
| 4:H:29:VAL:CG1    | 4:H:133:SER:HB3   | 2.26                     | 0.65              |
| 5:I:25:MET:HE1    | 23:B:438:LEU:HD11 | 1.77                     | 0.65              |
| 5:I:133:SER:OG    | 5:I:164:ILE:HG21  | 1.96                     | 0.65              |
| 8:M:87:LEU:HD22   | 8:M:131:PHE:CD2   | 2.30                     | 0.65              |
| 8:M:212:GLU:C     | 8:M:213:LEU:HD12  | 2.20                     | 0.65              |
| 9:V:259:LEU:HG    | 9:V:264:TYR:CE1   | 2.29                     | 0.65              |
| 13:Z:227:ILE:HG13 | 14:a:346:ILE:HD11 | 1.78                     | 0.65              |
| 14:a:112:ILE:HD13 | 14:a:138:VAL:CG2  | 2.21                     | 0.65              |
| 18:f:271:MET:CE   | 18:f:786:GLN:HB3  | 2.26                     | 0.65              |
| 25:F:185:TYR:CD1  | 25:F:239:ALA:HB1  | 2.32                     | 0.65              |
| 27:U:192:GLN:OE1  | 27:U:192:GLN:N    | 2.26                     | 0.65              |
| 27:U:227:GLN:O    | 27:U:230:SER:OG   | 2.08                     | 0.65              |
| 27:U:538:GLU:HG3  | 27:U:538:GLU:O    | 1.95                     | 0.65              |
| 27:U:873:PRO:HB3  | 27:U:876:GLN:HG3  | 1.77                     | 0.65              |
| 1:C:288:ASN:O     | 1:C:289:ILE:HD13  | 1.96                     | 0.65              |
| 9:V:113:LEU:O     | 9:V:117:VAL:HG13  | 1.95                     | 0.65              |
| 9:V:123:SER:HB2   | 9:V:125:ASN:CG    | 2.21                     | 0.65              |
| 14:a:79:ILE:O     | 14:a:83:VAL:HG23  | 1.96                     | 0.65              |
| 14:a:160:SER:CA   | 14:a:163:TYR:HB3  | 2.26                     | 0.65              |
| 14:a:245:VAL:O    | 14:a:246:GLU:HG3  | 1.97                     | 0.65              |
| 16:c:145:VAL:O    | 16:c:147:PRO:HD3  | 1.96                     | 0.65              |
| 27:U:902:PRO:HA   | 27:U:914:LEU:HA   | 1.78                     | 0.65              |
| 1:C:307:ARG:HG3   | 1:C:307:ARG:O     | 1.95                     | 0.65              |
| 1:C:351:MET:HG2   | 1:C:391:MET:HE3   | 1.77                     | 0.65              |
| 2:D:92:PHE:CE1    | 2:D:124:LEU:HD13  | 2.31                     | 0.65              |
| 3:G:232:GLU:H     | 3:G:232:GLU:CD    | 2.03                     | 0.65              |
| 4:H:74:LEU:HB2    | 4:H:83:TYR:OH     | 1.96                     | 0.65              |
| 6:J:183:THR:CB    | 6:J:186:LEU:HB2   | 2.26                     | 0.65              |
| 7:L:38:LEU:HD23   | 7:L:45:VAL:O      | 1.96                     | 0.65              |
| 7:L:56:LEU:HD23   | 7:L:56:LEU:H      | 1.61                     | 0.65              |
| 9:V:214:HIS:O     | 9:V:217:VAL:HG22  | 1.95                     | 0.65              |
| 12:Y:97:GLU:HA    | 12:Y:100:ILE:HD11 | 1.77                     | 0.65              |
| 13:Z:86:ASN:HB3   | 13:Z:89:GLU:OE1   | 1.96                     | 0.65              |
| 14:a:257:GLN:NE2  | 14:a:259:PRO:O    | 2.30                     | 0.65              |
| 15:b:48:ASN:HA    | 15:b:66:PRO:HA    | 1.76                     | 0.65              |
| 15:b:180:ALA:O    | 15:b:184:ILE:N    | 2.29                     | 0.65              |
| 17:d:163:SER:HA   | 17:d:166:ARG:HD2  | 1.79                     | 0.65              |
| 18:f:479:LEU:HD11 | 18:f:513:GLU:CG   | 2.25                     | 0.65              |
| 18:f:542:ILE:HD12 | 18:f:562:LEU:HD12 | 1.78                     | 0.65              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 18:f:833:PHE:HD1  | 18:f:839:PRO:HA   | 1.61                     | 0.65              |
| 19:g:128:LYS:C    | 19:g:129:ILE:HD13 | 2.22                     | 0.65              |
| 22:A:177:VAL:HG11 | 22:A:225:CYS:SG   | 2.37                     | 0.65              |
| 9:V:101:LEU:O     | 9:V:105:SER:N     | 2.29                     | 0.65              |
| 10:W:140:ILE:HD12 | 10:W:140:ILE:H    | 1.62                     | 0.65              |
| 11:X:93:LEU:HD22  | 11:X:129:LEU:CD1  | 2.26                     | 0.65              |
| 12:Y:17:LEU:HG    | 12:Y:213:LEU:HD13 | 1.77                     | 0.65              |
| 18:f:301:HIS:ND1  | 18:f:301:HIS:O    | 2.30                     | 0.65              |
| 18:f:562:LEU:HD22 | 18:f:595:VAL:CG1  | 2.27                     | 0.65              |
| 19:g:117:ALA:HA   | 19:g:122:LEU:HB2  | 1.77                     | 0.65              |
| 25:F:288:LEU:HB3  | 25:F:332:THR:OG1  | 1.95                     | 0.65              |
| 27:U:163:PHE:CE2  | 27:U:197:VAL:HG13 | 2.28                     | 0.65              |
| 27:U:188:MET:HE2  | 27:U:188:MET:CA   | 2.27                     | 0.65              |
| 27:U:412:HIS:O    | 27:U:449:ILE:HG12 | 1.96                     | 0.65              |
| 1:C:114:VAL:HG11  | 1:C:123:LEU:HD11  | 1.78                     | 0.65              |
| 3:G:37:LEU:HD12   | 3:G:68:HIS:CE1    | 2.31                     | 0.65              |
| 4:H:65:VAL:HG12   | 4:H:218:PHE:HZ    | 1.62                     | 0.65              |
| 7:L:112:ILE:O     | 7:L:116:THR:HG23  | 1.96                     | 0.65              |
| 10:W:112:VAL:HG13 | 10:W:121:LYS:HZ1  | 1.61                     | 0.65              |
| 10:W:171:VAL:HA   | 10:W:174:TYR:CD2  | 2.31                     | 0.65              |
| 10:W:270:VAL:HG22 | 10:W:290:ILE:HD12 | 1.79                     | 0.65              |
| 11:X:57:LEU:O     | 11:X:61:GLY:N     | 2.30                     | 0.65              |
| 11:X:208:ALA:HB1  | 11:X:239:TYR:CD2  | 2.31                     | 0.65              |
| 13:Z:37:GLY:HA3   | 13:Z:95:TYR:CE2   | 2.30                     | 0.65              |
| 14:a:84:VAL:HA    | 14:a:87:MET:CG    | 2.27                     | 0.65              |
| 16:c:177:THR:CB   | 27:U:774:PRO:HD3  | 2.26                     | 0.65              |
| 18:f:655:LEU:HD21 | 18:f:800:LEU:HB3  | 1.78                     | 0.65              |
| 18:f:830:LEU:CD2  | 18:f:846:VAL:HG21 | 2.26                     | 0.65              |
| 18:f:830:LEU:HD21 | 18:f:846:VAL:HG21 | 1.79                     | 0.65              |
| 19:g:128:LYS:O    | 19:g:129:ILE:HD13 | 1.96                     | 0.65              |
| 22:A:334:PRO:CB   | 25:F:398:ALA:HB2  | 2.26                     | 0.65              |
| 24:E:152:PRO:CG   | 24:E:274:LYS:HE2  | 2.27                     | 0.65              |
| 26:K:70:ILE:HB    | 26:K:74:ILE:HG23  | 1.78                     | 0.65              |
| 27:U:241:ASN:O    | 27:U:243:LEU:N    | 2.30                     | 0.65              |
| 1:C:214:VAL:CG1   | 1:C:219:LEU:HD21  | 2.26                     | 0.65              |
| 1:C:338:LEU:HD21  | 1:C:342:ILE:HG12  | 1.79                     | 0.65              |
| 2:D:236:VAL:O     | 2:D:236:VAL:HG12  | 1.96                     | 0.65              |
| 3:G:131:MET:HG2   | 8:M:125:TYR:HE1   | 1.61                     | 0.65              |
| 8:M:136:MET:HE1   | 8:M:148:LEU:HD21  | 1.79                     | 0.65              |
| 9:V:175:MET:O     | 9:V:180:ARG:N     | 2.28                     | 0.65              |
| 10:W:378:MET:HE1  | 10:W:393:LEU:HD22 | 1.79                     | 0.65              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 14:a:188:LEU:HD11 | 14:a:193:GLN:HG3  | 1.78                     | 0.65              |
| 15:b:26:LEU:HD11  | 15:b:80:PRO:HB3   | 1.77                     | 0.65              |
| 16:c:144:VAL:HG12 | 16:c:145:VAL:H    | 1.62                     | 0.65              |
| 17:d:259:PHE:HA   | 17:d:262:ILE:CD1  | 2.26                     | 0.65              |
| 23:B:332:ASN:OD1  | 23:B:332:ASN:N    | 2.29                     | 0.65              |
| 24:E:245:GLU:OE2  | 24:E:254:GLN:NE2  | 2.26                     | 0.65              |
| 25:F:69:MET:HG3   | 25:F:73:ILE:HD13  | 1.77                     | 0.65              |
| 25:F:268:VAL:HG11 | 25:F:313:LEU:CA   | 2.27                     | 0.65              |
| 28:e:18:GLU:OE1   | 28:e:18:GLU:N     | 2.21                     | 0.65              |
| 1:C:37:ASP:OD1    | 1:C:38:LYS:N      | 2.30                     | 0.65              |
| 1:C:271:ARG:CZ    | 23:B:305:ILE:HD13 | 2.26                     | 0.65              |
| 6:J:68:ASN:HA     | 6:J:211:MET:CE    | 2.26                     | 0.65              |
| 8:M:87:LEU:HD22   | 8:M:131:PHE:HD2   | 1.60                     | 0.65              |
| 10:W:60:MET:CA    | 10:W:97:LEU:HD12  | 2.27                     | 0.65              |
| 10:W:287:VAL:HA   | 10:W:290:ILE:HG22 | 1.78                     | 0.65              |
| 15:b:29:GLN:HB2   | 15:b:112:PHE:HD2  | 1.61                     | 0.65              |
| 15:b:157:VAL:CG2  | 15:b:170:LEU:HB2  | 2.25                     | 0.65              |
| 17:d:89:GLN:O     | 17:d:93:GLY:N     | 2.25                     | 0.65              |
| 17:d:223:ASN:CB   | 17:d:226:ILE:HD12 | 2.26                     | 0.65              |
| 18:f:56:LEU:O     | 18:f:60:VAL:HG12  | 1.97                     | 0.65              |
| 22:A:213:LEU:CB   | 22:A:337:LEU:HD13 | 2.26                     | 0.65              |
| 24:E:150:GLU:HG2  | 24:E:191:LEU:HD11 | 1.79                     | 0.65              |
| 24:E:165:ILE:CG2  | 24:E:166:PRO:HD2  | 2.26                     | 0.65              |
| 26:K:78:MET:HE2   | 26:K:85:ALA:CB    | 2.26                     | 0.65              |
| 27:U:247:GLN:HG2  | 27:U:913:ILE:CG1  | 2.25                     | 0.65              |
| 27:U:806:CYS:SG   | 27:U:874:ASN:HB3  | 2.37                     | 0.65              |
| 9:V:176:MET:HE3   | 9:V:217:VAL:HG13  | 1.79                     | 0.65              |
| 9:V:403:ILE:O     | 9:V:407:VAL:HG23  | 1.97                     | 0.65              |
| 10:W:239:SER:O    | 10:W:243:ILE:HG13 | 1.97                     | 0.65              |
| 10:W:274:VAL:HG11 | 10:W:290:ILE:HG21 | 1.79                     | 0.65              |
| 11:X:90:ARG:O     | 11:X:93:LEU:HG    | 1.97                     | 0.65              |
| 11:X:255:LEU:HD22 | 11:X:267:VAL:HG23 | 1.77                     | 0.65              |
| 12:Y:381:GLN:HA   | 12:Y:384:SER:OG   | 1.97                     | 0.65              |
| 18:f:66:LYS:HA    | 18:f:71:TYR:OH    | 1.97                     | 0.65              |
| 19:g:101:LEU:HD11 | 19:g:116:ILE:O    | 1.97                     | 0.65              |
| 23:B:46:ALA:HB3   | 23:B:179:ALA:HB2  | 1.78                     | 0.65              |
| 24:E:168:LYS:HA   | 24:E:274:LYS:HD2  | 1.78                     | 0.65              |
| 27:U:171:ASN:O    | 27:U:173:VAL:N    | 2.30                     | 0.65              |
| 27:U:221:ILE:CD1  | 27:U:256:ALA:HB2  | 2.27                     | 0.65              |
| 27:U:688:LEU:HD22 | 27:U:713:TYR:CE1  | 2.32                     | 0.65              |
| 27:U:888:GLN:OE1  | 27:U:888:GLN:N    | 2.29                     | 0.65              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:248:MET:HE1   | 1:C:276:LEU:HD12  | 1.79                     | 0.65              |
| 2:D:381:GLU:OE2   | 2:D:405:THR:HG21  | 1.97                     | 0.65              |
| 5:I:36:GLY:O      | 5:I:161:ALA:HA    | 1.96                     | 0.65              |
| 5:I:136:TYR:HE1   | 5:I:150:SER:HB2   | 1.61                     | 0.65              |
| 12:Y:48:ASN:HB3   | 12:Y:113:ARG:HG3  | 1.78                     | 0.65              |
| 13:Z:40:LEU:HD11  | 13:Z:54:PHE:CE2   | 2.32                     | 0.65              |
| 17:d:88:LEU:HD12  | 17:d:92:THR:HG23  | 1.79                     | 0.65              |
| 17:d:108:ASN:OD1  | 17:d:111:LYS:N    | 2.20                     | 0.65              |
| 18:f:160:ARG:NH2  | 18:f:203:GLU:OE2  | 2.30                     | 0.65              |
| 18:f:416:MET:HE2  | 18:f:819:TYR:HE1  | 1.62                     | 0.65              |
| 19:g:138:LEU:HD12 | 19:g:162:GLU:CG   | 2.27                     | 0.65              |
| 19:g:170:GLN:HA   | 19:g:173:GLU:CB   | 2.26                     | 0.65              |
| 22:A:48:VAL:HG21  | 23:B:62:LEU:CD1   | 2.27                     | 0.65              |
| 22:A:246:VAL:HG21 | 23:B:307:ARG:CD   | 2.26                     | 0.65              |
| 25:F:343:LEU:CD2  | 25:F:351:LYS:HD2  | 2.25                     | 0.65              |
| 27:U:902:PRO:HG3  | 27:U:906:LEU:CD2  | 2.26                     | 0.65              |
| 5:I:86:LEU:HD21   | 5:I:118:LYS:HZ2   | 1.61                     | 0.65              |
| 8:M:117:MET:HE2   | 8:M:117:MET:HA    | 1.76                     | 0.65              |
| 9:V:114:TYR:CE2   | 9:V:118:GLN:HG3   | 2.31                     | 0.65              |
| 10:W:20:TYR:O     | 10:W:24:VAL:HG12  | 1.97                     | 0.65              |
| 11:X:376:GLY:O    | 11:X:377:ILE:HG12 | 1.97                     | 0.65              |
| 12:Y:192:ARG:HD3  | 12:Y:294:TYR:CD2  | 2.31                     | 0.65              |
| 12:Y:316:LEU:HD22 | 12:Y:327:VAL:HG13 | 1.77                     | 0.65              |
| 14:a:61:GLU:HG3   | 14:a:79:ILE:HD13  | 1.79                     | 0.65              |
| 14:a:113:LEU:HA   | 14:a:116:THR:OG1  | 1.97                     | 0.65              |
| 15:b:38:HIS:O     | 15:b:42:ARG:HD3   | 1.97                     | 0.65              |
| 18:f:96:LEU:HD21  | 18:f:129:LEU:HA   | 1.77                     | 0.65              |
| 18:f:368:ALA:O    | 18:f:372:LEU:HG   | 1.97                     | 0.65              |
| 23:B:103:ARG:HA   | 23:B:160:ILE:CD1  | 2.26                     | 0.65              |
| 25:F:270:ASP:HA   | 25:F:273:ALA:HB3  | 1.77                     | 0.65              |
| 26:K:91:LYS:O     | 26:K:91:LYS:HD2   | 1.96                     | 0.65              |
| 27:U:142:LEU:HD22 | 27:U:169:GLU:OE1  | 1.97                     | 0.65              |
| 1:C:368:MET:HB3   | 2:D:329:ARG:HH22  | 1.62                     | 0.64              |
| 7:L:58:ALA:HB2    | 26:K:164:GLN:HE21 | 1.61                     | 0.64              |
| 7:L:104:PRO:HG3   | 7:L:107:ARG:HE    | 1.61                     | 0.64              |
| 10:W:87:ILE:HA    | 10:W:104:MET:HE1  | 1.79                     | 0.64              |
| 12:Y:50:MET:HG3   | 12:Y:113:ARG:O    | 1.97                     | 0.64              |
| 15:b:160:LEU:HD22 | 15:b:168:SER:HB2  | 1.78                     | 0.64              |
| 18:f:110:TYR:CE1  | 18:f:119:LYS:HE2  | 2.31                     | 0.64              |
| 18:f:110:TYR:CD1  | 18:f:119:LYS:HE2  | 2.32                     | 0.64              |
| 18:f:442:SER:HB3  | 18:f:476:THR:O    | 1.95                     | 0.64              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 18:f:470:VAL:HG12 | 18:f:481:SER:HB3  | 1.79                     | 0.64              |
| 18:f:590:PHE:HB2  | 18:f:649:HIS:CE1  | 2.32                     | 0.64              |
| 18:f:605:ASN:OD1  | 18:f:607:LEU:HB2  | 1.97                     | 0.64              |
| 23:B:187:ILE:HG22 | 23:B:234:LEU:CD2  | 2.27                     | 0.64              |
| 24:E:149:ILE:CD1  | 24:E:276:ILE:CD1  | 2.73                     | 0.64              |
| 25:F:204:LEU:HB2  | 25:F:205:PRO:HD3  | 1.79                     | 0.64              |
| 25:F:257:VAL:HG13 | 25:F:257:VAL:O    | 1.97                     | 0.64              |
| 1:C:199:LEU:HD23  | 1:C:199:LEU:O     | 1.96                     | 0.64              |
| 2:D:263:PHE:HA    | 2:D:308:ILE:O     | 1.98                     | 0.64              |
| 5:I:17:ARG:HA     | 23:B:439:TYR:OH   | 1.98                     | 0.64              |
| 5:I:45:LEU:HD22   | 5:I:65:ILE:CD1    | 2.28                     | 0.64              |
| 7:L:26:MET:HE1    | 7:L:149:PRO:HD2   | 1.77                     | 0.64              |
| 8:M:25:TYR:HA     | 8:M:28:LYS:HG2    | 1.78                     | 0.64              |
| 13:Z:101:LEU:HB3  | 13:Z:105:ASP:OD2  | 1.97                     | 0.64              |
| 14:a:202:LEU:O    | 14:a:206:LEU:HD23 | 1.96                     | 0.64              |
| 16:c:187:PRO:HB3  | 16:c:192:LEU:HD11 | 1.78                     | 0.64              |
| 18:f:483:PHE:HB2  | 18:f:517:VAL:HG11 | 1.78                     | 0.64              |
| 22:A:271:LEU:C    | 22:A:272:ILE:HD13 | 2.22                     | 0.64              |
| 23:B:201:VAL:HG11 | 23:B:328:ILE:HD11 | 1.80                     | 0.64              |
| 25:F:185:TYR:CE1  | 25:F:239:ALA:HB1  | 2.33                     | 0.64              |
| 27:U:150:ALA:O    | 27:U:154:ALA:N    | 2.27                     | 0.64              |
| 27:U:791:LEU:HD13 | 27:U:797:MET:HE1  | 1.78                     | 0.64              |
| 2:D:155:THR:HG23  | 2:D:158:GLN:OE1   | 1.97                     | 0.64              |
| 2:D:323:ARG:HH12  | 2:D:326:ARG:NH1   | 1.94                     | 0.64              |
| 3:G:164:LYS:HE2   | 4:H:57:TYR:O      | 1.96                     | 0.64              |
| 4:H:79:MET:HE2    | 4:H:82:ASP:OD2    | 1.97                     | 0.64              |
| 12:Y:98:SER:OG    | 12:Y:99:GLU:OE2   | 2.15                     | 0.64              |
| 14:a:16:PRO:O     | 14:a:21:VAL:HG13  | 1.97                     | 0.64              |
| 15:b:16:MET:HA    | 15:b:25:ARG:HE    | 1.63                     | 0.64              |
| 17:d:145:ARG:O    | 17:d:149:GLU:HB2  | 1.96                     | 0.64              |
| 18:f:183:PRO:O    | 18:f:186:THR:OG1  | 2.13                     | 0.64              |
| 18:f:333:LEU:HA   | 18:f:336:GLU:OE1  | 1.98                     | 0.64              |
| 23:B:180:PRO:O    | 23:B:241:ASN:ND2  | 2.28                     | 0.64              |
| 25:F:277:GLU:HB3  | 25:F:278:LYS:NZ   | 2.13                     | 0.64              |
| 27:U:353:LEU:HD11 | 27:U:373:ASN:CB   | 2.27                     | 0.64              |
| 1:C:148:TYR:CE1   | 1:C:158:ILE:HG23  | 2.32                     | 0.64              |
| 1:C:401:ILE:HD13  | 4:H:26:LEU:HD13   | 1.80                     | 0.64              |
| 3:G:231:THR:O     | 3:G:235:ILE:HD12  | 1.98                     | 0.64              |
| 4:H:44:VAL:HG21   | 4:H:145:TYR:O     | 1.97                     | 0.64              |
| 5:I:171:ALA:CB    | 5:I:200:THR:HG21  | 2.26                     | 0.64              |
| 5:I:197:LEU:HB2   | 5:I:206:LEU:HD11  | 1.79                     | 0.64              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 10:W:117:ASP:OD1  | 10:W:119:PRO:HD2  | 1.97                     | 0.64              |
| 12:Y:104:MET:HE1  | 12:Y:130:LYS:NZ   | 2.13                     | 0.64              |
| 13:Z:110:GLU:OE1  | 13:Z:113:LYS:HD3  | 1.97                     | 0.64              |
| 14:a:77:VAL:CA    | 14:a:80:ILE:HG12  | 2.27                     | 0.64              |
| 18:f:830:LEU:HD22 | 18:f:874:LEU:CD2  | 2.21                     | 0.64              |
| 22:A:217:PRO:HG2  | 22:A:345:LEU:HD21 | 1.79                     | 0.64              |
| 23:B:112:LEU:CD2  | 23:B:144:LEU:HG   | 2.27                     | 0.64              |
| 24:E:247:THR:H    | 24:E:250:ASP:HB2  | 1.61                     | 0.64              |
| 27:U:158:ARG:HD2  | 27:U:158:ARG:N    | 2.12                     | 0.64              |
| 27:U:249:CYS:SG   | 27:U:328:ILE:HG13 | 2.38                     | 0.64              |
| 2:D:250:VAL:CG1   | 2:D:262:ILE:HD13  | 2.26                     | 0.64              |
| 7:L:79:ALA:HA     | 26:K:121:LEU:HD13 | 1.78                     | 0.64              |
| 8:M:41:CYS:N      | 8:M:44:GLY:O      | 2.31                     | 0.64              |
| 9:V:67:LEU:CA     | 9:V:70:VAL:HG12   | 2.28                     | 0.64              |
| 9:V:108:LEU:HA    | 9:V:112:VAL:HG21  | 1.80                     | 0.64              |
| 10:W:72:LYS:HD3   | 10:W:111:TYR:OH   | 1.96                     | 0.64              |
| 10:W:224:LEU:O    | 10:W:228:ASN:HB2  | 1.97                     | 0.64              |
| 11:X:47:GLU:HG2   | 11:X:80:ILE:CG2   | 2.28                     | 0.64              |
| 14:a:70:ARG:NH1   | 15:b:17:ARG:HB3   | 2.13                     | 0.64              |
| 18:f:132:THR:OG1  | 22:A:32:LEU:HD11  | 1.97                     | 0.64              |
| 18:f:439:TYR:HA   | 18:f:477:MET:CE   | 2.21                     | 0.64              |
| 19:g:109:GLY:O    | 19:g:113:ARG:HD2  | 1.97                     | 0.64              |
| 23:B:112:LEU:HD12 | 23:B:123:VAL:HG12 | 1.79                     | 0.64              |
| 24:E:145:LEU:HD12 | 24:E:172:LEU:HD21 | 1.79                     | 0.64              |
| 25:F:187:ASP:O    | 25:F:368:ILE:HG21 | 1.97                     | 0.64              |
| 25:F:248:PHE:HA   | 25:F:282:ILE:HG12 | 1.80                     | 0.64              |
| 25:F:251:LEU:HD11 | 25:F:256:LEU:CD2  | 2.24                     | 0.64              |
| 25:F:364:ARG:O    | 25:F:368:ILE:HD12 | 1.96                     | 0.64              |
| 25:F:410:ARG:O    | 25:F:410:ARG:HG2  | 1.97                     | 0.64              |
| 27:U:524:LYS:O    | 27:U:524:LYS:HG3  | 1.97                     | 0.64              |
| 27:U:583:MET:HE2  | 27:U:618:ALA:HB2  | 1.79                     | 0.64              |
| 27:U:788:VAL:HA   | 27:U:910:GLY:O    | 1.97                     | 0.64              |
| 27:U:874:ASN:H    | 27:U:876:GLN:CD   | 2.06                     | 0.64              |
| 1:C:57:ARG:HG3    | 1:C:57:ARG:HH11   | 1.63                     | 0.64              |
| 1:C:97:VAL:HB     | 1:C:121:TYR:O     | 1.97                     | 0.64              |
| 2:D:230:VAL:HG11  | 2:D:235:PHE:CE1   | 2.32                     | 0.64              |
| 3:G:22:LEU:HD11   | 4:H:128:ARG:CD    | 2.28                     | 0.64              |
| 5:I:68:LEU:HD11   | 5:I:74:CYS:HB3    | 1.80                     | 0.64              |
| 6:J:10:PHE:CE1    | 6:J:16:LEU:HG     | 2.29                     | 0.64              |
| 9:V:264:TYR:CE2   | 17:d:213:GLU:HG3  | 2.31                     | 0.64              |
| 9:V:442:ILE:HD11  | 9:V:449:ALA:HB3   | 1.79                     | 0.64              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 10:W:140:ILE:HG22 | 10:W:144:ARG:HH22 | 1.63                     | 0.64              |
| 12:Y:376:LEU:O    | 12:Y:376:LEU:HD12 | 1.96                     | 0.64              |
| 13:Z:78:MET:HE2   | 16:c:98:MET:HE3   | 1.78                     | 0.64              |
| 14:a:221:VAL:HG23 | 14:a:222:LEU:H    | 1.62                     | 0.64              |
| 14:a:325:ASP:O    | 14:a:329:LYS:HA   | 1.98                     | 0.64              |
| 15:b:85:THR:HG23  | 15:b:85:THR:O     | 1.96                     | 0.64              |
| 18:f:114:ALA:CB   | 18:f:118:ASN:HB2  | 2.26                     | 0.64              |
| 18:f:478:ARG:NH1  | 18:f:507:ASP:OD2  | 2.29                     | 0.64              |
| 19:g:132:ASN:HB2  | 19:g:151:VAL:CG1  | 2.25                     | 0.64              |
| 19:g:161:SER:OG   | 19:g:163:GLU:OE1  | 2.13                     | 0.64              |
| 20:u:196:ILE:O    | 20:u:215:THR:HG22 | 1.97                     | 0.64              |
| 23:B:46:ALA:CB    | 23:B:179:ALA:HB2  | 2.28                     | 0.64              |
| 23:B:223:ILE:HG21 | 23:B:350:LYS:HG2  | 1.79                     | 0.64              |
| 27:U:31:VAL:HG22  | 27:U:38:ILE:HD13  | 1.79                     | 0.64              |
| 27:U:532:MET:HG2  | 27:U:548:LEU:CD1  | 2.27                     | 0.64              |
| 1:C:168:PRO:HA    | 1:C:175:PHE:CE1   | 2.32                     | 0.64              |
| 3:G:70:PHE:CD2    | 3:G:91:VAL:HG21   | 2.32                     | 0.64              |
| 9:V:470:ARG:HH12  | 9:V:474:LEU:HD13  | 1.61                     | 0.64              |
| 10:W:267:LEU:HA   | 10:W:270:VAL:CG1  | 2.28                     | 0.64              |
| 11:X:298:SER:OG   | 11:X:301:ASP:HB2  | 1.98                     | 0.64              |
| 13:Z:175:LEU:HD13 | 16:c:217:LEU:HD12 | 1.80                     | 0.64              |
| 15:b:9:CYS:HB3    | 15:b:54:LEU:HD21  | 1.78                     | 0.64              |
| 18:f:301:HIS:NE2  | 18:f:788:MET:O    | 2.30                     | 0.64              |
| 27:U:194:ARG:HD3  | 27:U:198:LEU:HD23 | 1.77                     | 0.64              |
| 27:U:805:ASN:HB2  | 27:U:891:VAL:O    | 1.98                     | 0.64              |
| 11:X:57:LEU:HD21  | 11:X:62:GLN:O     | 1.96                     | 0.64              |
| 11:X:65:GLU:O     | 11:X:69:LEU:N     | 2.27                     | 0.64              |
| 11:X:86:ALA:HB1   | 11:X:90:ARG:HH21  | 1.63                     | 0.64              |
| 11:X:183:LEU:HD11 | 11:X:220:ALA:HB3  | 1.79                     | 0.64              |
| 13:Z:13:PRO:HD3   | 13:Z:163:GLY:O    | 1.98                     | 0.64              |
| 13:Z:23:PHE:CD2   | 13:Z:126:VAL:HG11 | 2.32                     | 0.64              |
| 18:f:381:VAL:HG12 | 18:f:382:ASN:OD1  | 1.98                     | 0.64              |
| 18:f:560:LEU:HD11 | 18:f:798:THR:HA   | 1.79                     | 0.64              |
| 22:A:44:GLN:O     | 22:A:48:VAL:HG23  | 1.98                     | 0.64              |
| 23:B:174:MET:HE1  | 23:B:266:LEU:HD21 | 1.79                     | 0.64              |
| 26:K:230:THR:HG22 | 26:K:233:GLU:OE1  | 1.98                     | 0.64              |
| 27:U:322:THR:O    | 27:U:326:ILE:HG13 | 1.97                     | 0.64              |
| 27:U:348:THR:HG21 | 27:U:377:HIS:HD2  | 1.63                     | 0.64              |
| 27:U:501:LEU:CD1  | 27:U:544:ILE:HD11 | 2.27                     | 0.64              |
| 27:U:786:THR:OG1  | 27:U:884:VAL:O    | 2.15                     | 0.64              |
| 27:U:796:LYS:HG2  | 27:U:798:PRO:HD3  | 1.80                     | 0.64              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:G:76:ILE:HG12   | 3:G:111:VAL:HG22  | 1.79                     | 0.64              |
| 9:V:330:LYS:HD3   | 9:V:360:TYR:OH    | 1.97                     | 0.64              |
| 9:V:446:VAL:C     | 9:V:447:ILE:HD13  | 2.23                     | 0.64              |
| 11:X:368:MET:HE2  | 11:X:374:PHE:CD1  | 2.32                     | 0.64              |
| 17:d:123:LEU:O    | 17:d:127:ASN:N    | 2.31                     | 0.64              |
| 18:f:845:ARG:CG   | 18:f:865:PHE:HB2  | 2.27                     | 0.64              |
| 25:F:225:MET:HG2  | 25:F:352:ILE:CG2  | 2.28                     | 0.64              |
| 27:U:486:MET:HE1  | 27:U:781:LEU:HD21 | 1.80                     | 0.64              |
| 27:U:699:THR:OG1  | 27:U:701:ILE:HG22 | 1.98                     | 0.64              |
| 1:C:117:ARG:HG2   | 1:C:117:ARG:HH11  | 1.63                     | 0.64              |
| 2:D:370:ILE:HG21  | 2:D:407:ILE:HD11  | 1.77                     | 0.64              |
| 3:G:58:ASP:HB3    | 3:G:61:LEU:HD13   | 1.80                     | 0.64              |
| 4:H:39:LYS:HE2    | 4:H:144:PRO:O     | 1.98                     | 0.64              |
| 4:H:59:GLU:N      | 4:H:59:GLU:OE1    | 2.31                     | 0.64              |
| 7:L:15:PRO:HA     | 8:M:25:TYR:CD2    | 2.33                     | 0.64              |
| 8:M:31:GLU:OE1    | 8:M:169:ARG:HD3   | 1.98                     | 0.64              |
| 9:V:440:LYS:CE    | 9:V:443:ARG:HH21  | 2.10                     | 0.64              |
| 10:W:98:LYS:HD2   | 10:W:137:TYR:CE1  | 2.33                     | 0.64              |
| 11:X:345:VAL:HG13 | 11:X:350:ILE:HD11 | 1.80                     | 0.64              |
| 15:b:171:VAL:CG2  | 15:b:187:PRO:HG3  | 2.21                     | 0.64              |
| 18:f:89:MET:HE3   | 23:B:411:ARG:CD   | 2.27                     | 0.64              |
| 18:f:367:SER:HB3  | 18:f:370:MET:CG   | 2.27                     | 0.64              |
| 19:g:160:GLN:HB2  | 19:g:168:ASN:HB2  | 1.80                     | 0.64              |
| 22:A:158:ASP:HB3  | 22:A:161:VAL:HB   | 1.80                     | 0.64              |
| 26:K:228:MET:HA   | 26:K:228:MET:HE3  | 1.79                     | 0.64              |
| 27:U:351:MET:HA   | 27:U:351:MET:HE3  | 1.80                     | 0.64              |
| 5:I:36:GLY:HA2    | 5:I:44:LEU:O      | 1.98                     | 0.63              |
| 7:L:193:ARG:O     | 7:L:197:GLU:HG2   | 1.98                     | 0.63              |
| 8:M:37:ILE:HG12   | 8:M:48:GLY:O      | 1.98                     | 0.63              |
| 8:M:197:ILE:O     | 8:M:200:VAL:HG22  | 1.98                     | 0.63              |
| 9:V:175:MET:HB3   | 9:V:184:ALA:HB2   | 1.79                     | 0.63              |
| 9:V:363:LEU:CD2   | 9:V:395:ILE:HD12  | 2.27                     | 0.63              |
| 10:W:34:LEU:HB2   | 10:W:43:VAL:CG2   | 2.28                     | 0.63              |
| 10:W:406:VAL:HG12 | 10:W:413:ILE:HG12 | 1.79                     | 0.63              |
| 11:X:344:ARG:CG   | 11:X:386:ILE:HD12 | 2.17                     | 0.63              |
| 13:Z:106:ILE:HG12 | 13:Z:155:PHE:HE1  | 1.61                     | 0.63              |
| 14:a:17:GLY:O     | 14:a:21:VAL:HG22  | 1.97                     | 0.63              |
| 14:a:54:ASP:CG    | 14:a:86:GLN:HG3   | 2.23                     | 0.63              |
| 17:d:92:THR:HA    | 17:d:95:TYR:HB3   | 1.80                     | 0.63              |
| 18:f:293:GLN:OE1  | 18:f:293:GLN:HA   | 1.98                     | 0.63              |
| 18:f:683:GLU:HG2  | 18:f:686:LEU:CD1  | 2.28                     | 0.63              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 18:f:870:THR:HA   | 18:f:872:VAL:HG23 | 1.81                     | 0.63              |
| 18:f:881:GLU:HA   | 18:f:894:LEU:HD22 | 1.79                     | 0.63              |
| 26:K:185:TYR:HA   | 26:K:189:MET:CE   | 2.27                     | 0.63              |
| 27:U:73:ALA:HB1   | 27:U:75:GLU:OE2   | 1.98                     | 0.63              |
| 27:U:132:GLY:HA2  | 27:U:135:ASN:OD1  | 1.98                     | 0.63              |
| 27:U:147:TYR:O    | 27:U:151:ILE:HG22 | 1.98                     | 0.63              |
| 1:C:131:VAL:HG13  | 1:C:136:SER:HB2   | 1.78                     | 0.63              |
| 1:C:194:THR:HG21  | 1:C:317:PHE:HB3   | 1.81                     | 0.63              |
| 4:H:139:TRP:CZ2   | 4:H:142:GLY:HA2   | 2.33                     | 0.63              |
| 7:L:26:MET:HE2    | 7:L:149:PRO:HD2   | 1.79                     | 0.63              |
| 8:M:45:VAL:HG23   | 8:M:146:ALA:HB1   | 1.79                     | 0.63              |
| 9:V:101:LEU:HD23  | 9:V:209:LYS:HG2   | 1.79                     | 0.63              |
| 11:X:68:GLY:HA2   | 11:X:71:LYS:HG2   | 1.79                     | 0.63              |
| 14:a:321:LYS:O    | 14:a:334:THR:OG1  | 2.14                     | 0.63              |
| 18:f:502:LEU:O    | 18:f:505:MET:HG2  | 1.98                     | 0.63              |
| 22:A:174:TYR:OH   | 22:A:229:VAL:HG22 | 1.97                     | 0.63              |
| 24:E:194:ASN:O    | 24:E:228:CYS:HA   | 1.98                     | 0.63              |
| 24:E:238:ILE:HD12 | 24:E:238:ILE:N    | 2.13                     | 0.63              |
| 25:F:172:VAL:HG22 | 25:F:267:LEU:CD1  | 2.27                     | 0.63              |
| 25:F:188:ILE:CD1  | 25:F:239:ALA:HB2  | 2.28                     | 0.63              |
| 26:K:108:THR:O    | 26:K:111:SER:OG   | 2.12                     | 0.63              |
| 26:K:220:VAL:HA   | 26:K:228:MET:HE1  | 1.80                     | 0.63              |
| 27:U:357:LYS:HE2  | 27:U:385:PHE:HE2  | 1.64                     | 0.63              |
| 27:U:792:ASN:OD1  | 27:U:793:LYS:N    | 2.27                     | 0.63              |
| 27:U:803:LYS:CB   | 27:U:875:PHE:HA   | 2.28                     | 0.63              |
| 1:C:329:LEU:HD11  | 1:C:347:ILE:HG22  | 1.78                     | 0.63              |
| 11:X:89:VAL:CG1   | 11:X:125:LEU:HD11 | 2.28                     | 0.63              |
| 13:Z:185:GLY:O    | 13:Z:186:THR:OG1  | 2.08                     | 0.63              |
| 17:d:197:LEU:O    | 17:d:197:LEU:HD23 | 1.98                     | 0.63              |
| 17:d:206:ALA:O    | 17:d:210:THR:HG22 | 1.98                     | 0.63              |
| 18:f:467:SER:O    | 18:f:470:VAL:HG22 | 1.99                     | 0.63              |
| 23:B:225:TYR:CZ   | 23:B:352:GLU:HB2  | 2.33                     | 0.63              |
| 23:B:383:LEU:CD2  | 23:B:419:PHE:HB3  | 2.26                     | 0.63              |
| 26:K:44:GLU:HG3   | 26:K:191:LEU:HB2  | 1.81                     | 0.63              |
| 26:K:146:VAL:HG21 | 26:K:222:PRO:HA   | 1.79                     | 0.63              |
| 27:U:373:ASN:HD21 | 27:U:411:ILE:HD11 | 1.62                     | 0.63              |
| 27:U:811:PHE:O    | 27:U:812:ALA:HB3  | 1.98                     | 0.63              |
| 3:G:196:GLU:CB    | 3:G:242:LEU:HD21  | 2.29                     | 0.63              |
| 7:L:125:ARG:NH1   | 7:L:125:ARG:HG3   | 2.12                     | 0.63              |
| 9:V:408:ARG:HG2   | 9:V:408:ARG:HH11  | 1.64                     | 0.63              |
| 11:X:130:GLU:HG2  | 11:X:149:LEU:HD11 | 1.80                     | 0.63              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 12:Y:52:PRO:HG2   | 12:Y:114:ILE:CD1  | 2.29                     | 0.63              |
| 12:Y:145:LEU:CD2  | 12:Y:160:ASN:HB2  | 2.28                     | 0.63              |
| 12:Y:279:GLU:CG   | 12:Y:296:VAL:HG21 | 2.29                     | 0.63              |
| 13:Z:74:TYR:HE1   | 13:Z:78:MET:HE3   | 1.61                     | 0.63              |
| 16:c:177:THR:HB   | 27:U:773:PHE:HB2  | 1.78                     | 0.63              |
| 18:f:316:ASP:O    | 18:f:319:GLU:HG3  | 1.98                     | 0.63              |
| 18:f:444:ALA:O    | 18:f:448:CYS:N    | 2.25                     | 0.63              |
| 18:f:836:GLU:OE1  | 18:f:838:ARG:HG3  | 1.98                     | 0.63              |
| 18:f:862:ILE:HD12 | 18:f:881:GLU:CG   | 2.28                     | 0.63              |
| 19:g:93:LEU:HG    | 19:g:157:GLU:OE1  | 1.99                     | 0.63              |
| 24:E:142:ILE:HG12 | 24:E:183:LEU:HD13 | 1.79                     | 0.63              |
| 27:U:115:ASN:ND2  | 27:U:123:LYS:HG2  | 2.13                     | 0.63              |
| 2:D:357:GLU:OE1   | 2:D:357:GLU:N     | 2.26                     | 0.63              |
| 3:G:143:ILE:CG1   | 3:G:220:VAL:HG22  | 2.27                     | 0.63              |
| 6:J:64:ALA:HB2    | 6:J:217:LEU:CD2   | 2.26                     | 0.63              |
| 7:L:132:LEU:O     | 7:L:146:GLN:HA    | 1.98                     | 0.63              |
| 9:V:188:SER:O     | 9:V:192:MET:HG2   | 1.98                     | 0.63              |
| 9:V:348:PHE:CE2   | 9:V:361:PHE:HA    | 2.34                     | 0.63              |
| 11:X:137:TYR:HB3  | 11:X:146:ALA:HB2  | 1.80                     | 0.63              |
| 12:Y:259:TYR:CD2  | 12:Y:278:VAL:HG21 | 2.33                     | 0.63              |
| 13:Z:125:ASP:O    | 13:Z:128:PRO:HD2  | 1.98                     | 0.63              |
| 14:a:101:ARG:HD2  | 14:a:111:VAL:CG2  | 2.27                     | 0.63              |
| 14:a:112:ILE:HD13 | 14:a:138:VAL:HG11 | 1.80                     | 0.63              |
| 14:a:112:ILE:HA   | 14:a:115:LYS:HG3  | 1.80                     | 0.63              |
| 14:a:217:LEU:HA   | 14:a:223:GLU:OE1  | 1.98                     | 0.63              |
| 14:a:344:GLN:OE1  | 14:a:344:GLN:HA   | 1.97                     | 0.63              |
| 15:b:17:ARG:CG    | 15:b:80:PRO:HG2   | 2.28                     | 0.63              |
| 18:f:107:LYS:O    | 18:f:110:TYR:HB3  | 1.98                     | 0.63              |
| 24:E:98:VAL:HB    | 24:E:107:ILE:HG23 | 1.81                     | 0.63              |
| 25:F:197:GLU:OE2  | 25:F:350:ARG:NH2  | 2.31                     | 0.63              |
| 25:F:248:PHE:CD1  | 25:F:282:ILE:HD11 | 2.31                     | 0.63              |
| 26:K:31:ILE:HD11  | 26:K:140:ALA:HB3  | 1.80                     | 0.63              |
| 27:U:488:THR:HG23 | 27:U:490:ARG:N    | 2.11                     | 0.63              |
| 27:U:559:ARG:HB3  | 27:U:562:GLU:CB   | 2.24                     | 0.63              |
| 2:D:177:VAL:HG23  | 2:D:331:ILE:HD13  | 1.79                     | 0.63              |
| 4:H:93:LEU:CD1    | 4:H:113:ARG:HB3   | 2.26                     | 0.63              |
| 4:H:173:PHE:HD2   | 4:H:194:THR:HA    | 1.64                     | 0.63              |
| 8:M:37:ILE:HG22   | 8:M:164:ALA:HB2   | 1.80                     | 0.63              |
| 9:V:244:ALA:HB1   | 9:V:279:GLN:HE21  | 1.63                     | 0.63              |
| 10:W:122:LEU:O    | 10:W:125:ILE:HG13 | 1.99                     | 0.63              |
| 10:W:214:PHE:HA   | 10:W:219:THR:OG1  | 1.98                     | 0.63              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 11:X:70:LEU:HA    | 11:X:73:VAL:HG22  | 1.80                     | 0.63              |
| 13:Z:228:TYR:O    | 13:Z:231:GLN:HB3  | 1.99                     | 0.63              |
| 14:a:76:LEU:O     | 14:a:80:ILE:HG23  | 1.97                     | 0.63              |
| 14:a:130:VAL:O    | 14:a:134:THR:HG23 | 1.98                     | 0.63              |
| 15:b:51:LEU:O     | 15:b:52:ILE:HD13  | 1.98                     | 0.63              |
| 18:f:267:ARG:O    | 18:f:271:MET:HG3  | 1.99                     | 0.63              |
| 18:f:439:TYR:CD2  | 18:f:476:THR:HG21 | 2.33                     | 0.63              |
| 18:f:650:GLN:NE2  | 18:f:683:GLU:OE2  | 2.23                     | 0.63              |
| 19:g:107:ILE:HG13 | 19:g:115:LYS:NZ   | 2.12                     | 0.63              |
| 19:g:159:LYS:HB2  | 19:g:168:ASN:ND2  | 2.14                     | 0.63              |
| 23:B:133:VAL:HB   | 23:B:158:ALA:HA   | 1.80                     | 0.63              |
| 26:K:42:THR:HG22  | 26:K:189:MET:HB2  | 1.81                     | 0.63              |
| 26:K:210:LEU:CD1  | 26:K:215:ILE:HG12 | 2.23                     | 0.63              |
| 27:U:664:GLY:N    | 27:U:698:GLN:HE22 | 1.95                     | 0.63              |
| 1:C:339:THR:HG23  | 1:C:378:VAL:O     | 1.99                     | 0.63              |
| 1:C:354:ALA:O     | 1:C:356:GLY:N     | 2.31                     | 0.63              |
| 2:D:273:LYS:HZ3   | 2:D:319:PRO:HD3   | 1.62                     | 0.63              |
| 2:D:338:ARG:HD2   | 2:D:338:ARG:O     | 1.99                     | 0.63              |
| 11:X:81:SER:HB3   | 11:X:84:LYS:HD2   | 1.80                     | 0.63              |
| 11:X:299:LEU:HD21 | 11:X:331:LEU:HA   | 1.81                     | 0.63              |
| 12:Y:279:GLU:HB2  | 12:Y:296:VAL:HG21 | 1.80                     | 0.63              |
| 14:a:153:SER:O    | 14:a:157:ASP:N    | 2.21                     | 0.63              |
| 15:b:147:GLU:HG3  | 15:b:150:THR:HG23 | 1.80                     | 0.63              |
| 18:f:138:GLU:HA   | 18:f:141:LYS:HZ2  | 1.64                     | 0.63              |
| 18:f:344:VAL:HG12 | 18:f:345:PRO:HD2  | 1.81                     | 0.63              |
| 18:f:692:LEU:HD21 | 18:f:724:ASN:OD1  | 1.98                     | 0.63              |
| 19:g:128:LYS:HB3  | 19:g:158:LEU:CD1  | 2.29                     | 0.63              |
| 19:g:129:ILE:O    | 19:g:136:LEU:HG   | 1.99                     | 0.63              |
| 22:A:246:VAL:HG13 | 22:A:295:VAL:HG22 | 1.80                     | 0.63              |
| 26:K:88:LEU:HD13  | 26:K:116:VAL:CG1  | 2.28                     | 0.63              |
| 26:K:210:LEU:HD12 | 26:K:211:ASN:N    | 2.14                     | 0.63              |
| 27:U:485:ALA:HB1  | 27:U:488:THR:CG2  | 2.28                     | 0.63              |
| 27:U:529:ILE:O    | 27:U:533:VAL:HG22 | 1.99                     | 0.63              |
| 27:U:596:ASN:HA   | 27:U:599:ILE:CG2  | 2.29                     | 0.63              |
| 1:C:43:ARG:CZ     | 9:V:498:PRO:HB3   | 2.29                     | 0.63              |
| 1:C:203:VAL:O     | 1:C:207:THR:HB    | 1.99                     | 0.63              |
| 2:D:264:ILE:CG2   | 2:D:267:ILE:HD13  | 2.27                     | 0.63              |
| 4:H:71:HIS:CE1    | 4:H:72:ILE:HD11   | 2.34                     | 0.63              |
| 4:H:139:TRP:NE1   | 4:H:215:GLU:HG2   | 2.14                     | 0.63              |
| 8:M:72:HIS:CD2    | 8:M:105:ASN:HB3   | 2.33                     | 0.63              |
| 9:V:67:LEU:O      | 9:V:71:THR:HG23   | 1.99                     | 0.63              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 10:W:17:GLU:N     | 10:W:57:ALA:O     | 2.31                     | 0.63              |
| 14:a:212:ASN:N    | 14:a:212:ASN:OD1  | 2.31                     | 0.63              |
| 18:f:498:LEU:HD21 | 18:f:525:ILE:HG22 | 1.81                     | 0.63              |
| 18:f:590:PHE:HB2  | 18:f:649:HIS:ND1  | 2.13                     | 0.63              |
| 19:g:98:LYS:NZ    | 19:g:100:LEU:HD11 | 2.14                     | 0.63              |
| 24:E:252:GLU:OE1  | 24:E:252:GLU:HA   | 1.98                     | 0.63              |
| 27:U:423:MET:HA   | 27:U:423:MET:HE3  | 1.79                     | 0.63              |
| 27:U:678:ASP:HB3  | 27:U:683:VAL:HG13 | 1.80                     | 0.63              |
| 5:I:139:TRP:CD1   | 5:I:144:GLY:HA2   | 2.34                     | 0.63              |
| 6:J:71:MET:HE3    | 6:J:131:ALA:HB1   | 1.81                     | 0.63              |
| 8:M:33:SER:CB     | 8:M:79:GLY:HA2    | 2.28                     | 0.63              |
| 11:X:57:LEU:HD22  | 11:X:66:LEU:HB2   | 1.81                     | 0.63              |
| 11:X:63:ALA:O     | 11:X:67:GLY:N     | 2.22                     | 0.63              |
| 13:Z:212:LEU:CD1  | 14:a:346:ILE:HG23 | 2.28                     | 0.63              |
| 14:a:335:TRP:HE1  | 14:a:337:GLN:HB3  | 1.64                     | 0.63              |
| 16:c:127:ILE:HG23 | 16:c:162:LEU:HD21 | 1.81                     | 0.63              |
| 17:d:97:GLN:O     | 17:d:101:GLU:N    | 2.29                     | 0.63              |
| 17:d:228:HIS:CE1  | 17:d:232:LEU:HD22 | 2.33                     | 0.63              |
| 17:d:300:THR:CA   | 17:d:303:ALA:HB3  | 2.28                     | 0.63              |
| 18:f:141:LYS:O    | 18:f:145:VAL:HG22 | 1.99                     | 0.63              |
| 18:f:341:GLU:O    | 18:f:773:LYS:NZ   | 2.21                     | 0.63              |
| 18:f:539:LEU:HA   | 18:f:542:ILE:HD11 | 1.80                     | 0.63              |
| 22:A:285:PHE:CE2  | 22:A:287:ASP:HB2  | 2.34                     | 0.63              |
| 22:A:431:THR:HG23 | 22:A:432:TYR:CD1  | 2.34                     | 0.63              |
| 23:B:366:GLN:HA   | 23:B:369:THR:CG2  | 2.29                     | 0.63              |
| 24:E:200:SER:HB2  | 24:E:234:GLU:O    | 1.99                     | 0.63              |
| 25:F:120:LYS:O    | 25:F:137:ILE:HG23 | 1.98                     | 0.63              |
| 27:U:335:ILE:O    | 27:U:339:LEU:N    | 2.30                     | 0.63              |
| 27:U:661:ALA:O    | 27:U:746:ILE:HD11 | 1.99                     | 0.63              |
| 27:U:796:LYS:NZ   | 27:U:921:ILE:HB   | 2.14                     | 0.63              |
| 1:C:170:LYS:HE2   | 1:C:208:ASP:OD2   | 1.99                     | 0.62              |
| 2:D:71:GLU:HG3    | 27:U:644:TYR:CZ   | 2.34                     | 0.62              |
| 2:D:388:ARG:HH21  | 24:E:297:ARG:HH12 | 1.47                     | 0.62              |
| 4:H:196:LYS:HE2   | 4:H:203:MET:HE2   | 1.80                     | 0.62              |
| 5:I:135:LEU:HG    | 5:I:164:ILE:HD11  | 1.80                     | 0.62              |
| 10:W:106:GLN:O    | 10:W:110:THR:HG23 | 1.99                     | 0.62              |
| 10:W:144:ARG:HB2  | 10:W:144:ARG:CZ   | 2.28                     | 0.62              |
| 11:X:69:LEU:O     | 11:X:73:VAL:HG13  | 1.99                     | 0.62              |
| 13:Z:208:ILE:CG2  | 13:Z:230:LEU:HD11 | 2.29                     | 0.62              |
| 14:a:319:LEU:N    | 14:a:319:LEU:HD12 | 2.14                     | 0.62              |
| 15:b:35:ILE:HG23  | 15:b:188:ILE:CD1  | 2.28                     | 0.62              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 15:b:124:LEU:CD2  | 15:b:152:LYS:HB2  | 2.29                     | 0.62              |
| 15:b:173:VAL:HG22 | 15:b:174:PRO:HD2  | 1.80                     | 0.62              |
| 18:f:851:ASP:OD1  | 18:f:853:VAL:HG23 | 1.99                     | 0.62              |
| 19:g:112:LEU:HD11 | 19:g:116:ILE:CD1  | 2.29                     | 0.62              |
| 23:B:322:ARG:NH1  | 23:B:325:VAL:O    | 2.32                     | 0.62              |
| 24:E:39:GLN:HA    | 24:E:42:LYS:HE2   | 1.81                     | 0.62              |
| 24:E:168:LYS:HA   | 24:E:274:LYS:CD   | 2.29                     | 0.62              |
| 24:E:310:LEU:O    | 24:E:314:LYS:N    | 2.19                     | 0.62              |
| 25:F:251:LEU:N    | 25:F:284:PHE:O    | 2.25                     | 0.62              |
| 27:U:486:MET:CE   | 27:U:781:LEU:HD21 | 2.29                     | 0.62              |
| 1:C:248:MET:HE1   | 1:C:276:LEU:CD1   | 2.30                     | 0.62              |
| 2:D:230:VAL:HG11  | 2:D:235:PHE:CZ    | 2.34                     | 0.62              |
| 3:G:72:ILE:HD13   | 3:G:140:LEU:HD21  | 1.81                     | 0.62              |
| 3:G:76:ILE:HG23   | 3:G:111:VAL:HG22  | 1.81                     | 0.62              |
| 8:M:52:LEU:CD2    | 8:M:209:PHE:HB2   | 2.30                     | 0.62              |
| 9:V:190:ASP:O     | 9:V:194:LYS:HG2   | 1.98                     | 0.62              |
| 10:W:118:LEU:HB2  | 10:W:119:PRO:HD3  | 1.81                     | 0.62              |
| 10:W:304:ASP:O    | 10:W:307:LYS:HG2  | 1.99                     | 0.62              |
| 11:X:71:LYS:CA    | 11:X:74:ARG:HG3   | 2.28                     | 0.62              |
| 11:X:143:TYR:HE2  | 11:X:179:ALA:HB1  | 1.64                     | 0.62              |
| 11:X:143:TYR:CE2  | 11:X:179:ALA:HB1  | 2.34                     | 0.62              |
| 12:Y:319:MET:HE2  | 12:Y:330:ILE:HG13 | 1.81                     | 0.62              |
| 13:Z:106:ILE:HG12 | 13:Z:155:PHE:CE1  | 2.35                     | 0.62              |
| 17:d:171:LEU:HD21 | 17:d:191:LEU:HD13 | 1.81                     | 0.62              |
| 18:f:109:ILE:HG12 | 18:f:113:MET:CB   | 2.29                     | 0.62              |
| 18:f:433:LEU:CD2  | 19:g:173:GLU:HA   | 2.29                     | 0.62              |
| 18:f:556:ARG:HD3  | 18:f:590:PHE:CZ   | 2.35                     | 0.62              |
| 22:A:172:VAL:HG21 | 22:A:224:LEU:CD1  | 2.27                     | 0.62              |
| 22:A:339:ARG:HH11 | 22:A:339:ARG:HG3  | 1.64                     | 0.62              |
| 25:F:124:ILE:HG13 | 25:F:160:ILE:CD1  | 2.28                     | 0.62              |
| 25:F:292:GLY:HA2  | 25:F:310:MET:HE1  | 1.82                     | 0.62              |
| 27:U:368:ALA:HB1  | 27:U:731:ILE:CB   | 2.28                     | 0.62              |
| 27:U:902:PRO:HA   | 27:U:915:LYS:H    | 1.64                     | 0.62              |
| 1:C:175:PHE:HD2   | 1:C:180:ILE:HD11  | 1.65                     | 0.62              |
| 1:C:209:CYS:SG    | 1:C:243:PRO:HB2   | 2.39                     | 0.62              |
| 2:D:196:ILE:HG13  | 2:D:196:ILE:O     | 1.98                     | 0.62              |
| 3:G:243:ALA:O     | 10:W:92:LYS:HE3   | 2.00                     | 0.62              |
| 9:V:248:ALA:HA    | 9:V:276:PHE:HE1   | 1.64                     | 0.62              |
| 9:V:309:MET:CE    | 9:V:328:VAL:HG13  | 2.29                     | 0.62              |
| 10:W:326:MET:C    | 10:W:326:MET:HE3  | 2.25                     | 0.62              |
| 11:X:187:ARG:HH12 | 11:X:190:LEU:HD23 | 1.63                     | 0.62              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 15:b:35:ILE:C     | 15:b:188:ILE:HD11 | 2.24                     | 0.62              |
| 17:d:137:THR:HB   | 17:d:140:GLN:CB   | 2.27                     | 0.62              |
| 22:A:185:GLU:O    | 22:A:189:GLU:HG2  | 1.99                     | 0.62              |
| 22:A:348:LEU:O    | 22:A:352:THR:HG23 | 2.00                     | 0.62              |
| 25:F:225:MET:HA   | 25:F:352:ILE:CG2  | 2.28                     | 0.62              |
| 27:U:845:GLU:O    | 27:U:849:LYS:HG3  | 1.99                     | 0.62              |
| 27:U:879:ASP:CB   | 27:U:881:PRO:HD2  | 2.20                     | 0.62              |
| 27:U:901:GLN:O    | 27:U:915:LYS:N    | 2.32                     | 0.62              |
| 9:V:93:PHE:HA     | 9:V:96:ARG:HH21   | 1.65                     | 0.62              |
| 10:W:147:LYS:HE3  | 10:W:185:PHE:CE1  | 2.33                     | 0.62              |
| 11:X:377:ILE:HG21 | 12:Y:312:ARG:HB2  | 1.82                     | 0.62              |
| 12:Y:338:ILE:HD13 | 12:Y:345:CYS:O    | 1.98                     | 0.62              |
| 13:Z:114:ARG:CZ   | 13:Z:114:ARG:HB2  | 2.28                     | 0.62              |
| 15:b:35:ILE:HG13  | 15:b:188:ILE:CD1  | 2.28                     | 0.62              |
| 18:f:106:LEU:HA   | 18:f:109:ILE:HG22 | 1.81                     | 0.62              |
| 18:f:562:LEU:HD22 | 18:f:595:VAL:HG12 | 1.80                     | 0.62              |
| 18:f:654:VAL:CG2  | 18:f:678:LEU:HD23 | 2.29                     | 0.62              |
| 18:f:711:SER:HA   | 18:f:714:SER:HB3  | 1.81                     | 0.62              |
| 18:f:737:ASN:OD1  | 18:f:774:GLY:HA3  | 2.00                     | 0.62              |
| 24:E:356:ARG:O    | 24:E:357:ALA:C    | 2.42                     | 0.62              |
| 25:F:376:SER:HB2  | 25:F:414:GLU:CD   | 2.24                     | 0.62              |
| 26:K:142:LEU:HD23 | 26:K:155:HIS:HB2  | 1.81                     | 0.62              |
| 27:U:661:ALA:HB1  | 27:U:746:ILE:HD12 | 1.82                     | 0.62              |
| 1:C:370:ALA:HB2   | 1:C:375:ARG:HH21  | 1.64                     | 0.62              |
| 2:D:380:GLN:O     | 24:E:164:ILE:HD13 | 1.99                     | 0.62              |
| 3:G:179:LEU:HG    | 3:G:201:CYS:SG    | 2.40                     | 0.62              |
| 5:I:115:CYS:SG    | 5:I:156:TYR:HB3   | 2.40                     | 0.62              |
| 7:L:44:ALA:HB3    | 7:L:215:VAL:CG1   | 2.30                     | 0.62              |
| 7:L:47:VAL:CG1    | 7:L:195:LEU:HD12  | 2.27                     | 0.62              |
| 9:V:121:PHE:CE2   | 9:V:159:LEU:HD12  | 2.33                     | 0.62              |
| 9:V:135:LEU:HA    | 9:V:180:ARG:NH2   | 2.15                     | 0.62              |
| 9:V:440:LYS:HE2   | 9:V:444:ASP:OD2   | 2.00                     | 0.62              |
| 11:X:96:PHE:CE2   | 11:X:109:LEU:HD22 | 2.34                     | 0.62              |
| 13:Z:212:LEU:HD13 | 14:a:346:ILE:HG23 | 1.82                     | 0.62              |
| 14:a:17:GLY:O     | 14:a:21:VAL:N     | 2.28                     | 0.62              |
| 15:b:140:ILE:HG21 | 15:b:153:LEU:HD21 | 1.81                     | 0.62              |
| 17:d:104:ARG:NE   | 17:d:106:SER:OG   | 2.28                     | 0.62              |
| 17:d:119:LEU:O    | 17:d:122:VAL:HG22 | 1.99                     | 0.62              |
| 17:d:191:LEU:HA   | 17:d:194:LEU:CD1  | 2.29                     | 0.62              |
| 19:g:109:GLY:HA2  | 19:g:112:LEU:CB   | 2.29                     | 0.62              |
| 19:g:112:LEU:O    | 19:g:116:ILE:N    | 2.20                     | 0.62              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 25:F:343:LEU:HD23 | 25:F:351:LYS:CD   | 2.26                     | 0.62              |
| 27:U:250:PHE:HE2  | 27:U:911:ILE:HG21 | 1.63                     | 0.62              |
| 27:U:410:VAL:HG21 | 27:U:777:HIS:HB3  | 1.82                     | 0.62              |
| 1:C:21:ARG:HA     | 27:U:149:GLN:NE2  | 2.15                     | 0.62              |
| 1:C:113:ARG:HH22  | 2:D:102:ILE:HD13  | 1.65                     | 0.62              |
| 1:C:134:LEU:HD13  | 1:C:230:MET:CE    | 2.28                     | 0.62              |
| 1:C:262:GLY:HA2   | 23:B:295:TYR:CD2  | 2.33                     | 0.62              |
| 2:D:254:ALA:CB    | 2:D:262:ILE:HD11  | 2.28                     | 0.62              |
| 5:I:25:MET:HE1    | 23:B:438:LEU:CD1  | 2.30                     | 0.62              |
| 6:J:173:GLU:HG3   | 26:K:58:LEU:HD11  | 1.80                     | 0.62              |
| 9:V:72:LEU:HD11   | 9:V:116:ALA:CB    | 2.29                     | 0.62              |
| 11:X:62:GLN:O     | 11:X:66:LEU:N     | 2.24                     | 0.62              |
| 11:X:175:LYS:HA   | 11:X:213:GLN:NE2  | 2.15                     | 0.62              |
| 13:Z:33:LYS:HG3   | 13:Z:34:ARG:H     | 1.64                     | 0.62              |
| 13:Z:175:LEU:HD13 | 16:c:217:LEU:CD1  | 2.30                     | 0.62              |
| 15:b:36:VAL:HA    | 15:b:188:ILE:HD11 | 1.81                     | 0.62              |
| 15:b:140:ILE:CG2  | 15:b:153:LEU:HD21 | 2.30                     | 0.62              |
| 18:f:185:LEU:O    | 18:f:188:VAL:HG22 | 1.99                     | 0.62              |
| 19:g:116:ILE:HD13 | 19:g:129:ILE:CG1  | 2.29                     | 0.62              |
| 20:u:194:VAL:HG13 | 20:u:246:ILE:HG23 | 1.81                     | 0.62              |
| 22:A:278:ASP:HB2  | 23:B:310:LEU:CD2  | 2.30                     | 0.62              |
| 22:A:297:ARG:HD3  | 25:F:257:VAL:HG21 | 1.80                     | 0.62              |
| 22:A:384:GLU:CG   | 23:B:344:PRO:HG2  | 2.27                     | 0.62              |
| 26:K:37:ALA:HB2   | 26:K:50:VAL:HG22  | 1.81                     | 0.62              |
| 27:U:903:PHE:CB   | 27:U:915:LYS:HB2  | 2.24                     | 0.62              |
| 1:C:21:ARG:HA     | 1:C:24:TYR:HD2    | 1.65                     | 0.62              |
| 1:C:114:VAL:HB    | 1:C:123:LEU:HD21  | 1.82                     | 0.62              |
| 1:C:174:LEU:HD11  | 22:A:30:ILE:CD1   | 2.29                     | 0.62              |
| 2:D:412:GLN:HE22  | 24:E:283:ASP:HA   | 1.64                     | 0.62              |
| 8:M:8:ASP:O       | 8:M:8:ASP:OD1     | 2.18                     | 0.62              |
| 9:V:192:MET:HE3   | 9:V:214:HIS:CB    | 2.29                     | 0.62              |
| 11:X:157:LEU:HD11 | 11:X:165:LEU:HB3  | 1.81                     | 0.62              |
| 11:X:208:ALA:HB1  | 11:X:239:TYR:CE2  | 2.34                     | 0.62              |
| 14:a:70:ARG:CZ    | 15:b:17:ARG:HB3   | 2.30                     | 0.62              |
| 14:a:312:MET:HE2  | 14:a:312:MET:HA   | 1.81                     | 0.62              |
| 18:f:62:ARG:O     | 18:f:70:LEU:HD13  | 2.00                     | 0.62              |
| 18:f:545:LYS:HA   | 18:f:545:LYS:HE3  | 1.81                     | 0.62              |
| 18:f:564:LEU:HD23 | 18:f:567:LEU:HD21 | 1.81                     | 0.62              |
| 19:g:90:PRO:CB    | 19:g:157:GLU:HB2  | 2.30                     | 0.62              |
| 22:A:286:ASP:H    | 25:F:337:ILE:HD11 | 1.63                     | 0.62              |
| 27:U:12:LEU:HD22  | 27:U:45:ILE:HD12  | 1.81                     | 0.62              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 27:U:177:LEU:HD21 | 27:U:205:TYR:HH   | 1.64                     | 0.62              |
| 27:U:673:GLU:O    | 27:U:676:THR:HG22 | 1.99                     | 0.62              |
| 2:D:383:GLY:HA2   | 2:D:394:VAL:CG2   | 2.30                     | 0.62              |
| 3:G:167:ALA:O     | 3:G:172:GLN:HG3   | 1.99                     | 0.62              |
| 4:H:71:HIS:CD2    | 4:H:72:ILE:HG13   | 2.34                     | 0.62              |
| 6:J:55:ASP:OD1    | 6:J:55:ASP:N      | 2.26                     | 0.62              |
| 9:V:118:GLN:O     | 9:V:122:THR:HG21  | 1.99                     | 0.62              |
| 9:V:176:MET:HE1   | 9:V:216:ARG:HB3   | 1.82                     | 0.62              |
| 10:W:135:LYS:NZ   | 10:W:137:TYR:OH   | 2.17                     | 0.62              |
| 11:X:105:GLN:HA   | 11:X:108:GLU:HB2  | 1.82                     | 0.62              |
| 13:Z:184:VAL:HG23 | 13:Z:186:THR:HG23 | 1.80                     | 0.62              |
| 13:Z:243:GLN:NE2  | 13:Z:247:LYS:HE3  | 2.12                     | 0.62              |
| 14:a:38:THR:HA    | 14:a:41:VAL:HB    | 1.82                     | 0.62              |
| 16:c:307:VAL:CG2  | 17:d:332:SER:HB2  | 2.29                     | 0.62              |
| 18:f:110:TYR:O    | 18:f:119:LYS:HE3  | 2.00                     | 0.62              |
| 18:f:433:LEU:HD12 | 18:f:441:LYS:HG2  | 1.80                     | 0.62              |
| 22:A:421:ALA:O    | 22:A:422:LYS:HG3  | 2.00                     | 0.62              |
| 25:F:172:VAL:HG12 | 25:F:274:LEU:HD23 | 1.82                     | 0.62              |
| 25:F:428:GLN:HG3  | 25:F:430:LYS:HE2  | 1.81                     | 0.62              |
| 1:C:273:MET:CE    | 1:C:277:LEU:HD12  | 2.28                     | 0.62              |
| 3:G:165:ALA:CB    | 3:G:179:LEU:HD13  | 2.27                     | 0.62              |
| 3:G:174:GLU:HA    | 3:G:177:SER:OG    | 1.99                     | 0.62              |
| 4:H:19:LEU:CD1    | 5:I:79:ILE:HD11   | 2.30                     | 0.62              |
| 6:J:58:THR:HA     | 6:J:60:ARG:NH2    | 2.15                     | 0.62              |
| 7:L:33:SER:HB2    | 7:L:62:LYS:NZ     | 2.15                     | 0.62              |
| 9:V:173:ILE:HG12  | 9:V:213:TYR:CD2   | 2.35                     | 0.62              |
| 11:X:113:CYS:HB3  | 11:X:129:LEU:HG   | 1.80                     | 0.62              |
| 14:a:119:GLY:O    | 14:a:123:LEU:N    | 2.30                     | 0.62              |
| 17:d:128:PHE:C    | 17:d:129:LEU:HD23 | 2.25                     | 0.62              |
| 17:d:148:LEU:O    | 17:d:151:GLY:N    | 2.33                     | 0.62              |
| 17:d:271:ILE:O    | 17:d:275:ILE:HG13 | 2.00                     | 0.62              |
| 18:f:267:ARG:NH1  | 18:f:893:ILE:HB   | 2.14                     | 0.62              |
| 18:f:345:PRO:HD3  | 18:f:378:ASN:OD1  | 1.99                     | 0.62              |
| 18:f:426:LEU:HB3  | 19:g:156:LEU:CD2  | 2.30                     | 0.62              |
| 18:f:429:ILE:HG22 | 18:f:429:ILE:O    | 1.99                     | 0.62              |
| 18:f:613:LEU:HB2  | 23:B:74:MET:HE3   | 1.82                     | 0.62              |
| 18:f:834:ASP:N    | 18:f:838:ARG:O    | 2.30                     | 0.62              |
| 19:g:112:LEU:CD2  | 19:g:136:LEU:HD13 | 2.30                     | 0.62              |
| 19:g:112:LEU:HG   | 19:g:116:ILE:HD12 | 1.82                     | 0.62              |
| 22:A:193:THR:HG22 | 22:A:201:PHE:HE1  | 1.63                     | 0.62              |
| 24:E:71:VAL:HG21  | 24:E:107:ILE:HD11 | 1.82                     | 0.62              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 25:F:324:THR:OG1  | 25:F:326:VAL:HG23 | 1.98                     | 0.62              |
| 26:K:50:VAL:CG1   | 26:K:66:LYS:HE2   | 2.30                     | 0.62              |
| 26:K:203:LYS:HG3  | 26:K:210:LEU:CB   | 2.30                     | 0.62              |
| 27:U:181:LEU:HD11 | 27:U:219:CYS:SG   | 2.40                     | 0.62              |
| 27:U:489:ALA:HA   | 27:U:520:MET:HE1  | 1.81                     | 0.62              |
| 1:C:49:ARG:HD2    | 2:D:64:GLU:OE1    | 2.00                     | 0.62              |
| 1:C:57:ARG:HG3    | 1:C:57:ARG:NH1    | 2.15                     | 0.62              |
| 2:D:341:LYS:HD2   | 2:D:370:ILE:HD11  | 1.82                     | 0.62              |
| 9:V:67:LEU:HA     | 9:V:70:VAL:CG1    | 2.27                     | 0.62              |
| 9:V:171:VAL:O     | 9:V:175:MET:N     | 2.28                     | 0.62              |
| 9:V:273:LYS:N     | 9:V:273:LYS:HD2   | 2.15                     | 0.62              |
| 10:W:68:VAL:O     | 10:W:71:VAL:HG22  | 2.00                     | 0.62              |
| 10:W:194:LEU:HD12 | 10:W:229:LEU:HD22 | 1.81                     | 0.62              |
| 11:X:91:SER:O     | 11:X:95:LEU:HB2   | 2.00                     | 0.62              |
| 12:Y:56:ALA:HA    | 12:Y:59:LYS:CD    | 2.29                     | 0.62              |
| 14:a:36:GLN:OE1   | 14:a:36:GLN:N     | 2.18                     | 0.62              |
| 14:a:116:THR:HG21 | 14:a:154:ARG:CB   | 2.30                     | 0.62              |
| 16:c:176:GLN:HB3  | 27:U:399:TRP:HB2  | 1.82                     | 0.62              |
| 16:c:176:GLN:O    | 16:c:178:THR:HG22 | 2.00                     | 0.62              |
| 17:d:117:GLY:O    | 17:d:120:LYS:HG3  | 2.00                     | 0.62              |
| 17:d:166:ARG:HB2  | 27:U:14:GLU:OE2   | 2.00                     | 0.62              |
| 18:f:107:LYS:HE2  | 18:f:107:LYS:HA   | 1.82                     | 0.62              |
| 18:f:833:PHE:HA   | 18:f:840:LEU:H    | 1.63                     | 0.62              |
| 19:g:103:THR:HG21 | 19:g:115:LYS:HG3  | 1.81                     | 0.62              |
| 22:A:92:PRO:HG2   | 22:A:144:ARG:HD2  | 1.82                     | 0.62              |
| 25:F:124:ILE:CG1  | 25:F:160:ILE:HD11 | 2.29                     | 0.62              |
| 26:K:40:ILE:HD13  | 26:K:198:SER:HB3  | 1.81                     | 0.62              |
| 27:U:28:ASN:HB2   | 27:U:63:VAL:CG2   | 2.19                     | 0.62              |
| 27:U:391:GLU:HA   | 27:U:391:GLU:OE2  | 2.00                     | 0.62              |
| 27:U:602:LEU:CD2  | 27:U:618:ALA:HA   | 2.29                     | 0.62              |
| 27:U:788:VAL:HG21 | 27:U:906:LEU:HD11 | 1.81                     | 0.62              |
| 27:U:802:TYR:HB3  | 27:U:895:PRO:HB3  | 1.81                     | 0.62              |
| 1:C:21:ARG:HA     | 27:U:149:GLN:HE22 | 1.64                     | 0.61              |
| 1:C:119:ASP:HB2   | 16:c:193:ILE:CD1  | 2.30                     | 0.61              |
| 4:H:111:VAL:CG2   | 4:H:136:ILE:HD12  | 2.19                     | 0.61              |
| 7:L:36:VAL:HG21   | 7:L:194:ALA:CB    | 2.30                     | 0.61              |
| 8:M:215:TRP:CZ2   | 8:M:228:PRO:HD2   | 2.35                     | 0.61              |
| 10:W:201:ARG:O    | 10:W:204:ILE:HG22 | 2.00                     | 0.61              |
| 11:X:299:LEU:HD11 | 11:X:334:ASN:HD22 | 1.65                     | 0.61              |
| 12:Y:21:GLN:HA    | 12:Y:286:TRP:HB3  | 1.81                     | 0.61              |
| 13:Z:38:VAL:CG1   | 13:Z:91:ILE:HG23  | 2.30                     | 0.61              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 15:b:59:GLU:OE1   | 15:b:59:GLU:N     | 2.32                     | 0.61              |
| 16:c:52:GLU:OE1   | 20:u:289:HIS:HD2  | 1.79                     | 0.61              |
| 17:d:152:ALA:CB   | 17:d:191:LEU:HD22 | 2.30                     | 0.61              |
| 18:f:502:LEU:HD22 | 18:f:537:THR:OG1  | 2.00                     | 0.61              |
| 22:A:146:LYS:O    | 25:F:87:PRO:HG3   | 2.00                     | 0.61              |
| 24:E:49:ALA:HA    | 25:F:136:VAL:HG21 | 1.81                     | 0.61              |
| 24:E:112:PRO:HD2  | 25:F:97:LEU:CD1   | 2.22                     | 0.61              |
| 26:K:142:LEU:CD2  | 26:K:155:HIS:HB2  | 2.30                     | 0.61              |
| 27:U:91:ASN:OD1   | 27:U:97:VAL:HG21  | 2.00                     | 0.61              |
| 27:U:550:VAL:HG21 | 27:U:768:GLN:HG3  | 1.81                     | 0.61              |
| 27:U:803:LYS:HB2  | 27:U:874:ASN:O    | 1.99                     | 0.61              |
| 27:U:845:GLU:HG2  | 27:U:848:LYS:HZ1  | 1.63                     | 0.61              |
| 3:G:22:LEU:HD11   | 4:H:128:ARG:HD3   | 1.80                     | 0.61              |
| 9:V:71:THR:O      | 9:V:75:ILE:HG13   | 2.01                     | 0.61              |
| 9:V:181:TYR:O     | 9:V:185:GLN:N     | 2.33                     | 0.61              |
| 9:V:417:ILE:HD13  | 9:V:422:ILE:CG1   | 2.29                     | 0.61              |
| 10:W:171:VAL:HG23 | 10:W:172:GLU:OE2  | 2.00                     | 0.61              |
| 13:Z:20:VAL:HG22  | 13:Z:126:VAL:HG23 | 1.81                     | 0.61              |
| 13:Z:132:GLY:HA3  | 16:c:222:LYS:NZ   | 2.15                     | 0.61              |
| 14:a:31:LYS:O     | 14:a:31:LYS:HG2   | 1.99                     | 0.61              |
| 16:c:123:SER:HB2  | 20:u:289:HIS:CE1  | 2.34                     | 0.61              |
| 18:f:46:SER:H     | 18:f:49:ASP:HB2   | 1.65                     | 0.61              |
| 18:f:208:LEU:HD12 | 18:f:217:LEU:HD13 | 1.81                     | 0.61              |
| 18:f:217:LEU:HD21 | 18:f:229:VAL:CG2  | 2.30                     | 0.61              |
| 19:g:85:ILE:CD1   | 19:g:131:ILE:HD11 | 2.30                     | 0.61              |
| 19:g:128:LYS:HB2  | 19:g:158:LEU:HD22 | 1.81                     | 0.61              |
| 22:A:176:ASP:C    | 22:A:357:ILE:HD13 | 2.25                     | 0.61              |
| 24:E:56:ILE:HB    | 24:E:100:LEU:HD11 | 1.82                     | 0.61              |
| 24:E:275:MET:CG   | 24:E:295:LEU:HD21 | 2.04                     | 0.61              |
| 27:U:423:MET:HE3  | 27:U:423:MET:CA   | 2.29                     | 0.61              |
| 27:U:765:VAL:HG13 | 27:U:778:PHE:HB3  | 1.81                     | 0.61              |
| 1:C:46:GLN:OE1    | 27:U:639:LEU:HD13 | 2.00                     | 0.61              |
| 5:I:228:LEU:HB3   | 5:I:232:GLU:HG3   | 1.82                     | 0.61              |
| 8:M:23:VAL:HG11   | 8:M:154:SER:HB3   | 1.82                     | 0.61              |
| 8:M:27:MET:HG2    | 8:M:153:PRO:CD    | 2.29                     | 0.61              |
| 9:V:440:LYS:HE3   | 9:V:443:ARG:NH2   | 2.11                     | 0.61              |
| 10:W:41:GLN:O     | 10:W:45:GLU:HG2   | 1.99                     | 0.61              |
| 11:X:90:ARG:HA    | 11:X:93:LEU:CD2   | 2.30                     | 0.61              |
| 11:X:414:LEU:HD21 | 13:Z:273:HIS:CB   | 2.30                     | 0.61              |
| 14:a:68:GLU:HG3   | 14:a:69:HIS:N     | 2.14                     | 0.61              |
| 17:d:231:SER:HA   | 17:d:234:GLN:NE2  | 2.16                     | 0.61              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 17:d:300:THR:O    | 17:d:304:LYS:N    | 2.33                     | 0.61              |
| 17:d:301:ASP:O    | 17:d:305:LYS:N    | 2.30                     | 0.61              |
| 18:f:343:LYS:CD   | 18:f:773:LYS:HE2  | 2.30                     | 0.61              |
| 18:f:417:ILE:HG22 | 18:f:418:LEU:CD2  | 2.26                     | 0.61              |
| 23:B:278:ALA:CB   | 23:B:279:PRO:CD   | 2.78                     | 0.61              |
| 25:F:225:MET:HE1  | 25:F:236:LEU:CD2  | 2.29                     | 0.61              |
| 27:U:787:CYS:SG   | 27:U:789:ILE:HD11 | 2.41                     | 0.61              |
| 2:D:98:GLN:OE1    | 2:D:98:GLN:HA     | 2.01                     | 0.61              |
| 3:G:131:MET:CG    | 8:M:125:TYR:HE1   | 2.13                     | 0.61              |
| 5:I:71:ASP:HB2    | 5:I:223:THR:HG21  | 1.81                     | 0.61              |
| 10:W:440:ASN:HD22 | 16:c:226:MET:HE3  | 1.65                     | 0.61              |
| 11:X:107:VAL:O    | 11:X:111:LEU:HD23 | 2.00                     | 0.61              |
| 14:a:371:ALA:HB2  | 17:d:340:ILE:HD12 | 1.82                     | 0.61              |
| 15:b:150:THR:O    | 15:b:154:THR:HG22 | 1.99                     | 0.61              |
| 18:f:441:LYS:O    | 18:f:445:LEU:HG   | 1.99                     | 0.61              |
| 22:A:143:ASP:OD1  | 22:A:147:TYR:N    | 2.33                     | 0.61              |
| 23:B:197:ILE:HG21 | 23:B:235:LEU:CD2  | 2.08                     | 0.61              |
| 24:E:65:THR:OG1   | 24:E:66:GLU:N     | 2.29                     | 0.61              |
| 24:E:235:ILE:CD1  | 24:E:277:MET:CA   | 2.60                     | 0.61              |
| 25:F:181:PRO:HB2  | 25:F:183:GLU:OE2  | 1.99                     | 0.61              |
| 27:U:376:MET:HE2  | 27:U:734:GLN:O    | 2.00                     | 0.61              |
| 3:G:77:GLY:O      | 3:G:141:ILE:HG12  | 2.01                     | 0.61              |
| 7:L:193:ARG:HA    | 7:L:196:ARG:HG2   | 1.81                     | 0.61              |
| 9:V:108:LEU:O     | 9:V:108:LEU:HD12  | 1.99                     | 0.61              |
| 15:b:38:HIS:CE1   | 15:b:72:LEU:HD11  | 2.36                     | 0.61              |
| 15:b:100:ARG:HD2  | 15:b:105:HIS:HB2  | 1.80                     | 0.61              |
| 18:f:830:LEU:HB3  | 18:f:872:VAL:HB   | 1.82                     | 0.61              |
| 23:B:221:GLY:HA2  | 23:B:327:VAL:O    | 1.99                     | 0.61              |
| 25:F:182:THR:HG22 | 25:F:184:GLN:HG3  | 1.80                     | 0.61              |
| 25:F:310:MET:HE3  | 25:F:342:LEU:CD2  | 2.30                     | 0.61              |
| 27:U:84:ALA:HB3   | 27:U:88:PHE:HB2   | 1.82                     | 0.61              |
| 27:U:165:LYS:HZ2  | 27:U:165:LYS:HB3  | 1.65                     | 0.61              |
| 27:U:466:LYS:NZ   | 27:U:496:LEU:HD13 | 2.15                     | 0.61              |
| 2:D:103:VAL:HG11  | 2:D:132:LEU:HD21  | 1.81                     | 0.61              |
| 6:J:158:ALA:CB    | 6:J:172:LEU:HD21  | 2.31                     | 0.61              |
| 7:L:40:SER:OG     | 7:L:187:LEU:HD22  | 2.00                     | 0.61              |
| 9:V:240:LEU:HD11  | 27:U:69:TYR:CE1   | 2.36                     | 0.61              |
| 10:W:188:GLU:HA   | 10:W:188:GLU:OE2  | 2.01                     | 0.61              |
| 10:W:222:LEU:O    | 10:W:226:TYR:N    | 2.29                     | 0.61              |
| 11:X:125:LEU:O    | 11:X:128:ALA:HB3  | 2.01                     | 0.61              |
| 14:a:65:SER:HA    | 14:a:68:GLU:CD    | 2.24                     | 0.61              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 14:a:186:LYS:NZ   | 14:a:193:GLN:HB2  | 2.12                     | 0.61              |
| 14:a:251:LEU:O    | 14:a:254:ALA:HB3  | 2.01                     | 0.61              |
| 16:c:177:THR:HG22 | 27:U:773:PHE:HB2  | 1.83                     | 0.61              |
| 17:d:330:ILE:HD12 | 17:d:330:ILE:N    | 2.16                     | 0.61              |
| 22:A:214:LEU:HD12 | 22:A:214:LEU:H    | 1.64                     | 0.61              |
| 22:A:239:ARG:NE   | 23:B:320:ASP:OD2  | 2.33                     | 0.61              |
| 23:B:245:ALA:HB1  | 23:B:279:PRO:O    | 2.01                     | 0.61              |
| 25:F:95:GLU:O     | 25:F:96:LEU:HD12  | 2.01                     | 0.61              |
| 1:C:273:MET:HE1   | 1:C:277:LEU:CD1   | 2.30                     | 0.61              |
| 5:I:74:CYS:HA     | 5:I:135:LEU:O     | 2.01                     | 0.61              |
| 8:M:169:ARG:C     | 8:M:173:LYS:HZ3   | 2.08                     | 0.61              |
| 11:X:197:ALA:HB1  | 11:X:202:CYS:SG   | 2.40                     | 0.61              |
| 11:X:379:ASP:OD1  | 11:X:384:VAL:HG22 | 2.01                     | 0.61              |
| 13:Z:136:GLU:OE1  | 13:Z:136:GLU:HA   | 2.00                     | 0.61              |
| 14:a:191:SER:HA   | 14:a:194:GLN:HE21 | 1.64                     | 0.61              |
| 15:b:87:CYS:HB2   | 15:b:119:ASP:OD1  | 2.00                     | 0.61              |
| 15:b:130:ARG:O    | 15:b:133:LYS:HG2  | 2.01                     | 0.61              |
| 15:b:138:VAL:HG12 | 15:b:160:LEU:HD11 | 1.82                     | 0.61              |
| 17:d:231:SER:HA   | 17:d:234:GLN:HE21 | 1.66                     | 0.61              |
| 18:f:376:PHE:CE1  | 18:f:409:SER:HB3  | 2.36                     | 0.61              |
| 19:g:139:GLY:C    | 19:g:140:LYS:HD2  | 2.26                     | 0.61              |
| 22:A:120:LYS:O    | 25:F:90:VAL:HG12  | 2.00                     | 0.61              |
| 24:E:137:GLY:HA3  | 24:E:308:ALA:HB2  | 1.82                     | 0.61              |
| 1:C:48:GLN:HG2    | 2:D:65:GLN:OE1    | 2.01                     | 0.61              |
| 1:C:167:LEU:HB3   | 1:C:168:PRO:HD3   | 1.83                     | 0.61              |
| 7:L:72:ILE:HD13   | 7:L:132:LEU:HD22  | 1.81                     | 0.61              |
| 8:M:74:GLY:O      | 8:M:137:LEU:HD23  | 2.01                     | 0.61              |
| 9:V:192:MET:HE3   | 9:V:214:HIS:HB2   | 1.83                     | 0.61              |
| 9:V:350:GLN:O     | 9:V:354:LYS:HB2   | 2.01                     | 0.61              |
| 10:W:355:LYS:HE2  | 10:W:384:LEU:HD21 | 1.81                     | 0.61              |
| 11:X:57:LEU:HG    | 11:X:62:GLN:HB2   | 1.83                     | 0.61              |
| 11:X:171:LEU:HD22 | 11:X:210:LEU:CD2  | 2.24                     | 0.61              |
| 12:Y:149:LEU:HD23 | 12:Y:157:ILE:HD13 | 1.82                     | 0.61              |
| 12:Y:149:LEU:N    | 12:Y:157:ILE:HD11 | 2.15                     | 0.61              |
| 13:Z:43:TRP:HZ3   | 13:Z:46:LYS:HA    | 1.65                     | 0.61              |
| 13:Z:101:LEU:HD23 | 13:Z:123:ILE:HD11 | 1.82                     | 0.61              |
| 13:Z:125:ASP:C    | 13:Z:128:PRO:HD2  | 2.25                     | 0.61              |
| 14:a:76:LEU:HD21  | 14:a:100:THR:HB   | 1.83                     | 0.61              |
| 14:a:102:GLU:O    | 14:a:105:LYS:HG3  | 2.01                     | 0.61              |
| 14:a:157:ASP:OD1  | 14:a:196:ARG:NH2  | 2.34                     | 0.61              |
| 16:c:25:VAL:HG21  | 16:c:161:ARG:HE   | 1.65                     | 0.61              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 17:d:116:LEU:HD21 | 17:d:150:ILE:CG2  | 2.30                     | 0.61              |
| 18:f:711:SER:O    | 18:f:714:SER:N    | 2.24                     | 0.61              |
| 18:f:828:ARG:NH1  | 18:f:874:LEU:HD12 | 2.16                     | 0.61              |
| 18:f:843:SER:O    | 18:f:883:ALA:HB3  | 2.00                     | 0.61              |
| 19:g:164:ASP:HA   | 19:g:167:LYS:HD2  | 1.82                     | 0.61              |
| 22:A:139:ARG:NH2  | 22:A:156:LYS:HA   | 2.15                     | 0.61              |
| 25:F:198:LEU:HD23 | 25:F:202:ILE:HB   | 1.81                     | 0.61              |
| 26:K:23:GLN:OE1   | 26:K:23:GLN:HA    | 1.98                     | 0.61              |
| 1:C:404:LEU:CD2   | 4:H:152:SER:HB2   | 2.31                     | 0.61              |
| 9:V:194:LYS:O     | 9:V:198:GLN:HG2   | 2.01                     | 0.61              |
| 10:W:27:ARG:NH2   | 10:W:46:THR:HG21  | 2.16                     | 0.61              |
| 11:X:364:LYS:NZ   | 11:X:367:GLN:OE1  | 2.27                     | 0.61              |
| 18:f:433:LEU:HB3  | 19:g:172:GLU:HA   | 1.82                     | 0.61              |
| 18:f:654:VAL:HG22 | 18:f:678:LEU:HD23 | 1.83                     | 0.61              |
| 18:f:890:VAL:HG23 | 18:f:899:ILE:O    | 2.00                     | 0.61              |
| 19:g:80:THR:HG23  | 19:g:82:ILE:HG12  | 1.81                     | 0.61              |
| 19:g:128:LYS:HD2  | 19:g:129:ILE:H    | 1.65                     | 0.61              |
| 19:g:162:GLU:O    | 19:g:166:ARG:N    | 2.34                     | 0.61              |
| 20:u:182:PHE:CZ   | 20:u:246:ILE:HG21 | 2.35                     | 0.61              |
| 25:F:175:MET:HB3  | 25:F:249:LEU:CD1  | 2.30                     | 0.61              |
| 27:U:198:LEU:CB   | 27:U:223:LEU:HG   | 2.30                     | 0.61              |
| 27:U:481:LEU:HD11 | 27:U:493:VAL:CG2  | 2.31                     | 0.61              |
| 27:U:833:LEU:HA   | 27:U:836:THR:HG22 | 1.83                     | 0.61              |
| 27:U:836:THR:HG23 | 27:U:837:ALA:N    | 2.16                     | 0.61              |
| 2:D:186:THR:OG1   | 2:D:187:HIS:N     | 2.34                     | 0.61              |
| 3:G:29:PHE:CZ     | 3:G:156:PRO:HD2   | 2.35                     | 0.61              |
| 4:H:37:GLY:O      | 4:H:160:ALA:HA    | 2.01                     | 0.61              |
| 4:H:68:ILE:HD11   | 4:H:74:LEU:HG     | 1.83                     | 0.61              |
| 4:H:89:ARG:HB3    | 4:H:89:ARG:HH11   | 1.66                     | 0.61              |
| 5:I:65:ILE:CD1    | 5:I:75:SER:HB2    | 2.30                     | 0.61              |
| 7:L:26:MET:CE     | 7:L:148:CYS:HB2   | 2.19                     | 0.61              |
| 7:L:196:ARG:HH12  | 7:L:239:ARG:CA    | 2.13                     | 0.61              |
| 9:V:467:TYR:HA    | 9:V:472:PRO:HG2   | 1.83                     | 0.61              |
| 11:X:84:LYS:HA    | 11:X:87:ARG:NH1   | 2.16                     | 0.61              |
| 12:Y:279:GLU:OE1  | 28:e:52:PHE:HB3   | 2.01                     | 0.61              |
| 14:a:216:LEU:HD13 | 14:a:237:LEU:CB   | 2.30                     | 0.61              |
| 15:b:58:CYS:HB3   | 15:b:92:VAL:HG11  | 1.83                     | 0.61              |
| 17:d:129:LEU:CB   | 17:d:130:PRO:HD2  | 2.31                     | 0.61              |
| 17:d:145:ARG:NH2  | 17:d:188:MET:HB3  | 2.16                     | 0.61              |
| 18:f:59:LEU:CD1   | 18:f:74:ALA:HA    | 2.31                     | 0.61              |
| 24:E:97:ARG:NH2   | 25:F:95:GLU:OE2   | 2.24                     | 0.61              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 24:E:327:ASP:O    | 24:E:329:GLU:N    | 2.34                     | 0.61              |
| 27:U:3:THR:O      | 27:U:34:PHE:HZ    | 1.84                     | 0.61              |
| 27:U:489:ALA:HA   | 27:U:520:MET:HE2  | 1.83                     | 0.61              |
| 27:U:580:ARG:HG2  | 27:U:617:ALA:CB   | 2.30                     | 0.61              |
| 27:U:842:LYS:O    | 27:U:846:LYS:HE3  | 2.00                     | 0.61              |
| 1:C:213:ARG:HG3   | 1:C:213:ARG:O     | 2.01                     | 0.60              |
| 1:C:401:ILE:HD13  | 4:H:26:LEU:CD1    | 2.30                     | 0.60              |
| 9:V:110:HIS:HB3   | 9:V:136:GLU:O     | 2.01                     | 0.60              |
| 9:V:383:GLY:HA2   | 9:V:386:PHE:CD2   | 2.36                     | 0.60              |
| 9:V:416:ARG:HG3   | 9:V:457:TYR:CD1   | 2.36                     | 0.60              |
| 13:Z:12:HIS:O     | 13:Z:15:VAL:HG12  | 2.01                     | 0.60              |
| 13:Z:20:VAL:HA    | 13:Z:126:VAL:HG21 | 1.83                     | 0.60              |
| 13:Z:127:LYS:O    | 13:Z:129:LYS:NZ   | 2.34                     | 0.60              |
| 14:a:40:GLN:HG3   | 14:a:44:PHE:CE2   | 2.34                     | 0.60              |
| 17:d:137:THR:N    | 17:d:140:GLN:OE1  | 2.34                     | 0.60              |
| 18:f:297:MET:HE1  | 18:f:782:HIS:CD2  | 2.36                     | 0.60              |
| 19:g:89:LEU:HA    | 19:g:155:VAL:HB   | 1.82                     | 0.60              |
| 19:g:113:ARG:HB3  | 19:g:138:LEU:CD1  | 2.31                     | 0.60              |
| 19:g:116:ILE:HG22 | 19:g:127:ILE:HD11 | 1.82                     | 0.60              |
| 23:B:245:ALA:HB1  | 23:B:279:PRO:C    | 2.26                     | 0.60              |
| 26:K:35:SER:OG    | 26:K:66:LYS:NZ    | 2.28                     | 0.60              |
| 27:U:353:LEU:HD11 | 27:U:373:ASN:HB3  | 1.83                     | 0.60              |
| 27:U:904:LYS:CG   | 27:U:905:PRO:HD2  | 2.31                     | 0.60              |
| 2:D:235:PHE:CD1   | 2:D:246:MET:HG2   | 2.36                     | 0.60              |
| 10:W:203:GLN:HG2  | 10:W:233:LEU:CD2  | 2.22                     | 0.60              |
| 10:W:407:ASP:OD1  | 11:X:344:ARG:HD3  | 2.02                     | 0.60              |
| 13:Z:130:ASP:N    | 13:Z:130:ASP:OD1  | 2.33                     | 0.60              |
| 14:a:100:THR:HA   | 14:a:103:LYS:CD   | 2.31                     | 0.60              |
| 15:b:109:ILE:HB   | 15:b:138:VAL:HG23 | 1.82                     | 0.60              |
| 16:c:180:ASN:OD1  | 16:c:180:ASN:N    | 2.34                     | 0.60              |
| 17:d:136:LEU:HB3  | 17:d:140:GLN:OE1  | 2.01                     | 0.60              |
| 17:d:166:ARG:O    | 17:d:170:GLN:NE2  | 2.26                     | 0.60              |
| 18:f:316:ASP:HA   | 18:f:319:GLU:CG   | 2.31                     | 0.60              |
| 18:f:407:MET:CE   | 18:f:440:ILE:HG21 | 2.31                     | 0.60              |
| 18:f:726:ILE:CG1  | 18:f:762:VAL:HG22 | 2.30                     | 0.60              |
| 19:g:106:HIS:ND1  | 19:g:107:ILE:HG23 | 2.17                     | 0.60              |
| 23:B:190:LEU:HA   | 23:B:193:GLN:OE1  | 2.01                     | 0.60              |
| 24:E:55:GLN:OE1   | 24:E:55:GLN:N     | 2.33                     | 0.60              |
| 27:U:474:ARG:HE   | 27:U:500:ASN:CG   | 2.09                     | 0.60              |
| 27:U:596:ASN:HA   | 27:U:599:ILE:HG22 | 1.84                     | 0.60              |
| 1:C:36:ASN:HD21   | 9:V:89:LYS:HB3    | 1.65                     | 0.60              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:87:VAL:HG21   | 1:C:116:LEU:HD11  | 1.83                     | 0.60              |
| 3:G:50:ILE:HD13   | 3:G:141:ILE:CD1   | 2.32                     | 0.60              |
| 4:H:73:GLY:O      | 4:H:74:LEU:HD23   | 2.01                     | 0.60              |
| 10:W:203:GLN:O    | 10:W:207:LYS:HD3  | 2.02                     | 0.60              |
| 11:X:54:GLY:CA    | 11:X:66:LEU:HD11  | 2.31                     | 0.60              |
| 11:X:142:ARG:HB3  | 11:X:145:GLU:OE1  | 2.01                     | 0.60              |
| 11:X:373:LYS:HA   | 11:X:373:LYS:NZ   | 2.16                     | 0.60              |
| 12:Y:52:PRO:HD2   | 12:Y:114:ILE:O    | 2.01                     | 0.60              |
| 14:a:72:ASN:ND2   | 14:a:74:LEU:HB2   | 2.16                     | 0.60              |
| 14:a:127:ASP:O    | 14:a:131:THR:HG21 | 2.01                     | 0.60              |
| 17:d:90:ALA:O     | 17:d:94:MET:HG3   | 2.01                     | 0.60              |
| 17:d:124:LEU:HD22 | 27:U:22:PHE:HD2   | 1.66                     | 0.60              |
| 18:f:330:PHE:HZ   | 18:f:776:LEU:HD21 | 1.65                     | 0.60              |
| 18:f:644:ALA:O    | 18:f:647:GLY:N    | 2.34                     | 0.60              |
| 19:g:161:SER:OG   | 19:g:162:GLU:OE1  | 2.19                     | 0.60              |
| 20:u:130:ILE:HG23 | 20:u:169:VAL:CG1  | 2.31                     | 0.60              |
| 22:A:71:GLY:HA3   | 23:B:162:VAL:CG1  | 2.31                     | 0.60              |
| 23:B:251:VAL:O    | 23:B:251:VAL:HG22 | 2.02                     | 0.60              |
| 27:U:160:LEU:HD11 | 27:U:196:LYS:HD2  | 1.83                     | 0.60              |
| 27:U:811:PHE:CD1  | 27:U:885:MET:HE1  | 2.35                     | 0.60              |
| 2:D:181:VAL:HG11  | 2:D:308:ILE:CG1   | 2.32                     | 0.60              |
| 5:I:86:LEU:HD21   | 5:I:118:LYS:HZ1   | 1.63                     | 0.60              |
| 10:W:112:VAL:HG13 | 10:W:121:LYS:NZ   | 2.16                     | 0.60              |
| 10:W:138:VAL:HA   | 10:W:141:GLU:OE1  | 2.01                     | 0.60              |
| 12:Y:301:ILE:HG23 | 12:Y:343:LEU:HD11 | 1.82                     | 0.60              |
| 14:a:75:SER:HA    | 14:a:78:GLU:HB2   | 1.82                     | 0.60              |
| 15:b:27:GLN:O     | 15:b:31:ASP:N     | 2.21                     | 0.60              |
| 15:b:53:THR:HB    | 15:b:61:LEU:HD11  | 1.82                     | 0.60              |
| 17:d:127:ASN:ND2  | 17:d:136:LEU:HD11 | 2.13                     | 0.60              |
| 17:d:142:ILE:HG22 | 17:d:146:ASP:CG   | 2.27                     | 0.60              |
| 18:f:261:ARG:HA   | 18:f:261:ARG:HE   | 1.65                     | 0.60              |
| 18:f:305:LEU:HD12 | 18:f:305:LEU:O    | 2.01                     | 0.60              |
| 22:A:333:ARG:NH1  | 22:A:335:GLY:HA3  | 2.17                     | 0.60              |
| 27:U:549:ALA:O    | 27:U:581:SER:OG   | 2.12                     | 0.60              |
| 27:U:678:ASP:OD1  | 27:U:679:PRO:HD2  | 2.01                     | 0.60              |
| 1:C:391:MET:HG3   | 1:C:391:MET:O     | 2.01                     | 0.60              |
| 3:G:76:ILE:CG2    | 3:G:111:VAL:HG22  | 2.31                     | 0.60              |
| 3:G:215:ILE:CD1   | 3:G:217:VAL:HG23  | 2.31                     | 0.60              |
| 5:I:33:THR:OG1    | 5:I:166:ASN:O     | 2.19                     | 0.60              |
| 7:L:58:ALA:CB     | 26:K:164:GLN:HG3  | 2.31                     | 0.60              |
| 7:L:66:VAL:HB     | 7:L:70:ILE:O      | 2.01                     | 0.60              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 8:M:216:VAL:HG12  | 8:M:223:ARG:O     | 2.02                     | 0.60              |
| 9:V:62:HIS:O      | 9:V:65:ARG:HG2    | 2.01                     | 0.60              |
| 9:V:375:PHE:O     | 9:V:379:LEU:HG    | 2.02                     | 0.60              |
| 11:X:80:ILE:HG13  | 11:X:85:ALA:HB2   | 1.83                     | 0.60              |
| 13:Z:67:VAL:CG1   | 15:b:91:ARG:HB2   | 2.31                     | 0.60              |
| 14:a:70:ARG:HH22  | 15:b:17:ARG:NE    | 2.00                     | 0.60              |
| 14:a:96:PHE:O     | 14:a:99:LYS:HG2   | 2.02                     | 0.60              |
| 14:a:277:LEU:O    | 14:a:280:MET:HG3  | 2.01                     | 0.60              |
| 15:b:53:THR:C     | 15:b:54:LEU:HD23  | 2.26                     | 0.60              |
| 15:b:104:ASN:OD1  | 15:b:105:HIS:N    | 2.34                     | 0.60              |
| 18:f:333:LEU:HD12 | 18:f:337:LEU:HD13 | 1.83                     | 0.60              |
| 18:f:395:GLY:HA3  | 18:f:432:TYR:HE2  | 1.67                     | 0.60              |
| 18:f:538:ILE:O    | 18:f:542:ILE:HG23 | 2.01                     | 0.60              |
| 22:A:52:ILE:HD13  | 23:B:72:LEU:HD12  | 1.84                     | 0.60              |
| 22:A:229:VAL:O    | 22:A:233:THR:HG23 | 2.01                     | 0.60              |
| 24:E:150:GLU:OE2  | 24:E:154:THR:HG21 | 2.00                     | 0.60              |
| 25:F:188:ILE:HG12 | 25:F:235:LEU:CD2  | 2.32                     | 0.60              |
| 27:U:42:VAL:HG12  | 27:U:68:PHE:CE1   | 2.36                     | 0.60              |
| 4:H:159:LYS:HB2   | 5:I:55:LEU:O      | 2.02                     | 0.60              |
| 12:Y:149:LEU:HD23 | 12:Y:157:ILE:CD1  | 2.32                     | 0.60              |
| 16:c:63:ASP:OD1   | 16:c:65:TYR:N     | 2.35                     | 0.60              |
| 18:f:267:ARG:HH21 | 18:f:891:THR:CG2  | 2.14                     | 0.60              |
| 19:g:112:LEU:HD23 | 19:g:138:LEU:CD2  | 2.31                     | 0.60              |
| 19:g:130:VAL:O    | 19:g:153:ALA:HA   | 2.02                     | 0.60              |
| 22:A:254:ALA:HB1  | 22:A:301:GLU:HG2  | 1.82                     | 0.60              |
| 22:A:425:ALA:O    | 22:A:429:TYR:N    | 2.33                     | 0.60              |
| 1:C:229:ARG:NH1   | 1:C:229:ARG:HG2   | 2.17                     | 0.60              |
| 3:G:36:GLY:O      | 3:G:37:LEU:HD23   | 2.02                     | 0.60              |
| 5:I:76:VAL:HG11   | 5:I:83:ALA:CB     | 2.31                     | 0.60              |
| 5:I:116:ASP:OD1   | 6:J:81:ARG:NH2    | 2.33                     | 0.60              |
| 6:J:26:VAL:HG21   | 6:J:130:SER:HB3   | 1.84                     | 0.60              |
| 6:J:210:VAL:HG12  | 6:J:220:LEU:HD21  | 1.82                     | 0.60              |
| 10:W:241:LEU:HD21 | 10:W:282:GLU:HG2  | 1.84                     | 0.60              |
| 10:W:408:ARG:HD2  | 11:X:342:PHE:HE2  | 1.65                     | 0.60              |
| 12:Y:42:MET:HE2   | 12:Y:63:TRP:CZ3   | 2.36                     | 0.60              |
| 13:Z:212:LEU:HB3  | 14:a:350:LYS:HB3  | 1.82                     | 0.60              |
| 14:a:61:GLU:CD    | 14:a:79:ILE:HD13  | 2.27                     | 0.60              |
| 15:b:121:GLU:O    | 15:b:124:LEU:HG   | 2.01                     | 0.60              |
| 16:c:278:GLN:O    | 16:c:282:ARG:NH2  | 2.34                     | 0.60              |
| 18:f:498:LEU:HD13 | 18:f:534:VAL:HG21 | 1.83                     | 0.60              |
| 19:g:109:GLY:HA2  | 19:g:112:LEU:HB3  | 1.83                     | 0.60              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:A:333:ARG:CG   | 22:A:334:PRO:HD2  | 2.31                     | 0.60              |
| 24:E:173:TYR:CZ   | 24:E:300:HIS:HB2  | 2.36                     | 0.60              |
| 25:F:223:VAL:HA   | 25:F:350:ARG:O    | 2.00                     | 0.60              |
| 25:F:252:ALA:HA   | 25:F:286:ASP:H    | 1.66                     | 0.60              |
| 26:K:99:HIS:O     | 26:K:103:TYR:HB2  | 2.01                     | 0.60              |
| 3:G:155:ASP:OD2   | 3:G:159:TYR:HB3   | 2.01                     | 0.60              |
| 5:I:105:ILE:HD11  | 5:I:110:LEU:CA    | 2.31                     | 0.60              |
| 5:I:179:TYR:OH    | 5:I:181:GLU:HB2   | 2.01                     | 0.60              |
| 7:L:125:ARG:HH21  | 7:L:128:TYR:HE1   | 1.50                     | 0.60              |
| 9:V:223:LYS:O     | 9:V:261:TYR:OH    | 2.19                     | 0.60              |
| 10:W:105:VAL:HG21 | 10:W:138:VAL:CG2  | 2.30                     | 0.60              |
| 10:W:323:ASP:HB3  | 10:W:324:TYR:HD1  | 1.67                     | 0.60              |
| 10:W:383:ASP:C    | 10:W:384:LEU:HD23 | 2.26                     | 0.60              |
| 11:X:47:GLU:HA    | 11:X:76:PHE:CZ    | 2.28                     | 0.60              |
| 11:X:68:GLY:HA2   | 11:X:71:LYS:CG    | 2.31                     | 0.60              |
| 12:Y:26:LEU:HG    | 12:Y:37:VAL:CG1   | 2.32                     | 0.60              |
| 14:a:211:PHE:CE2  | 14:a:319:LEU:HD21 | 2.36                     | 0.60              |
| 18:f:432:TYR:H    | 19:g:172:GLU:CB   | 2.14                     | 0.60              |
| 18:f:484:GLY:HA2  | 18:f:487:LEU:HD12 | 1.83                     | 0.60              |
| 22:A:158:ASP:OD1  | 22:A:159:PRO:HD2  | 2.01                     | 0.60              |
| 22:A:187:LEU:HD11 | 22:A:318:LEU:HD21 | 1.83                     | 0.60              |
| 23:B:54:PRO:HG3   | 23:B:60:LEU:HB3   | 1.83                     | 0.60              |
| 23:B:197:ILE:O    | 23:B:201:VAL:HG22 | 2.01                     | 0.60              |
| 25:F:315:ASN:HB3  | 25:F:316:GLN:NE2  | 2.17                     | 0.60              |
| 26:K:97:GLN:HA    | 26:K:97:GLN:OE1   | 2.02                     | 0.60              |
| 27:U:245:ALA:HB1  | 27:U:325:MET:CE   | 2.32                     | 0.60              |
| 27:U:493:VAL:HG13 | 27:U:519:VAL:HG21 | 1.83                     | 0.60              |
| 27:U:713:TYR:O    | 27:U:717:ILE:HG22 | 2.02                     | 0.60              |
| 27:U:879:ASP:OD2  | 27:U:925:VAL:HG11 | 2.01                     | 0.60              |
| 1:C:165:ILE:HD11  | 1:C:292:ILE:CG1   | 2.32                     | 0.60              |
| 8:M:186:CYS:CA    | 8:M:189:ILE:HB    | 2.23                     | 0.60              |
| 9:V:451:ILE:HG12  | 9:V:458:VAL:HG22  | 1.83                     | 0.60              |
| 14:a:94:LEU:CD1   | 14:a:118:ILE:HB   | 2.32                     | 0.60              |
| 16:c:177:THR:CG2  | 27:U:773:PHE:HB2  | 2.32                     | 0.60              |
| 17:d:180:GLU:CD   | 17:d:180:GLU:H    | 2.10                     | 0.60              |
| 18:f:430:ASP:HB2  | 19:g:168:ASN:O    | 2.02                     | 0.60              |
| 18:f:670:MET:HE3  | 23:B:68:ILE:HG23  | 1.83                     | 0.60              |
| 24:E:141:GLN:HG2  | 24:E:300:HIS:O    | 2.02                     | 0.60              |
| 24:E:308:ALA:O    | 24:E:309:ARG:C    | 2.45                     | 0.60              |
| 25:F:219:PRO:O    | 25:F:327:LYS:NZ   | 2.35                     | 0.60              |
| 25:F:223:VAL:HG23 | 25:F:329:ILE:HG12 | 1.83                     | 0.60              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 26:K:220:VAL:HB   | 26:K:228:MET:CE   | 2.31                     | 0.60              |
| 27:U:132:GLY:O    | 27:U:136:LYS:HB3  | 2.01                     | 0.60              |
| 2:D:277:ALA:HB1   | 2:D:283:ARG:HG2   | 1.83                     | 0.60              |
| 3:G:13:ILE:CD1    | 3:G:126:THR:HA    | 2.23                     | 0.60              |
| 3:G:207:SER:O     | 3:G:208:ILE:HD13  | 2.02                     | 0.60              |
| 4:H:19:LEU:H      | 4:H:19:LEU:HD12   | 1.67                     | 0.60              |
| 4:H:50:LYS:HG2    | 4:H:52:GLN:NE2    | 2.15                     | 0.60              |
| 4:H:89:ARG:O      | 4:H:93:LEU:HB2    | 2.02                     | 0.60              |
| 7:L:117:GLN:OE1   | 7:L:118:ILE:HD13  | 2.01                     | 0.60              |
| 9:V:70:VAL:HA     | 9:V:73:GLU:OE1    | 2.02                     | 0.60              |
| 9:V:182:LYS:O     | 9:V:186:LYS:HG2   | 2.02                     | 0.60              |
| 9:V:191:LEU:O     | 9:V:195:ILE:HG23  | 2.02                     | 0.60              |
| 9:V:273:LYS:HA    | 9:V:273:LYS:HE3   | 1.83                     | 0.60              |
| 9:V:381:GLN:HG2   | 9:V:382:PHE:CD1   | 2.37                     | 0.60              |
| 10:W:364:ARG:C    | 10:W:368:LYS:HE2  | 2.26                     | 0.60              |
| 10:W:370:TYR:OH   | 14:a:308:GLU:HG3  | 2.02                     | 0.60              |
| 14:a:189:PRO:CG   | 14:a:192:GLU:HB2  | 2.31                     | 0.60              |
| 14:a:274:LEU:HD23 | 14:a:278:MET:HE1  | 1.83                     | 0.60              |
| 15:b:71:ILE:H     | 15:b:71:ILE:HD12  | 1.67                     | 0.60              |
| 15:b:180:ALA:O    | 15:b:184:ILE:HG23 | 2.01                     | 0.60              |
| 17:d:117:GLY:HA3  | 17:d:118:ARG:NH2  | 2.16                     | 0.60              |
| 17:d:302:TYR:O    | 17:d:307:GLY:N    | 2.35                     | 0.60              |
| 18:f:329:ASN:O    | 18:f:333:LEU:N    | 2.29                     | 0.60              |
| 18:f:497:VAL:O    | 18:f:501:LEU:HD23 | 2.01                     | 0.60              |
| 18:f:542:ILE:CD1  | 18:f:580:LEU:HD21 | 2.30                     | 0.60              |
| 18:f:579:ALA:O    | 18:f:582:VAL:HG23 | 2.02                     | 0.60              |
| 18:f:830:LEU:CB   | 18:f:872:VAL:HB   | 2.32                     | 0.60              |
| 19:g:112:LEU:HD22 | 19:g:142:LEU:HG   | 1.82                     | 0.60              |
| 22:A:284:ARG:HG2  | 22:A:296:GLN:HG3  | 1.84                     | 0.60              |
| 24:E:87:LEU:HD23  | 24:E:92:LEU:HD11  | 1.81                     | 0.60              |
| 24:E:138:LEU:HB3  | 24:E:142:ILE:HG13 | 1.84                     | 0.60              |
| 24:E:251:ARG:HG3  | 24:E:255:ARG:NH1  | 2.17                     | 0.60              |
| 25:F:134:LEU:HD11 | 25:F:159:LEU:CA   | 2.26                     | 0.60              |
| 27:U:88:PHE:CE1   | 27:U:90:VAL:HG23  | 2.37                     | 0.60              |
| 27:U:171:ASN:HB2  | 27:U:176:MET:SD   | 2.41                     | 0.60              |
| 2:D:46:LYS:HE3    | 27:U:187:LEU:HD11 | 1.83                     | 0.59              |
| 7:L:46:LEU:HD12   | 7:L:63:ILE:HD11   | 1.83                     | 0.59              |
| 7:L:81:ALA:HA     | 7:L:130:VAL:HG21  | 1.83                     | 0.59              |
| 8:M:117:MET:HE2   | 8:M:117:MET:CA    | 2.32                     | 0.59              |
| 8:M:136:MET:CE    | 8:M:163:CYS:HB3   | 2.32                     | 0.59              |
| 9:V:79:VAL:HG13   | 9:V:163:VAL:HG11  | 1.84                     | 0.59              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 9:V:201:ARG:NH1   | 9:V:241:ARG:HD3   | 2.17                     | 0.59              |
| 9:V:324:PHE:HB2   | 28:e:19:PHE:HD2   | 1.67                     | 0.59              |
| 9:V:410:ILE:HG12  | 9:V:426:LEU:HD11  | 1.84                     | 0.59              |
| 10:W:272:LEU:HD21 | 10:W:341:PHE:CD2  | 2.37                     | 0.59              |
| 11:X:334:ASN:HD22 | 11:X:354:ILE:HD13 | 1.67                     | 0.59              |
| 11:X:348:GLU:O    | 11:X:351:SER:OG   | 2.18                     | 0.59              |
| 13:Z:14:LEU:HD12  | 13:Z:14:LEU:O     | 2.02                     | 0.59              |
| 18:f:333:LEU:HD13 | 18:f:831:VAL:CG2  | 2.32                     | 0.59              |
| 18:f:613:LEU:CB   | 23:B:74:MET:HE3   | 2.32                     | 0.59              |
| 19:g:113:ARG:HE   | 19:g:138:LEU:HD13 | 1.66                     | 0.59              |
| 19:g:165:ALA:CB   | 19:g:169:PHE:H    | 2.15                     | 0.59              |
| 22:A:348:LEU:HD23 | 22:A:348:LEU:C    | 2.27                     | 0.59              |
| 23:B:187:ILE:HG22 | 23:B:234:LEU:HG   | 1.84                     | 0.59              |
| 25:F:208:HIS:HD2  | 25:F:211:LYS:HG2  | 1.67                     | 0.59              |
| 27:U:86:ASP:O     | 27:U:90:VAL:HB    | 2.01                     | 0.59              |
| 27:U:239:GLU:OE1  | 27:U:241:ASN:HB2  | 2.01                     | 0.59              |
| 27:U:351:MET:HE1  | 27:U:354:LYS:HD3  | 1.84                     | 0.59              |
| 27:U:609:ASP:OD1  | 27:U:610:VAL:N    | 2.34                     | 0.59              |
| 1:C:193:GLY:HA3   | 2:D:323:ARG:CD    | 2.31                     | 0.59              |
| 2:D:138:ALA:O     | 2:D:140:VAL:HG13  | 2.02                     | 0.59              |
| 2:D:218:ALA:O     | 2:D:220:ALA:N     | 2.35                     | 0.59              |
| 8:M:69:VAL:O      | 8:M:92:ARG:HG2    | 2.02                     | 0.59              |
| 8:M:190:VAL:HG21  | 8:M:215:TRP:CE3   | 2.37                     | 0.59              |
| 9:V:174:PHE:HA    | 9:V:177:ASN:HB2   | 1.83                     | 0.59              |
| 10:W:366:MET:HE2  | 10:W:373:ILE:CD1  | 2.32                     | 0.59              |
| 10:W:377:ARG:O    | 10:W:381:LEU:HG   | 2.02                     | 0.59              |
| 11:X:114:ILE:O    | 11:X:118:LYS:HG2  | 2.01                     | 0.59              |
| 11:X:160:MET:HE2  | 11:X:161:ASP:O    | 2.01                     | 0.59              |
| 12:Y:58:CYS:SG    | 12:Y:65:ILE:HG12  | 2.43                     | 0.59              |
| 12:Y:80:GLU:O     | 12:Y:84:LEU:HG    | 2.00                     | 0.59              |
| 12:Y:338:ILE:HD11 | 12:Y:345:CYS:SG   | 2.42                     | 0.59              |
| 13:Z:32:GLN:OE1   | 13:Z:33:LYS:N     | 2.22                     | 0.59              |
| 13:Z:58:PHE:HE2   | 13:Z:108:ILE:HD13 | 1.67                     | 0.59              |
| 14:a:84:VAL:HG21  | 14:a:93:ALA:HB1   | 1.84                     | 0.59              |
| 14:a:137:ASP:OD1  | 14:a:138:VAL:N    | 2.35                     | 0.59              |
| 15:b:17:ARG:HD3   | 15:b:81:LYS:HZ2   | 1.64                     | 0.59              |
| 17:d:259:PHE:O    | 17:d:262:ILE:N    | 2.34                     | 0.59              |
| 18:f:45:LEU:CG    | 18:f:49:ASP:HB3   | 2.31                     | 0.59              |
| 22:A:230:ALA:HA   | 22:A:233:THR:CG2  | 2.32                     | 0.59              |
| 22:A:262:GLU:O    | 22:A:266:THR:HG23 | 2.01                     | 0.59              |
| 25:F:274:LEU:CD1  | 25:F:278:LYS:HZ3  | 2.14                     | 0.59              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:187:LEU:HD22  | 1:C:306:LEU:HD22  | 1.84                     | 0.59              |
| 3:G:111:VAL:HG21  | 3:G:142:GLY:HA3   | 1.84                     | 0.59              |
| 3:G:139:ILE:HA    | 3:G:152:TYR:O     | 2.01                     | 0.59              |
| 4:H:110:LEU:O     | 4:H:114:VAL:N     | 2.31                     | 0.59              |
| 4:H:139:TRP:CZ2   | 4:H:215:GLU:HG2   | 2.37                     | 0.59              |
| 6:J:132:LEU:HG    | 6:J:161:ILE:HD13  | 1.84                     | 0.59              |
| 7:L:167:SER:O     | 7:L:170:THR:HG22  | 2.02                     | 0.59              |
| 8:M:175:GLU:O     | 8:M:196:ILE:HD11  | 2.03                     | 0.59              |
| 9:V:117:VAL:HG11  | 9:V:131:LEU:CD1   | 2.32                     | 0.59              |
| 11:X:325:LYS:O    | 11:X:325:LYS:HD3  | 2.01                     | 0.59              |
| 14:a:152:HIS:HB3  | 14:a:156:TYR:OH   | 2.02                     | 0.59              |
| 14:a:243:GLY:C    | 14:a:272:ILE:HD11 | 2.27                     | 0.59              |
| 18:f:408:LEU:HD13 | 18:f:442:SER:OG   | 2.02                     | 0.59              |
| 18:f:470:VAL:CG1  | 18:f:481:SER:HB3  | 2.33                     | 0.59              |
| 18:f:861:THR:HB   | 18:f:879:ARG:HH22 | 1.66                     | 0.59              |
| 27:U:403:THR:HG23 | 27:U:777:HIS:NE2  | 2.16                     | 0.59              |
| 2:D:414:HIS:HB3   | 2:D:416:PHE:CE1   | 2.37                     | 0.59              |
| 6:J:90:GLU:HG2    | 6:J:110:TYR:CG    | 2.37                     | 0.59              |
| 9:V:100:MET:N     | 9:V:100:MET:HE3   | 2.17                     | 0.59              |
| 9:V:434:ALA:O     | 9:V:438:VAL:HG23  | 2.01                     | 0.59              |
| 10:W:271:VAL:HG11 | 10:W:302:TYR:HB3  | 1.83                     | 0.59              |
| 12:Y:183:TYR:CE1  | 12:Y:213:LEU:HD21 | 2.38                     | 0.59              |
| 14:a:97:LEU:HD22  | 14:a:117:ALA:HB3  | 1.83                     | 0.59              |
| 14:a:374:ILE:HD13 | 17:d:347:GLU:HG3  | 1.84                     | 0.59              |
| 15:b:63:THR:HG22  | 15:b:64:LEU:H     | 1.67                     | 0.59              |
| 18:f:190:GLU:C    | 18:f:193:PRO:HD2  | 2.28                     | 0.59              |
| 18:f:219:LYS:HA   | 18:f:258:LYS:HZ3  | 1.67                     | 0.59              |
| 18:f:429:ILE:O    | 19:g:172:GLU:HB3  | 2.02                     | 0.59              |
| 18:f:439:TYR:CA   | 18:f:477:MET:HE1  | 2.22                     | 0.59              |
| 18:f:645:ASP:O    | 18:f:649:HIS:NE2  | 2.34                     | 0.59              |
| 18:f:718:ASP:HB3  | 18:f:721:VAL:CG1  | 2.30                     | 0.59              |
| 18:f:784:ASP:H    | 18:f:895:GLU:CD   | 2.08                     | 0.59              |
| 19:g:89:LEU:HD23  | 19:g:155:VAL:CG2  | 2.32                     | 0.59              |
| 23:B:69:LYS:HE3   | 23:B:73:LEU:HD11  | 1.84                     | 0.59              |
| 24:E:200:SER:HB3  | 24:E:238:ILE:CD1  | 2.32                     | 0.59              |
| 25:F:251:LEU:HG   | 25:F:256:LEU:HD11 | 1.83                     | 0.59              |
| 27:U:586:VAL:HG11 | 27:U:602:LEU:HD12 | 1.82                     | 0.59              |
| 1:C:21:ARG:HA     | 1:C:24:TYR:CE2    | 2.38                     | 0.59              |
| 1:C:82:LYS:HD2    | 1:C:105:ILE:HG21  | 1.83                     | 0.59              |
| 1:C:131:VAL:HG22  | 1:C:135:VAL:HG13  | 1.83                     | 0.59              |
| 3:G:143:ILE:CG2   | 3:G:222:VAL:HA    | 2.25                     | 0.59              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:G:191:PHE:HE1   | 3:G:219:VAL:HG11  | 1.67                     | 0.59              |
| 4:H:113:ARG:O     | 4:H:117:VAL:HG23  | 2.03                     | 0.59              |
| 9:V:121:PHE:CD2   | 9:V:159:LEU:HD12  | 2.36                     | 0.59              |
| 9:V:123:SER:OG    | 9:V:155:ALA:O     | 2.09                     | 0.59              |
| 9:V:269:LYS:HB3   | 27:U:36:ALA:HB1   | 1.84                     | 0.59              |
| 10:W:260:SER:HA   | 10:W:263:TRP:CD1  | 2.37                     | 0.59              |
| 14:a:32:LYS:HG3   | 14:a:34:TRP:CH2   | 2.38                     | 0.59              |
| 14:a:350:LYS:HG3  | 14:a:351:ASP:N    | 2.18                     | 0.59              |
| 15:b:97:LEU:HG    | 15:b:107:MET:CE   | 2.33                     | 0.59              |
| 18:f:84:SER:O     | 18:f:88:SER:OG    | 2.19                     | 0.59              |
| 18:f:138:GLU:HA   | 18:f:141:LYS:HG2  | 1.82                     | 0.59              |
| 18:f:214:VAL:HG22 | 18:f:214:VAL:O    | 2.03                     | 0.59              |
| 19:g:112:LEU:CD1  | 19:g:142:LEU:HD11 | 2.32                     | 0.59              |
| 22:A:121:PHE:CZ   | 22:A:147:TYR:HE2  | 2.21                     | 0.59              |
| 22:A:339:ARG:NH2  | 25:F:402:GLU:OE2  | 2.35                     | 0.59              |
| 23:B:107:MET:HE3  | 23:B:151:LEU:HD22 | 1.85                     | 0.59              |
| 27:U:87:LEU:HD23  | 27:U:87:LEU:H     | 1.67                     | 0.59              |
| 27:U:794:ASP:N    | 27:U:794:ASP:OD1  | 2.34                     | 0.59              |
| 3:G:29:PHE:O      | 3:G:32:ILE:HB     | 2.02                     | 0.59              |
| 3:G:29:PHE:CE2    | 3:G:155:ASP:HB2   | 2.37                     | 0.59              |
| 3:G:100:ASN:O     | 3:G:104:LYS:HB2   | 2.02                     | 0.59              |
| 4:H:100:VAL:HG12  | 4:H:101:TYR:CD1   | 2.38                     | 0.59              |
| 4:H:213:CYS:SG    | 4:H:218:PHE:HB2   | 2.43                     | 0.59              |
| 4:H:224:THR:O     | 4:H:227:LYS:N     | 2.35                     | 0.59              |
| 5:I:100:GLN:HG2   | 5:I:101:TYR:HE1   | 1.62                     | 0.59              |
| 5:I:143:TYR:HB2   | 5:I:146:GLN:HE21  | 1.67                     | 0.59              |
| 6:J:45:VAL:HG22   | 6:J:61:LYS:HD3    | 1.84                     | 0.59              |
| 10:W:245:LYS:NZ   | 10:W:282:GLU:OE2  | 2.35                     | 0.59              |
| 11:X:57:LEU:HG    | 11:X:62:GLN:OE1   | 2.03                     | 0.59              |
| 13:Z:121:LEU:HG   | 13:Z:138:TYR:HB2  | 1.84                     | 0.59              |
| 14:a:41:VAL:HG12  | 14:a:79:ILE:CD1   | 2.31                     | 0.59              |
| 15:b:13:SER:O     | 15:b:16:MET:HB2   | 2.03                     | 0.59              |
| 17:d:153:GLN:O    | 17:d:157:LEU:HG   | 2.02                     | 0.59              |
| 18:f:330:PHE:CZ   | 18:f:776:LEU:HD21 | 2.37                     | 0.59              |
| 18:f:379:GLY:CA   | 18:f:416:MET:HE3  | 2.32                     | 0.59              |
| 18:f:562:LEU:HD13 | 18:f:595:VAL:HG11 | 1.84                     | 0.59              |
| 18:f:583:VAL:HG13 | 18:f:588:ARG:HB2  | 1.83                     | 0.59              |
| 19:g:83:ALA:HB3   | 19:g:149:HIS:HB3  | 1.84                     | 0.59              |
| 19:g:165:ALA:O    | 19:g:170:GLN:N    | 2.34                     | 0.59              |
| 22:A:433:ASN:HD21 | 26:K:64:ILE:HG23  | 1.68                     | 0.59              |
| 23:B:186:ASP:O    | 23:B:367:ILE:HG21 | 2.03                     | 0.59              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 24:E:111:LEU:HD11 | 25:F:133:PHE:CD2  | 2.38                     | 0.59              |
| 25:F:279:ALA:CB   | 25:F:280:PRO:HD2  | 2.27                     | 0.59              |
| 26:K:89:ILE:O     | 26:K:92:ALA:N     | 2.31                     | 0.59              |
| 27:U:24:LEU:HD21  | 27:U:45:ILE:HG23  | 1.83                     | 0.59              |
| 27:U:137:MET:O    | 27:U:141:CYS:N    | 2.30                     | 0.59              |
| 5:I:38:LEU:CD2    | 5:I:160:LYS:HB3   | 2.29                     | 0.59              |
| 5:I:227:VAL:HG23  | 5:I:227:VAL:O     | 2.03                     | 0.59              |
| 7:L:10:VAL:HG21   | 7:L:120:THR:HA    | 1.84                     | 0.59              |
| 7:L:109:VAL:HG22  | 7:L:134:ILE:CD1   | 2.33                     | 0.59              |
| 9:V:161:PRO:HA    | 9:V:164:GLU:CD    | 2.28                     | 0.59              |
| 10:W:135:LYS:HB2  | 10:W:138:VAL:HG12 | 1.84                     | 0.59              |
| 10:W:407:ASP:OD1  | 11:X:344:ARG:HB2  | 2.01                     | 0.59              |
| 10:W:408:ARG:NH1  | 11:X:346:GLN:OE1  | 2.32                     | 0.59              |
| 13:Z:220:LEU:HG   | 13:Z:221:PRO:HD2  | 1.85                     | 0.59              |
| 14:a:249:GLN:O    | 14:a:253:THR:N    | 2.28                     | 0.59              |
| 15:b:151:GLU:HA   | 15:b:154:THR:HG22 | 1.84                     | 0.59              |
| 18:f:45:LEU:HB2   | 18:f:50:LYS:HE2   | 1.83                     | 0.59              |
| 18:f:433:LEU:HG   | 19:g:173:GLU:HA   | 1.85                     | 0.59              |
| 22:A:166:VAL:O    | 22:A:166:VAL:HG13 | 2.01                     | 0.59              |
| 22:A:276:GLU:OE1  | 22:A:276:GLU:HA   | 2.01                     | 0.59              |
| 25:F:287:GLU:N    | 25:F:331:ALA:O    | 2.36                     | 0.59              |
| 25:F:375:VAL:HG11 | 25:F:381:TYR:OH   | 2.03                     | 0.59              |
| 27:U:164:GLU:HG2  | 27:U:168:LEU:HD13 | 1.83                     | 0.59              |
| 27:U:566:LEU:O    | 27:U:570:LEU:HB2  | 2.03                     | 0.59              |
| 5:I:180:LYS:HD2   | 5:I:183:GLU:O     | 2.03                     | 0.59              |
| 7:L:52:ALA:HB2    | 7:L:59:HIS:ND1    | 2.18                     | 0.59              |
| 7:L:134:ILE:N     | 7:L:145:PHE:O     | 2.33                     | 0.59              |
| 9:V:326:GLN:O     | 9:V:330:LYS:HG3   | 2.03                     | 0.59              |
| 10:W:268:LYS:HA   | 10:W:302:TYR:CD2  | 2.37                     | 0.59              |
| 10:W:396:LEU:HD22 | 10:W:401:THR:HG21 | 1.84                     | 0.59              |
| 13:Z:29:VAL:HG23  | 13:Z:30:GLY:H     | 1.67                     | 0.59              |
| 13:Z:186:THR:O    | 13:Z:190:ARG:HG2  | 2.03                     | 0.59              |
| 14:a:116:THR:HA   | 14:a:119:GLY:HA3  | 1.83                     | 0.59              |
| 14:a:252:LYS:HA   | 14:a:255:TRP:NE1  | 2.17                     | 0.59              |
| 14:a:374:ILE:HD13 | 17:d:347:GLU:CB   | 2.32                     | 0.59              |
| 22:A:174:TYR:HD2  | 22:A:232:ARG:HD3  | 1.66                     | 0.59              |
| 25:F:350:ARG:HB3  | 25:F:350:ARG:NH1  | 2.18                     | 0.59              |
| 27:U:193:PHE:O    | 27:U:197:VAL:HG23 | 2.03                     | 0.59              |
| 27:U:673:GLU:OE2  | 27:U:673:GLU:HA   | 2.03                     | 0.59              |
| 3:G:79:VAL:HG12   | 3:G:139:ILE:HD12  | 1.84                     | 0.59              |
| 5:I:159:TRP:CE3   | 6:J:54:GLN:HB3    | 2.38                     | 0.59              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:L:188:VAL:CG2   | 7:L:212:ILE:HG21  | 2.33                     | 0.59              |
| 8:M:161:TRP:CE2   | 8:M:182:LYS:HE3   | 2.38                     | 0.59              |
| 10:W:296:LEU:HD23 | 10:W:303:LYS:HD2  | 1.85                     | 0.59              |
| 14:a:157:ASP:HA   | 14:a:160:SER:OG   | 2.03                     | 0.59              |
| 14:a:366:LEU:HD23 | 14:a:366:LEU:O    | 2.03                     | 0.59              |
| 15:b:23:PRO:HG2   | 15:b:27:GLN:NE2   | 2.16                     | 0.59              |
| 18:f:372:LEU:CD2  | 18:f:406:GLY:HA2  | 2.32                     | 0.59              |
| 19:g:85:ILE:HD11  | 19:g:131:ILE:HD11 | 1.85                     | 0.59              |
| 19:g:104:ARG:C    | 19:g:105:LEU:HD22 | 2.28                     | 0.59              |
| 22:A:72:LEU:HD11  | 23:B:103:ARG:HH22 | 1.66                     | 0.59              |
| 22:A:105:ASP:OD1  | 22:A:108:ASP:N    | 2.30                     | 0.59              |
| 23:B:167:THR:OG1  | 23:B:272:ARG:NH2  | 2.35                     | 0.59              |
| 25:F:225:MET:HE1  | 25:F:236:LEU:HD22 | 1.83                     | 0.59              |
| 25:F:253:GLY:N    | 25:F:286:ASP:O    | 2.32                     | 0.59              |
| 27:U:142:LEU:HD21 | 27:U:166:THR:HG22 | 1.84                     | 0.59              |
| 27:U:323:LEU:O    | 27:U:327:LYS:HG2  | 2.03                     | 0.59              |
| 1:C:275:GLU:OE2   | 23:B:251:VAL:HG11 | 2.03                     | 0.59              |
| 2:D:235:PHE:HD1   | 2:D:246:MET:HG2   | 1.68                     | 0.59              |
| 2:D:269:ALA:HB2   | 24:E:258:MET:CE   | 2.32                     | 0.59              |
| 2:D:309:MET:CE    | 2:D:327:LEU:HD11  | 2.30                     | 0.59              |
| 2:D:378:ILE:CG1   | 2:D:406:VAL:HB    | 2.33                     | 0.59              |
| 3:G:113:MET:O     | 3:G:116:LYS:N     | 2.36                     | 0.59              |
| 5:I:140:ASP:OD1   | 5:I:143:TYR:N     | 2.26                     | 0.59              |
| 7:L:33:SER:HB2    | 7:L:62:LYS:HZ1    | 1.67                     | 0.59              |
| 7:L:116:THR:O     | 7:L:119:PRO:HD2   | 2.03                     | 0.59              |
| 9:V:181:TYR:HB2   | 9:V:221:LEU:HD21  | 1.83                     | 0.59              |
| 9:V:182:LYS:HA    | 9:V:185:GLN:CB    | 2.31                     | 0.59              |
| 10:W:198:ASP:OD2  | 10:W:201:ARG:NH1  | 2.36                     | 0.59              |
| 11:X:141:LYS:HE2  | 11:X:141:LYS:HA   | 1.85                     | 0.59              |
| 11:X:380:GLN:HB3  | 12:Y:314:LEU:HA   | 1.83                     | 0.59              |
| 12:Y:105:MET:SD   | 12:Y:140:ILE:HD11 | 2.43                     | 0.59              |
| 14:a:76:LEU:O     | 14:a:80:ILE:HG12  | 2.02                     | 0.59              |
| 15:b:26:LEU:HD21  | 15:b:80:PRO:HD3   | 1.85                     | 0.59              |
| 15:b:108:ARG:HA   | 15:b:137:ASN:O    | 2.02                     | 0.59              |
| 18:f:159:VAL:HG11 | 18:f:194:TYR:CD2  | 2.38                     | 0.59              |
| 18:f:416:MET:HB2  | 18:f:450:ILE:HD13 | 1.84                     | 0.59              |
| 18:f:703:ARG:HB3  | 18:f:706:ILE:CG2  | 2.33                     | 0.59              |
| 24:E:184:ALA:HB2  | 24:E:276:ILE:HG21 | 1.85                     | 0.59              |
| 24:E:276:ILE:O    | 24:E:276:ILE:CG2  | 2.51                     | 0.59              |
| 24:E:317:ALA:HA   | 24:E:347:CYS:SG   | 2.43                     | 0.59              |
| 26:K:146:VAL:HG12 | 26:K:151:PRO:CA   | 2.32                     | 0.59              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 27:U:142:LEU:CD2  | 27:U:166:THR:HG22 | 2.33                     | 0.59              |
| 27:U:602:LEU:HD22 | 27:U:618:ALA:O    | 2.03                     | 0.59              |
| 27:U:646:PRO:HB3  | 27:U:680:VAL:HG21 | 1.85                     | 0.59              |
| 10:W:125:ILE:HG22 | 10:W:145:LEU:CD1  | 2.33                     | 0.58              |
| 11:X:219:ALA:O    | 11:X:322:HIS:NE2  | 2.32                     | 0.58              |
| 12:Y:14:ASN:HD21  | 12:Y:113:ARG:HH11 | 1.51                     | 0.58              |
| 13:Z:246:VAL:HG13 | 17:d:330:ILE:HD11 | 1.83                     | 0.58              |
| 14:a:54:ASP:OD2   | 14:a:86:GLN:HG3   | 2.02                     | 0.58              |
| 14:a:137:ASP:OD1  | 14:a:138:VAL:HG23 | 2.03                     | 0.58              |
| 14:a:148:VAL:CG1  | 14:a:151:VAL:HG22 | 2.31                     | 0.58              |
| 15:b:7:MET:HE3    | 15:b:64:LEU:HG    | 1.85                     | 0.58              |
| 17:d:91:ALA:O     | 17:d:95:TYR:N     | 2.32                     | 0.58              |
| 17:d:282:ILE:HB   | 17:d:318:PHE:CE2  | 2.38                     | 0.58              |
| 18:f:391:LEU:CG   | 18:f:414:LEU:HG   | 2.33                     | 0.58              |
| 18:f:609:VAL:CG1  | 23:B:74:MET:HE1   | 2.30                     | 0.58              |
| 22:A:190:VAL:CG2  | 22:A:209:PRO:HB2  | 2.33                     | 0.58              |
| 23:B:223:ILE:CB   | 23:B:347:ILE:HG21 | 2.33                     | 0.58              |
| 24:E:171:LEU:HD11 | 24:E:279:THR:CG2  | 2.31                     | 0.58              |
| 27:U:9:ILE:HA     | 27:U:12:LEU:HD13  | 1.85                     | 0.58              |
| 1:C:139:MET:HE1   | 1:C:241:HIS:ND1   | 2.18                     | 0.58              |
| 1:C:329:LEU:HD23  | 1:C:363:CYS:SG    | 2.43                     | 0.58              |
| 2:D:152:MET:HB3   | 2:D:229:ARG:HH12  | 1.68                     | 0.58              |
| 2:D:348:ILE:HD13  | 2:D:376:ASN:HA    | 1.86                     | 0.58              |
| 4:H:34:PRO:HG2    | 4:H:49:GLU:HG2    | 1.84                     | 0.58              |
| 4:H:67:PRO:O      | 4:H:91:ARG:NH2    | 2.33                     | 0.58              |
| 5:I:76:VAL:HG11   | 5:I:83:ALA:HB1    | 1.85                     | 0.58              |
| 5:I:118:LYS:HZ3   | 5:I:118:LYS:HB2   | 1.68                     | 0.58              |
| 7:L:83:LEU:HD11   | 26:K:125:GLU:HB3  | 1.85                     | 0.58              |
| 7:L:155:ASP:HB2   | 8:M:62:SER:CB     | 2.32                     | 0.58              |
| 12:Y:320:ALA:HB1  | 12:Y:325:VAL:O    | 2.02                     | 0.58              |
| 12:Y:381:GLN:O    | 12:Y:385:ARG:HG2  | 2.03                     | 0.58              |
| 13:Z:195:VAL:HG23 | 14:a:367:VAL:HG12 | 1.85                     | 0.58              |
| 14:a:83:VAL:HG12  | 14:a:87:MET:HG2   | 1.83                     | 0.58              |
| 14:a:210:VAL:O    | 14:a:271:LYS:NZ   | 2.36                     | 0.58              |
| 18:f:422:VAL:O    | 18:f:426:LEU:HB2  | 2.03                     | 0.58              |
| 18:f:437:GLU:HG2  | 18:f:439:TYR:HB3  | 1.84                     | 0.58              |
| 18:f:542:ILE:CD1  | 18:f:562:LEU:HD12 | 2.34                     | 0.58              |
| 18:f:543:MET:HA   | 18:f:543:MET:CE   | 2.24                     | 0.58              |
| 18:f:669:GLU:OE1  | 23:B:50:PRO:HG3   | 2.03                     | 0.58              |
| 18:f:785:ARG:HH21 | 18:f:877:GLY:H    | 1.50                     | 0.58              |
| 19:g:107:ILE:HD11 | 19:g:115:LYS:HD3  | 1.84                     | 0.58              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:A:120:LYS:HB2  | 25:F:90:VAL:HG11  | 1.83                     | 0.58              |
| 22:A:322:ASN:OD1  | 22:A:322:ASN:N    | 2.37                     | 0.58              |
| 23:B:366:GLN:HA   | 23:B:369:THR:HG22 | 1.85                     | 0.58              |
| 24:E:361:PHE:CE1  | 24:E:366:ASP:CB   | 2.86                     | 0.58              |
| 1:C:215:SER:O     | 1:C:218:GLU:HG3   | 2.03                     | 0.58              |
| 4:H:120:GLU:O     | 4:H:123:GLN:HG2   | 2.04                     | 0.58              |
| 5:I:4:ARG:NH2     | 5:I:23:TYR:OH     | 2.36                     | 0.58              |
| 6:J:108:THR:CG2   | 6:J:153:TYR:HB2   | 2.33                     | 0.58              |
| 7:L:164:ARG:HD2   | 7:L:198:THR:O     | 2.03                     | 0.58              |
| 9:V:67:LEU:O      | 9:V:70:VAL:HG12   | 2.03                     | 0.58              |
| 9:V:118:GLN:HA    | 9:V:122:THR:CG2   | 2.33                     | 0.58              |
| 9:V:176:MET:HE3   | 9:V:217:VAL:CG1   | 2.33                     | 0.58              |
| 12:Y:225:TYR:OH   | 12:Y:281:GLU:OE2  | 2.21                     | 0.58              |
| 12:Y:313:SER:HA   | 12:Y:354:VAL:O    | 2.03                     | 0.58              |
| 14:a:8:LEU:HA     | 14:a:22:TRP:CZ3   | 2.38                     | 0.58              |
| 14:a:197:ALA:HB3  | 14:a:226:ARG:HD2  | 1.84                     | 0.58              |
| 15:b:71:ILE:HD12  | 15:b:71:ILE:N     | 2.19                     | 0.58              |
| 17:d:168:MET:HE2  | 17:d:195:ASN:ND2  | 2.18                     | 0.58              |
| 18:f:231:LEU:CD2  | 18:f:853:VAL:HA   | 2.33                     | 0.58              |
| 18:f:388:ASP:O    | 18:f:392:THR:OG1  | 2.21                     | 0.58              |
| 22:A:393:GLY:C    | 23:B:216:ILE:HD11 | 2.28                     | 0.58              |
| 23:B:395:ILE:HA   | 23:B:398:ILE:CG2  | 2.33                     | 0.58              |
| 25:F:277:GLU:HB3  | 25:F:278:LYS:HZ2  | 1.68                     | 0.58              |
| 27:U:137:MET:HE2  | 27:U:137:MET:CA   | 2.33                     | 0.58              |
| 27:U:241:ASN:ND2  | 27:U:244:MET:HB2  | 2.17                     | 0.58              |
| 27:U:243:LEU:HD23 | 27:U:913:ILE:CD1  | 2.28                     | 0.58              |
| 27:U:352:ILE:HA   | 27:U:355:ASN:HD21 | 1.69                     | 0.58              |
| 27:U:354:LYS:HA   | 27:U:357:LYS:HG2  | 1.85                     | 0.58              |
| 1:C:29:GLU:OE2    | 9:V:200:ARG:HA    | 2.04                     | 0.58              |
| 1:C:84:LYS:HD3    | 1:C:96:VAL:HG12   | 1.85                     | 0.58              |
| 1:C:271:ARG:CZ    | 1:C:271:ARG:HB2   | 2.33                     | 0.58              |
| 3:G:208:ILE:HG22  | 3:G:210:PHE:H     | 1.68                     | 0.58              |
| 7:L:40:SER:HB3    | 7:L:187:LEU:HD22  | 1.84                     | 0.58              |
| 7:L:44:ALA:HB3    | 7:L:215:VAL:HG13  | 1.85                     | 0.58              |
| 9:V:117:VAL:O     | 9:V:122:THR:HG23  | 2.03                     | 0.58              |
| 10:W:276:LEU:CD2  | 10:W:354:LEU:HD13 | 2.34                     | 0.58              |
| 11:X:213:GLN:NE2  | 11:X:217:ILE:HD11 | 2.19                     | 0.58              |
| 13:Z:97:THR:HA    | 13:Z:124:ILE:O    | 2.03                     | 0.58              |
| 14:a:74:LEU:HA    | 14:a:77:VAL:HG12  | 1.85                     | 0.58              |
| 14:a:148:VAL:HG11 | 14:a:151:VAL:HG13 | 1.85                     | 0.58              |
| 14:a:281:THR:HG23 | 14:a:335:TRP:CZ3  | 2.37                     | 0.58              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 15:b:75:LEU:O     | 15:b:78:VAL:HB    | 2.04                     | 0.58              |
| 22:A:333:ARG:HG3  | 22:A:334:PRO:HD2  | 1.86                     | 0.58              |
| 22:A:348:LEU:O    | 22:A:348:LEU:HD23 | 2.03                     | 0.58              |
| 24:E:310:LEU:CD2  | 24:E:328:TYR:HB3  | 2.33                     | 0.58              |
| 26:K:37:ALA:HB3   | 26:K:170:ILE:HG12 | 1.84                     | 0.58              |
| 1:C:257:SER:O     | 2:D:283:ARG:NH2   | 2.36                     | 0.58              |
| 2:D:161:ASP:OD1   | 2:D:161:ASP:O     | 2.21                     | 0.58              |
| 5:I:148:TYR:HD1   | 5:I:158:GLY:HA2   | 1.68                     | 0.58              |
| 7:L:192:LEU:CD2   | 7:L:210:VAL:HG11  | 2.34                     | 0.58              |
| 8:M:196:ILE:CA    | 8:M:199:ILE:HD12  | 2.29                     | 0.58              |
| 9:V:235:LEU:HD11  | 9:V:251:LEU:HD13  | 1.84                     | 0.58              |
| 10:W:251:TYR:HB2  | 10:W:266:ALA:CB   | 2.34                     | 0.58              |
| 14:a:214:GLY:HA2  | 14:a:340:VAL:CG1  | 2.31                     | 0.58              |
| 17:d:85:GLY:O     | 17:d:89:GLN:HG3   | 2.04                     | 0.58              |
| 24:E:33:LEU:CD2   | 25:F:66:LEU:HA    | 2.32                     | 0.58              |
| 24:E:352:MET:HA   | 24:E:355:ILE:HD12 | 1.85                     | 0.58              |
| 25:F:280:PRO:CA   | 25:F:325:GLN:HB3  | 2.34                     | 0.58              |
| 27:U:465:LEU:HD22 | 27:U:496:LEU:CD2  | 2.33                     | 0.58              |
| 2:D:282:ASP:O     | 2:D:286:GLN:HG2   | 2.03                     | 0.58              |
| 4:H:109:GLN:HB3   | 4:H:113:ARG:NH2   | 2.18                     | 0.58              |
| 7:L:155:ASP:O     | 8:M:59:GLU:N      | 2.36                     | 0.58              |
| 9:V:428:LEU:HD12  | 9:V:434:ALA:HB2   | 1.83                     | 0.58              |
| 10:W:133:GLU:HA   | 10:W:142:ARG:NE   | 2.18                     | 0.58              |
| 11:X:267:VAL:HG11 | 11:X:291:ALA:HB1  | 1.85                     | 0.58              |
| 11:X:363:ARG:NH2  | 12:Y:266:CYS:HB3  | 2.18                     | 0.58              |
| 12:Y:111:LEU:O    | 12:Y:114:ILE:HG13 | 2.04                     | 0.58              |
| 12:Y:279:GLU:CB   | 12:Y:296:VAL:HG21 | 2.34                     | 0.58              |
| 13:Z:47:VAL:HG23  | 13:Z:47:VAL:O     | 2.03                     | 0.58              |
| 17:d:218:LYS:C    | 17:d:218:LYS:HD3  | 2.28                     | 0.58              |
| 18:f:726:ILE:CD1  | 18:f:748:LEU:HD13 | 2.32                     | 0.58              |
| 19:g:114:SER:O    | 19:g:118:GLU:HB3  | 2.03                     | 0.58              |
| 23:B:256:ILE:CD1  | 23:B:305:ILE:HG23 | 2.34                     | 0.58              |
| 23:B:415:THR:OG1  | 23:B:416:ASN:N    | 2.37                     | 0.58              |
| 24:E:33:LEU:CD1   | 25:F:65:GLU:HB2   | 2.32                     | 0.58              |
| 25:F:198:LEU:HD21 | 25:F:329:ILE:HD11 | 1.84                     | 0.58              |
| 2:D:341:LYS:HD3   | 2:D:370:ILE:HG13  | 1.86                     | 0.58              |
| 2:D:388:ARG:HH22  | 24:E:147:GLU:CG   | 2.04                     | 0.58              |
| 3:G:51:VAL:CG1    | 3:G:217:VAL:HG22  | 2.31                     | 0.58              |
| 5:I:84:ASN:O      | 5:I:87:THR:HG22   | 2.04                     | 0.58              |
| 7:L:34:ALA:HA     | 7:L:162:GLY:CA    | 2.29                     | 0.58              |
| 7:L:46:LEU:HD23   | 7:L:135:ALA:CB    | 2.33                     | 0.58              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 8:M:77:VAL:CG1    | 8:M:84:ALA:HB1    | 2.33                     | 0.58              |
| 9:V:123:SER:HB2   | 9:V:125:ASN:OD1   | 2.04                     | 0.58              |
| 9:V:337:LEU:HD22  | 9:V:367:VAL:CG2   | 2.32                     | 0.58              |
| 9:V:345:ARG:HD3   | 9:V:345:ARG:C     | 2.29                     | 0.58              |
| 10:W:251:TYR:HB2  | 10:W:266:ALA:HB1  | 1.86                     | 0.58              |
| 11:X:234:GLU:HA   | 11:X:234:GLU:OE2  | 2.02                     | 0.58              |
| 14:a:134:THR:O    | 14:a:138:VAL:HG23 | 2.03                     | 0.58              |
| 15:b:38:HIS:HE1   | 15:b:72:LEU:HD11  | 1.69                     | 0.58              |
| 15:b:113:VAL:HG21 | 15:b:140:ILE:HD12 | 1.84                     | 0.58              |
| 17:d:130:PRO:HG3  | 27:U:3:THR:HG23   | 1.84                     | 0.58              |
| 18:f:62:ARG:NH2   | 18:f:70:LEU:HD23  | 2.18                     | 0.58              |
| 18:f:180:GLN:O    | 18:f:183:PRO:HG2  | 2.03                     | 0.58              |
| 22:A:105:ASP:O    | 22:A:106:SER:HB2  | 2.03                     | 0.58              |
| 22:A:240:VAL:HG21 | 22:A:274:PHE:CD1  | 2.39                     | 0.58              |
| 22:A:393:GLY:O    | 22:A:396:ALA:N    | 2.37                     | 0.58              |
| 23:B:49:LEU:HD13  | 23:B:68:ILE:HG21  | 1.85                     | 0.58              |
| 23:B:187:ILE:CG2  | 23:B:234:LEU:HG   | 2.33                     | 0.58              |
| 25:F:278:LYS:HD3  | 25:F:278:LYS:N    | 2.17                     | 0.58              |
| 27:U:88:PHE:CG    | 27:U:89:ASN:N     | 2.71                     | 0.58              |
| 28:e:21:GLU:CD    | 28:e:21:GLU:H     | 2.12                     | 0.58              |
| 1:C:89:VAL:HG12   | 1:C:91:PRO:HD2    | 1.84                     | 0.58              |
| 1:C:308:PRO:HB3   | 23:B:397:ALA:CB   | 2.33                     | 0.58              |
| 2:D:113:VAL:HB    | 2:D:138:ALA:HA    | 1.85                     | 0.58              |
| 3:G:29:PHE:CE2    | 3:G:156:PRO:HD2   | 2.38                     | 0.58              |
| 9:V:131:LEU:HB2   | 9:V:171:VAL:HG11  | 1.84                     | 0.58              |
| 9:V:408:ARG:HG2   | 9:V:408:ARG:NH1   | 2.18                     | 0.58              |
| 9:V:470:ARG:O     | 9:V:470:ARG:HG2   | 2.04                     | 0.58              |
| 10:W:72:LYS:O     | 10:W:76:GLU:HG2   | 2.03                     | 0.58              |
| 12:Y:55:GLU:OE1   | 12:Y:65:ILE:HD13  | 2.03                     | 0.58              |
| 14:a:154:ARG:O    | 14:a:158:LEU:HB3  | 2.03                     | 0.58              |
| 16:c:181:LEU:CD2  | 27:U:725:MET:HE2  | 2.33                     | 0.58              |
| 18:f:678:LEU:O    | 18:f:682:GLY:HA3  | 2.03                     | 0.58              |
| 18:f:880:ALA:O    | 18:f:894:LEU:HD22 | 2.04                     | 0.58              |
| 19:g:128:LYS:CB   | 19:g:158:LEU:HD22 | 2.34                     | 0.58              |
| 20:u:189:GLN:O    | 20:u:259:ARG:N    | 2.37                     | 0.58              |
| 23:B:86:LYS:HD2   | 23:B:87:PRO:CD    | 2.20                     | 0.58              |
| 24:E:145:LEU:CD1  | 24:E:172:LEU:HD11 | 2.33                     | 0.58              |
| 24:E:200:SER:HB3  | 24:E:238:ILE:HD13 | 1.86                     | 0.58              |
| 26:K:220:VAL:HB   | 26:K:228:MET:HE2  | 1.86                     | 0.58              |
| 27:U:419:ALA:CA   | 27:U:422:LEU:HB3  | 2.33                     | 0.58              |
| 27:U:599:ILE:CD1  | 27:U:626:LEU:HD11 | 2.33                     | 0.58              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:D:204:MET:HE2   | 2:D:308:ILE:CG2   | 2.34                     | 0.58              |
| 2:D:254:ALA:HB2   | 2:D:262:ILE:HD11  | 1.83                     | 0.58              |
| 2:D:397:LYS:HG3   | 2:D:398:ASP:OD1   | 2.03                     | 0.58              |
| 3:G:172:GLN:HA    | 3:G:175:SER:OG    | 2.03                     | 0.58              |
| 4:H:132:VAL:HG23  | 4:H:132:VAL:O     | 2.03                     | 0.58              |
| 7:L:146:GLN:OE1   | 7:L:159:MET:HG2   | 2.03                     | 0.58              |
| 8:M:52:LEU:HD11   | 8:M:206:ASP:HB3   | 1.85                     | 0.58              |
| 9:V:161:PRO:HA    | 9:V:164:GLU:OE2   | 2.04                     | 0.58              |
| 10:W:108:CYS:CB   | 10:W:128:LEU:HD21 | 2.34                     | 0.58              |
| 10:W:278:PRO:HG3  | 10:W:357:ARG:NH2  | 2.16                     | 0.58              |
| 10:W:414:ASN:C    | 10:W:414:ASN:OD1  | 2.47                     | 0.58              |
| 12:Y:56:ALA:HA    | 12:Y:59:LYS:CE    | 2.34                     | 0.58              |
| 14:a:110:ALA:HA   | 14:a:113:LEU:CD1  | 2.33                     | 0.58              |
| 15:b:73:SER:HA    | 25:F:61:ARG:HD2   | 1.83                     | 0.58              |
| 18:f:62:ARG:NH1   | 18:f:74:ALA:HB2   | 2.17                     | 0.58              |
| 18:f:143:ARG:NH1  | 18:f:148:GLN:O    | 2.37                     | 0.58              |
| 18:f:339:ILE:O    | 18:f:773:LYS:NZ   | 2.37                     | 0.58              |
| 18:f:371:ASN:O    | 18:f:375:SER:N    | 2.34                     | 0.58              |
| 18:f:654:VAL:HG22 | 18:f:678:LEU:CD2  | 2.33                     | 0.58              |
| 19:g:108:THR:HG22 | 19:g:109:GLY:N    | 2.19                     | 0.58              |
| 22:A:119:ALA:HB3  | 22:A:121:PHE:CE1  | 2.39                     | 0.58              |
| 23:B:69:LYS:HE2   | 27:U:833:LEU:HD22 | 1.85                     | 0.58              |
| 23:B:397:ALA:O    | 23:B:426:VAL:HG21 | 2.04                     | 0.58              |
| 24:E:259:GLU:OE1  | 24:E:259:GLU:HA   | 2.04                     | 0.58              |
| 27:U:136:LYS:O    | 27:U:140:ARG:N    | 2.36                     | 0.58              |
| 27:U:606:ALA:HB2  | 27:U:618:ALA:CB   | 2.34                     | 0.58              |
| 27:U:789:ILE:N    | 27:U:789:ILE:HD12 | 2.18                     | 0.58              |
| 27:U:804:SER:HA   | 27:U:892:LEU:HA   | 1.86                     | 0.58              |
| 4:H:176:LYS:NZ    | 11:X:200:ILE:O    | 2.37                     | 0.58              |
| 7:L:126:ARG:HH11  | 7:L:126:ARG:HG3   | 1.69                     | 0.58              |
| 8:M:111:LEU:HD12  | 8:M:111:LEU:O     | 2.03                     | 0.58              |
| 9:V:114:TYR:CG    | 9:V:138:PRO:HD2   | 2.38                     | 0.58              |
| 9:V:127:THR:O     | 9:V:131:LEU:HD23  | 2.04                     | 0.58              |
| 9:V:289:LEU:HB3   | 9:V:312:ALA:HB2   | 1.85                     | 0.58              |
| 9:V:495:ARG:HA    | 9:V:495:ARG:HE    | 1.69                     | 0.58              |
| 10:W:214:PHE:HB3  | 10:W:223:LYS:CB   | 2.33                     | 0.58              |
| 10:W:369:TYR:HD2  | 14:a:312:MET:SD   | 2.27                     | 0.58              |
| 11:X:118:LYS:CD   | 11:X:126:ARG:HG3  | 2.34                     | 0.58              |
| 13:Z:6:VAL:HG12   | 13:Z:43:TRP:CH2   | 2.39                     | 0.58              |
| 13:Z:22:HIS:CE1   | 13:Z:35:VAL:HB    | 2.39                     | 0.58              |
| 14:a:309:LEU:HD12 | 14:a:312:MET:HB3  | 1.85                     | 0.58              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 15:b:29:GLN:HB2   | 15:b:112:PHE:CD2  | 2.38                     | 0.58              |
| 17:d:119:LEU:HD13 | 17:d:147:ILE:CG1  | 2.33                     | 0.58              |
| 17:d:258:PHE:CE2  | 17:d:262:ILE:HD11 | 2.38                     | 0.58              |
| 18:f:409:SER:OG   | 18:f:815:HIS:HB2  | 2.04                     | 0.58              |
| 18:f:683:GLU:H    | 18:f:686:LEU:HD12 | 1.68                     | 0.58              |
| 22:A:415:LYS:HA   | 22:A:419:SER:HB2  | 1.86                     | 0.58              |
| 24:E:65:THR:HG22  | 24:E:68:LYS:HB2   | 1.85                     | 0.58              |
| 25:F:230:GLY:HA3  | 25:F:392:ASN:HB2  | 1.85                     | 0.58              |
| 25:F:286:ASP:HA   | 25:F:331:ALA:HB3  | 1.84                     | 0.58              |
| 26:K:88:LEU:HD13  | 26:K:116:VAL:HG12 | 1.86                     | 0.58              |
| 26:K:203:LYS:HG3  | 26:K:210:LEU:HB3  | 1.86                     | 0.58              |
| 27:U:245:ALA:HB1  | 27:U:325:MET:HE3  | 1.84                     | 0.58              |
| 27:U:443:LEU:CD2  | 27:U:477:GLY:HA2  | 2.30                     | 0.58              |
| 27:U:699:THR:HG21 | 27:U:812:ALA:H    | 1.69                     | 0.58              |
| 27:U:803:LYS:HB2  | 27:U:875:PHE:HD1  | 1.68                     | 0.58              |
| 27:U:811:PHE:HD1  | 27:U:885:MET:HE1  | 1.69                     | 0.58              |
| 1:C:25:LEU:O      | 1:C:28:ILE:HG12   | 2.03                     | 0.57              |
| 1:C:114:VAL:HG21  | 1:C:123:LEU:CD1   | 2.33                     | 0.57              |
| 5:I:121:TYR:CE1   | 5:I:127:LYS:HD2   | 2.39                     | 0.57              |
| 6:J:45:VAL:HG11   | 6:J:61:LYS:HD2    | 1.85                     | 0.57              |
| 9:V:237:THR:HG22  | 9:V:241:ARG:HH22  | 1.68                     | 0.57              |
| 9:V:260:HIS:O     | 9:V:260:HIS:ND1   | 2.35                     | 0.57              |
| 10:W:63:THR:O     | 10:W:67:LEU:HB2   | 2.04                     | 0.57              |
| 10:W:166:LEU:HD23 | 10:W:192:LEU:CD1  | 2.34                     | 0.57              |
| 10:W:289:ARG:HB3  | 10:W:289:ARG:NH1  | 2.18                     | 0.57              |
| 11:X:212:MET:HE1  | 11:X:250:SER:CA   | 2.28                     | 0.57              |
| 14:a:179:PHE:CD2  | 14:a:180:LEU:HD23 | 2.39                     | 0.57              |
| 15:b:11:ASP:OD2   | 15:b:84:ILE:HD12  | 2.04                     | 0.57              |
| 15:b:35:ILE:O     | 15:b:39:SER:HB3   | 2.04                     | 0.57              |
| 17:d:301:ASP:HA   | 17:d:304:LYS:HZ2  | 1.69                     | 0.57              |
| 18:f:67:ASP:HB3   | 18:f:70:LEU:HD12  | 1.85                     | 0.57              |
| 18:f:107:LYS:HE3  | 18:f:142:TYR:CZ   | 2.39                     | 0.57              |
| 18:f:298:LEU:HD22 | 18:f:303:VAL:HB   | 1.86                     | 0.57              |
| 18:f:512:MET:HE2  | 18:f:512:MET:HA   | 1.85                     | 0.57              |
| 18:f:585:GLU:HB3  | 18:f:586:PRO:HA   | 1.85                     | 0.57              |
| 19:g:106:HIS:CE1  | 19:g:107:ILE:HG23 | 2.39                     | 0.57              |
| 19:g:131:ILE:CG1  | 19:g:147:VAL:HG13 | 2.26                     | 0.57              |
| 22:A:96:ALA:HB1   | 22:A:114:ASN:O    | 2.04                     | 0.57              |
| 22:A:333:ARG:HH12 | 22:A:335:GLY:HA3  | 1.69                     | 0.57              |
| 23:B:264:PRO:O    | 23:B:267:VAL:HG22 | 2.04                     | 0.57              |
| 23:B:356:PRO:HB2  | 23:B:361:LYS:HG2  | 1.86                     | 0.57              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 25:F:89:LEU:O     | 25:F:153:VAL:HG22 | 2.04                     | 0.57              |
| 25:F:91:SER:O     | 25:F:150:LEU:HD13 | 2.04                     | 0.57              |
| 25:F:224:LEU:CD2  | 25:F:343:LEU:HD21 | 2.32                     | 0.57              |
| 27:U:198:LEU:O    | 27:U:202:VAL:HG12 | 2.04                     | 0.57              |
| 27:U:419:ALA:HB2  | 27:U:449:ILE:HG21 | 1.87                     | 0.57              |
| 1:C:76:VAL:HG22   | 1:C:87:VAL:HG12   | 1.86                     | 0.57              |
| 1:C:194:THR:CG2   | 1:C:317:PHE:HB3   | 2.33                     | 0.57              |
| 6:J:133:ILE:CD1   | 6:J:147:THR:HG23  | 2.31                     | 0.57              |
| 7:L:84:LEU:HD22   | 7:L:112:ILE:HD11  | 1.86                     | 0.57              |
| 7:L:168:ALA:HB2   | 7:L:198:THR:CG2   | 2.33                     | 0.57              |
| 8:M:46:VAL:HG12   | 8:M:193:VAL:HG21  | 1.85                     | 0.57              |
| 8:M:78:ALA:HB3    | 8:M:165:ILE:CG2   | 2.35                     | 0.57              |
| 10:W:315:MET:CE   | 10:W:358:VAL:HG22 | 2.29                     | 0.57              |
| 12:Y:14:ASN:ND2   | 12:Y:113:ARG:HD3  | 2.18                     | 0.57              |
| 12:Y:42:MET:HE1   | 12:Y:54:TYR:CZ    | 2.39                     | 0.57              |
| 12:Y:104:MET:HE1  | 12:Y:130:LYS:CE   | 2.34                     | 0.57              |
| 14:a:248:PHE:O    | 14:a:252:LYS:N    | 2.34                     | 0.57              |
| 15:b:16:MET:O     | 15:b:25:ARG:HB2   | 2.04                     | 0.57              |
| 16:c:38:LEU:HD11  | 16:c:155:VAL:HG11 | 1.85                     | 0.57              |
| 17:d:153:GLN:HA   | 17:d:156:ILE:CG1  | 2.33                     | 0.57              |
| 17:d:172:LYS:HE3  | 17:d:195:ASN:ND2  | 2.19                     | 0.57              |
| 17:d:302:TYR:HD1  | 17:d:306:ARG:CG   | 2.16                     | 0.57              |
| 18:f:208:LEU:HD11 | 18:f:217:LEU:HD13 | 1.84                     | 0.57              |
| 18:f:459:CYS:SG   | 19:g:154:MET:HB2  | 2.44                     | 0.57              |
| 18:f:502:LEU:HD22 | 18:f:537:THR:HG21 | 1.87                     | 0.57              |
| 27:U:251:ASP:HA   | 27:U:254:GLU:OE2  | 2.04                     | 0.57              |
| 27:U:351:MET:HE3  | 27:U:351:MET:CA   | 2.34                     | 0.57              |
| 1:C:91:PRO:HG3    | 2:D:109:SER:OG    | 2.03                     | 0.57              |
| 1:C:146:SER:O     | 1:C:202:ALA:HA    | 2.03                     | 0.57              |
| 2:D:104:GLY:HA2   | 2:D:110:ASN:HA    | 1.85                     | 0.57              |
| 3:G:161:CYS:HB3   | 3:G:163:PHE:CE1   | 2.40                     | 0.57              |
| 7:L:56:LEU:CD1    | 26:K:167:ALA:HB3  | 2.34                     | 0.57              |
| 8:M:75:MET:HE1    | 8:M:88:ALA:CA     | 2.34                     | 0.57              |
| 8:M:83:ASP:OD1    | 8:M:129:ARG:NH2   | 2.23                     | 0.57              |
| 8:M:136:MET:CE    | 8:M:150:MET:HB2   | 2.26                     | 0.57              |
| 9:V:467:TYR:HH    | 11:X:397:TYR:HE2  | 1.50                     | 0.57              |
| 10:W:436:MET:HG2  | 16:c:225:TRP:CH2  | 2.38                     | 0.57              |
| 11:X:414:LEU:HD21 | 13:Z:273:HIS:HB2  | 1.86                     | 0.57              |
| 13:Z:36:VAL:HG13  | 13:Z:94:TRP:HE3   | 1.70                     | 0.57              |
| 14:a:321:LYS:HG3  | 14:a:336:VAL:HG22 | 1.85                     | 0.57              |
| 17:d:256:TYR:O    | 17:d:260:ILE:HG12 | 2.04                     | 0.57              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 17:d:301:ASP:HA   | 17:d:304:LYS:NZ   | 2.19                     | 0.57              |
| 18:f:173:LEU:HD22 | 18:f:180:GLN:HB2  | 1.85                     | 0.57              |
| 18:f:700:SER:O    | 18:f:700:SER:OG   | 2.18                     | 0.57              |
| 19:g:161:SER:HB3  | 19:g:164:ASP:N    | 2.14                     | 0.57              |
| 22:A:52:ILE:CD1   | 23:B:72:LEU:HD12  | 2.34                     | 0.57              |
| 22:A:352:THR:HG22 | 22:A:374:ALA:HB2  | 1.86                     | 0.57              |
| 22:A:431:THR:HG23 | 22:A:432:TYR:HD1  | 1.67                     | 0.57              |
| 23:B:383:LEU:O    | 23:B:423:LYS:NZ   | 2.36                     | 0.57              |
| 25:F:332:THR:HG22 | 25:F:334:ARG:H    | 1.68                     | 0.57              |
| 26:K:74:ILE:HD12  | 26:K:109:VAL:HB   | 1.87                     | 0.57              |
| 27:U:748:LEU:HB3  | 27:U:760:VAL:HG23 | 1.86                     | 0.57              |
| 1:C:161:ILE:O     | 1:C:161:ILE:HG13  | 2.04                     | 0.57              |
| 1:C:258:ARG:HB3   | 1:C:270:GLN:OE1   | 2.05                     | 0.57              |
| 2:D:64:GLU:O      | 2:D:68:LEU:HD13   | 2.05                     | 0.57              |
| 2:D:230:VAL:O     | 2:D:264:ILE:HA    | 2.04                     | 0.57              |
| 4:H:212:ILE:HG13  | 4:H:212:ILE:O     | 2.03                     | 0.57              |
| 5:I:161:ALA:HB1   | 5:I:175:LEU:CD2   | 2.19                     | 0.57              |
| 6:J:212:ARG:HD2   | 6:J:215:GLN:OE1   | 2.04                     | 0.57              |
| 7:L:96:ARG:O      | 7:L:100:ASP:HA    | 2.04                     | 0.57              |
| 9:V:113:LEU:CD1   | 9:V:171:VAL:HA    | 2.34                     | 0.57              |
| 9:V:150:ARG:NH1   | 9:V:157:THR:O     | 2.36                     | 0.57              |
| 9:V:181:TYR:O     | 9:V:185:GLN:HB2   | 2.04                     | 0.57              |
| 9:V:237:THR:O     | 9:V:241:ARG:NH1   | 2.37                     | 0.57              |
| 9:V:314:ARG:HG2   | 9:V:314:ARG:HH11  | 1.69                     | 0.57              |
| 10:W:203:GLN:CG   | 10:W:233:LEU:HD21 | 2.24                     | 0.57              |
| 10:W:244:CYS:HB2  | 10:W:273:TYR:CB   | 2.33                     | 0.57              |
| 10:W:370:TYR:CD2  | 10:W:373:ILE:HB   | 2.40                     | 0.57              |
| 11:X:89:VAL:HA    | 11:X:92:LEU:HB2   | 1.85                     | 0.57              |
| 11:X:126:ARG:HH21 | 11:X:127:GLN:HE21 | 1.53                     | 0.57              |
| 12:Y:26:LEU:HD13  | 12:Y:63:TRP:HZ2   | 1.70                     | 0.57              |
| 13:Z:67:VAL:HG13  | 15:b:91:ARG:HB2   | 1.86                     | 0.57              |
| 13:Z:145:HIS:HE1  | 13:Z:151:THR:HA   | 1.65                     | 0.57              |
| 14:a:36:GLN:H     | 14:a:36:GLN:CD    | 2.09                     | 0.57              |
| 14:a:160:SER:C    | 14:a:163:TYR:HB3  | 2.28                     | 0.57              |
| 15:b:130:ARG:HD2  | 15:b:134:GLU:OE2  | 2.03                     | 0.57              |
| 17:d:98:LEU:HB2   | 17:d:115:GLU:HG2  | 1.87                     | 0.57              |
| 17:d:275:ILE:HA   | 17:d:279:TYR:CE2  | 2.40                     | 0.57              |
| 18:f:233:LEU:O    | 18:f:237:VAL:HG22 | 2.04                     | 0.57              |
| 18:f:423:ASP:O    | 18:f:427:THR:HG23 | 2.05                     | 0.57              |
| 18:f:796:LEU:H    | 18:f:796:LEU:HD12 | 1.70                     | 0.57              |
| 19:g:112:LEU:HA   | 19:g:115:LYS:HG2  | 1.86                     | 0.57              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:A:240:VAL:HG21 | 22:A:274:PHE:CE1  | 2.38                     | 0.57              |
| 24:E:152:PRO:HB3  | 24:E:166:PRO:HB2  | 1.86                     | 0.57              |
| 24:E:359:HIS:CE1  | 25:F:214:ASN:HD22 | 2.23                     | 0.57              |
| 25:F:310:MET:HE3  | 25:F:342:LEU:HG   | 1.87                     | 0.57              |
| 27:U:871:PRO:HA   | 27:U:875:PHE:HE2  | 1.70                     | 0.57              |
| 5:I:21:VAL:HG12   | 23:B:438:LEU:HD21 | 1.85                     | 0.57              |
| 5:I:240:HIS:NE2   | 5:I:244:GLU:OE2   | 2.37                     | 0.57              |
| 6:J:6:ALA:HB3     | 6:J:9:VAL:CG2     | 2.34                     | 0.57              |
| 11:X:57:LEU:HA    | 11:X:60:THR:OG1   | 2.05                     | 0.57              |
| 11:X:248:ILE:HD13 | 11:X:279:TYR:HB3  | 1.85                     | 0.57              |
| 11:X:346:GLN:HA   | 11:X:383:GLY:O    | 2.05                     | 0.57              |
| 11:X:407:MET:CA   | 11:X:410:VAL:HG12 | 2.34                     | 0.57              |
| 12:Y:104:MET:HG2  | 12:Y:127:THR:OG1  | 2.04                     | 0.57              |
| 12:Y:121:LEU:HD11 | 12:Y:156:LEU:HD21 | 1.86                     | 0.57              |
| 13:Z:10:VAL:HA    | 13:Z:161:GLU:O    | 2.05                     | 0.57              |
| 13:Z:195:VAL:CG2  | 14:a:367:VAL:HG12 | 2.34                     | 0.57              |
| 14:a:82:HIS:O     | 14:a:86:GLN:HB2   | 2.05                     | 0.57              |
| 14:a:93:ALA:CB    | 14:a:121:LEU:HD22 | 2.34                     | 0.57              |
| 16:c:118:PHE:HB3  | 16:c:121:TRP:HZ2  | 1.69                     | 0.57              |
| 17:d:104:ARG:NE   | 17:d:106:SER:O    | 2.37                     | 0.57              |
| 17:d:129:LEU:CD1  | 27:U:26:LYS:HG2   | 2.35                     | 0.57              |
| 22:A:52:ILE:HD11  | 23:B:69:LYS:CA    | 2.34                     | 0.57              |
| 22:A:334:PRO:HB2  | 25:F:398:ALA:HB2  | 1.86                     | 0.57              |
| 22:A:388:VAL:HG23 | 22:A:416:VAL:HG11 | 1.84                     | 0.57              |
| 26:K:99:HIS:CD2   | 26:K:107:MET:HG3  | 2.40                     | 0.57              |
| 2:D:150:SER:HB3   | 2:D:253:LEU:CD2   | 2.35                     | 0.57              |
| 2:D:154:LEU:HD12  | 2:D:227:PHE:CB    | 2.21                     | 0.57              |
| 2:D:301:GLN:OE1   | 2:D:301:GLN:HA    | 2.03                     | 0.57              |
| 3:G:32:ILE:HD11   | 3:G:156:PRO:HG3   | 1.86                     | 0.57              |
| 3:G:77:GLY:HA3    | 3:G:227:PHE:CE1   | 2.39                     | 0.57              |
| 6:J:36:ARG:HB3    | 6:J:144:LEU:HD23  | 1.87                     | 0.57              |
| 9:V:79:VAL:HA     | 9:V:82:LEU:HB2    | 1.86                     | 0.57              |
| 10:W:103:LYS:HA   | 10:W:106:GLN:OE1  | 2.04                     | 0.57              |
| 10:W:191:ARG:HG2  | 10:W:191:ARG:HH11 | 1.69                     | 0.57              |
| 11:X:418:ALA:HB2  | 13:Z:276:ILE:HD13 | 1.85                     | 0.57              |
| 13:Z:222:ILE:HD11 | 14:a:343:LEU:CD2  | 2.34                     | 0.57              |
| 14:a:34:TRP:CB    | 14:a:70:ARG:HB2   | 2.35                     | 0.57              |
| 14:a:245:VAL:C    | 14:a:246:GLU:HG3  | 2.30                     | 0.57              |
| 18:f:226:TYR:HA   | 18:f:229:VAL:HG12 | 1.86                     | 0.57              |
| 18:f:417:ILE:O    | 18:f:418:LEU:HD22 | 2.04                     | 0.57              |
| 18:f:501:LEU:HB3  | 18:f:522:CYS:SG   | 2.44                     | 0.57              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 19:g:89:LEU:HD23  | 19:g:155:VAL:HG21 | 1.87                     | 0.57              |
| 24:E:187:VAL:HG13 | 24:E:229:ILE:HD13 | 1.86                     | 0.57              |
| 24:E:235:ILE:HG22 | 24:E:235:ILE:O    | 2.04                     | 0.57              |
| 25:F:211:LYS:HG3  | 25:F:212:PHE:N    | 2.18                     | 0.57              |
| 25:F:251:LEU:O    | 25:F:251:LEU:HG   | 2.04                     | 0.57              |
| 25:F:350:ARG:HB3  | 25:F:350:ARG:CZ   | 2.35                     | 0.57              |
| 27:U:88:PHE:CE2   | 27:U:89:ASN:HB2   | 2.39                     | 0.57              |
| 3:G:111:VAL:HG13  | 3:G:140:LEU:HB3   | 1.87                     | 0.57              |
| 7:L:196:ARG:NH2   | 7:L:239:ARG:HB2   | 2.18                     | 0.57              |
| 8:M:149:TYR:HD1   | 8:M:159:GLY:HA2   | 1.70                     | 0.57              |
| 10:W:40:LEU:HD22  | 10:W:79:GLU:HG3   | 1.87                     | 0.57              |
| 10:W:40:LEU:CD2   | 10:W:82:LEU:HD22  | 2.30                     | 0.57              |
| 10:W:172:GLU:HA   | 10:W:182:ARG:HD3  | 1.86                     | 0.57              |
| 10:W:201:ARG:NH1  | 10:W:201:ARG:HB2  | 2.20                     | 0.57              |
| 13:Z:136:GLU:HG3  | 13:Z:138:TYR:CE1  | 2.39                     | 0.57              |
| 13:Z:175:LEU:HD11 | 16:c:35:SER:HB2   | 1.87                     | 0.57              |
| 13:Z:176:LEU:O    | 13:Z:178:ASP:N    | 2.38                     | 0.57              |
| 14:a:42:LEU:CD1   | 14:a:78:GLU:HB3   | 2.35                     | 0.57              |
| 18:f:240:VAL:HG13 | 18:f:241:PRO:HD2  | 1.86                     | 0.57              |
| 18:f:322:SER:OG   | 18:f:324:VAL:HG13 | 2.05                     | 0.57              |
| 18:f:325:GLN:HG3  | 18:f:329:ASN:HD21 | 1.69                     | 0.57              |
| 22:A:101:ILE:HG23 | 22:A:101:ILE:O    | 2.04                     | 0.57              |
| 24:E:33:LEU:HD21  | 25:F:66:LEU:N     | 2.20                     | 0.57              |
| 24:E:308:ALA:O    | 24:E:311:ASP:N    | 2.37                     | 0.57              |
| 25:F:224:LEU:O    | 25:F:352:ILE:HG22 | 2.04                     | 0.57              |
| 27:U:563:ALA:C    | 27:U:565:ALA:H    | 2.12                     | 0.57              |
| 27:U:713:TYR:CE2  | 27:U:733:ALA:HB1  | 2.39                     | 0.57              |
| 2:D:309:MET:HE3   | 2:D:327:LEU:CD1   | 2.31                     | 0.57              |
| 4:H:179:ASN:HB3   | 4:H:182:LEU:CD2   | 2.33                     | 0.57              |
| 8:M:200:VAL:O     | 8:M:201:HIS:HB3   | 2.04                     | 0.57              |
| 9:V:113:LEU:HD11  | 9:V:174:PHE:CB    | 2.34                     | 0.57              |
| 10:W:119:PRO:O    | 10:W:123:ARG:HG2  | 2.05                     | 0.57              |
| 10:W:363:ILE:HD11 | 10:W:378:MET:HE2  | 1.85                     | 0.57              |
| 10:W:445:LEU:CB   | 13:Z:226:ILE:HG21 | 2.35                     | 0.57              |
| 14:a:114:CYS:CA   | 14:a:117:ALA:HB3  | 2.30                     | 0.57              |
| 14:a:119:GLY:O    | 14:a:123:LEU:CB   | 2.53                     | 0.57              |
| 17:d:197:LEU:HD12 | 17:d:256:TYR:HD1  | 1.70                     | 0.57              |
| 17:d:283:LEU:HD13 | 17:d:315:TYR:CE1  | 2.35                     | 0.57              |
| 17:d:283:LEU:HD12 | 17:d:284:PHE:N    | 2.20                     | 0.57              |
| 18:f:420:TRP:CD1  | 18:f:455:VAL:HG13 | 2.40                     | 0.57              |
| 18:f:589:SER:OG   | 18:f:649:HIS:NE2  | 2.38                     | 0.57              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 18:f:741:LEU:O    | 18:f:741:LEU:HD12 | 2.05                     | 0.57              |
| 19:g:116:ILE:CD1  | 19:g:136:LEU:HD11 | 2.34                     | 0.57              |
| 23:B:236:ALA:O    | 23:B:239:VAL:HG12 | 2.04                     | 0.57              |
| 24:E:320:ILE:HG23 | 25:F:215:LEU:HD12 | 1.86                     | 0.57              |
| 25:F:310:MET:HE3  | 25:F:342:LEU:HD21 | 1.87                     | 0.57              |
| 26:K:185:TYR:HA   | 26:K:189:MET:HE2  | 1.84                     | 0.57              |
| 27:U:88:PHE:HE1   | 27:U:90:VAL:HG23  | 1.69                     | 0.57              |
| 27:U:638:SER:HA   | 27:U:671:LEU:CD1  | 2.33                     | 0.57              |
| 27:U:768:GLN:O    | 27:U:775:LEU:HD12 | 2.05                     | 0.57              |
| 2:D:116:LEU:HB3   | 2:D:119:ILE:CD1   | 2.34                     | 0.57              |
| 2:D:414:HIS:C     | 2:D:415:GLU:HG3   | 2.29                     | 0.57              |
| 6:J:212:ARG:HB2   | 6:J:215:GLN:CG    | 2.35                     | 0.57              |
| 7:L:104:PRO:CG    | 7:L:107:ARG:HE    | 2.17                     | 0.57              |
| 7:L:189:LYS:HE3   | 7:L:235:GLY:C     | 2.30                     | 0.57              |
| 8:M:22:GLN:OE1    | 8:M:22:GLN:HA     | 2.05                     | 0.57              |
| 10:W:26:GLN:HG3   | 10:W:27:ARG:N     | 2.18                     | 0.57              |
| 10:W:178:GLU:OE2  | 10:W:180:LYS:HB3  | 2.04                     | 0.57              |
| 10:W:440:ASN:HD22 | 16:c:226:MET:CE   | 2.18                     | 0.57              |
| 11:X:349:HIS:NE2  | 11:X:353:LEU:HD11 | 2.20                     | 0.57              |
| 11:X:379:ASP:CG   | 11:X:384:VAL:HG22 | 2.29                     | 0.57              |
| 11:X:407:MET:SD   | 11:X:410:VAL:HG11 | 2.45                     | 0.57              |
| 12:Y:124:PHE:HD1  | 12:Y:140:ILE:HD12 | 1.70                     | 0.57              |
| 12:Y:309:GLU:OE2  | 12:Y:358:ARG:HD3  | 2.04                     | 0.57              |
| 13:Z:220:LEU:HG   | 13:Z:221:PRO:CD   | 2.35                     | 0.57              |
| 14:a:135:ILE:HD11 | 14:a:158:LEU:HG   | 1.86                     | 0.57              |
| 14:a:185:ILE:HG22 | 14:a:187:ASP:OD2  | 2.05                     | 0.57              |
| 17:d:85:GLY:CA    | 17:d:88:LEU:HB3   | 2.31                     | 0.57              |
| 22:A:384:GLU:HG2  | 23:B:344:PRO:CG   | 2.28                     | 0.57              |
| 23:B:174:MET:SD   | 23:B:250:VAL:HG12 | 2.45                     | 0.57              |
| 23:B:225:TYR:HA   | 23:B:331:THR:O    | 2.05                     | 0.57              |
| 23:B:278:ALA:CB   | 23:B:279:PRO:HD2  | 2.33                     | 0.57              |
| 23:B:322:ARG:HD2  | 23:B:325:VAL:CG1  | 2.31                     | 0.57              |
| 27:U:236:LEU:HD23 | 27:U:245:ALA:CB   | 2.34                     | 0.57              |
| 27:U:535:TYR:O    | 27:U:539:THR:HG22 | 2.04                     | 0.57              |
| 27:U:627:PHE:CE1  | 27:U:748:LEU:HB2  | 2.40                     | 0.57              |
| 27:U:671:LEU:O    | 27:U:674:PRO:HD2  | 2.05                     | 0.57              |
| 2:D:150:SER:HB3   | 2:D:253:LEU:HD22  | 1.85                     | 0.57              |
| 2:D:353:ASN:OD1   | 2:D:393:ILE:HG12  | 2.05                     | 0.57              |
| 2:D:360:LEU:O     | 2:D:364:VAL:HG13  | 2.04                     | 0.57              |
| 7:L:196:ARG:HB3   | 7:L:205:LEU:CG    | 2.35                     | 0.57              |
| 9:V:86:VAL:CG1    | 9:V:200:ARG:HH12  | 2.17                     | 0.57              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 9:V:324:PHE:HD2   | 28:e:19:PHE:HE2   | 1.52                     | 0.57              |
| 10:W:212:LYS:HE2  | 10:W:212:LYS:HA   | 1.86                     | 0.57              |
| 10:W:265:GLN:OE1  | 10:W:336:PRO:HG2  | 2.05                     | 0.57              |
| 13:Z:208:ILE:HG23 | 13:Z:230:LEU:HD11 | 1.87                     | 0.57              |
| 14:a:86:GLN:O     | 14:a:88:THR:HG23  | 2.04                     | 0.57              |
| 14:a:348:GLY:O    | 14:a:352:ARG:HG3  | 2.05                     | 0.57              |
| 17:d:95:TYR:OH    | 17:d:146:ASP:HB3  | 2.04                     | 0.57              |
| 17:d:137:THR:HG22 | 17:d:140:GLN:H    | 1.68                     | 0.57              |
| 17:d:169:ALA:HB3  | 27:U:10:SER:OG    | 2.05                     | 0.57              |
| 18:f:235:SER:OG   | 18:f:853:VAL:HG21 | 2.04                     | 0.57              |
| 18:f:239:TYR:CZ   | 23:B:64:LYS:HG2   | 2.39                     | 0.57              |
| 18:f:447:ALA:HA   | 18:f:450:ILE:CG2  | 2.33                     | 0.57              |
| 18:f:499:THR:O    | 18:f:503:PRO:HD3  | 2.04                     | 0.57              |
| 18:f:662:MET:HE2  | 18:f:781:TYR:HE1  | 1.69                     | 0.57              |
| 22:A:95:VAL:CG1   | 22:A:139:ARG:HD2  | 2.35                     | 0.57              |
| 22:A:227:ARG:HG2  | 23:B:319:PHE:CE1  | 2.39                     | 0.57              |
| 23:B:174:MET:CE   | 23:B:266:LEU:HD21 | 2.35                     | 0.57              |
| 23:B:223:ILE:HG23 | 23:B:223:ILE:O    | 2.05                     | 0.57              |
| 26:K:37:ALA:O     | 26:K:169:ALA:HA   | 2.04                     | 0.57              |
| 27:U:481:LEU:CD2  | 27:U:493:VAL:HG23 | 2.29                     | 0.57              |
| 27:U:586:VAL:CG1  | 27:U:602:LEU:HD12 | 2.35                     | 0.57              |
| 27:U:593:SER:O    | 27:U:595:ASN:N    | 2.37                     | 0.57              |
| 27:U:789:ILE:HB   | 27:U:911:ILE:HG23 | 1.87                     | 0.57              |
| 1:C:76:VAL:HG11   | 1:C:108:VAL:HG12  | 1.87                     | 0.56              |
| 1:C:237:MET:O     | 1:C:237:MET:HG2   | 2.03                     | 0.56              |
| 1:C:280:LEU:HD21  | 1:C:291:VAL:HG11  | 1.87                     | 0.56              |
| 1:C:355:SER:CB    | 1:C:358:GLU:HG3   | 2.35                     | 0.56              |
| 4:H:179:ASN:O     | 4:H:182:LEU:HG    | 2.05                     | 0.56              |
| 4:H:212:ILE:HG12  | 4:H:221:LEU:HD21  | 1.87                     | 0.56              |
| 5:I:92:LEU:HD23   | 5:I:92:LEU:C      | 2.30                     | 0.56              |
| 7:L:91:GLU:OE2    | 7:L:108:LEU:HD13  | 2.04                     | 0.56              |
| 8:M:161:TRP:HB3   | 8:M:181:MET:CE    | 2.36                     | 0.56              |
| 8:M:229:LYS:O     | 8:M:233:GLU:HG2   | 2.04                     | 0.56              |
| 9:V:110:HIS:CD2   | 9:V:136:GLU:HB2   | 2.40                     | 0.56              |
| 10:W:132:THR:HG22 | 10:W:138:VAL:HG21 | 1.87                     | 0.56              |
| 10:W:317:TRP:CZ3  | 10:W:355:LYS:HA   | 2.40                     | 0.56              |
| 10:W:378:MET:SD   | 10:W:413:ILE:HD12 | 2.45                     | 0.56              |
| 11:X:84:LYS:HA    | 11:X:87:ARG:HH12  | 1.70                     | 0.56              |
| 12:Y:334:LEU:CD2  | 12:Y:343:LEU:HD23 | 2.35                     | 0.56              |
| 14:a:211:PHE:CZ   | 14:a:319:LEU:HD21 | 2.40                     | 0.56              |
| 14:a:315:LEU:HD12 | 14:a:315:LEU:O    | 2.05                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 15:b:52:ILE:HG23  | 15:b:59:GLU:O     | 2.05                     | 0.56              |
| 18:f:122:ALA:O    | 18:f:126:ILE:HG13 | 2.05                     | 0.56              |
| 19:g:112:LEU:HD23 | 19:g:138:LEU:HD21 | 1.87                     | 0.56              |
| 22:A:306:LEU:HD21 | 22:A:317:VAL:HG21 | 1.87                     | 0.56              |
| 22:A:372:LEU:CD1  | 22:A:376:LEU:HD11 | 2.35                     | 0.56              |
| 24:E:267:PHE:O    | 24:E:268:ASP:C    | 2.48                     | 0.56              |
| 27:U:52:GLU:HA    | 27:U:57:ARG:HE    | 1.69                     | 0.56              |
| 2:D:398:ASP:O     | 2:D:402:ALA:N     | 2.29                     | 0.56              |
| 6:J:145:TYR:HE1   | 6:J:155:ALA:HB2   | 1.68                     | 0.56              |
| 9:V:91:PRO:O      | 9:V:94:VAL:HG22   | 2.05                     | 0.56              |
| 9:V:162:GLU:HG3   | 9:V:206:VAL:HG21  | 1.87                     | 0.56              |
| 9:V:300:LEU:O     | 9:V:300:LEU:HD23  | 2.05                     | 0.56              |
| 11:X:378:LEU:O    | 12:Y:311:TYR:HA   | 2.05                     | 0.56              |
| 12:Y:52:PRO:HG2   | 12:Y:114:ILE:HD12 | 1.87                     | 0.56              |
| 13:Z:224:HIS:HB2  | 14:a:218:MET:SD   | 2.45                     | 0.56              |
| 17:d:116:LEU:HD23 | 17:d:147:ILE:HG23 | 1.86                     | 0.56              |
| 18:f:437:GLU:O    | 18:f:440:ILE:HG23 | 2.05                     | 0.56              |
| 18:f:498:LEU:HD22 | 18:f:534:VAL:CG2  | 2.35                     | 0.56              |
| 18:f:677:HIS:CD2  | 23:B:79:ILE:HD11  | 2.40                     | 0.56              |
| 18:f:803:PHE:CE1  | 18:f:810:ILE:HG13 | 2.39                     | 0.56              |
| 23:B:81:ASN:O     | 23:B:85:MET:HB3   | 2.05                     | 0.56              |
| 23:B:387:LYS:HA   | 23:B:387:LYS:CE   | 2.19                     | 0.56              |
| 27:U:137:MET:HA   | 27:U:137:MET:HE2  | 1.86                     | 0.56              |
| 27:U:213:PHE:HA   | 27:U:216:VAL:CG1  | 2.34                     | 0.56              |
| 27:U:247:GLN:NE2  | 27:U:251:ASP:OD1  | 2.38                     | 0.56              |
| 28:e:62:LYS:HA    | 28:e:65:TYR:CE2   | 2.40                     | 0.56              |
| 1:C:55:LYS:HB3    | 1:C:55:LYS:HZ2    | 1.70                     | 0.56              |
| 2:D:378:ILE:HD13  | 2:D:403:TYR:HD1   | 1.69                     | 0.56              |
| 2:D:392:TYR:CZ    | 10:W:200:ILE:HG21 | 2.41                     | 0.56              |
| 3:G:174:GLU:OE1   | 3:G:174:GLU:N     | 2.33                     | 0.56              |
| 3:G:183:VAL:HG11  | 4:H:56:LEU:HD23   | 1.87                     | 0.56              |
| 3:G:208:ILE:HD12  | 24:E:306:GLU:OE2  | 1.95                     | 0.56              |
| 4:H:70:LYS:HG3    | 4:H:70:LYS:O      | 2.03                     | 0.56              |
| 6:J:52:LYS:O      | 6:J:52:LYS:HG2    | 2.05                     | 0.56              |
| 7:L:7:ASP:O       | 7:L:7:ASP:CG      | 2.48                     | 0.56              |
| 7:L:59:HIS:HD2    | 7:L:208:LYS:O     | 1.88                     | 0.56              |
| 7:L:137:TYR:HE1   | 7:L:141:GLY:HA2   | 1.70                     | 0.56              |
| 7:L:189:LYS:HG2   | 7:L:236:LEU:CD1   | 2.35                     | 0.56              |
| 8:M:52:LEU:CD1    | 8:M:206:ASP:HB3   | 2.35                     | 0.56              |
| 9:V:121:PHE:CZ    | 9:V:164:GLU:HA    | 2.40                     | 0.56              |
| 9:V:416:ARG:O     | 12:Y:350:VAL:HG23 | 2.05                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 10:W:72:LYS:HD2   | 10:W:76:GLU:OE2   | 2.04                     | 0.56              |
| 10:W:83:LEU:O     | 10:W:87:ILE:HD12  | 2.05                     | 0.56              |
| 10:W:112:VAL:CG1  | 10:W:121:LYS:HZ1  | 2.18                     | 0.56              |
| 10:W:171:VAL:HG11 | 10:W:185:PHE:CB   | 2.35                     | 0.56              |
| 10:W:377:ARG:NE   | 10:W:381:LEU:HD21 | 2.18                     | 0.56              |
| 11:X:68:GLY:O     | 11:X:72:TYR:N     | 2.33                     | 0.56              |
| 11:X:358:LYS:NZ   | 11:X:358:LYS:HB3  | 2.18                     | 0.56              |
| 11:X:379:ASP:OD1  | 11:X:379:ASP:O    | 2.23                     | 0.56              |
| 12:Y:26:LEU:HD13  | 12:Y:63:TRP:CZ2   | 2.40                     | 0.56              |
| 12:Y:42:MET:HE2   | 12:Y:63:TRP:HZ3   | 1.70                     | 0.56              |
| 12:Y:293:ARG:HG2  | 12:Y:293:ARG:HH11 | 1.70                     | 0.56              |
| 13:Z:242:LEU:HD12 | 13:Z:243:GLN:N    | 2.21                     | 0.56              |
| 14:a:19:PRO:HA    | 14:a:23:HIS:CD2   | 2.40                     | 0.56              |
| 14:a:142:LEU:HD22 | 14:a:151:VAL:CG2  | 2.35                     | 0.56              |
| 14:a:243:GLY:CA   | 14:a:272:ILE:HD11 | 2.35                     | 0.56              |
| 14:a:312:MET:HE2  | 14:a:312:MET:CA   | 2.35                     | 0.56              |
| 15:b:17:ARG:HG2   | 15:b:80:PRO:HG2   | 1.85                     | 0.56              |
| 15:b:37:CYS:SG    | 15:b:72:LEU:HD21  | 2.45                     | 0.56              |
| 15:b:112:PHE:CD1  | 15:b:141:ILE:HD11 | 2.40                     | 0.56              |
| 16:c:114:SER:O    | 16:c:115:HIS:HD2  | 1.88                     | 0.56              |
| 17:d:216:PRO:HG2  | 17:d:219:ASP:CG   | 2.31                     | 0.56              |
| 17:d:280:GLU:HG2  | 17:d:281:LYS:N    | 2.20                     | 0.56              |
| 18:f:214:VAL:HG13 | 18:f:251:CYS:SG   | 2.45                     | 0.56              |
| 18:f:274:ASP:HB3  | 18:f:277:LEU:HD12 | 1.86                     | 0.56              |
| 18:f:325:GLN:HE21 | 18:f:329:ASN:CG   | 2.13                     | 0.56              |
| 18:f:498:LEU:HD21 | 18:f:525:ILE:CG2  | 2.35                     | 0.56              |
| 18:f:564:LEU:CD2  | 18:f:794:ALA:HA   | 2.36                     | 0.56              |
| 18:f:830:LEU:HB3  | 18:f:872:VAL:CB   | 2.35                     | 0.56              |
| 18:f:831:VAL:HA   | 18:f:871:PRO:CA   | 2.35                     | 0.56              |
| 19:g:128:LYS:HB3  | 19:g:158:LEU:HD13 | 1.87                     | 0.56              |
| 19:g:166:ARG:O    | 19:g:170:GLN:HB2  | 2.06                     | 0.56              |
| 22:A:170:PRO:HG2  | 22:A:230:ALA:HB3  | 1.87                     | 0.56              |
| 22:A:195:LEU:HD22 | 22:A:314:ASN:HD21 | 1.69                     | 0.56              |
| 24:E:56:ILE:HD11  | 24:E:102:MET:HA   | 1.85                     | 0.56              |
| 25:F:90:VAL:O     | 25:F:90:VAL:HG13  | 2.05                     | 0.56              |
| 25:F:314:LEU:C    | 25:F:347:ARG:HH12 | 2.13                     | 0.56              |
| 25:F:391:PHE:CD1  | 25:F:395:GLN:HB3  | 2.40                     | 0.56              |
| 26:K:173:ALA:HB1  | 26:K:205:VAL:HG21 | 1.87                     | 0.56              |
| 27:U:164:GLU:OE2  | 27:U:203:LYS:HD3  | 2.05                     | 0.56              |
| 27:U:357:LYS:HE2  | 27:U:385:PHE:CE2  | 2.40                     | 0.56              |
| 27:U:516:LEU:HD23 | 27:U:532:MET:CG   | 2.36                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 27:U:557:TYR:HA   | 27:U:588:MET:O    | 2.05                     | 0.56              |
| 27:U:636:VAL:HG13 | 27:U:637:VAL:HG23 | 1.87                     | 0.56              |
| 27:U:872:GLU:HB2  | 27:U:873:PRO:HD2  | 1.87                     | 0.56              |
| 3:G:101:TRP:HB3   | 3:G:109:ILE:HB    | 1.87                     | 0.56              |
| 7:L:31:GLN:OE1    | 7:L:31:GLN:HA     | 2.04                     | 0.56              |
| 7:L:146:GLN:O     | 7:L:153:TYR:HA    | 2.05                     | 0.56              |
| 9:V:479:ARG:NH1   | 12:Y:370:ILE:HD13 | 2.14                     | 0.56              |
| 10:W:55:ARG:NH1   | 10:W:93:ARG:HD3   | 2.21                     | 0.56              |
| 10:W:112:VAL:O    | 10:W:121:LYS:NZ   | 2.36                     | 0.56              |
| 10:W:363:ILE:CD1  | 10:W:378:MET:HE2  | 2.36                     | 0.56              |
| 11:X:339:ILE:HD11 | 11:X:350:ILE:HD11 | 1.87                     | 0.56              |
| 12:Y:173:ASP:N    | 12:Y:173:ASP:OD1  | 2.39                     | 0.56              |
| 15:b:51:LEU:C     | 15:b:52:ILE:HD13  | 2.30                     | 0.56              |
| 17:d:298:LYS:O    | 17:d:301:ASP:HB2  | 2.05                     | 0.56              |
| 18:f:93:PRO:CB    | 18:f:96:LEU:HD12  | 2.34                     | 0.56              |
| 18:f:141:LYS:HA   | 18:f:144:LEU:HB3  | 1.87                     | 0.56              |
| 18:f:301:HIS:CD2  | 18:f:787:LEU:HD21 | 2.39                     | 0.56              |
| 18:f:801:VAL:HA   | 18:f:804:LEU:CD1  | 2.35                     | 0.56              |
| 18:f:855:GLN:OE1  | 18:f:859:PRO:HB3  | 2.05                     | 0.56              |
| 19:g:122:LEU:CB   | 19:g:127:ILE:HD13 | 2.35                     | 0.56              |
| 22:A:53:GLN:OE1   | 22:A:53:GLN:HA    | 2.06                     | 0.56              |
| 22:A:121:PHE:CE2  | 22:A:147:TYR:HE2  | 2.23                     | 0.56              |
| 23:B:222:VAL:HG23 | 23:B:224:LEU:CD1  | 2.35                     | 0.56              |
| 25:F:368:ILE:HD12 | 25:F:368:ILE:H    | 1.69                     | 0.56              |
| 27:U:159:ARG:HB3  | 27:U:162:VAL:HG12 | 1.86                     | 0.56              |
| 1:C:36:ASN:ND2    | 9:V:89:LYS:HB3    | 2.20                     | 0.56              |
| 1:C:277:LEU:HD23  | 1:C:310:ARG:CD    | 2.35                     | 0.56              |
| 1:C:306:LEU:CB    | 23:B:429:LYS:HG3  | 2.36                     | 0.56              |
| 2:D:274:ARG:HG3   | 2:D:318:ASP:OD2   | 2.04                     | 0.56              |
| 4:H:19:LEU:HD11   | 5:I:79:ILE:HD11   | 1.87                     | 0.56              |
| 4:H:116:SER:O     | 4:H:120:GLU:HG3   | 2.05                     | 0.56              |
| 7:L:231:PRO:O     | 7:L:234:GLU:HG3   | 2.05                     | 0.56              |
| 9:V:63:SER:O      | 9:V:67:LEU:N      | 2.29                     | 0.56              |
| 9:V:224:LEU:HG    | 9:V:257:ASN:OD1   | 2.05                     | 0.56              |
| 10:W:132:THR:HA   | 10:W:138:VAL:HG11 | 1.87                     | 0.56              |
| 10:W:146:THR:O    | 10:W:149:LEU:HB3  | 2.05                     | 0.56              |
| 13:Z:121:LEU:C    | 13:Z:121:LEU:HD12 | 2.30                     | 0.56              |
| 14:a:83:VAL:C     | 14:a:87:MET:HG2   | 2.31                     | 0.56              |
| 14:a:111:VAL:HG22 | 14:a:115:LYS:CG   | 2.36                     | 0.56              |
| 14:a:118:ILE:HD11 | 14:a:122:LYS:HD2  | 1.87                     | 0.56              |
| 14:a:205:LEU:HB3  | 14:a:268:LEU:HD11 | 1.87                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 14:a:287:ASN:OD1  | 14:a:288:HIS:N    | 2.38                     | 0.56              |
| 14:a:321:LYS:HD2  | 14:a:336:VAL:CG1  | 2.35                     | 0.56              |
| 15:b:20:ASP:OD1   | 15:b:21:PHE:N     | 2.38                     | 0.56              |
| 17:d:216:PRO:HG2  | 17:d:219:ASP:OD2  | 2.05                     | 0.56              |
| 18:f:399:LEU:HD11 | 18:f:432:TYR:CD2  | 2.41                     | 0.56              |
| 23:B:112:LEU:HD22 | 23:B:144:LEU:HG   | 1.86                     | 0.56              |
| 23:B:246:THR:HG23 | 23:B:280:SER:CB   | 2.34                     | 0.56              |
| 24:E:111:LEU:HD13 | 25:F:97:LEU:HD12  | 1.87                     | 0.56              |
| 25:F:93:VAL:HG22  | 25:F:124:ILE:HD11 | 1.87                     | 0.56              |
| 26:K:37:ALA:CB    | 26:K:50:VAL:HG22  | 2.35                     | 0.56              |
| 27:U:588:MET:HA   | 27:U:588:MET:HE3  | 1.87                     | 0.56              |
| 27:U:791:LEU:HD12 | 27:U:796:LYS:O    | 2.06                     | 0.56              |
| 2:D:242:GLU:OE1   | 2:D:245:ARG:NH2   | 2.38                     | 0.56              |
| 2:D:268:ASP:OD2   | 2:D:313:ARG:HB2   | 2.06                     | 0.56              |
| 2:D:368:ASP:OD2   | 2:D:403:TYR:OH    | 2.18                     | 0.56              |
| 4:H:65:VAL:HG22   | 4:H:75:VAL:HG12   | 1.86                     | 0.56              |
| 6:J:102:VAL:HG11  | 6:J:107:ILE:HD13  | 1.88                     | 0.56              |
| 7:L:101:ARG:HG2   | 7:L:102:PRO:N     | 2.20                     | 0.56              |
| 8:M:38:GLY:O      | 8:M:162:GLY:HA2   | 2.05                     | 0.56              |
| 9:V:86:VAL:HG21   | 9:V:160:LEU:HD13  | 1.87                     | 0.56              |
| 9:V:434:ALA:O     | 9:V:437:ILE:HG22  | 2.04                     | 0.56              |
| 10:W:256:ILE:HD13 | 10:W:259:GLU:OE2  | 2.05                     | 0.56              |
| 12:Y:45:VAL:HG13  | 12:Y:50:MET:HB2   | 1.88                     | 0.56              |
| 12:Y:257:ARG:HH11 | 12:Y:257:ARG:HG2  | 1.70                     | 0.56              |
| 17:d:162:PRO:HA   | 17:d:165:GLU:OE1  | 2.05                     | 0.56              |
| 18:f:138:GLU:HG3  | 18:f:141:LYS:HE3  | 1.88                     | 0.56              |
| 18:f:167:ALA:O    | 18:f:171:GLN:HG3  | 2.06                     | 0.56              |
| 18:f:182:GLU:O    | 18:f:186:THR:HG23 | 2.06                     | 0.56              |
| 18:f:256:PHE:CZ   | 18:f:264:GLU:HB3  | 2.40                     | 0.56              |
| 18:f:380:PHE:CD1  | 18:f:771:LEU:HD21 | 2.41                     | 0.56              |
| 19:g:112:LEU:HD13 | 19:g:142:LEU:CD1  | 2.35                     | 0.56              |
| 22:A:54:GLN:HE22  | 22:A:58:LYS:HD2   | 1.71                     | 0.56              |
| 23:B:209:GLU:O    | 23:B:213:GLU:HB3  | 2.06                     | 0.56              |
| 23:B:429:LYS:HG2  | 23:B:429:LYS:O    | 2.04                     | 0.56              |
| 25:F:81:LYS:HG3   | 25:F:82:VAL:N     | 2.20                     | 0.56              |
| 26:K:70:ILE:HD11  | 26:K:89:ILE:HD13  | 1.88                     | 0.56              |
| 27:U:221:ILE:HD11 | 27:U:256:ALA:HB2  | 1.87                     | 0.56              |
| 27:U:520:MET:HE2  | 27:U:520:MET:HA   | 1.86                     | 0.56              |
| 27:U:649:ARG:NH1  | 27:U:678:ASP:OD1  | 2.39                     | 0.56              |
| 1:C:217:SER:HB3   | 2:D:287:ARG:HG2   | 1.87                     | 0.56              |
| 1:C:358:GLU:HG2   | 2:D:324:PRO:HD2   | 1.87                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:D:245:ARG:HA    | 2:D:248:ARG:HH12  | 1.70                     | 0.56              |
| 2:D:315:ASP:OD1   | 2:D:316:THR:N     | 2.38                     | 0.56              |
| 8:M:190:VAL:HG11  | 8:M:227:VAL:HG21  | 1.87                     | 0.56              |
| 9:V:153:LYS:O     | 9:V:157:THR:HG23  | 2.06                     | 0.56              |
| 10:W:97:LEU:O     | 10:W:101:VAL:HG23 | 2.05                     | 0.56              |
| 10:W:259:GLU:OE1  | 10:W:262:LYS:HE2  | 2.05                     | 0.56              |
| 11:X:57:LEU:HD22  | 11:X:66:LEU:HD22  | 1.87                     | 0.56              |
| 11:X:125:LEU:HD12 | 11:X:128:ALA:HB3  | 1.87                     | 0.56              |
| 11:X:194:ARG:HG3  | 11:X:194:ARG:HH11 | 1.70                     | 0.56              |
| 12:Y:34:ASP:OD2   | 12:Y:37:VAL:HG23  | 2.06                     | 0.56              |
| 12:Y:45:VAL:HG13  | 12:Y:50:MET:CB    | 2.35                     | 0.56              |
| 14:a:116:THR:HG21 | 14:a:154:ARG:HB2  | 1.87                     | 0.56              |
| 17:d:97:GLN:O     | 17:d:101:GLU:HB2  | 2.06                     | 0.56              |
| 17:d:119:LEU:HB3  | 17:d:147:ILE:HD13 | 1.87                     | 0.56              |
| 18:f:140:LEU:HD13 | 18:f:169:GLU:HB2  | 1.88                     | 0.56              |
| 18:f:217:LEU:HD21 | 18:f:229:VAL:HG21 | 1.88                     | 0.56              |
| 18:f:460:ASP:HB3  | 19:g:133:LYS:CB   | 2.35                     | 0.56              |
| 18:f:662:MET:HE1  | 18:f:780:PRO:CG   | 2.35                     | 0.56              |
| 20:u:200:LEU:HD12 | 20:u:245:THR:HG21 | 1.87                     | 0.56              |
| 22:A:186:LYS:HZ2  | 22:A:186:LYS:HB3  | 1.71                     | 0.56              |
| 22:A:372:LEU:HD13 | 22:A:376:LEU:CD1  | 2.36                     | 0.56              |
| 24:E:184:ALA:CB   | 24:E:276:ILE:HG21 | 2.36                     | 0.56              |
| 25:F:425:LEU:HD13 | 25:F:432:LYS:HB2  | 1.88                     | 0.56              |
| 27:U:27:LEU:C     | 27:U:31:VAL:HG23  | 2.31                     | 0.56              |
| 27:U:247:GLN:HG3  | 27:U:904:LYS:HD2  | 1.88                     | 0.56              |
| 27:U:401:LYS:NZ   | 27:U:435:SER:HG   | 2.02                     | 0.56              |
| 27:U:560:MET:HG3  | 27:U:560:MET:O    | 2.06                     | 0.56              |
| 27:U:906:LEU:HD13 | 27:U:912:ILE:HG12 | 1.86                     | 0.56              |
| 1:C:50:ASN:ND2    | 27:U:639:LEU:HD11 | 2.20                     | 0.56              |
| 1:C:351:MET:HG3   | 1:C:387:VAL:HG23  | 1.88                     | 0.56              |
| 2:D:46:LYS:CE     | 27:U:187:LEU:HD11 | 2.35                     | 0.56              |
| 7:L:38:LEU:CD2    | 7:L:45:VAL:HG13   | 2.36                     | 0.56              |
| 7:L:155:ASP:HB2   | 8:M:62:SER:HB3    | 1.87                     | 0.56              |
| 8:M:152:ASP:OD1   | 8:M:154:SER:OG    | 2.24                     | 0.56              |
| 8:M:228:PRO:HG2   | 8:M:231:ILE:HD13  | 1.86                     | 0.56              |
| 9:V:209:LYS:HE3   | 9:V:213:TYR:CZ    | 2.41                     | 0.56              |
| 9:V:216:ARG:HA    | 9:V:219:GLU:CB    | 2.36                     | 0.56              |
| 9:V:216:ARG:HA    | 9:V:219:GLU:HB2   | 1.88                     | 0.56              |
| 9:V:468:SER:OG    | 13:Z:247:LYS:HB3  | 2.05                     | 0.56              |
| 10:W:216:GLU:H    | 10:W:219:THR:HG21 | 1.70                     | 0.56              |
| 11:X:193:ALA:HA   | 11:X:196:THR:HG22 | 1.87                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 13:Z:167:ALA:O    | 13:Z:170:VAL:HG12 | 2.05                     | 0.56              |
| 13:Z:209:ARG:HB2  | 14:a:353:LEU:CD2  | 2.34                     | 0.56              |
| 14:a:25:LEU:HD13  | 14:a:37:LEU:CD1   | 2.29                     | 0.56              |
| 14:a:40:GLN:HA    | 14:a:43:ASP:HB3   | 1.88                     | 0.56              |
| 14:a:89:ASP:CG    | 14:a:92:VAL:HG12  | 2.30                     | 0.56              |
| 14:a:148:VAL:HG13 | 14:a:149:THR:H    | 1.71                     | 0.56              |
| 14:a:364:GLU:HG2  | 14:a:368:GLU:OE2  | 2.05                     | 0.56              |
| 18:f:326:LEU:C    | 18:f:326:LEU:HD23 | 2.31                     | 0.56              |
| 18:f:389:LYS:O    | 18:f:390:LEU:HD22 | 2.06                     | 0.56              |
| 18:f:442:SER:O    | 18:f:446:LEU:HG   | 2.06                     | 0.56              |
| 18:f:662:MET:HE2  | 18:f:781:TYR:CE1  | 2.41                     | 0.56              |
| 18:f:836:GLU:O    | 18:f:837:LEU:HB2  | 2.06                     | 0.56              |
| 18:f:882:LEU:HG   | 18:f:882:LEU:O    | 2.04                     | 0.56              |
| 19:g:112:LEU:HD11 | 19:g:116:ILE:HG13 | 1.88                     | 0.56              |
| 24:E:173:TYR:OH   | 24:E:300:HIS:HB2  | 2.06                     | 0.56              |
| 25:F:254:PRO:O    | 25:F:257:VAL:HG12 | 2.05                     | 0.56              |
| 25:F:365:ILE:HG12 | 29:F:501:ATP:C6   | 2.40                     | 0.56              |
| 26:K:50:VAL:HG11  | 26:K:66:LYS:HE2   | 1.87                     | 0.56              |
| 26:K:202:LEU:HG   | 26:K:206:MET:HE2  | 1.87                     | 0.56              |
| 27:U:245:ALA:O    | 27:U:325:MET:HE1  | 2.05                     | 0.56              |
| 1:C:24:TYR:CE1    | 27:U:153:ILE:HG13 | 2.40                     | 0.56              |
| 1:C:93:GLY:HA3    | 23:B:126:SER:CB   | 2.33                     | 0.56              |
| 1:C:386:ALA:O     | 1:C:390:VAL:HG12  | 2.05                     | 0.56              |
| 2:D:218:ALA:O     | 2:D:221:HIS:N     | 2.38                     | 0.56              |
| 4:H:39:LYS:HG2    | 4:H:39:LYS:O      | 2.04                     | 0.56              |
| 5:I:144:GLY:O     | 5:I:146:GLN:HG3   | 2.05                     | 0.56              |
| 6:J:60:ARG:HG2    | 6:J:60:ARG:O      | 2.06                     | 0.56              |
| 7:L:171:TYR:CD1   | 7:L:172:LEU:HD23  | 2.39                     | 0.56              |
| 9:V:170:LEU:HD12  | 9:V:173:ILE:HD12  | 1.88                     | 0.56              |
| 10:W:361:HIS:HA   | 10:W:364:ARG:NH2  | 2.19                     | 0.56              |
| 11:X:194:ARG:HB2  | 11:X:194:ARG:CZ   | 2.35                     | 0.56              |
| 11:X:332:GLU:HG2  | 11:X:368:MET:SD   | 2.46                     | 0.56              |
| 11:X:390:GLU:O    | 11:X:390:GLU:HG2  | 2.05                     | 0.56              |
| 12:Y:85:ASP:O     | 12:Y:89:GLU:HG2   | 2.06                     | 0.56              |
| 14:a:148:VAL:HG13 | 14:a:149:THR:N    | 2.21                     | 0.56              |
| 14:a:193:GLN:OE1  | 14:a:225:LEU:HD21 | 2.06                     | 0.56              |
| 15:b:118:GLU:N    | 15:b:118:GLU:OE1  | 2.38                     | 0.56              |
| 16:c:141:VAL:HG23 | 16:c:161:ARG:HH12 | 1.71                     | 0.56              |
| 19:g:158:LEU:HD23 | 19:g:165:ALA:HB1  | 1.87                     | 0.56              |
| 26:K:88:LEU:HD21  | 26:K:119:LEU:HB3  | 1.88                     | 0.56              |
| 27:U:109:THR:O    | 27:U:113:VAL:HG23 | 2.05                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 27:U:348:THR:HG21 | 27:U:377:HIS:CD2  | 2.41                     | 0.56              |
| 27:U:458:ILE:HD11 | 27:U:485:ALA:N    | 2.20                     | 0.56              |
| 27:U:483:LEU:CD1  | 27:U:778:PHE:HE1  | 2.17                     | 0.56              |
| 1:C:24:TYR:O      | 2:D:40:LEU:HD11   | 2.06                     | 0.56              |
| 1:C:365:GLU:OE2   | 2:D:329:ARG:NH1   | 2.39                     | 0.56              |
| 1:C:404:LEU:HD23  | 4:H:152:SER:HB2   | 1.87                     | 0.56              |
| 2:D:204:MET:HB3   | 2:D:333:PHE:CE1   | 2.41                     | 0.56              |
| 2:D:309:MET:HE3   | 2:D:327:LEU:CD2   | 2.33                     | 0.56              |
| 2:D:354:LEU:HB3   | 2:D:358:VAL:CG1   | 2.37                     | 0.56              |
| 3:G:13:ILE:HA     | 3:G:24:GLN:HB2    | 1.88                     | 0.56              |
| 3:G:93:ARG:NH1    | 3:G:93:ARG:O      | 2.40                     | 0.56              |
| 3:G:219:VAL:CG2   | 3:G:230:LEU:HD21  | 2.36                     | 0.56              |
| 5:I:216:LEU:O     | 5:I:216:LEU:HD23  | 2.05                     | 0.56              |
| 7:L:43:HIS:CD2    | 7:L:216:GLY:HA3   | 2.41                     | 0.56              |
| 8:M:51:LYS:HE3    | 8:M:210:GLU:OE1   | 2.05                     | 0.56              |
| 8:M:140:TYR:CB    | 8:M:217:GLY:HA2   | 2.36                     | 0.56              |
| 9:V:168:GLN:HG2   | 9:V:187:ILE:HG23  | 1.87                     | 0.56              |
| 11:X:264:PRO:O    | 11:X:267:VAL:HG12 | 2.05                     | 0.56              |
| 12:Y:114:ILE:HD11 | 12:Y:116:ASP:CB   | 2.34                     | 0.56              |
| 14:a:136:GLU:O    | 14:a:139:GLU:HG3  | 2.06                     | 0.56              |
| 14:a:193:GLN:HB3  | 14:a:225:LEU:CD1  | 2.36                     | 0.56              |
| 15:b:79:GLN:C     | 15:b:81:LYS:HE2   | 2.31                     | 0.56              |
| 16:c:233:ASP:OD1  | 16:c:234:TYR:N    | 2.39                     | 0.56              |
| 18:f:238:ASN:HB3  | 18:f:664:GLU:OE2  | 2.06                     | 0.56              |
| 18:f:478:ARG:NH1  | 18:f:510:SER:HG   | 2.02                     | 0.56              |
| 18:f:669:GLU:CD   | 23:B:50:PRO:HG3   | 2.31                     | 0.56              |
| 18:f:759:LEU:HD12 | 18:f:759:LEU:O    | 2.06                     | 0.56              |
| 19:g:98:LYS:HE2   | 19:g:100:LEU:HD11 | 1.88                     | 0.56              |
| 25:F:195:ILE:O    | 25:F:199:VAL:HG23 | 2.06                     | 0.56              |
| 25:F:236:LEU:C    | 25:F:236:LEU:HD23 | 2.31                     | 0.56              |
| 25:F:291:ILE:HG21 | 25:F:309:THR:HG21 | 1.86                     | 0.56              |
| 25:F:436:GLN:HE22 | 26:K:28:ILE:CD1   | 2.19                     | 0.56              |
| 26:K:52:LYS:HB2   | 26:K:214:ASN:O    | 2.06                     | 0.56              |
| 26:K:121:LEU:HD21 | 26:K:160:GLY:HA3  | 1.87                     | 0.56              |
| 26:K:205:VAL:HG22 | 26:K:205:VAL:O    | 2.05                     | 0.56              |
| 27:U:85:GLY:N     | 27:U:88:PHE:HB3   | 2.20                     | 0.56              |
| 27:U:357:LYS:NZ   | 27:U:389:ASN:HD22 | 2.04                     | 0.56              |
| 27:U:638:SER:CA   | 27:U:671:LEU:HD11 | 2.33                     | 0.56              |
| 27:U:879:ASP:C    | 27:U:881:PRO:HD2  | 2.31                     | 0.56              |
| 1:C:114:VAL:HG21  | 1:C:123:LEU:HD11  | 1.88                     | 0.55              |
| 1:C:338:LEU:HD22  | 1:C:342:ILE:HG12  | 1.87                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:351:MET:HE3   | 1:C:354:ALA:CB    | 2.36                     | 0.55              |
| 2:D:329:ARG:HH11  | 2:D:329:ARG:HG3   | 1.71                     | 0.55              |
| 2:D:378:ILE:HA    | 2:D:406:VAL:HG21  | 1.88                     | 0.55              |
| 4:H:36:VAL:HG22   | 4:H:47:ALA:HB3    | 1.88                     | 0.55              |
| 6:J:183:THR:CB    | 6:J:186:LEU:HD22  | 2.36                     | 0.55              |
| 9:V:139:MET:H     | 9:V:139:MET:CE    | 2.19                     | 0.55              |
| 9:V:165:ALA:O     | 9:V:169:LEU:N     | 2.23                     | 0.55              |
| 9:V:218:TYR:HA    | 9:V:221:LEU:HB2   | 1.87                     | 0.55              |
| 10:W:187:LEU:CD1  | 10:W:229:LEU:HD12 | 2.36                     | 0.55              |
| 10:W:309:PHE:HE1  | 10:W:315:MET:HE1  | 1.64                     | 0.55              |
| 10:W:373:ILE:CG2  | 10:W:415:PHE:HE1  | 2.18                     | 0.55              |
| 11:X:54:GLY:HA2   | 11:X:66:LEU:CD1   | 2.35                     | 0.55              |
| 12:Y:148:GLY:HA3  | 12:Y:157:ILE:HG13 | 1.88                     | 0.55              |
| 14:a:148:VAL:HG22 | 14:a:150:SER:H    | 1.71                     | 0.55              |
| 15:b:24:THR:HG22  | 15:b:26:LEU:N     | 2.21                     | 0.55              |
| 15:b:180:ALA:HA   | 15:b:183:LEU:HD13 | 1.88                     | 0.55              |
| 18:f:427:THR:HG23 | 19:g:156:LEU:CD1  | 2.36                     | 0.55              |
| 18:f:704:LEU:HD11 | 18:f:740:ARG:CD   | 2.36                     | 0.55              |
| 22:A:352:THR:HG22 | 22:A:374:ALA:CB   | 2.35                     | 0.55              |
| 23:B:246:THR:HG23 | 23:B:280:SER:HB2  | 1.88                     | 0.55              |
| 23:B:334:ILE:O    | 23:B:334:ILE:HG12 | 2.05                     | 0.55              |
| 24:E:145:LEU:CG   | 24:E:149:ILE:HD12 | 2.35                     | 0.55              |
| 27:U:248:ILE:O    | 27:U:252:LEU:HB2  | 2.07                     | 0.55              |
| 27:U:356:THR:CG2  | 27:U:731:ILE:HD12 | 2.36                     | 0.55              |
| 27:U:435:SER:HB3  | 27:U:438:GLN:HB3  | 1.87                     | 0.55              |
| 27:U:491:GLN:OE1  | 27:U:491:GLN:HA   | 2.05                     | 0.55              |
| 27:U:641:SER:HB2  | 27:U:675:MET:CE   | 2.33                     | 0.55              |
| 1:C:271:ARG:NH2   | 23:B:305:ILE:HD13 | 2.20                     | 0.55              |
| 2:D:60:TYR:CD1    | 27:U:607:VAL:HG21 | 2.42                     | 0.55              |
| 2:D:273:LYS:HZ3   | 2:D:319:PRO:CD    | 2.19                     | 0.55              |
| 5:I:33:THR:HG23   | 5:I:163:CYS:SG    | 2.46                     | 0.55              |
| 7:L:46:LEU:HD11   | 7:L:63:ILE:HG12   | 1.88                     | 0.55              |
| 7:L:84:LEU:HD12   | 7:L:130:VAL:CG1   | 2.36                     | 0.55              |
| 10:W:75:TYR:O     | 10:W:78:LYS:NZ    | 2.31                     | 0.55              |
| 11:X:57:LEU:HD21  | 11:X:62:GLN:C     | 2.31                     | 0.55              |
| 11:X:89:VAL:HG11  | 11:X:125:LEU:HD11 | 1.88                     | 0.55              |
| 11:X:226:LYS:HG3  | 11:X:261:LEU:HD11 | 1.87                     | 0.55              |
| 11:X:271:VAL:HG11 | 11:X:288:LYS:HD3  | 1.88                     | 0.55              |
| 11:X:385:LEU:HD21 | 11:X:387:ILE:HD11 | 1.86                     | 0.55              |
| 13:Z:7:GLN:CG     | 13:Z:47:VAL:HG12  | 2.36                     | 0.55              |
| 13:Z:34:ARG:HD2   | 13:Z:102:HIS:NE2  | 2.21                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 13:Z:34:ARG:HH21  | 13:Z:96:HIS:CG    | 2.23                     | 0.55              |
| 15:b:80:PRO:N     | 15:b:81:LYS:HE2   | 2.21                     | 0.55              |
| 17:d:330:ILE:HD12 | 17:d:330:ILE:H    | 1.70                     | 0.55              |
| 18:f:136:GLU:OE2  | 18:f:137:ARG:NH2  | 2.38                     | 0.55              |
| 18:f:217:LEU:CD2  | 18:f:229:VAL:HG21 | 2.36                     | 0.55              |
| 18:f:305:LEU:O    | 18:f:321:MET:HE1  | 2.06                     | 0.55              |
| 18:f:326:LEU:HA   | 18:f:329:ASN:HD22 | 1.71                     | 0.55              |
| 18:f:886:GLU:HB3  | 18:f:887:PHE:CD1  | 2.41                     | 0.55              |
| 19:g:164:ASP:HA   | 19:g:167:LYS:HB2  | 1.89                     | 0.55              |
| 22:A:278:ASP:HB2  | 23:B:310:LEU:HD21 | 1.88                     | 0.55              |
| 24:E:133:SER:O    | 24:E:315:ILE:HD13 | 2.05                     | 0.55              |
| 25:F:134:LEU:CD1  | 25:F:159:LEU:HA   | 2.27                     | 0.55              |
| 26:K:39:GLY:N     | 26:K:168:ARG:O    | 2.39                     | 0.55              |
| 27:U:527:GLN:O    | 27:U:531:ASP:HB2  | 2.04                     | 0.55              |
| 27:U:602:LEU:HD11 | 27:U:621:SER:HB3  | 1.88                     | 0.55              |
| 27:U:625:ILE:HG13 | 27:U:626:LEU:HD23 | 1.86                     | 0.55              |
| 1:C:84:LYS:HD3    | 1:C:96:VAL:CG1    | 2.35                     | 0.55              |
| 1:C:214:VAL:HG21  | 1:C:234:LEU:CD2   | 2.35                     | 0.55              |
| 2:D:85:ILE:CD1    | 24:E:68:LYS:HG2   | 2.36                     | 0.55              |
| 3:G:153:LYS:HD3   | 3:G:166:THR:OG1   | 2.06                     | 0.55              |
| 5:I:124:PHE:HE1   | 6:J:118:TYR:HE1   | 1.54                     | 0.55              |
| 5:I:174:MET:CE    | 5:I:196:VAL:HA    | 2.35                     | 0.55              |
| 7:L:214:ILE:HD13  | 7:L:232:PHE:CZ    | 2.41                     | 0.55              |
| 11:X:72:TYR:O     | 11:X:75:PRO:HD2   | 2.07                     | 0.55              |
| 11:X:173:GLU:HA   | 11:X:176:THR:CG2  | 2.36                     | 0.55              |
| 11:X:384:VAL:CG2  | 11:X:386:ILE:HD11 | 2.37                     | 0.55              |
| 12:Y:90:ASP:OD1   | 12:Y:94:ASN:ND2   | 2.37                     | 0.55              |
| 12:Y:220:VAL:HG21 | 12:Y:249:VAL:HG11 | 1.88                     | 0.55              |
| 13:Z:17:LEU:HD21  | 16:c:35:SER:C     | 2.31                     | 0.55              |
| 13:Z:48:LEU:HD23  | 13:Z:120:VAL:HG11 | 1.89                     | 0.55              |
| 15:b:4:GLU:OE2    | 15:b:40:LYS:HE2   | 2.05                     | 0.55              |
| 15:b:16:MET:O     | 15:b:26:LEU:HD12  | 2.06                     | 0.55              |
| 15:b:22:LEU:HB2   | 15:b:23:PRO:CD    | 2.35                     | 0.55              |
| 15:b:26:LEU:HD11  | 15:b:80:PRO:CB    | 2.35                     | 0.55              |
| 15:b:53:THR:CG2   | 15:b:61:LEU:HD11  | 2.36                     | 0.55              |
| 16:c:115:HIS:O    | 16:c:117:GLY:N    | 2.39                     | 0.55              |
| 18:f:93:PRO:O     | 18:f:96:LEU:N     | 2.39                     | 0.55              |
| 18:f:512:MET:HG2  | 18:f:552:ASP:OD2  | 2.06                     | 0.55              |
| 18:f:785:ARG:NH2  | 18:f:876:HIS:HA   | 2.20                     | 0.55              |
| 23:B:186:ASP:C    | 23:B:367:ILE:HD13 | 2.32                     | 0.55              |
| 27:U:756:HIS:ND1  | 27:U:759:SER:HB2  | 2.20                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 27:U:793:LYS:NZ   | 27:U:916:ASP:OD2  | 2.35                     | 0.55              |
| 27:U:845:GLU:HG2  | 27:U:848:LYS:NZ   | 2.22                     | 0.55              |
| 27:U:879:ASP:HB3  | 27:U:881:PRO:CD   | 2.23                     | 0.55              |
| 3:G:101:TRP:CB    | 3:G:109:ILE:HB    | 2.37                     | 0.55              |
| 3:G:138:MET:O     | 3:G:153:LYS:HA    | 2.06                     | 0.55              |
| 5:I:176:LYS:O     | 5:I:179:TYR:HB3   | 2.07                     | 0.55              |
| 7:L:233:LEU:O     | 7:L:236:LEU:HB2   | 2.05                     | 0.55              |
| 8:M:122:TYR:CG    | 8:M:131:PHE:HE1   | 2.23                     | 0.55              |
| 9:V:470:ARG:NH1   | 9:V:474:LEU:HD13  | 2.21                     | 0.55              |
| 12:Y:121:LEU:HD11 | 12:Y:156:LEU:CD2  | 2.37                     | 0.55              |
| 12:Y:273:GLN:OE1  | 12:Y:273:GLN:HA   | 2.05                     | 0.55              |
| 13:Z:9:VAL:O      | 13:Z:9:VAL:HG12   | 2.05                     | 0.55              |
| 13:Z:109:ASN:ND2  | 13:Z:140:SER:HB2  | 2.22                     | 0.55              |
| 13:Z:121:LEU:HD23 | 13:Z:155:PHE:CE2  | 2.41                     | 0.55              |
| 14:a:142:LEU:HD21 | 14:a:152:HIS:NE2  | 2.22                     | 0.55              |
| 15:b:171:VAL:HG21 | 15:b:187:PRO:CG   | 2.26                     | 0.55              |
| 16:c:121:TRP:HZ3  | 16:c:123:SER:HG   | 1.54                     | 0.55              |
| 18:f:300:ARG:HA   | 18:f:300:ARG:HE   | 1.72                     | 0.55              |
| 18:f:523:GLY:O    | 18:f:527:VAL:HG13 | 2.06                     | 0.55              |
| 18:f:539:LEU:O    | 18:f:542:ILE:HG12 | 2.06                     | 0.55              |
| 18:f:794:ALA:O    | 18:f:798:THR:HG23 | 2.07                     | 0.55              |
| 18:f:857:GLY:C    | 18:f:859:PRO:HD3  | 2.31                     | 0.55              |
| 24:E:134:GLU:HA   | 24:E:315:ILE:HG21 | 1.88                     | 0.55              |
| 25:F:175:MET:SD   | 25:F:251:LEU:HA   | 2.47                     | 0.55              |
| 25:F:246:ALA:HB1  | 25:F:281:SER:HA   | 1.88                     | 0.55              |
| 25:F:284:PHE:CE2  | 25:F:286:ASP:HB2  | 2.41                     | 0.55              |
| 3:G:32:ILE:HD11   | 3:G:156:PRO:CG    | 2.37                     | 0.55              |
| 5:I:180:LYS:HD2   | 5:I:184:MET:HA    | 1.89                     | 0.55              |
| 6:J:43:LEU:HD13   | 6:J:134:VAL:CG1   | 2.37                     | 0.55              |
| 7:L:121:GLN:HG3   | 8:M:129:ARG:CZ    | 2.36                     | 0.55              |
| 8:M:187:ARG:HG2   | 8:M:219:LEU:CD1   | 2.37                     | 0.55              |
| 9:V:71:THR:HA     | 9:V:74:ASP:HB2    | 1.88                     | 0.55              |
| 9:V:214:HIS:CD2   | 9:V:230:PHE:HE2   | 2.25                     | 0.55              |
| 10:W:205:ILE:O    | 10:W:209:ILE:HG22 | 2.07                     | 0.55              |
| 11:X:74:ARG:HB2   | 11:X:75:PRO:HD3   | 1.87                     | 0.55              |
| 12:Y:145:LEU:HD23 | 12:Y:160:ASN:HB2  | 1.88                     | 0.55              |
| 12:Y:280:GLN:OE1  | 12:Y:280:GLN:HA   | 2.06                     | 0.55              |
| 13:Z:129:LYS:HD3  | 16:c:212:LEU:HA   | 1.88                     | 0.55              |
| 14:a:58:LYS:HB2   | 14:a:58:LYS:HZ3   | 1.71                     | 0.55              |
| 14:a:312:MET:HE1  | 14:a:324:ILE:HD13 | 1.87                     | 0.55              |
| 15:b:16:MET:HA    | 15:b:25:ARG:NE    | 2.20                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 18:f:250:ARG:HH11 | 18:f:272:LEU:HD11 | 1.72                     | 0.55              |
| 24:E:135:ILE:HG12 | 24:E:182:LEU:HG   | 1.87                     | 0.55              |
| 27:U:368:ALA:HA   | 27:U:371:ILE:HG22 | 1.88                     | 0.55              |
| 27:U:368:ALA:O    | 27:U:372:ALA:N    | 2.34                     | 0.55              |
| 27:U:912:ILE:C    | 27:U:912:ILE:HD12 | 2.32                     | 0.55              |
| 2:D:391:ARG:NH1   | 2:D:397:LYS:HD2   | 2.21                     | 0.55              |
| 3:G:202:LEU:HG    | 3:G:210:PHE:CZ    | 2.34                     | 0.55              |
| 7:L:143:HIS:HB3   | 7:L:145:PHE:CE1   | 2.42                     | 0.55              |
| 8:M:195:LYS:HG3   | 8:M:196:ILE:N     | 2.22                     | 0.55              |
| 9:V:333:ILE:HD13  | 9:V:348:PHE:CZ    | 2.41                     | 0.55              |
| 10:W:276:LEU:HD23 | 10:W:354:LEU:HD13 | 1.88                     | 0.55              |
| 10:W:375:MET:SD   | 10:W:413:ILE:HD11 | 2.47                     | 0.55              |
| 11:X:103:THR:OG1  | 11:X:105:GLN:HG2  | 2.07                     | 0.55              |
| 11:X:407:MET:HA   | 11:X:410:VAL:CG1  | 2.33                     | 0.55              |
| 13:Z:34:ARG:HB2   | 13:Z:96:HIS:HB2   | 1.87                     | 0.55              |
| 13:Z:201:LEU:HB2  | 16:c:225:TRP:HZ3  | 1.72                     | 0.55              |
| 14:a:176:ALA:HB3  | 14:a:200:LEU:CD1  | 2.33                     | 0.55              |
| 14:a:342:ASP:HB3  | 14:a:345:GLN:CG   | 2.36                     | 0.55              |
| 15:b:109:ILE:CG2  | 15:b:138:VAL:HG23 | 2.37                     | 0.55              |
| 16:c:69:VAL:HG12  | 16:c:109:VAL:HG11 | 1.87                     | 0.55              |
| 16:c:211:GLU:OE1  | 27:U:574:LYS:NZ   | 2.40                     | 0.55              |
| 17:d:304:LYS:HZ2  | 17:d:304:LYS:HB2  | 1.71                     | 0.55              |
| 18:f:430:ASP:O    | 19:g:171:LEU:HB2  | 2.07                     | 0.55              |
| 18:f:433:LEU:HG   | 19:g:173:GLU:CA   | 2.37                     | 0.55              |
| 19:g:101:LEU:HD21 | 19:g:116:ILE:O    | 2.07                     | 0.55              |
| 20:u:168:THR:OG1  | 20:u:245:THR:HG22 | 2.06                     | 0.55              |
| 22:A:101:ILE:HD11 | 22:A:111:TYR:CE2  | 2.41                     | 0.55              |
| 22:A:415:LYS:O    | 22:A:419:SER:HB3  | 2.06                     | 0.55              |
| 24:E:280:ASN:OD1  | 24:E:280:ASN:O    | 2.24                     | 0.55              |
| 27:U:535:TYR:CE1  | 27:U:539:THR:HB   | 2.42                     | 0.55              |
| 1:C:355:SER:HB3   | 1:C:358:GLU:HG3   | 1.87                     | 0.55              |
| 2:D:414:HIS:HB3   | 2:D:416:PHE:CD1   | 2.41                     | 0.55              |
| 7:L:40:SER:HB3    | 7:L:187:LEU:HD13  | 1.88                     | 0.55              |
| 8:M:164:ALA:O     | 8:M:165:ILE:HD13  | 2.06                     | 0.55              |
| 8:M:169:ARG:O     | 8:M:173:LYS:HG3   | 2.07                     | 0.55              |
| 8:M:216:VAL:HG12  | 8:M:224:HIS:HA    | 1.88                     | 0.55              |
| 10:W:268:LYS:HG2  | 10:W:302:TYR:CE2  | 2.42                     | 0.55              |
| 10:W:451:MET:SD   | 13:Z:100:LYS:HA   | 2.46                     | 0.55              |
| 12:Y:224:VAL:HG11 | 12:Y:256:VAL:HG13 | 1.88                     | 0.55              |
| 12:Y:244:ALA:HB3  | 12:Y:245:GLU:OE1  | 2.05                     | 0.55              |
| 13:Z:144:VAL:HG21 | 14:a:178:ARG:CD   | 2.36                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 14:a:210:VAL:O    | 14:a:210:VAL:HG23 | 2.06                     | 0.55              |
| 16:c:118:PHE:HB3  | 16:c:121:TRP:CZ2  | 2.42                     | 0.55              |
| 17:d:94:MET:O     | 17:d:98:LEU:N     | 2.21                     | 0.55              |
| 17:d:109:LEU:HD13 | 17:d:158:ARG:HG3  | 1.88                     | 0.55              |
| 18:f:47:GLU:O     | 18:f:51:GLN:HB2   | 2.06                     | 0.55              |
| 18:f:63:LEU:HB2   | 18:f:105:LYS:NZ   | 2.22                     | 0.55              |
| 18:f:567:LEU:HB2  | 18:f:790:GLN:HE22 | 1.68                     | 0.55              |
| 18:f:662:MET:HE1  | 18:f:780:PRO:HG3  | 1.89                     | 0.55              |
| 18:f:846:VAL:HG22 | 18:f:880:ALA:CA   | 2.36                     | 0.55              |
| 19:g:128:LYS:HZ3  | 19:g:129:ILE:C    | 2.15                     | 0.55              |
| 19:g:130:VAL:CG2  | 19:g:154:MET:HB3  | 2.37                     | 0.55              |
| 22:A:87:LEU:CD1   | 23:B:156:VAL:HB   | 2.36                     | 0.55              |
| 22:A:195:LEU:HD11 | 22:A:316:LYS:CG   | 2.36                     | 0.55              |
| 22:A:213:LEU:O    | 22:A:213:LEU:HG   | 2.06                     | 0.55              |
| 22:A:292:ASP:HB2  | 23:B:300:GLY:HA3  | 1.87                     | 0.55              |
| 25:F:94:ILE:CG1   | 25:F:125:LYS:HB2  | 2.36                     | 0.55              |
| 25:F:226:TYR:CE1  | 25:F:353:GLU:HA   | 2.42                     | 0.55              |
| 25:F:385:ALA:HA   | 25:F:388:THR:OG1  | 2.07                     | 0.55              |
| 27:U:675:MET:O    | 27:U:678:ASP:HB2  | 2.06                     | 0.55              |
| 2:D:64:GLU:HG3    | 27:U:607:VAL:HG13 | 1.88                     | 0.55              |
| 2:D:204:MET:HE1   | 2:D:216:ALA:HB2   | 1.88                     | 0.55              |
| 3:G:66:VAL:O      | 3:G:66:VAL:HG12   | 2.06                     | 0.55              |
| 5:I:224:VAL:HG22  | 5:I:226:ARG:HG2   | 1.89                     | 0.55              |
| 7:L:154:PHE:CB    | 8:M:58:TYR:HD2    | 2.20                     | 0.55              |
| 8:M:50:GLU:OE1    | 8:M:201:HIS:HB2   | 2.06                     | 0.55              |
| 8:M:215:TRP:CZ3   | 8:M:219:LEU:HD23  | 2.42                     | 0.55              |
| 9:V:353:LEU:HB3   | 9:V:357:LEU:HD12  | 1.88                     | 0.55              |
| 10:W:276:LEU:O    | 10:W:357:ARG:HG3  | 2.06                     | 0.55              |
| 13:Z:81:MET:HE1   | 16:c:95:MET:N     | 2.21                     | 0.55              |
| 13:Z:242:LEU:HD12 | 13:Z:243:GLN:H    | 1.72                     | 0.55              |
| 16:c:27:THR:HG23  | 16:c:175:ARG:CB   | 2.37                     | 0.55              |
| 16:c:75:MET:HE1   | 16:c:88:ASP:H     | 1.71                     | 0.55              |
| 18:f:114:ALA:HB3  | 18:f:118:ASN:CB   | 2.35                     | 0.55              |
| 18:f:132:THR:HG21 | 22:A:32:LEU:HD21  | 1.89                     | 0.55              |
| 18:f:266:LEU:HD22 | 18:f:294:MET:CB   | 2.33                     | 0.55              |
| 18:f:830:LEU:HD23 | 18:f:872:VAL:HB   | 1.88                     | 0.55              |
| 18:f:885:GLU:HG3  | 18:f:906:TYR:CD2  | 2.41                     | 0.55              |
| 23:B:248:LEU:HD13 | 23:B:274:ALA:HB2  | 1.88                     | 0.55              |
| 23:B:383:LEU:HB3  | 23:B:423:LYS:HE3  | 1.88                     | 0.55              |
| 24:E:233:ASP:O    | 24:E:234:GLU:C    | 2.49                     | 0.55              |
| 25:F:192:ASP:O    | 25:F:195:ILE:N    | 2.39                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 26:K:171:GLY:O    | 26:K:174:SER:OG   | 2.18                     | 0.55              |
| 27:U:39:SER:O     | 27:U:42:VAL:HG13  | 2.06                     | 0.55              |
| 27:U:356:THR:HG23 | 27:U:731:ILE:HD12 | 1.89                     | 0.55              |
| 27:U:545:LEU:CB   | 27:U:577:ILE:HG21 | 2.37                     | 0.55              |
| 27:U:740:GLY:HA3  | 27:U:744:VAL:HG22 | 1.88                     | 0.55              |
| 1:C:79:ALA:HB1    | 22:A:65:ILE:HD13  | 1.88                     | 0.55              |
| 1:C:135:VAL:O     | 1:C:135:VAL:HG22  | 2.07                     | 0.55              |
| 3:G:196:GLU:CA    | 3:G:242:LEU:HD21  | 2.37                     | 0.55              |
| 7:L:38:LEU:HD21   | 7:L:45:VAL:HG13   | 1.88                     | 0.55              |
| 8:M:98:PHE:CD1    | 8:M:106:ILE:HB    | 2.42                     | 0.55              |
| 9:V:131:LEU:HD12  | 9:V:171:VAL:HG21  | 1.87                     | 0.55              |
| 9:V:134:PHE:CG    | 9:V:183:GLU:HB3   | 2.42                     | 0.55              |
| 9:V:192:MET:HA    | 9:V:195:ILE:CG1   | 2.32                     | 0.55              |
| 10:W:267:LEU:O    | 10:W:270:VAL:HG12 | 2.07                     | 0.55              |
| 11:X:363:ARG:O    | 11:X:366:SER:N    | 2.40                     | 0.55              |
| 14:a:131:THR:O    | 14:a:134:THR:OG1  | 2.11                     | 0.55              |
| 17:d:194:LEU:O    | 17:d:197:LEU:N    | 2.40                     | 0.55              |
| 18:f:395:GLY:HA3  | 18:f:432:TYR:CE2  | 2.42                     | 0.55              |
| 18:f:733:GLY:HA3  | 18:f:741:LEU:CD2  | 2.33                     | 0.55              |
| 18:f:833:PHE:CD1  | 18:f:839:PRO:HA   | 2.41                     | 0.55              |
| 19:g:170:GLN:HA   | 19:g:173:GLU:CA   | 2.36                     | 0.55              |
| 23:B:232:LYS:HZ3  | 23:B:232:LYS:HB2  | 1.71                     | 0.55              |
| 24:E:235:ILE:HD12 | 24:E:277:MET:C    | 2.32                     | 0.55              |
| 25:F:228:PRO:HG3  | 25:F:356:MET:HG3  | 1.87                     | 0.55              |
| 25:F:232:GLY:HA2  | 29:F:501:ATP:O1A  | 2.06                     | 0.55              |
| 26:K:9:ASP:HB3    | 26:K:22:PHE:HB3   | 1.89                     | 0.55              |
| 27:U:338:HIS:O    | 27:U:342:LEU:HD23 | 2.06                     | 0.55              |
| 27:U:368:ALA:HA   | 27:U:371:ILE:CG2  | 2.37                     | 0.55              |
| 1:C:31:LEU:O      | 1:C:34:ILE:HG22   | 2.06                     | 0.55              |
| 2:D:173:GLN:OE1   | 2:D:173:GLN:N     | 2.37                     | 0.55              |
| 8:M:197:ILE:HD13  | 8:M:211:LEU:HD13  | 1.88                     | 0.55              |
| 9:V:67:LEU:C      | 9:V:70:VAL:HG12   | 2.32                     | 0.55              |
| 9:V:192:MET:HE3   | 9:V:214:HIS:CG    | 2.42                     | 0.55              |
| 10:W:171:VAL:O    | 10:W:182:ARG:HD3  | 2.07                     | 0.55              |
| 11:X:252:LYS:HD2  | 11:X:283:GLN:HB3  | 1.89                     | 0.55              |
| 11:X:397:TYR:CE2  | 13:Z:258:VAL:HG11 | 2.42                     | 0.55              |
| 12:Y:70:LEU:HD12  | 12:Y:74:LYS:HG3   | 1.88                     | 0.55              |
| 14:a:58:LYS:HG3   | 14:a:83:VAL:HG11  | 1.88                     | 0.55              |
| 15:b:6:THR:O      | 15:b:49:VAL:HA    | 2.06                     | 0.55              |
| 17:d:98:LEU:CD2   | 17:d:150:ILE:HG21 | 2.28                     | 0.55              |
| 18:f:124:ASP:OD2  | 18:f:147:SER:HB3  | 2.06                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 18:f:267:ARG:NH2  | 18:f:297:MET:HE3  | 2.22                     | 0.55              |
| 18:f:411:ALA:HA   | 18:f:414:LEU:HD12 | 1.89                     | 0.55              |
| 18:f:433:LEU:HD22 | 18:f:444:ALA:HB3  | 1.88                     | 0.55              |
| 19:g:113:ARG:HE   | 19:g:138:LEU:CD1  | 2.20                     | 0.55              |
| 22:A:95:VAL:HG22  | 22:A:153:LEU:HD22 | 1.88                     | 0.55              |
| 22:A:102:ILE:HD12 | 25:F:165:PRO:HG2  | 1.88                     | 0.55              |
| 23:B:153:ASN:OD1  | 23:B:154:HIS:N    | 2.40                     | 0.55              |
| 23:B:203:LEU:N    | 23:B:204:PRO:HD2  | 2.22                     | 0.55              |
| 24:E:147:GLU:CA   | 24:E:151:LEU:HD13 | 2.32                     | 0.55              |
| 25:F:202:ILE:HG22 | 25:F:203:VAL:H    | 1.72                     | 0.55              |
| 26:K:24:VAL:HG11  | 26:K:159:SER:HA   | 1.89                     | 0.55              |
| 27:U:364:VAL:HG12 | 27:U:724:VAL:CG1  | 2.32                     | 0.55              |
| 27:U:631:GLU:O    | 27:U:634:PRO:HD2  | 2.07                     | 0.55              |
| 27:U:919:GLU:HG3  | 27:U:920:ASP:H    | 1.72                     | 0.55              |
| 1:C:148:TYR:HE1   | 1:C:158:ILE:HG23  | 1.72                     | 0.54              |
| 3:G:73:THR:HG22   | 3:G:74:GLU:N      | 2.22                     | 0.54              |
| 6:J:133:ILE:O     | 6:J:145:TYR:N     | 2.27                     | 0.54              |
| 9:V:101:LEU:HD13  | 9:V:166:TYR:CE1   | 2.42                     | 0.54              |
| 9:V:169:LEU:O     | 9:V:173:ILE:HG13  | 2.07                     | 0.54              |
| 9:V:412:LEU:HD22  | 12:Y:339:ALA:HA   | 1.88                     | 0.54              |
| 10:W:34:LEU:HD12  | 10:W:43:VAL:CG2   | 2.37                     | 0.54              |
| 10:W:60:MET:H     | 10:W:60:MET:CE    | 2.12                     | 0.54              |
| 10:W:117:ASP:HB3  | 10:W:120:ILE:HB   | 1.89                     | 0.54              |
| 10:W:170:GLN:O    | 10:W:173:THR:OG1  | 2.23                     | 0.54              |
| 10:W:172:GLU:CG   | 10:W:208:LYS:HD2  | 2.37                     | 0.54              |
| 10:W:365:ILE:HD13 | 10:W:368:LYS:HE3  | 1.89                     | 0.54              |
| 13:Z:79:TYR:CE2   | 13:Z:83:LYS:HE3   | 2.42                     | 0.54              |
| 13:Z:246:VAL:HG22 | 17:d:330:ILE:CD1  | 2.37                     | 0.54              |
| 14:a:62:ASN:O     | 14:a:66:GLU:HG3   | 2.07                     | 0.54              |
| 14:a:185:ILE:CG2  | 14:a:187:ASP:HB3  | 2.37                     | 0.54              |
| 14:a:321:LYS:CD   | 14:a:336:VAL:HG11 | 2.35                     | 0.54              |
| 15:b:44:ASN:OD1   | 15:b:45:PRO:HD2   | 2.06                     | 0.54              |
| 18:f:233:LEU:O    | 18:f:237:VAL:HG13 | 2.07                     | 0.54              |
| 19:g:108:THR:O    | 19:g:112:LEU:N    | 2.40                     | 0.54              |
| 20:u:229:GLY:O    | 20:u:230:ILE:HD13 | 2.07                     | 0.54              |
| 22:A:190:VAL:HG22 | 22:A:209:PRO:HB2  | 1.88                     | 0.54              |
| 23:B:286:GLU:HA   | 23:B:286:GLU:OE2  | 2.06                     | 0.54              |
| 24:E:236:ASP:N    | 24:E:236:ASP:OD1  | 2.39                     | 0.54              |
| 25:F:247:THR:HB   | 25:F:281:SER:HB3  | 1.89                     | 0.54              |
| 26:K:70:ILE:HD12  | 26:K:92:ALA:CB    | 2.38                     | 0.54              |
| 27:U:813:TYR:HE1  | 27:U:883:ARG:HD2  | 1.71                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:35:VAL:CG1    | 2:D:51:LEU:HB2    | 2.34                     | 0.54              |
| 2:D:184:PRO:HG3   | 2:D:191:TYR:CE2   | 2.42                     | 0.54              |
| 4:H:203:MET:SD    | 4:H:208:ILE:HG13  | 2.47                     | 0.54              |
| 5:I:97:TYR:CZ     | 5:I:106:PRO:HD3   | 2.42                     | 0.54              |
| 6:J:85:ASN:C      | 6:J:85:ASN:OD1    | 2.50                     | 0.54              |
| 6:J:212:ARG:O     | 6:J:215:GLN:HB2   | 2.08                     | 0.54              |
| 7:L:68:ASN:HB3    | 7:L:220:GLU:HG2   | 1.88                     | 0.54              |
| 9:V:198:GLN:HB2   | 9:V:203:LEU:CD2   | 2.38                     | 0.54              |
| 10:W:124:LEU:HD12 | 10:W:124:LEU:O    | 2.07                     | 0.54              |
| 11:X:69:LEU:O     | 11:X:73:VAL:HG22  | 2.07                     | 0.54              |
| 12:Y:297:ARG:HB3  | 12:Y:297:ARG:HH11 | 1.71                     | 0.54              |
| 13:Z:165:GLU:HG2  | 13:Z:166:GLU:H    | 1.72                     | 0.54              |
| 13:Z:169:GLU:HA   | 13:Z:169:GLU:OE2  | 2.07                     | 0.54              |
| 15:b:35:ILE:O     | 15:b:39:SER:N     | 2.37                     | 0.54              |
| 15:b:183:LEU:O    | 15:b:187:PRO:HD2  | 2.07                     | 0.54              |
| 16:c:150:SER:HB3  | 16:c:156:VAL:HG22 | 1.88                     | 0.54              |
| 22:A:377:CYS:SG   | 22:A:417:ILE:HG13 | 2.46                     | 0.54              |
| 23:B:225:TYR:OH   | 23:B:352:GLU:HB2  | 2.07                     | 0.54              |
| 27:U:96:TYR:CE1   | 27:U:100:ILE:HG13 | 2.42                     | 0.54              |
| 27:U:108:TYR:CB   | 27:U:134:VAL:HG21 | 2.37                     | 0.54              |
| 27:U:344:ARG:HE   | 27:U:927:PRO:HG2  | 1.72                     | 0.54              |
| 27:U:662:GLY:O    | 27:U:698:GLN:NE2  | 2.40                     | 0.54              |
| 2:D:218:ALA:C     | 2:D:220:ALA:N     | 2.64                     | 0.54              |
| 3:G:62:ASP:OD2    | 8:M:40:ARG:NH1    | 2.40                     | 0.54              |
| 3:G:132:ARG:HG3   | 8:M:12:SER:O      | 2.07                     | 0.54              |
| 5:I:197:LEU:CB    | 5:I:206:LEU:HD11  | 2.37                     | 0.54              |
| 7:L:209:ASN:OD1   | 7:L:210:VAL:HG23  | 2.07                     | 0.54              |
| 8:M:164:ALA:CB    | 8:M:172:ALA:HB3   | 2.37                     | 0.54              |
| 9:V:375:PHE:HE2   | 9:V:398:LEU:HD23  | 1.70                     | 0.54              |
| 10:W:24:VAL:HG13  | 10:W:65:ARG:NH2   | 2.22                     | 0.54              |
| 10:W:61:VAL:HG23  | 10:W:62:SER:H     | 1.71                     | 0.54              |
| 10:W:187:LEU:HD12 | 10:W:225:LYS:HG2  | 1.88                     | 0.54              |
| 10:W:265:GLN:OE1  | 10:W:268:LYS:HD2  | 2.06                     | 0.54              |
| 12:Y:28:LEU:HD22  | 12:Y:29:PRO:HD2   | 1.89                     | 0.54              |
| 13:Z:121:LEU:HD11 | 13:Z:123:ILE:HG13 | 1.88                     | 0.54              |
| 14:a:8:LEU:HD12   | 14:a:9:GLN:OE1    | 2.08                     | 0.54              |
| 14:a:65:SER:HA    | 14:a:68:GLU:CG    | 2.37                     | 0.54              |
| 14:a:112:ILE:HA   | 14:a:115:LYS:HB2  | 1.87                     | 0.54              |
| 17:d:94:MET:HB2   | 17:d:119:LEU:CD2  | 2.35                     | 0.54              |
| 19:g:87:VAL:C     | 19:g:88:PHE:HD1   | 2.15                     | 0.54              |
| 19:g:141:THR:HG22 | 19:g:144:GLU:HG2  | 1.90                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 19:g:156:LEU:C    | 19:g:158:LEU:HD12 | 2.32                     | 0.54              |
| 22:A:190:VAL:HG11 | 22:A:212:VAL:HG13 | 1.89                     | 0.54              |
| 22:A:402:LYS:O    | 23:B:214:MET:HE1  | 2.08                     | 0.54              |
| 26:K:77:ALA:HB3   | 26:K:142:LEU:HB2  | 1.89                     | 0.54              |
| 26:K:199:LEU:CD1  | 26:K:210:LEU:HD21 | 2.37                     | 0.54              |
| 27:U:497:LEU:HD13 | 27:U:515:ALA:CB   | 2.37                     | 0.54              |
| 27:U:532:MET:SD   | 27:U:552:ILE:HG22 | 2.47                     | 0.54              |
| 1:C:21:ARG:CA     | 27:U:149:GLN:HE22 | 2.20                     | 0.54              |
| 3:G:219:VAL:HG21  | 3:G:230:LEU:HD21  | 1.89                     | 0.54              |
| 4:H:74:LEU:HB3    | 4:H:134:LEU:HD22  | 1.88                     | 0.54              |
| 5:I:197:LEU:HA    | 5:I:200:THR:OG1   | 2.07                     | 0.54              |
| 9:V:180:ARG:HG2   | 9:V:183:GLU:CD    | 2.31                     | 0.54              |
| 9:V:196:SER:HB3   | 9:V:234:ARG:HH22  | 1.72                     | 0.54              |
| 9:V:348:PHE:HE2   | 9:V:361:PHE:HA    | 1.73                     | 0.54              |
| 11:X:69:LEU:O     | 11:X:73:VAL:N     | 2.30                     | 0.54              |
| 12:Y:194:PHE:CD2  | 12:Y:229:ILE:HD13 | 2.42                     | 0.54              |
| 12:Y:387:ILE:CG1  | 13:Z:276:ILE:HG12 | 2.32                     | 0.54              |
| 14:a:92:VAL:HA    | 14:a:95:THR:OG1   | 2.08                     | 0.54              |
| 15:b:85:THR:O     | 15:b:85:THR:CG2   | 2.56                     | 0.54              |
| 15:b:141:ILE:HG13 | 15:b:143:PHE:CZ   | 2.42                     | 0.54              |
| 19:g:102:GLU:O    | 19:g:119:THR:HG21 | 2.08                     | 0.54              |
| 19:g:105:LEU:HB2  | 19:g:149:HIS:CE1  | 2.42                     | 0.54              |
| 20:u:127:MET:HA   | 20:u:130:ILE:HD12 | 1.89                     | 0.54              |
| 20:u:204:MET:HE3  | 20:u:208:GLU:HG2  | 1.90                     | 0.54              |
| 22:A:195:LEU:CD2  | 22:A:314:ASN:HD21 | 2.21                     | 0.54              |
| 22:A:249:TYR:HB2  | 22:A:252:GLU:OE1  | 2.07                     | 0.54              |
| 25:F:198:LEU:CD2  | 25:F:202:ILE:HB   | 2.38                     | 0.54              |
| 26:K:157:ASP:OD1  | 26:K:161:THR:HG22 | 2.08                     | 0.54              |
| 27:U:345:ASN:HD21 | 27:U:883:ARG:HG2  | 1.72                     | 0.54              |
| 27:U:361:ARG:NH1  | 27:U:720:LYS:HE3  | 2.21                     | 0.54              |
| 27:U:364:VAL:O    | 27:U:367:THR:HG22 | 2.07                     | 0.54              |
| 1:C:339:THR:HG21  | 1:C:379:THR:HG22  | 1.88                     | 0.54              |
| 1:C:368:MET:SD    | 2:D:196:ILE:HD11  | 2.47                     | 0.54              |
| 4:H:139:TRP:CZ3   | 4:H:144:PRO:HD3   | 2.34                     | 0.54              |
| 5:I:45:LEU:HD22   | 5:I:65:ILE:HD12   | 1.89                     | 0.54              |
| 6:J:208:LEU:O     | 6:J:220:LEU:HG    | 2.07                     | 0.54              |
| 8:M:73:VAL:HG21   | 8:M:111:LEU:HD23  | 1.89                     | 0.54              |
| 8:M:152:ASP:OD1   | 8:M:152:ASP:C     | 2.50                     | 0.54              |
| 9:V:109:ASN:H     | 9:V:112:VAL:CG2   | 2.20                     | 0.54              |
| 9:V:175:MET:O     | 9:V:179:LYS:N     | 2.40                     | 0.54              |
| 9:V:486:ILE:HD13  | 9:V:489:MET:HE2   | 1.89                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 10:W:263:TRP:CE3  | 10:W:295:LYS:HD3  | 2.42                     | 0.54              |
| 10:W:334:GLU:OE1  | 10:W:334:GLU:N    | 2.40                     | 0.54              |
| 10:W:420:ASP:OD1  | 10:W:420:ASP:N    | 2.34                     | 0.54              |
| 11:X:125:LEU:O    | 11:X:129:LEU:HD22 | 2.07                     | 0.54              |
| 11:X:141:LYS:HA   | 11:X:143:TYR:CE1  | 2.42                     | 0.54              |
| 12:Y:36:ALA:HA    | 12:Y:39:ASP:OD2   | 2.07                     | 0.54              |
| 13:Z:173:GLU:OE2  | 13:Z:180:LYS:HE2  | 2.07                     | 0.54              |
| 14:a:68:GLU:CG    | 14:a:69:HIS:H     | 2.20                     | 0.54              |
| 14:a:250:THR:O    | 14:a:254:ALA:HB2  | 2.07                     | 0.54              |
| 15:b:143:PHE:CE1  | 15:b:183:LEU:HD21 | 2.43                     | 0.54              |
| 17:d:228:HIS:O    | 17:d:232:LEU:HB2  | 2.08                     | 0.54              |
| 18:f:63:LEU:HB2   | 18:f:105:LYS:HZ2  | 1.72                     | 0.54              |
| 18:f:141:LYS:NZ   | 18:f:142:TYR:HE1  | 2.06                     | 0.54              |
| 18:f:460:ASP:CB   | 19:g:133:LYS:HD2  | 2.37                     | 0.54              |
| 18:f:474:SER:CB   | 18:f:477:MET:HG2  | 2.21                     | 0.54              |
| 18:f:681:TYR:OH   | 22:A:63:THR:OG1   | 2.05                     | 0.54              |
| 18:f:799:VAL:HA   | 18:f:802:SER:OG   | 2.08                     | 0.54              |
| 18:f:828:ARG:HD2  | 18:f:874:LEU:CB   | 2.37                     | 0.54              |
| 18:f:887:PHE:CE2  | 18:f:902:LYS:HG2  | 2.42                     | 0.54              |
| 19:g:108:THR:HA   | 19:g:141:THR:CA   | 2.34                     | 0.54              |
| 22:A:387:SER:HA   | 22:A:390:THR:HG22 | 1.90                     | 0.54              |
| 23:B:356:PRO:HB2  | 23:B:361:LYS:HG3  | 1.88                     | 0.54              |
| 24:E:235:ILE:HD11 | 24:E:277:MET:HA   | 1.86                     | 0.54              |
| 25:F:196:GLN:O    | 25:F:200:GLU:HG3  | 2.08                     | 0.54              |
| 25:F:197:GLU:HA   | 25:F:200:GLU:CD   | 2.33                     | 0.54              |
| 26:K:70:ILE:HD12  | 26:K:92:ALA:HB3   | 1.90                     | 0.54              |
| 27:U:205:TYR:O    | 27:U:211:PRO:HB3  | 2.08                     | 0.54              |
| 27:U:902:PRO:HG3  | 27:U:906:LEU:HD22 | 1.88                     | 0.54              |
| 2:D:120:ASP:HB2   | 2:D:123:LEU:HG    | 1.89                     | 0.54              |
| 3:G:16:PHE:HB2    | 4:H:21:GLN:OE1    | 2.08                     | 0.54              |
| 3:G:86:ASP:OD2    | 3:G:132:ARG:NH2   | 2.39                     | 0.54              |
| 3:G:190:THR:O     | 3:G:193:GLN:N     | 2.41                     | 0.54              |
| 5:I:4:ARG:HE      | 5:I:19:TYR:HE2    | 1.55                     | 0.54              |
| 6:J:43:LEU:HD12   | 6:J:72:ALA:CB     | 2.37                     | 0.54              |
| 10:W:267:LEU:CA   | 10:W:270:VAL:HG12 | 2.33                     | 0.54              |
| 11:X:96:PHE:CD2   | 11:X:97:LEU:HD22  | 2.43                     | 0.54              |
| 11:X:297:ARG:CZ   | 11:X:297:ARG:HB2  | 2.38                     | 0.54              |
| 12:Y:79:ASP:OD1   | 12:Y:80:GLU:N     | 2.40                     | 0.54              |
| 12:Y:323:PHE:O    | 12:Y:325:VAL:HG13 | 2.07                     | 0.54              |
| 14:a:131:THR:HA   | 14:a:134:THR:CG2  | 2.38                     | 0.54              |
| 14:a:203:ALA:O    | 14:a:207:GLY:N    | 2.40                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 17:d:91:ALA:O     | 17:d:95:TYR:HB2   | 2.06                     | 0.54              |
| 17:d:175:TYR:OH   | 17:d:191:LEU:HB2  | 2.08                     | 0.54              |
| 17:d:218:LYS:HD3  | 17:d:219:ASP:N    | 2.22                     | 0.54              |
| 18:f:140:LEU:HD12 | 18:f:165:GLU:C    | 2.33                     | 0.54              |
| 18:f:556:ARG:HH11 | 18:f:556:ARG:HG2  | 1.72                     | 0.54              |
| 18:f:828:ARG:HD2  | 18:f:874:LEU:N    | 2.22                     | 0.54              |
| 18:f:868:HIS:HB2  | 18:f:872:VAL:HG21 | 1.87                     | 0.54              |
| 19:g:117:ALA:HB1  | 19:g:122:LEU:C    | 2.32                     | 0.54              |
| 19:g:122:LEU:HD23 | 19:g:127:ILE:HG21 | 1.89                     | 0.54              |
| 22:A:58:LYS:O     | 22:A:62:LEU:HG    | 2.08                     | 0.54              |
| 22:A:239:ARG:O    | 22:A:239:ARG:HD2  | 2.08                     | 0.54              |
| 23:B:425:ASN:HA   | 23:B:428:TYR:CZ   | 2.42                     | 0.54              |
| 24:E:111:LEU:HD22 | 25:F:97:LEU:HD12  | 1.89                     | 0.54              |
| 25:F:185:TYR:CZ   | 25:F:243:GLN:HB3  | 2.43                     | 0.54              |
| 27:U:209:GLU:HG2  | 27:U:210:LYS:N    | 2.23                     | 0.54              |
| 27:U:258:GLN:HA   | 27:U:261:LEU:HD12 | 1.89                     | 0.54              |
| 3:G:77:GLY:HA3    | 3:G:227:PHE:CD1   | 2.42                     | 0.54              |
| 3:G:201:CYS:O     | 3:G:205:VAL:HG22  | 2.07                     | 0.54              |
| 4:H:173:PHE:CD2   | 4:H:194:THR:HA    | 2.43                     | 0.54              |
| 5:I:39:ALA:HB3    | 5:I:42:GLY:O      | 2.06                     | 0.54              |
| 8:M:117:MET:HE2   | 8:M:117:MET:N     | 2.23                     | 0.54              |
| 9:V:68:ASP:HA     | 9:V:71:THR:OG1    | 2.08                     | 0.54              |
| 9:V:128:ARG:O     | 9:V:132:LEU:HB2   | 2.07                     | 0.54              |
| 9:V:128:ARG:HA    | 9:V:132:LEU:HD23  | 1.89                     | 0.54              |
| 10:W:430:GLN:HA   | 10:W:430:GLN:OE1  | 2.06                     | 0.54              |
| 11:X:47:GLU:HG2   | 11:X:80:ILE:HG22  | 1.88                     | 0.54              |
| 12:Y:45:VAL:HA    | 12:Y:50:MET:HE3   | 1.88                     | 0.54              |
| 13:Z:6:VAL:HG23   | 13:Z:158:VAL:HG21 | 1.90                     | 0.54              |
| 14:a:83:VAL:O     | 14:a:86:GLN:N     | 2.40                     | 0.54              |
| 14:a:93:ALA:HB3   | 14:a:121:LEU:HD22 | 1.89                     | 0.54              |
| 14:a:115:LYS:O    | 14:a:118:ILE:HG23 | 2.07                     | 0.54              |
| 14:a:222:LEU:HD12 | 14:a:222:LEU:O    | 2.07                     | 0.54              |
| 17:d:142:ILE:HG22 | 17:d:146:ASP:OD2  | 2.08                     | 0.54              |
| 17:d:241:TYR:CD2  | 17:d:271:ILE:HG12 | 2.43                     | 0.54              |
| 18:f:100:ARG:N    | 18:f:101:PRO:HD3  | 2.23                     | 0.54              |
| 18:f:609:VAL:HG12 | 23:B:74:MET:SD    | 2.47                     | 0.54              |
| 18:f:726:ILE:CG2  | 18:f:762:VAL:HA   | 2.37                     | 0.54              |
| 23:B:112:LEU:HB2  | 23:B:150:VAL:CG1  | 2.38                     | 0.54              |
| 26:K:154:PHE:CE1  | 26:K:164:GLN:HB3  | 2.43                     | 0.54              |
| 1:C:162:LYS:CG    | 1:C:166:GLU:HB2   | 2.38                     | 0.54              |
| 2:D:205:TYR:CB    | 2:D:314:ALA:HB2   | 2.38                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:D:291:GLU:OE1   | 2:D:291:GLU:HA    | 2.08                     | 0.54              |
| 6:J:130:SER:O     | 6:J:161:ILE:HD12  | 2.08                     | 0.54              |
| 7:L:26:MET:HE1    | 7:L:148:CYS:CB    | 2.20                     | 0.54              |
| 7:L:143:HIS:HB3   | 7:L:145:PHE:HE1   | 1.72                     | 0.54              |
| 7:L:192:LEU:HD13  | 7:L:233:LEU:HD23  | 1.89                     | 0.54              |
| 9:V:414:TYR:OH    | 9:V:425:LYS:HE3   | 2.08                     | 0.54              |
| 9:V:472:PRO:HB3   | 12:Y:366:TYR:CE1  | 2.43                     | 0.54              |
| 10:W:78:LYS:N     | 10:W:78:LYS:HD2   | 2.21                     | 0.54              |
| 10:W:212:LYS:O    | 10:W:212:LYS:HD3  | 2.07                     | 0.54              |
| 10:W:278:PRO:CG   | 10:W:357:ARG:HH21 | 2.16                     | 0.54              |
| 10:W:327:GLU:OE1  | 10:W:327:GLU:C    | 2.51                     | 0.54              |
| 10:W:404:ALA:O    | 10:W:405:LYS:HD3  | 2.07                     | 0.54              |
| 11:X:200:ILE:CG1  | 11:X:201:TYR:H    | 2.20                     | 0.54              |
| 11:X:339:ILE:CD1  | 11:X:345:VAL:HG11 | 2.37                     | 0.54              |
| 13:Z:11:VAL:HG13  | 13:Z:15:VAL:CG1   | 2.38                     | 0.54              |
| 13:Z:16:LEU:HD13  | 16:c:216:MET:CG   | 2.38                     | 0.54              |
| 13:Z:39:LEU:O     | 13:Z:92:VAL:HG22  | 2.08                     | 0.54              |
| 14:a:217:LEU:HA   | 14:a:223:GLU:CD   | 2.33                     | 0.54              |
| 14:a:252:LYS:HA   | 14:a:255:TRP:CD1  | 2.42                     | 0.54              |
| 15:b:4:GLU:OE1    | 15:b:108:ARG:HB3  | 2.08                     | 0.54              |
| 15:b:41:THR:HG23  | 15:b:42:ARG:HD2   | 1.90                     | 0.54              |
| 18:f:753:ALA:HA   | 18:f:759:LEU:HD22 | 1.90                     | 0.54              |
| 18:f:830:LEU:HB3  | 18:f:872:VAL:N    | 2.22                     | 0.54              |
| 19:g:169:PHE:O    | 19:g:173:GLU:HB3  | 2.08                     | 0.54              |
| 22:A:72:LEU:HD11  | 23:B:103:ARG:NH2  | 2.22                     | 0.54              |
| 22:A:112:ILE:HG12 | 22:A:122:VAL:HG22 | 1.90                     | 0.54              |
| 24:E:151:LEU:HB3  | 24:E:159:PHE:CZ   | 2.43                     | 0.54              |
| 27:U:12:LEU:H     | 27:U:12:LEU:HD12  | 1.72                     | 0.54              |
| 27:U:703:CYS:O    | 27:U:706:VAL:HG12 | 2.08                     | 0.54              |
| 1:C:81:ASP:O      | 1:C:82:LYS:HB2    | 2.07                     | 0.54              |
| 7:L:160:SER:O     | 7:L:165:SER:HB2   | 2.08                     | 0.54              |
| 8:M:15:SER:OG     | 8:M:17:ASP:OD1    | 2.16                     | 0.54              |
| 9:V:177:ASN:O     | 9:V:179:LYS:NZ    | 2.38                     | 0.54              |
| 10:W:132:THR:HB   | 10:W:138:VAL:CG1  | 2.38                     | 0.54              |
| 10:W:166:LEU:HD23 | 10:W:192:LEU:HD12 | 1.90                     | 0.54              |
| 11:X:57:LEU:CD2   | 11:X:66:LEU:HB2   | 2.37                     | 0.54              |
| 11:X:91:SER:O     | 11:X:95:LEU:HD23  | 2.08                     | 0.54              |
| 12:Y:152:MET:HG3  | 12:Y:152:MET:O    | 2.08                     | 0.54              |
| 13:Z:173:GLU:OE2  | 13:Z:173:GLU:HA   | 2.08                     | 0.54              |
| 13:Z:199:LYS:HA   | 14:a:364:GLU:OE1  | 2.07                     | 0.54              |
| 14:a:37:LEU:HD21  | 14:a:64:ILE:CD1   | 2.38                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 14:a:243:GLY:HA2  | 14:a:272:ILE:HD12 | 1.90                     | 0.54              |
| 14:a:247:ARG:HD2  | 14:a:301:LYS:HD3  | 1.90                     | 0.54              |
| 14:a:371:ALA:HB1  | 14:a:374:ILE:CG2  | 2.37                     | 0.54              |
| 14:a:371:ALA:O    | 14:a:375:LEU:HB2  | 2.07                     | 0.54              |
| 18:f:191:ILE:HD13 | 18:f:207:LEU:HD21 | 1.89                     | 0.54              |
| 18:f:350:LYS:O    | 18:f:350:LYS:HG2  | 2.08                     | 0.54              |
| 18:f:433:LEU:CD1  | 18:f:441:LYS:HA   | 2.36                     | 0.54              |
| 24:E:83:CYS:SG    | 24:E:89:LYS:NZ    | 2.63                     | 0.54              |
| 24:E:125:GLU:HB2  | 25:F:344:ARG:NH2  | 2.22                     | 0.54              |
| 24:E:305:ASN:HB2  | 24:E:308:ALA:HB2  | 1.90                     | 0.54              |
| 25:F:80:ILE:O     | 25:F:84:LYS:HG2   | 2.07                     | 0.54              |
| 25:F:268:VAL:HG11 | 25:F:313:LEU:HA   | 1.90                     | 0.54              |
| 27:U:247:GLN:HG3  | 27:U:904:LYS:CD   | 2.38                     | 0.54              |
| 27:U:649:ARG:HH11 | 27:U:678:ASP:CG   | 2.16                     | 0.54              |
| 1:C:310:ARG:O     | 1:C:311:ILE:HD13  | 2.08                     | 0.54              |
| 2:D:147:ALA:HB1   | 2:D:253:LEU:HD11  | 1.89                     | 0.54              |
| 2:D:402:ALA:O     | 2:D:405:THR:HG22  | 2.08                     | 0.54              |
| 3:G:15:ILE:HD13   | 4:H:8:PHE:HB3     | 1.88                     | 0.54              |
| 4:H:177:ARG:HG2   | 4:H:177:ARG:HH11  | 1.72                     | 0.54              |
| 5:I:178:ASP:C     | 5:I:178:ASP:OD1   | 2.51                     | 0.54              |
| 6:J:109:ARG:HH11  | 6:J:109:ARG:HG3   | 1.72                     | 0.54              |
| 9:V:365:GLN:NE2   | 28:e:46:ASP:HB3   | 2.22                     | 0.54              |
| 10:W:140:ILE:CG2  | 10:W:144:ARG:HH22 | 2.21                     | 0.54              |
| 11:X:67:GLY:O     | 11:X:71:LYS:HG2   | 2.08                     | 0.54              |
| 11:X:173:GLU:CA   | 11:X:176:THR:HG22 | 2.38                     | 0.54              |
| 11:X:306:LEU:HD11 | 11:X:314:ARG:NE   | 2.22                     | 0.54              |
| 11:X:397:TYR:O    | 11:X:401:LEU:HD23 | 2.07                     | 0.54              |
| 12:Y:58:CYS:O     | 12:Y:62:ASP:N     | 2.41                     | 0.54              |
| 13:Z:223:ASN:O    | 13:Z:224:HIS:HB3  | 2.07                     | 0.54              |
| 14:a:21:VAL:HA    | 14:a:44:PHE:CE2   | 2.43                     | 0.54              |
| 14:a:58:LYS:NZ    | 14:a:58:LYS:HB2   | 2.23                     | 0.54              |
| 14:a:61:GLU:CG    | 14:a:79:ILE:HD13  | 2.38                     | 0.54              |
| 14:a:317:VAL:HB   | 14:a:319:LEU:CD1  | 2.38                     | 0.54              |
| 15:b:130:ARG:HB3  | 15:b:130:ARG:CZ   | 2.36                     | 0.54              |
| 15:b:154:THR:HA   | 15:b:170:LEU:CD2  | 2.38                     | 0.54              |
| 16:c:75:MET:HE1   | 16:c:88:ASP:N     | 2.22                     | 0.54              |
| 17:d:98:LEU:HG    | 17:d:150:ILE:HD13 | 1.90                     | 0.54              |
| 18:f:66:LYS:HA    | 18:f:71:TYR:CZ    | 2.43                     | 0.54              |
| 18:f:386:GLY:C    | 18:f:418:LEU:HD21 | 2.33                     | 0.54              |
| 18:f:390:LEU:HB3  | 18:f:398:TRP:CZ3  | 2.43                     | 0.54              |
| 18:f:539:LEU:HD11 | 18:f:579:ALA:HB1  | 1.89                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 18:f:745:LEU:HD13 | 18:f:766:GLN:N    | 2.23                     | 0.54              |
| 18:f:833:PHE:C    | 18:f:840:LEU:HB3  | 2.33                     | 0.54              |
| 19:g:164:ASP:C    | 19:g:168:ASN:H    | 2.15                     | 0.54              |
| 22:A:111:TYR:CD1  | 22:A:125:LEU:HD21 | 2.43                     | 0.54              |
| 26:K:108:THR:N    | 26:K:111:SER:OG   | 2.41                     | 0.54              |
| 26:K:112:VAL:O    | 26:K:115:ALA:N    | 2.41                     | 0.54              |
| 27:U:452:ASN:ND2  | 27:U:758:PRO:HG3  | 2.23                     | 0.54              |
| 27:U:549:ALA:CA   | 27:U:581:SER:HB2  | 2.36                     | 0.54              |
| 27:U:638:SER:CB   | 27:U:671:LEU:HD11 | 2.38                     | 0.54              |
| 27:U:646:PRO:CG   | 27:U:680:VAL:HG21 | 2.38                     | 0.54              |
| 27:U:699:THR:O    | 27:U:702:THR:N    | 2.39                     | 0.54              |
| 1:C:37:ASP:OD1    | 1:C:38:LYS:HE3    | 2.09                     | 0.53              |
| 1:C:163:GLU:HB3   | 23:B:404:LEU:HD13 | 1.90                     | 0.53              |
| 1:C:314:LYS:CE    | 23:B:429:LYS:HB3  | 2.38                     | 0.53              |
| 6:J:103:THR:HG23  | 6:J:106:TYR:H     | 1.73                     | 0.53              |
| 8:M:163:CYS:SG    | 8:M:164:ALA:N     | 2.82                     | 0.53              |
| 9:V:121:PHE:HZ    | 9:V:164:GLU:HA    | 1.73                     | 0.53              |
| 10:W:20:TYR:HB3   | 10:W:23:THR:OG1   | 2.08                     | 0.53              |
| 10:W:131:VAL:O    | 10:W:135:LYS:HD2  | 2.08                     | 0.53              |
| 10:W:256:ILE:HA   | 10:W:259:GLU:OE2  | 2.08                     | 0.53              |
| 10:W:272:LEU:HD21 | 10:W:341:PHE:CE2  | 2.42                     | 0.53              |
| 13:Z:65:ASP:OD1   | 13:Z:103:LYS:HD2  | 2.07                     | 0.53              |
| 13:Z:135:THR:HG21 | 13:Z:162:ILE:HD11 | 1.90                     | 0.53              |
| 14:a:109:GLU:HG3  | 14:a:151:VAL:CG1  | 2.39                     | 0.53              |
| 16:c:188:SER:O    | 16:c:192:LEU:HD13 | 2.07                     | 0.53              |
| 16:c:291:LEU:O    | 16:c:295:ASN:ND2  | 2.40                     | 0.53              |
| 18:f:422:VAL:HG11 | 18:f:461:PRO:HG2  | 1.89                     | 0.53              |
| 18:f:513:GLU:HB2  | 18:f:554:TYR:CD2  | 2.43                     | 0.53              |
| 19:g:89:LEU:HB3   | 19:g:90:PRO:CD    | 2.38                     | 0.53              |
| 19:g:130:VAL:HG12 | 19:g:135:GLN:HE21 | 1.73                     | 0.53              |
| 22:A:119:ALA:HB1  | 25:F:89:LEU:HD11  | 1.90                     | 0.53              |
| 22:A:209:PRO:HD3  | 25:F:405:MET:HE3  | 1.89                     | 0.53              |
| 22:A:425:ALA:O    | 22:A:429:TYR:HB2  | 2.08                     | 0.53              |
| 24:E:277:MET:HE1  | 24:E:289:LEU:HD22 | 1.89                     | 0.53              |
| 25:F:136:VAL:HG23 | 25:F:159:LEU:HD11 | 1.88                     | 0.53              |
| 26:K:69:GLU:HG3   | 26:K:71:ASP:O     | 2.08                     | 0.53              |
| 2:D:133:HIS:O     | 2:D:137:ASN:HA    | 2.08                     | 0.53              |
| 2:D:377:SER:C     | 2:D:379:CYS:N     | 2.65                     | 0.53              |
| 3:G:10:ASP:OD2    | 8:M:7:TYR:HE2     | 1.91                     | 0.53              |
| 4:H:44:VAL:HB     | 4:H:213:CYS:HB2   | 1.91                     | 0.53              |
| 4:H:119:GLN:HG3   | 5:I:81:SER:HB2    | 1.90                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:I:35:LEU:HA     | 5:I:162:THR:O     | 2.09                     | 0.53              |
| 5:I:71:ASP:HB3    | 5:I:223:THR:HG21  | 1.90                     | 0.53              |
| 6:J:83:VAL:HG11   | 6:J:129:ILE:HD11  | 1.88                     | 0.53              |
| 7:L:36:VAL:CG1    | 7:L:47:VAL:HB     | 2.38                     | 0.53              |
| 9:V:217:VAL:O     | 9:V:221:LEU:HG    | 2.09                     | 0.53              |
| 9:V:276:PHE:HD1   | 9:V:277:PRO:CD    | 2.21                     | 0.53              |
| 9:V:379:LEU:O     | 9:V:383:GLY:HA3   | 2.09                     | 0.53              |
| 10:W:385:SER:OG   | 10:W:388:GLU:HG3  | 2.07                     | 0.53              |
| 10:W:385:SER:N    | 10:W:388:GLU:OE2  | 2.29                     | 0.53              |
| 11:X:57:LEU:CG    | 11:X:62:GLN:HB2   | 2.38                     | 0.53              |
| 11:X:96:PHE:CE2   | 11:X:109:LEU:HD13 | 2.43                     | 0.53              |
| 13:Z:129:LYS:HD2  | 16:c:215:LYS:HG3  | 1.89                     | 0.53              |
| 14:a:221:VAL:HB   | 14:a:225:LEU:HD12 | 1.91                     | 0.53              |
| 16:c:292:MET:SD   | 17:d:346:LEU:HD22 | 2.48                     | 0.53              |
| 17:d:192:LEU:HD12 | 17:d:215:LEU:HD21 | 1.88                     | 0.53              |
| 18:f:411:ALA:O    | 18:f:414:LEU:HB2  | 2.07                     | 0.53              |
| 18:f:434:TYR:HB2  | 19:g:170:GLN:O    | 2.08                     | 0.53              |
| 19:g:112:LEU:CG   | 19:g:142:LEU:HD11 | 2.37                     | 0.53              |
| 19:g:116:ILE:HG21 | 19:g:129:ILE:CG1  | 2.38                     | 0.53              |
| 19:g:131:ILE:HG21 | 19:g:147:VAL:CG2  | 2.34                     | 0.53              |
| 22:A:274:PHE:HB2  | 22:A:319:MET:HG3  | 1.91                     | 0.53              |
| 25:F:129:ARG:HH11 | 25:F:129:ARG:HG3  | 1.73                     | 0.53              |
| 26:K:195:ILE:HD12 | 26:K:217:LEU:CD1  | 2.38                     | 0.53              |
| 27:U:252:LEU:HD23 | 27:U:329:LEU:CD2  | 2.38                     | 0.53              |
| 27:U:496:LEU:HD12 | 27:U:496:LEU:O    | 2.08                     | 0.53              |
| 27:U:606:ALA:HB2  | 27:U:618:ALA:HB3  | 1.88                     | 0.53              |
| 27:U:698:GLN:O    | 27:U:706:VAL:HG21 | 2.07                     | 0.53              |
| 27:U:736:ILE:HD11 | 27:U:779:LEU:HD23 | 1.90                     | 0.53              |
| 1:C:156:LYS:NZ    | 1:C:160:GLU:OE2   | 2.42                     | 0.53              |
| 1:C:225:GLY:HA3   | 23:B:256:ILE:O    | 2.08                     | 0.53              |
| 2:D:399:PHE:O     | 2:D:403:TYR:N     | 2.39                     | 0.53              |
| 4:H:148:GLN:HB3   | 4:H:156:PHE:HD2   | 1.73                     | 0.53              |
| 5:I:148:TYR:CD1   | 5:I:158:GLY:HA2   | 2.43                     | 0.53              |
| 9:V:61:GLU:CA     | 9:V:64:GLN:HB3    | 2.38                     | 0.53              |
| 9:V:263:LEU:N     | 9:V:263:LEU:HD12  | 2.24                     | 0.53              |
| 9:V:417:ILE:CD1   | 9:V:422:ILE:HG13  | 2.36                     | 0.53              |
| 10:W:49:SER:HA    | 10:W:52:LYS:NZ    | 2.23                     | 0.53              |
| 10:W:319:THR:O    | 10:W:323:ASP:HB2  | 2.08                     | 0.53              |
| 12:Y:179:ARG:HG3  | 12:Y:210:SER:HB3  | 1.91                     | 0.53              |
| 12:Y:314:LEU:HD13 | 12:Y:319:MET:HG3  | 1.91                     | 0.53              |
| 13:Z:67:VAL:HG21  | 15:b:91:ARG:CD    | 2.31                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 13:Z:201:LEU:HB2  | 16:c:225:TRP:CZ3  | 2.43                     | 0.53              |
| 14:a:25:LEU:HD22  | 14:a:37:LEU:CD1   | 2.36                     | 0.53              |
| 14:a:122:LYS:O    | 14:a:122:LYS:HG2  | 2.09                     | 0.53              |
| 15:b:109:ILE:CB   | 15:b:138:VAL:HG23 | 2.38                     | 0.53              |
| 15:b:109:ILE:HG22 | 15:b:138:VAL:HG23 | 1.91                     | 0.53              |
| 16:c:29:GLU:OE2   | 16:c:161:ARG:NH2  | 2.41                     | 0.53              |
| 17:d:337:LYS:HB2  | 17:d:337:LYS:HZ3  | 1.73                     | 0.53              |
| 18:f:702:PRO:CG   | 18:f:736:THR:HG21 | 2.38                     | 0.53              |
| 22:A:397:ILE:CD1  | 23:B:210:TYR:HB3  | 2.31                     | 0.53              |
| 24:E:317:ALA:HB1  | 24:E:322:LYS:HE3  | 1.91                     | 0.53              |
| 25:F:226:TYR:HB2  | 25:F:335:VAL:HG21 | 1.90                     | 0.53              |
| 25:F:238:ARG:O    | 25:F:242:ALA:N    | 2.37                     | 0.53              |
| 25:F:347:ARG:O    | 25:F:349:ASP:N    | 2.41                     | 0.53              |
| 26:K:74:ILE:HG23  | 26:K:74:ILE:O     | 2.08                     | 0.53              |
| 27:U:134:VAL:O    | 27:U:138:PHE:N    | 2.29                     | 0.53              |
| 27:U:426:TYR:C    | 27:U:427:LEU:HD22 | 2.33                     | 0.53              |
| 27:U:629:THR:HG23 | 27:U:629:THR:O    | 2.08                     | 0.53              |
| 27:U:805:ASN:HB3  | 27:U:891:VAL:HB   | 1.89                     | 0.53              |
| 1:C:180:ILE:HD12  | 1:C:180:ILE:C     | 2.33                     | 0.53              |
| 1:C:306:LEU:O     | 23:B:429:LYS:HG3  | 2.09                     | 0.53              |
| 1:C:350:LEU:HD23  | 1:C:387:VAL:CG1   | 2.38                     | 0.53              |
| 4:H:174:LEU:C     | 4:H:176:LYS:H     | 2.15                     | 0.53              |
| 6:J:33:VAL:HG23   | 6:J:159:ASN:O     | 2.08                     | 0.53              |
| 8:M:189:ILE:O     | 8:M:192:GLU:N     | 2.39                     | 0.53              |
| 9:V:289:LEU:CB    | 9:V:312:ALA:HB2   | 2.38                     | 0.53              |
| 10:W:166:LEU:HD12 | 10:W:166:LEU:O    | 2.09                     | 0.53              |
| 10:W:194:LEU:CD2  | 10:W:202:THR:HG21 | 2.35                     | 0.53              |
| 10:W:263:TRP:CH2  | 10:W:295:LYS:HD3  | 2.43                     | 0.53              |
| 10:W:355:LYS:O    | 10:W:359:VAL:HG23 | 2.09                     | 0.53              |
| 11:X:414:LEU:HD21 | 13:Z:273:HIS:CG   | 2.42                     | 0.53              |
| 12:Y:70:LEU:CD1   | 12:Y:74:LYS:HG3   | 2.39                     | 0.53              |
| 14:a:189:PRO:CD   | 14:a:192:GLU:HB2  | 2.39                     | 0.53              |
| 14:a:247:ARG:HD3  | 14:a:301:LYS:NZ   | 2.22                     | 0.53              |
| 14:a:320:VAL:HG13 | 14:a:333:MET:SD   | 2.48                     | 0.53              |
| 14:a:331:VAL:O    | 14:a:331:VAL:HG12 | 2.08                     | 0.53              |
| 15:b:52:ILE:HD12  | 15:b:60:VAL:HG13  | 1.91                     | 0.53              |
| 16:c:63:ASP:OD1   | 16:c:63:ASP:C     | 2.50                     | 0.53              |
| 18:f:459:CYS:O    | 19:g:133:LYS:HA   | 2.08                     | 0.53              |
| 18:f:704:LEU:HD11 | 18:f:740:ARG:HD2  | 1.90                     | 0.53              |
| 18:f:787:LEU:HD23 | 18:f:787:LEU:O    | 2.08                     | 0.53              |
| 19:g:112:LEU:CG   | 19:g:116:ILE:HD12 | 2.38                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 19:g:132:ASN:C    | 19:g:133:LYS:HG2  | 2.34                     | 0.53              |
| 22:A:245:LEU:HD12 | 22:A:280:ILE:CD1  | 2.38                     | 0.53              |
| 24:E:111:LEU:HD22 | 25:F:97:LEU:CD1   | 2.37                     | 0.53              |
| 25:F:333:ASN:C    | 25:F:333:ASN:OD1  | 2.52                     | 0.53              |
| 27:U:177:LEU:HD21 | 27:U:205:TYR:CZ   | 2.43                     | 0.53              |
| 27:U:532:MET:HG2  | 27:U:548:LEU:HD11 | 1.89                     | 0.53              |
| 1:C:266:ASP:HB3   | 1:C:269:VAL:HG12  | 1.90                     | 0.53              |
| 2:D:40:LEU:HD23   | 27:U:149:GLN:CD   | 2.32                     | 0.53              |
| 2:D:383:GLY:HA2   | 2:D:394:VAL:HG22  | 1.90                     | 0.53              |
| 4:H:36:VAL:HG13   | 4:H:195:LEU:CD2   | 2.38                     | 0.53              |
| 4:H:72:ILE:HG21   | 4:H:110:LEU:HD23  | 1.90                     | 0.53              |
| 7:L:95:SER:OG     | 7:L:103:LEU:HD13  | 2.09                     | 0.53              |
| 8:M:161:TRP:HB3   | 8:M:181:MET:HE1   | 1.90                     | 0.53              |
| 10:W:112:VAL:HG21 | 10:W:145:LEU:HD21 | 1.91                     | 0.53              |
| 10:W:122:LEU:HA   | 10:W:125:ILE:CD1  | 2.37                     | 0.53              |
| 10:W:183:VAL:O    | 10:W:187:LEU:HD23 | 2.07                     | 0.53              |
| 11:X:182:ASN:OD1  | 11:X:185:LYS:HB2  | 2.08                     | 0.53              |
| 13:Z:40:LEU:HD11  | 13:Z:54:PHE:CD2   | 2.43                     | 0.53              |
| 14:a:118:ILE:O    | 14:a:122:LYS:CB   | 2.56                     | 0.53              |
| 15:b:33:VAL:HG11  | 15:b:75:LEU:CD1   | 2.36                     | 0.53              |
| 15:b:53:THR:CB    | 15:b:61:LEU:HD11  | 2.39                     | 0.53              |
| 17:d:207:GLU:HA   | 17:d:210:THR:CG2  | 2.38                     | 0.53              |
| 18:f:137:ARG:HA   | 18:f:137:ARG:NE   | 2.23                     | 0.53              |
| 18:f:375:SER:HA   | 18:f:398:TRP:CZ2  | 2.43                     | 0.53              |
| 18:f:566:HIS:O    | 18:f:599:ALA:HA   | 2.09                     | 0.53              |
| 18:f:670:MET:HE3  | 23:B:68:ILE:HA    | 1.91                     | 0.53              |
| 18:f:764:LEU:HD11 | 18:f:818:LEU:CD2  | 2.37                     | 0.53              |
| 19:g:105:LEU:CD1  | 19:g:142:LEU:HD23 | 2.39                     | 0.53              |
| 22:A:166:VAL:CG1  | 22:A:237:PHE:HB3  | 2.38                     | 0.53              |
| 22:A:171:ASP:OD1  | 22:A:171:ASP:N    | 2.26                     | 0.53              |
| 24:E:110:TYR:O    | 24:E:111:LEU:HD23 | 2.08                     | 0.53              |
| 25:F:230:GLY:O    | 25:F:393:GLY:N    | 2.41                     | 0.53              |
| 26:K:99:HIS:HD2   | 26:K:107:MET:HE3  | 1.74                     | 0.53              |
| 26:K:168:ARG:HA   | 26:K:178:GLN:HE22 | 1.73                     | 0.53              |
| 27:U:399:TRP:O    | 27:U:402:PHE:N    | 2.37                     | 0.53              |
| 27:U:791:LEU:CD1  | 27:U:797:MET:HE1  | 2.38                     | 0.53              |
| 1:C:384:GLU:HA    | 1:C:387:VAL:CG1   | 2.37                     | 0.53              |
| 3:G:101:TRP:CE3   | 3:G:109:ILE:HD12  | 2.44                     | 0.53              |
| 7:L:109:VAL:HG21  | 7:L:145:PHE:CG    | 2.43                     | 0.53              |
| 7:L:233:LEU:CD2   | 7:L:236:LEU:HD22  | 2.37                     | 0.53              |
| 8:M:67:PHE:HZ     | 8:M:85:ARG:HD2    | 1.72                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 8:M:160:TYR:CD2   | 8:M:163:CYS:HB2   | 2.43                     | 0.53              |
| 9:V:421:ASP:OD2   | 12:Y:349:LYS:HG2  | 2.08                     | 0.53              |
| 10:W:428:TRP:CD1  | 13:Z:238:PRO:HB3  | 2.43                     | 0.53              |
| 10:W:451:MET:HE2  | 13:Z:100:LYS:CD   | 2.38                     | 0.53              |
| 12:Y:236:LEU:HD12 | 12:Y:240:VAL:HB   | 1.91                     | 0.53              |
| 14:a:275:LEU:HA   | 14:a:278:MET:HE3  | 1.90                     | 0.53              |
| 14:a:281:THR:HA   | 14:a:284:ARG:HG3  | 1.89                     | 0.53              |
| 17:d:141:LEU:HG   | 17:d:182:LEU:HD21 | 1.91                     | 0.53              |
| 18:f:241:PRO:HG3  | 27:U:835:ILE:CG2  | 2.38                     | 0.53              |
| 18:f:562:LEU:HD23 | 18:f:562:LEU:C    | 2.33                     | 0.53              |
| 22:A:433:ASN:C    | 26:K:66:LYS:HD3   | 2.33                     | 0.53              |
| 23:B:214:MET:O    | 23:B:214:MET:HG3  | 2.07                     | 0.53              |
| 23:B:406:ALA:HB1  | 23:B:411:ARG:O    | 2.08                     | 0.53              |
| 26:K:74:ILE:CD1   | 26:K:109:VAL:HG23 | 2.38                     | 0.53              |
| 27:U:153:ILE:HD12 | 27:U:156:GLU:OE1  | 2.09                     | 0.53              |
| 27:U:160:LEU:HD11 | 27:U:196:LYS:CD   | 2.38                     | 0.53              |
| 27:U:321:GLN:OE1  | 27:U:324:LYS:HB3  | 2.09                     | 0.53              |
| 27:U:346:ASN:OD1  | 27:U:348:THR:HG23 | 2.09                     | 0.53              |
| 27:U:446:LEU:O    | 27:U:446:LEU:HD23 | 2.07                     | 0.53              |
| 27:U:603:LEU:HG   | 27:U:622:LEU:HD21 | 1.91                     | 0.53              |
| 27:U:761:VAL:O    | 27:U:765:VAL:HG12 | 2.09                     | 0.53              |
| 1:C:368:MET:CA    | 1:C:368:MET:HE3   | 2.38                     | 0.53              |
| 2:D:45:LYS:CB     | 27:U:187:LEU:HD13 | 2.36                     | 0.53              |
| 5:I:43:VAL:CG1    | 5:I:137:ILE:HB    | 2.39                     | 0.53              |
| 5:I:153:SER:HG    | 5:I:155:ASN:ND2   | 2.06                     | 0.53              |
| 6:J:68:ASN:CA     | 6:J:211:MET:HE1   | 2.37                     | 0.53              |
| 6:J:158:ALA:HB1   | 6:J:172:LEU:HD21  | 1.89                     | 0.53              |
| 7:L:158:ALA:HB1   | 7:L:172:LEU:CD1   | 2.39                     | 0.53              |
| 9:V:345:ARG:HG2   | 28:e:41:ASP:O     | 2.09                     | 0.53              |
| 10:W:125:ILE:HD12 | 10:W:149:LEU:HD13 | 1.90                     | 0.53              |
| 12:Y:101:ARG:HD2  | 12:Y:131:THR:CA   | 2.38                     | 0.53              |
| 12:Y:114:ILE:CD1  | 12:Y:116:ASP:HB2  | 2.34                     | 0.53              |
| 13:Z:74:TYR:O     | 13:Z:74:TYR:HD1   | 1.92                     | 0.53              |
| 13:Z:125:ASP:HB2  | 13:Z:128:PRO:CG   | 2.37                     | 0.53              |
| 13:Z:227:ILE:CG1  | 14:a:346:ILE:HD11 | 2.39                     | 0.53              |
| 14:a:8:LEU:HA     | 14:a:22:TRP:HZ3   | 1.73                     | 0.53              |
| 15:b:73:SER:HA    | 25:F:61:ARG:NE    | 2.24                     | 0.53              |
| 16:c:303:MET:CE   | 17:d:335:LEU:HD13 | 2.39                     | 0.53              |
| 18:f:93:PRO:HG2   | 18:f:96:LEU:HB2   | 1.91                     | 0.53              |
| 18:f:465:LEU:HD11 | 19:g:173:GLU:CG   | 2.39                     | 0.53              |
| 18:f:723:TYR:CE2  | 18:f:811:LEU:HD11 | 2.44                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 18:f:783:SER:HB3  | 18:f:787:LEU:HB3  | 1.90                     | 0.53              |
| 22:A:101:ILE:O    | 22:A:101:ILE:CG2  | 2.57                     | 0.53              |
| 23:B:430:LYS:HZ3  | 23:B:430:LYS:HA   | 1.73                     | 0.53              |
| 24:E:133:SER:O    | 24:E:315:ILE:CD1  | 2.57                     | 0.53              |
| 25:F:251:LEU:CG   | 25:F:256:LEU:HD11 | 2.38                     | 0.53              |
| 27:U:21:GLU:OE1   | 27:U:56:SER:HB2   | 2.08                     | 0.53              |
| 27:U:62:LEU:O     | 27:U:66:LYS:HG3   | 2.09                     | 0.53              |
| 27:U:348:THR:HG22 | 27:U:741:GLY:CA   | 2.39                     | 0.53              |
| 27:U:497:LEU:CD1  | 27:U:515:ALA:HB1  | 2.39                     | 0.53              |
| 27:U:646:PRO:HB2  | 27:U:682:TYR:OH   | 2.09                     | 0.53              |
| 27:U:655:ALA:O    | 27:U:659:CYS:HB3  | 2.08                     | 0.53              |
| 1:C:175:PHE:CD2   | 1:C:180:ILE:HD11  | 2.44                     | 0.53              |
| 1:C:188:LEU:HD22  | 1:C:317:PHE:CE1   | 2.44                     | 0.53              |
| 1:C:345:ARG:HG3   | 1:C:345:ARG:NH1   | 2.21                     | 0.53              |
| 4:H:71:HIS:CE1    | 4:H:104:PRO:HB3   | 2.44                     | 0.53              |
| 5:I:90:LEU:HG     | 5:I:114:LEU:CD2   | 2.25                     | 0.53              |
| 7:L:46:LEU:HD12   | 7:L:46:LEU:O      | 2.09                     | 0.53              |
| 9:V:443:ARG:CG    | 17:d:277:LYS:HE2  | 2.39                     | 0.53              |
| 9:V:469:THR:HG22  | 9:V:470:ARG:N     | 2.19                     | 0.53              |
| 10:W:187:LEU:HD13 | 10:W:229:LEU:HD12 | 1.89                     | 0.53              |
| 11:X:75:PRO:HA    | 11:X:78:ASN:OD1   | 2.08                     | 0.53              |
| 11:X:414:LEU:HD11 | 13:Z:273:HIS:CB   | 2.34                     | 0.53              |
| 12:Y:233:ARG:NH2  | 12:Y:264:TYR:O    | 2.32                     | 0.53              |
| 12:Y:349:LYS:HG3  | 12:Y:349:LYS:O    | 2.08                     | 0.53              |
| 14:a:7:PHE:CE2    | 14:a:60:TYR:HA    | 2.38                     | 0.53              |
| 14:a:68:GLU:CG    | 14:a:69:HIS:N     | 2.71                     | 0.53              |
| 14:a:154:ARG:HA   | 14:a:157:ASP:HB2  | 1.90                     | 0.53              |
| 14:a:186:LYS:CE   | 14:a:190:VAL:HA   | 2.39                     | 0.53              |
| 14:a:285:PRO:O    | 14:a:286:ALA:HB3  | 2.09                     | 0.53              |
| 14:a:374:ILE:CD1  | 17:d:347:GLU:HG3  | 2.38                     | 0.53              |
| 15:b:11:ASP:CG    | 15:b:84:ILE:HD12  | 2.34                     | 0.53              |
| 15:b:16:MET:CE    | 15:b:26:LEU:HD12  | 2.39                     | 0.53              |
| 17:d:258:PHE:CZ   | 17:d:262:ILE:HD11 | 2.44                     | 0.53              |
| 17:d:310:LEU:HA   | 17:d:316:TYR:HA   | 1.90                     | 0.53              |
| 18:f:247:ALA:HA   | 18:f:250:ARG:NE   | 2.24                     | 0.53              |
| 18:f:267:ARG:CZ   | 18:f:893:ILE:HD13 | 2.39                     | 0.53              |
| 19:g:107:ILE:HG13 | 19:g:115:LYS:HZ2  | 1.72                     | 0.53              |
| 19:g:109:GLY:HA3  | 19:g:145:GLN:HE22 | 1.74                     | 0.53              |
| 24:E:236:ASP:HB3  | 24:E:281:ARG:HG3  | 1.90                     | 0.53              |
| 25:F:247:THR:H    | 25:F:281:SER:HA   | 1.74                     | 0.53              |
| 25:F:283:ILE:HB   | 25:F:328:VAL:HG23 | 1.91                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 26:K:81:LEU:CD1   | 26:K:138:GLY:HA3  | 2.37                     | 0.53              |
| 26:K:85:ALA:HB2   | 26:K:139:VAL:HG21 | 1.91                     | 0.53              |
| 26:K:107:MET:HE2  | 26:K:111:SER:HB2  | 1.90                     | 0.53              |
| 26:K:190:THR:CG2  | 26:K:193:GLU:H    | 2.21                     | 0.53              |
| 27:U:490:ARG:CB   | 27:U:493:VAL:HG12 | 2.39                     | 0.53              |
| 1:C:94:LYS:HE3    | 23:B:166:ASP:OD1  | 2.09                     | 0.53              |
| 1:C:131:VAL:CG1   | 1:C:136:SER:HB2   | 2.37                     | 0.53              |
| 6:J:6:ALA:HB3     | 6:J:9:VAL:HG22    | 1.91                     | 0.53              |
| 6:J:24:GLU:HA     | 6:J:24:GLU:OE2    | 2.09                     | 0.53              |
| 6:J:65:LEU:HD13   | 6:J:87:ALA:HB1    | 1.89                     | 0.53              |
| 8:M:31:GLU:OE1    | 8:M:169:ARG:NH1   | 2.41                     | 0.53              |
| 9:V:324:PHE:CE1   | 9:V:328:VAL:CG2   | 2.92                     | 0.53              |
| 10:W:165:ILE:O    | 10:W:168:GLU:HG2  | 2.09                     | 0.53              |
| 11:X:390:GLU:OE1  | 11:X:390:GLU:N    | 2.41                     | 0.53              |
| 14:a:221:VAL:HG23 | 14:a:222:LEU:N    | 2.24                     | 0.53              |
| 17:d:170:GLN:OE1  | 27:U:11:LEU:HD23  | 2.08                     | 0.53              |
| 22:A:300:LEU:HA   | 22:A:303:ILE:HG22 | 1.90                     | 0.53              |
| 24:E:271:HIS:C    | 24:E:272:ARG:NH2  | 2.67                     | 0.53              |
| 24:E:309:ARG:NH2  | 24:E:335:SER:O    | 2.42                     | 0.53              |
| 25:F:431:LYS:O    | 25:F:431:LYS:HG3  | 2.09                     | 0.53              |
| 26:K:32:LYS:O     | 26:K:172:SER:HB3  | 2.08                     | 0.53              |
| 3:G:50:ILE:CG2    | 3:G:141:ILE:HD13  | 2.39                     | 0.53              |
| 3:G:65:THR:O      | 3:G:65:THR:HG22   | 2.08                     | 0.53              |
| 6:J:133:ILE:N     | 6:J:145:TYR:O     | 2.40                     | 0.53              |
| 8:M:49:VAL:CG2    | 8:M:65:ARG:HE     | 2.21                     | 0.53              |
| 8:M:73:VAL:HG13   | 8:M:108:LEU:CD1   | 2.38                     | 0.53              |
| 9:V:115:LYS:NZ    | 9:V:146:GLN:HA    | 2.24                     | 0.53              |
| 9:V:189:ASP:OD1   | 9:V:190:ASP:N     | 2.40                     | 0.53              |
| 9:V:416:ARG:O     | 9:V:416:ARG:HG2   | 2.09                     | 0.53              |
| 10:W:377:ARG:HE   | 10:W:381:LEU:CD2  | 2.18                     | 0.53              |
| 11:X:384:VAL:HG23 | 11:X:386:ILE:CD1  | 2.39                     | 0.53              |
| 12:Y:18:ARG:HD2   | 12:Y:18:ARG:O     | 2.09                     | 0.53              |
| 12:Y:191:ILE:O    | 12:Y:191:ILE:HG13 | 2.07                     | 0.53              |
| 13:Z:246:VAL:HG13 | 17:d:330:ILE:CD1  | 2.39                     | 0.53              |
| 14:a:41:VAL:O     | 14:a:45:VAL:N     | 2.42                     | 0.53              |
| 14:a:109:GLU:HG3  | 14:a:112:ILE:CG2  | 2.39                     | 0.53              |
| 14:a:171:SER:HA   | 14:a:174:LYS:HZ2  | 1.73                     | 0.53              |
| 14:a:281:THR:OG1  | 14:a:333:MET:HG2  | 2.09                     | 0.53              |
| 16:c:261:GLU:OE2  | 16:c:263:ASP:N    | 2.37                     | 0.53              |
| 17:d:129:LEU:CD1  | 27:U:8:ILE:HD11   | 2.39                     | 0.53              |
| 17:d:300:THR:O    | 17:d:304:LYS:HG3  | 2.09                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 18:f:167:ALA:HB1  | 18:f:210:GLU:HB3  | 1.92                     | 0.53              |
| 18:f:372:LEU:HA   | 18:f:375:SER:OG   | 2.09                     | 0.53              |
| 18:f:416:MET:CE   | 18:f:819:TYR:HE1  | 2.21                     | 0.53              |
| 18:f:449:GLY:HA3  | 18:f:484:GLY:O    | 2.06                     | 0.53              |
| 18:f:526:ALA:O    | 18:f:565:ASN:ND2  | 2.41                     | 0.53              |
| 18:f:594:LEU:HD12 | 18:f:652:VAL:CG1  | 2.33                     | 0.53              |
| 18:f:606:VAL:HG21 | 23:B:70:ASP:HB3   | 1.89                     | 0.53              |
| 19:g:98:LYS:CE    | 19:g:100:LEU:HD11 | 2.38                     | 0.53              |
| 19:g:103:THR:OG1  | 19:g:115:LYS:HB2  | 2.09                     | 0.53              |
| 20:u:146:PHE:HA   | 20:u:157:LEU:HD12 | 1.91                     | 0.53              |
| 22:A:372:LEU:O    | 22:A:376:LEU:HD12 | 2.08                     | 0.53              |
| 23:B:123:VAL:HG21 | 23:B:152:LEU:HD22 | 1.91                     | 0.53              |
| 23:B:223:ILE:CG2  | 23:B:350:LYS:HA   | 2.38                     | 0.53              |
| 27:U:164:GLU:O    | 27:U:168:LEU:HD13 | 2.09                     | 0.53              |
| 27:U:796:LYS:HE2  | 27:U:798:PRO:HB3  | 1.90                     | 0.53              |
| 27:U:889:LEU:HD23 | 27:U:890:LYS:N    | 2.23                     | 0.53              |
| 1:C:21:ARG:HD2    | 1:C:21:ARG:O      | 2.09                     | 0.52              |
| 1:C:49:ARG:O      | 1:C:52:LEU:N      | 2.42                     | 0.52              |
| 3:G:137:CYS:SG    | 3:G:155:ASP:HA    | 2.49                     | 0.52              |
| 4:H:38:ILE:HD13   | 4:H:191:ALA:CB    | 2.38                     | 0.52              |
| 5:I:6:ASP:C       | 5:I:6:ASP:OD1     | 2.52                     | 0.52              |
| 11:X:183:LEU:HD11 | 11:X:220:ALA:CB   | 2.39                     | 0.52              |
| 11:X:347:ILE:HD11 | 11:X:378:LEU:HD22 | 1.90                     | 0.52              |
| 12:Y:262:SER:OG   | 12:Y:271:PHE:HB2  | 2.09                     | 0.52              |
| 12:Y:334:LEU:CB   | 12:Y:347:ILE:HD11 | 2.39                     | 0.52              |
| 13:Z:20:VAL:CG2   | 13:Z:126:VAL:HG23 | 2.39                     | 0.52              |
| 14:a:171:SER:HA   | 14:a:174:LYS:NZ   | 2.24                     | 0.52              |
| 14:a:201:GLY:O    | 14:a:205:LEU:HD23 | 2.10                     | 0.52              |
| 16:c:163:ILE:HG22 | 16:c:199:HIS:C    | 2.34                     | 0.52              |
| 18:f:160:ARG:HD3  | 22:A:39:SER:HA    | 1.90                     | 0.52              |
| 18:f:282:PHE:CE2  | 18:f:305:LEU:HD11 | 2.44                     | 0.52              |
| 18:f:499:THR:HA   | 18:f:502:LEU:CD1  | 2.39                     | 0.52              |
| 18:f:589:SER:HG   | 18:f:649:HIS:CE1  | 2.27                     | 0.52              |
| 18:f:726:ILE:HG21 | 18:f:762:VAL:HA   | 1.90                     | 0.52              |
| 18:f:873:LEU:C    | 18:f:874:LEU:HD23 | 2.34                     | 0.52              |
| 20:u:167:ILE:HG23 | 20:u:167:ILE:O    | 2.09                     | 0.52              |
| 22:A:109:PRO:HB2  | 22:A:111:TYR:CE1  | 2.44                     | 0.52              |
| 24:E:291:ARG:HB3  | 24:E:292:PRO:HD2  | 1.91                     | 0.52              |
| 25:F:315:ASN:HB3  | 25:F:316:GLN:HE21 | 1.74                     | 0.52              |
| 27:U:811:PHE:O    | 27:U:812:ALA:CB   | 2.57                     | 0.52              |
| 1:C:295:THR:OG1   | 1:C:296:ASN:N     | 2.40                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:306:LEU:HB2   | 23:B:429:LYS:HG3  | 1.90                     | 0.52              |
| 1:C:378:VAL:HG13  | 1:C:382:ASP:OD2   | 2.09                     | 0.52              |
| 3:G:165:ALA:O     | 4:H:56:LEU:HB3    | 2.09                     | 0.52              |
| 4:H:112:GLN:HG2   | 4:H:155:TYR:CE2   | 2.44                     | 0.52              |
| 6:J:16:LEU:HD12   | 26:K:81:LEU:CD2   | 2.39                     | 0.52              |
| 6:J:90:GLU:HG2    | 6:J:110:TYR:CD2   | 2.45                     | 0.52              |
| 6:J:110:TYR:HA    | 6:J:113:SER:OG    | 2.09                     | 0.52              |
| 7:L:227:ASP:O     | 7:L:231:PRO:HD3   | 2.08                     | 0.52              |
| 8:M:40:ARG:HB3    | 8:M:45:VAL:HG22   | 1.91                     | 0.52              |
| 9:V:69:THR:HA     | 9:V:72:LEU:HB2    | 1.91                     | 0.52              |
| 9:V:162:GLU:OE2   | 9:V:203:LEU:HA    | 2.09                     | 0.52              |
| 9:V:410:ILE:HG21  | 9:V:422:ILE:HG12  | 1.90                     | 0.52              |
| 11:X:347:ILE:CD1  | 11:X:378:LEU:HD22 | 2.39                     | 0.52              |
| 14:a:44:PHE:HA    | 14:a:47:ASP:HB3   | 1.91                     | 0.52              |
| 17:d:258:PHE:O    | 17:d:262:ILE:HG13 | 2.09                     | 0.52              |
| 18:f:177:GLU:OE1  | 18:f:180:GLN:HG3  | 2.09                     | 0.52              |
| 18:f:327:ASN:C    | 18:f:327:ASN:OD1  | 2.51                     | 0.52              |
| 18:f:343:LYS:CG   | 18:f:773:LYS:HE2  | 2.39                     | 0.52              |
| 18:f:546:SER:O    | 18:f:550:LEU:HG   | 2.10                     | 0.52              |
| 18:f:564:LEU:HD21 | 18:f:794:ALA:HA   | 1.91                     | 0.52              |
| 18:f:670:MET:HE1  | 23:B:50:PRO:HD2   | 1.90                     | 0.52              |
| 18:f:792:ALA:HA   | 18:f:824:ALA:HB2  | 1.90                     | 0.52              |
| 22:A:166:VAL:HG12 | 22:A:237:PHE:HB3  | 1.91                     | 0.52              |
| 22:A:193:THR:HG22 | 22:A:201:PHE:CE1  | 2.44                     | 0.52              |
| 22:A:213:LEU:HD11 | 22:A:321:THR:HG22 | 1.89                     | 0.52              |
| 22:A:394:MET:CE   | 23:B:199:GLU:HB3  | 2.39                     | 0.52              |
| 23:B:414:VAL:CG2  | 23:B:418:ASP:HB2  | 2.37                     | 0.52              |
| 24:E:35:GLU:HA    | 24:E:38:LYS:CE    | 2.39                     | 0.52              |
| 25:F:285:ILE:O    | 25:F:331:ALA:N    | 2.38                     | 0.52              |
| 25:F:425:LEU:HD13 | 25:F:432:LYS:CB   | 2.39                     | 0.52              |
| 27:U:806:CYS:H    | 27:U:874:ASN:HB2  | 1.74                     | 0.52              |
| 1:C:24:TYR:O      | 1:C:28:ILE:HG23   | 2.08                     | 0.52              |
| 1:C:165:ILE:HG23  | 1:C:245:ILE:CD1   | 2.39                     | 0.52              |
| 2:D:106:THR:HG22  | 24:E:77:PRO:HA    | 1.92                     | 0.52              |
| 2:D:119:ILE:O     | 2:D:121:ARG:NH1   | 2.42                     | 0.52              |
| 7:L:5:GLN:OE1     | 8:M:9:LEU:HD11    | 2.09                     | 0.52              |
| 7:L:33:SER:HG     | 7:L:51:ARG:NE     | 2.07                     | 0.52              |
| 8:M:87:LEU:HD13   | 8:M:131:PHE:HE2   | 1.75                     | 0.52              |
| 8:M:187:ARG:HG2   | 8:M:219:LEU:HD13  | 1.91                     | 0.52              |
| 9:V:61:GLU:O      | 9:V:65:ARG:HD2    | 2.09                     | 0.52              |
| 9:V:175:MET:HB3   | 9:V:180:ARG:O     | 2.10                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 9:V:244:ALA:HB1   | 9:V:279:GLN:NE2   | 2.24                     | 0.52              |
| 9:V:281:ASN:OD1   | 9:V:281:ASN:C     | 2.51                     | 0.52              |
| 9:V:483:CYS:SG    | 12:Y:377:LEU:HD11 | 2.49                     | 0.52              |
| 10:W:135:LYS:HD3  | 10:W:137:TYR:HE2  | 1.72                     | 0.52              |
| 11:X:406:ASN:HD21 | 16:c:253:LYS:CD   | 2.22                     | 0.52              |
| 14:a:116:THR:CG2  | 14:a:154:ARG:HB3  | 2.39                     | 0.52              |
| 14:a:216:LEU:CD2  | 14:a:238:TYR:HA   | 2.37                     | 0.52              |
| 14:a:250:THR:HA   | 14:a:253:THR:CG2  | 2.38                     | 0.52              |
| 17:d:218:LYS:HD3  | 17:d:219:ASP:OD1  | 2.10                     | 0.52              |
| 18:f:89:MET:C     | 18:f:91:SER:H     | 2.15                     | 0.52              |
| 18:f:498:LEU:O    | 18:f:502:LEU:HG   | 2.09                     | 0.52              |
| 24:E:252:GLU:O    | 24:E:256:THR:HG22 | 2.09                     | 0.52              |
| 26:K:210:LEU:HD12 | 26:K:211:ASN:H    | 1.74                     | 0.52              |
| 27:U:217:CYS:SG   | 27:U:248:ILE:HD12 | 2.49                     | 0.52              |
| 3:G:202:LEU:HB3   | 3:G:210:PHE:HE2   | 1.74                     | 0.52              |
| 3:G:224:ASN:O     | 3:G:226:LYS:N     | 2.43                     | 0.52              |
| 5:I:28:ILE:HD12   | 5:I:77:ALA:O      | 2.09                     | 0.52              |
| 5:I:192:LEU:HA    | 5:I:195:LYS:HB3   | 1.90                     | 0.52              |
| 6:J:70:CYS:CB     | 6:J:217:LEU:HD21  | 2.39                     | 0.52              |
| 6:J:140:GLY:O     | 6:J:213:ARG:NH2   | 2.43                     | 0.52              |
| 7:L:95:SER:HB3    | 7:L:103:LEU:HB2   | 1.90                     | 0.52              |
| 7:L:140:MET:O     | 7:L:140:MET:HG3   | 2.09                     | 0.52              |
| 7:L:158:ALA:HB1   | 7:L:172:LEU:HD13  | 1.91                     | 0.52              |
| 8:M:33:SER:OG     | 8:M:34:SER:N      | 2.41                     | 0.52              |
| 9:V:150:ARG:HD3   | 9:V:159:LEU:HD21  | 1.91                     | 0.52              |
| 9:V:249:THR:O     | 9:V:253:LEU:HD23  | 2.10                     | 0.52              |
| 9:V:258:TYR:CE2   | 9:V:266:GLN:HG3   | 2.45                     | 0.52              |
| 9:V:300:LEU:O     | 9:V:300:LEU:CD2   | 2.57                     | 0.52              |
| 10:W:80:TRP:HA    | 10:W:80:TRP:CE3   | 2.44                     | 0.52              |
| 10:W:96:GLN:HG3   | 10:W:101:VAL:HG23 | 1.90                     | 0.52              |
| 10:W:296:LEU:HB3  | 10:W:303:LYS:HD3  | 1.91                     | 0.52              |
| 10:W:377:ARG:NH2  | 10:W:381:LEU:HD21 | 2.23                     | 0.52              |
| 10:W:396:LEU:HD22 | 10:W:401:THR:CB   | 2.39                     | 0.52              |
| 12:Y:149:LEU:CA   | 12:Y:157:ILE:HD11 | 2.40                     | 0.52              |
| 14:a:365:MET:HA   | 14:a:368:GLU:OE2  | 2.10                     | 0.52              |
| 17:d:161:ILE:HD12 | 17:d:161:ILE:H    | 1.74                     | 0.52              |
| 18:f:211:ILE:O    | 18:f:212:GLU:HG2  | 2.09                     | 0.52              |
| 18:f:246:SER:HA   | 18:f:249:LEU:HD12 | 1.92                     | 0.52              |
| 18:f:408:LEU:HD12 | 18:f:443:GLY:HA2  | 1.90                     | 0.52              |
| 18:f:499:THR:HA   | 18:f:502:LEU:CG   | 2.37                     | 0.52              |
| 22:A:195:LEU:HD21 | 22:A:316:LYS:CD   | 2.35                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 23:B:235:LEU:HD12 | 23:B:235:LEU:O    | 2.09                     | 0.52              |
| 24:E:257:LEU:C    | 24:E:257:LEU:HD23 | 2.34                     | 0.52              |
| 25:F:202:ILE:HG22 | 25:F:203:VAL:N    | 2.25                     | 0.52              |
| 25:F:253:GLY:C    | 25:F:290:ALA:HB3  | 2.35                     | 0.52              |
| 26:K:211:ASN:C    | 26:K:211:ASN:OD1  | 2.52                     | 0.52              |
| 27:U:108:TYR:CD2  | 27:U:134:VAL:HG21 | 2.45                     | 0.52              |
| 27:U:213:PHE:C    | 27:U:248:ILE:HD11 | 2.35                     | 0.52              |
| 27:U:342:LEU:HD21 | 27:U:785:PRO:HB3  | 1.90                     | 0.52              |
| 27:U:465:LEU:CD2  | 27:U:496:LEU:HD11 | 2.40                     | 0.52              |
| 27:U:532:MET:CB   | 27:U:552:ILE:HG22 | 2.36                     | 0.52              |
| 2:D:403:TYR:CE1   | 2:D:407:ILE:CD1   | 2.93                     | 0.52              |
| 2:D:418:LYS:NZ    | 4:H:80:GLY:HA3    | 2.24                     | 0.52              |
| 3:G:16:PHE:N      | 4:H:21:GLN:OE1    | 2.40                     | 0.52              |
| 4:H:120:GLU:HA    | 4:H:123:GLN:NE2   | 2.25                     | 0.52              |
| 6:J:110:TYR:O     | 6:J:114:LEU:N     | 2.42                     | 0.52              |
| 7:L:13:TRP:H      | 8:M:22:GLN:HE22   | 1.57                     | 0.52              |
| 7:L:66:VAL:CG2    | 7:L:72:ILE:HG23   | 2.38                     | 0.52              |
| 9:V:324:PHE:HD2   | 28:e:19:PHE:CE2   | 2.26                     | 0.52              |
| 10:W:289:ARG:HB3  | 10:W:289:ARG:CZ   | 2.39                     | 0.52              |
| 10:W:373:ILE:HG22 | 10:W:415:PHE:CE1  | 2.44                     | 0.52              |
| 11:X:76:PHE:O     | 11:X:79:SER:OG    | 2.25                     | 0.52              |
| 13:Z:202:ASN:HB2  | 14:a:360:VAL:HG13 | 1.92                     | 0.52              |
| 14:a:13:ASN:HA    | 14:a:18:GLN:OE1   | 2.10                     | 0.52              |
| 14:a:56:LEU:O     | 14:a:60:TYR:N     | 2.25                     | 0.52              |
| 15:b:16:MET:HE3   | 15:b:25:ARG:HB2   | 1.91                     | 0.52              |
| 15:b:142:ASN:O    | 15:b:173:VAL:HG12 | 2.09                     | 0.52              |
| 16:c:167:MET:N    | 16:c:167:MET:SD   | 2.82                     | 0.52              |
| 18:f:241:PRO:CB   | 27:U:835:ILE:HG21 | 2.40                     | 0.52              |
| 18:f:316:ASP:HA   | 18:f:319:GLU:HG2  | 1.91                     | 0.52              |
| 18:f:322:SER:HB2  | 18:f:456:ARG:O    | 2.10                     | 0.52              |
| 18:f:460:ASP:HB2  | 19:g:133:LYS:HD2  | 1.91                     | 0.52              |
| 18:f:564:LEU:HA   | 18:f:567:LEU:CD2  | 2.36                     | 0.52              |
| 18:f:566:HIS:CB   | 18:f:573:ILE:HD11 | 2.40                     | 0.52              |
| 19:g:87:VAL:CG2   | 19:g:155:VAL:HG23 | 2.39                     | 0.52              |
| 20:u:126:LEU:HD13 | 20:u:175:VAL:HG21 | 1.91                     | 0.52              |
| 22:A:54:GLN:HE22  | 22:A:58:LYS:CD    | 2.23                     | 0.52              |
| 22:A:433:ASN:ND2  | 26:K:64:ILE:HG23  | 2.23                     | 0.52              |
| 23:B:125:THR:CG2  | 23:B:126:SER:N    | 2.73                     | 0.52              |
| 25:F:183:GLU:OE1  | 25:F:183:GLU:N    | 2.42                     | 0.52              |
| 25:F:193:LYS:HB2  | 25:F:193:LYS:NZ   | 2.24                     | 0.52              |
| 25:F:391:PHE:HD1  | 25:F:395:GLN:HB3  | 1.73                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 26:K:70:ILE:HD11  | 26:K:89:ILE:CD1   | 2.40                     | 0.52              |
| 27:U:369:THR:N    | 27:U:731:ILE:HG21 | 2.25                     | 0.52              |
| 27:U:560:MET:O    | 27:U:561:GLU:HG3  | 2.09                     | 0.52              |
| 27:U:560:MET:SD   | 27:U:593:SER:HB2  | 2.49                     | 0.52              |
| 27:U:805:ASN:HA   | 27:U:874:ASN:HD22 | 1.73                     | 0.52              |
| 5:I:5:TYR:HE2     | 6:J:4:ASP:OD1     | 1.92                     | 0.52              |
| 5:I:32:GLY:HA2    | 5:I:50:ARG:HD2    | 1.90                     | 0.52              |
| 9:V:266:GLN:NE2   | 27:U:37:GLU:OE2   | 2.41                     | 0.52              |
| 10:W:144:ARG:HB2  | 10:W:144:ARG:NH1  | 2.24                     | 0.52              |
| 11:X:140:THR:CG2  | 11:X:140:THR:O    | 2.58                     | 0.52              |
| 12:Y:319:MET:CE   | 12:Y:330:ILE:HG13 | 2.39                     | 0.52              |
| 13:Z:216:ALA:HB1  | 14:a:347:LYS:CE   | 2.39                     | 0.52              |
| 14:a:60:TYR:O     | 14:a:64:ILE:HB    | 2.09                     | 0.52              |
| 14:a:274:LEU:HD23 | 14:a:274:LEU:C    | 2.34                     | 0.52              |
| 15:b:7:MET:HA     | 15:b:7:MET:HE2    | 1.91                     | 0.52              |
| 15:b:97:LEU:HD22  | 15:b:109:ILE:HD11 | 1.88                     | 0.52              |
| 16:c:174:PRO:O    | 16:c:176:GLN:NE2  | 2.43                     | 0.52              |
| 18:f:460:ASP:CB   | 19:g:133:LYS:HB3  | 2.36                     | 0.52              |
| 18:f:683:GLU:HG2  | 18:f:686:LEU:HD12 | 1.91                     | 0.52              |
| 18:f:707:LEU:HG   | 18:f:732:VAL:HG11 | 1.91                     | 0.52              |
| 18:f:813:LYS:N    | 18:f:813:LYS:HD3  | 2.23                     | 0.52              |
| 19:g:158:LEU:HB3  | 19:g:165:ALA:HB3  | 1.92                     | 0.52              |
| 22:A:274:PHE:CD2  | 22:A:319:MET:HE3  | 2.45                     | 0.52              |
| 22:A:339:ARG:HG3  | 22:A:339:ARG:NH1  | 2.23                     | 0.52              |
| 25:F:151:VAL:HG12 | 25:F:163:THR:HA   | 1.92                     | 0.52              |
| 25:F:173:LYS:HA   | 25:F:274:LEU:HD21 | 1.92                     | 0.52              |
| 25:F:313:LEU:O    | 25:F:313:LEU:HD23 | 2.10                     | 0.52              |
| 26:K:91:LYS:NZ    | 26:K:95:GLU:HG3   | 2.22                     | 0.52              |
| 26:K:186:HIS:CE1  | 26:K:189:MET:SD   | 3.02                     | 0.52              |
| 27:U:619:VAL:HG12 | 27:U:651:GLY:C    | 2.34                     | 0.52              |
| 27:U:796:LYS:O    | 27:U:797:MET:HE2  | 2.10                     | 0.52              |
| 1:C:62:GLU:OE2    | 2:D:117:SER:OG    | 2.27                     | 0.52              |
| 2:D:45:LYS:O      | 2:D:49:GLN:HG2    | 2.09                     | 0.52              |
| 3:G:87:SER:HA     | 3:G:136:CYS:SG    | 2.50                     | 0.52              |
| 5:I:111:VAL:HG21  | 5:I:148:TYR:CD2   | 2.45                     | 0.52              |
| 5:I:173:SER:O     | 5:I:176:LYS:HB2   | 2.10                     | 0.52              |
| 6:J:129:ILE:HG13  | 6:J:129:ILE:O     | 2.08                     | 0.52              |
| 7:L:56:LEU:HD11   | 26:K:167:ALA:HB3  | 1.92                     | 0.52              |
| 8:M:52:LEU:HD23   | 8:M:209:PHE:HB2   | 1.92                     | 0.52              |
| 9:V:407:VAL:HG11  | 9:V:441:ALA:CB    | 2.40                     | 0.52              |
| 10:W:287:VAL:HG13 | 10:W:306:LEU:HD11 | 1.91                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 11:X:368:MET:HA   | 11:X:373:LYS:HG3  | 1.92                     | 0.52              |
| 12:Y:26:LEU:HG    | 12:Y:37:VAL:HG11  | 1.90                     | 0.52              |
| 13:Z:201:LEU:HG   | 14:a:360:VAL:HG21 | 1.92                     | 0.52              |
| 13:Z:216:ALA:HB1  | 14:a:347:LYS:HZ3  | 1.75                     | 0.52              |
| 14:a:28:LEU:CD1   | 14:a:33:LEU:HD21  | 2.37                     | 0.52              |
| 17:d:109:LEU:HD22 | 17:d:158:ARG:HB2  | 1.91                     | 0.52              |
| 18:f:893:ILE:HD12 | 18:f:893:ILE:H    | 1.74                     | 0.52              |
| 19:g:112:LEU:HB3  | 19:g:138:LEU:CD2  | 2.33                     | 0.52              |
| 20:u:229:GLY:C    | 20:u:230:ILE:HD13 | 2.34                     | 0.52              |
| 23:B:93:GLU:HG3   | 23:B:94:GLU:HG3   | 1.92                     | 0.52              |
| 23:B:268:ARG:HG2  | 23:B:315:GLN:NE2  | 2.25                     | 0.52              |
| 27:U:21:GLU:CD    | 27:U:56:SER:HB2   | 2.34                     | 0.52              |
| 27:U:52:GLU:HA    | 27:U:57:ARG:NE    | 2.24                     | 0.52              |
| 27:U:204:ILE:HA   | 27:U:207:ASN:ND2  | 2.21                     | 0.52              |
| 27:U:341:PHE:CE2  | 27:U:787:CYS:CB   | 2.93                     | 0.52              |
| 27:U:419:ALA:CB   | 27:U:449:ILE:HG21 | 2.40                     | 0.52              |
| 27:U:748:LEU:HB3  | 27:U:760:VAL:HG22 | 1.90                     | 0.52              |
| 1:C:223:PHE:HA    | 21:v:17:UNK:O     | 2.10                     | 0.52              |
| 2:D:40:LEU:HD12   | 2:D:40:LEU:O      | 2.10                     | 0.52              |
| 3:G:32:ILE:CD1    | 3:G:137:CYS:SG    | 2.98                     | 0.52              |
| 3:G:132:ARG:HG2   | 3:G:133:PRO:HD2   | 1.92                     | 0.52              |
| 5:I:232:GLU:O     | 5:I:235:GLN:HG3   | 2.09                     | 0.52              |
| 7:L:189:LYS:HE3   | 7:L:235:GLY:O     | 2.10                     | 0.52              |
| 9:V:295:ILE:O     | 9:V:299:GLN:HG2   | 2.10                     | 0.52              |
| 10:W:109:CYS:HA   | 10:W:112:VAL:CB   | 2.40                     | 0.52              |
| 10:W:191:ARG:HG2  | 10:W:191:ARG:NH1  | 2.22                     | 0.52              |
| 13:Z:16:LEU:CD2   | 13:Z:162:ILE:HD12 | 2.40                     | 0.52              |
| 13:Z:211:TYR:O    | 13:Z:215:VAL:HG23 | 2.09                     | 0.52              |
| 14:a:74:LEU:O     | 14:a:78:GLU:HB2   | 2.09                     | 0.52              |
| 14:a:232:TRP:CZ2  | 14:a:257:GLN:HB2  | 2.45                     | 0.52              |
| 17:d:122:VAL:O    | 17:d:126:LEU:N    | 2.32                     | 0.52              |
| 18:f:105:LYS:HG3  | 18:f:106:LEU:N    | 2.24                     | 0.52              |
| 18:f:231:LEU:CD2  | 18:f:853:VAL:HG22 | 2.40                     | 0.52              |
| 18:f:711:SER:HB2  | 18:f:729:MET:CE   | 2.40                     | 0.52              |
| 19:g:111:GLU:O    | 19:g:115:LYS:N    | 2.42                     | 0.52              |
| 22:A:277:ILE:HG22 | 22:A:321:THR:HB   | 1.91                     | 0.52              |
| 24:E:277:MET:SD   | 24:E:295:LEU:HD13 | 2.25                     | 0.52              |
| 27:U:54:PHE:HB3   | 27:U:57:ARG:CG    | 2.39                     | 0.52              |
| 27:U:489:ALA:CA   | 27:U:520:MET:HE1  | 2.39                     | 0.52              |
| 27:U:543:LYS:HE3  | 27:U:772:TRP:CZ3  | 2.45                     | 0.52              |
| 1:C:83:LYS:O      | 1:C:84:LYS:HG2    | 2.10                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:86:LEU:CD1    | 23:B:163:LEU:HD21 | 2.40                     | 0.52              |
| 2:D:167:ILE:HG13  | 2:D:174:LYS:HD2   | 1.91                     | 0.52              |
| 2:D:378:ILE:HG12  | 2:D:406:VAL:HB    | 1.91                     | 0.52              |
| 6:J:43:LEU:HD12   | 6:J:72:ALA:HB2    | 1.91                     | 0.52              |
| 10:W:122:LEU:HA   | 10:W:125:ILE:CG1  | 2.40                     | 0.52              |
| 10:W:209:ILE:HD11 | 10:W:214:PHE:CE1  | 2.45                     | 0.52              |
| 10:W:442:THR:OG1  | 13:Z:229:GLN:OE1  | 2.17                     | 0.52              |
| 11:X:418:ALA:HB2  | 13:Z:276:ILE:CD1  | 2.40                     | 0.52              |
| 12:Y:49:ASN:C     | 12:Y:73:MET:HE2   | 2.35                     | 0.52              |
| 12:Y:202:LEU:CD1  | 12:Y:231:LEU:HD11 | 2.38                     | 0.52              |
| 12:Y:259:TYR:CE2  | 12:Y:278:VAL:HG21 | 2.44                     | 0.52              |
| 13:Z:84:LYS:HD2   | 16:c:76:PRO:HG3   | 1.92                     | 0.52              |
| 13:Z:101:LEU:HD21 | 13:Z:123:ILE:HD11 | 1.92                     | 0.52              |
| 14:a:42:LEU:O     | 14:a:46:GLN:HB2   | 2.10                     | 0.52              |
| 14:a:135:ILE:HD13 | 14:a:155:PHE:CD1  | 2.45                     | 0.52              |
| 18:f:200:ALA:HB1  | 18:f:203:GLU:OE1  | 2.10                     | 0.52              |
| 18:f:246:SER:O    | 18:f:250:ARG:HG2  | 2.09                     | 0.52              |
| 18:f:342:PRO:HB3  | 18:f:387:GLN:O    | 2.10                     | 0.52              |
| 18:f:833:PHE:HD1  | 18:f:839:PRO:CA   | 2.23                     | 0.52              |
| 20:u:118:ASP:O    | 20:u:119:ILE:HG13 | 2.09                     | 0.52              |
| 22:A:23:ARG:HH11  | 22:A:23:ARG:HG3   | 1.75                     | 0.52              |
| 22:A:125:LEU:HB3  | 22:A:129:VAL:HG11 | 1.91                     | 0.52              |
| 23:B:364:ILE:HD11 | 29:B:501:ATP:N6   | 2.25                     | 0.52              |
| 24:E:40:TYR:O     | 24:E:44:GLU:HG2   | 2.09                     | 0.52              |
| 24:E:325:GLU:O    | 24:E:364:GLN:NE2  | 2.43                     | 0.52              |
| 26:K:9:ASP:CB     | 26:K:22:PHE:HB3   | 2.40                     | 0.52              |
| 26:K:103:TYR:O    | 26:K:105:GLU:HG2  | 2.09                     | 0.52              |
| 26:K:184:VAL:HG11 | 26:K:197:SER:HB3  | 1.92                     | 0.52              |
| 27:U:250:PHE:HE1  | 27:U:328:ILE:CG2  | 2.23                     | 0.52              |
| 27:U:341:PHE:CD1  | 27:U:341:PHE:C    | 2.87                     | 0.52              |
| 1:C:85:VAL:HG11   | 1:C:108:VAL:HG11  | 1.92                     | 0.52              |
| 1:C:151:ILE:HD11  | 1:C:202:ALA:HB2   | 1.92                     | 0.52              |
| 2:D:252:ARG:HG2   | 2:D:252:ARG:HH11  | 1.75                     | 0.52              |
| 2:D:380:GLN:HE22  | 24:E:165:ILE:H    | 1.58                     | 0.52              |
| 5:I:24:ALA:O      | 5:I:27:ALA:HB3    | 2.10                     | 0.52              |
| 9:V:114:TYR:HA    | 9:V:117:VAL:HG22  | 1.92                     | 0.52              |
| 9:V:240:LEU:CD1   | 27:U:69:TYR:HE1   | 2.22                     | 0.52              |
| 9:V:329:HIS:CE1   | 9:V:347:GLN:HG2   | 2.44                     | 0.52              |
| 9:V:362:LEU:N     | 9:V:362:LEU:HD23  | 2.25                     | 0.52              |
| 9:V:462:GLU:H     | 9:V:462:GLU:CD    | 2.18                     | 0.52              |
| 9:V:479:ARG:HH22  | 12:Y:370:ILE:CD1  | 2.23                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 10:W:34:LEU:HA    | 10:W:37:GLU:OE2   | 2.09                     | 0.52              |
| 10:W:122:LEU:HB3  | 10:W:123:ARG:HH21 | 1.75                     | 0.52              |
| 10:W:274:VAL:HG22 | 10:W:287:VAL:CG2  | 2.40                     | 0.52              |
| 11:X:57:LEU:HD22  | 11:X:66:LEU:CD1   | 2.40                     | 0.52              |
| 11:X:328:ASP:OD1  | 11:X:364:LYS:HE2  | 2.10                     | 0.52              |
| 11:X:397:TYR:CZ   | 13:Z:258:VAL:HG21 | 2.44                     | 0.52              |
| 13:Z:267:ARG:NH1  | 17:d:346:LEU:HD23 | 2.25                     | 0.52              |
| 14:a:83:VAL:O     | 14:a:87:MET:HG2   | 2.10                     | 0.52              |
| 14:a:131:THR:HA   | 14:a:134:THR:HG23 | 1.92                     | 0.52              |
| 15:b:23:PRO:HG2   | 15:b:27:GLN:CG    | 2.39                     | 0.52              |
| 15:b:127:LEU:HD23 | 15:b:130:ARG:NH2  | 2.11                     | 0.52              |
| 16:c:58:LEU:HD21  | 16:c:96:LEU:HD21  | 1.91                     | 0.52              |
| 17:d:161:ILE:O    | 17:d:165:GLU:HG3  | 2.09                     | 0.52              |
| 18:f:56:LEU:HD12  | 18:f:99:LEU:CD2   | 2.37                     | 0.52              |
| 18:f:276:GLU:OE1  | 18:f:276:GLU:N    | 2.37                     | 0.52              |
| 18:f:316:ASP:HA   | 18:f:319:GLU:HG3  | 1.91                     | 0.52              |
| 18:f:438:ASP:HB2  | 18:f:441:LYS:HE3  | 1.91                     | 0.52              |
| 19:g:89:LEU:CD1   | 19:g:99:ASN:HD22  | 2.14                     | 0.52              |
| 19:g:128:LYS:H    | 19:g:158:LEU:HD13 | 1.74                     | 0.52              |
| 22:A:59:ILE:HD13  | 23:B:79:ILE:HD12  | 1.91                     | 0.52              |
| 23:B:395:ILE:O    | 23:B:398:ILE:HG23 | 2.10                     | 0.52              |
| 25:F:181:PRO:HD2  | 25:F:238:ARG:CD   | 2.39                     | 0.52              |
| 25:F:226:TYR:HE2  | 25:F:351:LYS:HE3  | 1.74                     | 0.52              |
| 25:F:254:PRO:HD3  | 25:F:287:GLU:CB   | 2.37                     | 0.52              |
| 26:K:51:GLU:OE2   | 26:K:206:MET:HG2  | 2.10                     | 0.52              |
| 27:U:115:ASN:HB3  | 27:U:123:LYS:CD   | 2.38                     | 0.52              |
| 27:U:549:ALA:HA   | 27:U:581:SER:CB   | 2.37                     | 0.52              |
| 27:U:803:LYS:HE3  | 27:U:875:PHE:CD1  | 2.45                     | 0.52              |
| 1:C:90:HIS:HB3    | 1:C:91:PRO:HD3    | 1.91                     | 0.51              |
| 1:C:199:LEU:HD13  | 1:C:317:PHE:HZ    | 1.74                     | 0.51              |
| 2:D:178:ARG:HE    | 2:D:182:GLU:CD    | 2.18                     | 0.51              |
| 3:G:94:ALA:HB2    | 3:G:118:ILE:CD1   | 2.26                     | 0.51              |
| 4:H:103:GLU:HG3   | 4:H:104:PRO:HD2   | 1.91                     | 0.51              |
| 7:L:46:LEU:HD23   | 7:L:135:ALA:HB2   | 1.93                     | 0.51              |
| 7:L:154:PHE:HB3   | 8:M:58:TYR:CD2    | 2.45                     | 0.51              |
| 8:M:21:PHE:O      | 8:M:25:TYR:HD1    | 1.93                     | 0.51              |
| 8:M:63:ASN:HB2    | 8:M:81:LEU:CD2    | 2.40                     | 0.51              |
| 8:M:65:ARG:HA     | 8:M:67:PHE:HE1    | 1.74                     | 0.51              |
| 8:M:216:VAL:HG13  | 8:M:224:HIS:CD2   | 2.45                     | 0.51              |
| 9:V:61:GLU:O      | 9:V:64:GLN:HB3    | 2.10                     | 0.51              |
| 9:V:65:ARG:HA     | 9:V:68:ASP:HB2    | 1.92                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 11:X:62:GLN:CB    | 11:X:65:GLU:HB2   | 2.39                     | 0.51              |
| 11:X:394:ASP:OD2  | 12:Y:362:LYS:HG2  | 2.11                     | 0.51              |
| 11:X:419:LYS:O    | 11:X:421:LEU:HG   | 2.10                     | 0.51              |
| 12:Y:121:LEU:HD21 | 12:Y:156:LEU:HD21 | 1.93                     | 0.51              |
| 14:a:28:LEU:HB3   | 14:a:33:LEU:CG    | 2.39                     | 0.51              |
| 14:a:292:THR:HG22 | 14:a:294:GLU:H    | 1.75                     | 0.51              |
| 17:d:92:THR:HA    | 17:d:95:TYR:CB    | 2.40                     | 0.51              |
| 17:d:124:LEU:HD22 | 27:U:22:PHE:CD2   | 2.44                     | 0.51              |
| 18:f:56:LEU:HD12  | 18:f:99:LEU:HD11  | 1.92                     | 0.51              |
| 18:f:347:ASP:OD1  | 18:f:348:ILE:N    | 2.43                     | 0.51              |
| 19:g:115:LYS:CE   | 19:g:142:LEU:HD22 | 2.40                     | 0.51              |
| 25:F:289:ASP:OD2  | 25:F:332:THR:HG23 | 2.10                     | 0.51              |
| 27:U:63:VAL:O     | 27:U:67:VAL:HG23  | 2.10                     | 0.51              |
| 27:U:267:ASN:N    | 27:U:267:ASN:HD22 | 2.07                     | 0.51              |
| 27:U:560:MET:HA   | 27:U:589:ALA:O    | 2.10                     | 0.51              |
| 1:C:246:ILE:O     | 1:C:291:VAL:HA    | 2.09                     | 0.51              |
| 2:D:116:LEU:HD23  | 2:D:119:ILE:HG13  | 1.92                     | 0.51              |
| 6:J:51:ALA:O      | 6:J:52:LYS:HB3    | 2.10                     | 0.51              |
| 9:V:65:ARG:HA     | 9:V:68:ASP:CG     | 2.35                     | 0.51              |
| 9:V:131:LEU:HD23  | 9:V:131:LEU:H     | 1.75                     | 0.51              |
| 9:V:336:GLU:OE1   | 9:V:343:PRO:HA    | 2.10                     | 0.51              |
| 9:V:403:ILE:HG12  | 9:V:428:LEU:HD21  | 1.92                     | 0.51              |
| 11:X:73:VAL:HG21  | 11:X:92:LEU:CD1   | 2.40                     | 0.51              |
| 11:X:400:ALA:O    | 11:X:404:ILE:HG12 | 2.10                     | 0.51              |
| 13:Z:58:PHE:HE2   | 13:Z:108:ILE:CD1  | 2.23                     | 0.51              |
| 14:a:65:SER:O     | 14:a:68:GLU:HG2   | 2.10                     | 0.51              |
| 15:b:91:ARG:NH1   | 15:b:127:LEU:HD21 | 2.26                     | 0.51              |
| 15:b:122:LYS:O    | 15:b:125:VAL:HG22 | 2.10                     | 0.51              |
| 18:f:391:LEU:O    | 18:f:414:LEU:HD21 | 2.11                     | 0.51              |
| 18:f:489:TYR:CE2  | 18:f:497:VAL:HG21 | 2.46                     | 0.51              |
| 19:g:109:GLY:N    | 19:g:140:LYS:O    | 2.40                     | 0.51              |
| 19:g:140:LYS:HB2  | 19:g:145:GLN:CB   | 2.34                     | 0.51              |
| 22:A:365:GLU:CD   | 22:A:405:THR:HG22 | 2.35                     | 0.51              |
| 23:B:246:THR:HG22 | 23:B:279:PRO:O    | 2.10                     | 0.51              |
| 25:F:266:LYS:O    | 25:F:270:ASP:HB2  | 2.11                     | 0.51              |
| 25:F:321:GLN:HG2  | 25:F:322:PRO:O    | 2.09                     | 0.51              |
| 26:K:166:ASP:HB3  | 26:K:185:TYR:OH   | 2.09                     | 0.51              |
| 27:U:46:GLU:O     | 27:U:50:GLU:HG2   | 2.10                     | 0.51              |
| 27:U:249:CYS:SG   | 27:U:329:LEU:HG   | 2.51                     | 0.51              |
| 27:U:637:VAL:O    | 27:U:637:VAL:HG12 | 2.11                     | 0.51              |
| 27:U:672:LEU:HD11 | 27:U:690:ALA:CB   | 2.41                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:49:ARG:NH1    | 27:U:639:LEU:HD23 | 2.26                     | 0.51              |
| 1:C:147:THR:HG22  | 1:C:150:MET:HG3   | 1.91                     | 0.51              |
| 2:D:236:VAL:HG21  | 24:E:255:ARG:HD3  | 1.93                     | 0.51              |
| 2:D:345:PHE:HB3   | 2:D:360:LEU:HD13  | 1.93                     | 0.51              |
| 4:H:74:LEU:HD13   | 4:H:134:LEU:HD13  | 1.93                     | 0.51              |
| 5:I:34:CYS:HA     | 5:I:46:ALA:O      | 2.09                     | 0.51              |
| 5:I:138:GLY:O     | 5:I:145:PHE:HA    | 2.10                     | 0.51              |
| 8:M:31:GLU:O      | 8:M:167:LYS:HG3   | 2.10                     | 0.51              |
| 8:M:140:TYR:CD2   | 8:M:217:GLY:HA2   | 2.46                     | 0.51              |
| 10:W:248:ARG:HG2  | 10:W:270:VAL:HG21 | 1.91                     | 0.51              |
| 10:W:317:TRP:HE3  | 10:W:358:VAL:HG11 | 1.75                     | 0.51              |
| 10:W:422:ASN:O    | 10:W:426:ASN:HB2  | 2.10                     | 0.51              |
| 12:Y:228:MET:SD   | 12:Y:260:LEU:HA   | 2.51                     | 0.51              |
| 12:Y:228:MET:C    | 12:Y:299:MET:HE3  | 2.35                     | 0.51              |
| 12:Y:321:GLU:OE1  | 12:Y:321:GLU:HA   | 2.09                     | 0.51              |
| 15:b:131:LEU:HD13 | 15:b:134:GLU:OE2  | 2.11                     | 0.51              |
| 16:c:87:VAL:HG11  | 20:u:278:PHE:CE2  | 2.46                     | 0.51              |
| 18:f:115:PRO:HB3  | 18:f:119:LYS:NZ   | 2.25                     | 0.51              |
| 18:f:201:GLU:HA   | 18:f:204:ALA:HB3  | 1.92                     | 0.51              |
| 18:f:465:LEU:HD11 | 19:g:173:GLU:HG2  | 1.91                     | 0.51              |
| 18:f:490:ALA:HA   | 18:f:524:MET:O    | 2.10                     | 0.51              |
| 18:f:766:GLN:O    | 18:f:769:THR:HG22 | 2.11                     | 0.51              |
| 22:A:209:PRO:CD   | 25:F:405:MET:HE3  | 2.40                     | 0.51              |
| 22:A:291:GLY:O    | 22:A:294:GLU:HB3  | 2.10                     | 0.51              |
| 23:B:194:ILE:HA   | 23:B:197:ILE:CG2  | 2.41                     | 0.51              |
| 25:F:168:TYR:CD2  | 25:F:274:LEU:HD13 | 2.45                     | 0.51              |
| 25:F:191:LEU:HD21 | 25:F:355:PRO:HD2  | 1.93                     | 0.51              |
| 25:F:406:ILE:HD13 | 25:F:422:GLU:CB   | 2.36                     | 0.51              |
| 26:K:195:ILE:HD12 | 26:K:217:LEU:HD13 | 1.91                     | 0.51              |
| 27:U:236:LEU:HD23 | 27:U:245:ALA:CA   | 2.41                     | 0.51              |
| 27:U:254:GLU:OE1  | 27:U:751:ARG:HD3  | 2.09                     | 0.51              |
| 27:U:678:ASP:OD2  | 27:U:683:VAL:HG21 | 2.09                     | 0.51              |
| 27:U:804:SER:C    | 27:U:874:ASN:HB2  | 2.35                     | 0.51              |
| 3:G:27:TYR:CD2    | 8:M:16:PRO:HA     | 2.45                     | 0.51              |
| 5:I:44:LEU:HB3    | 5:I:215:THR:HG22  | 1.91                     | 0.51              |
| 6:J:31:THR:HG22   | 6:J:163:ARG:O     | 2.10                     | 0.51              |
| 7:L:37:GLY:O      | 7:L:158:ALA:HA    | 2.09                     | 0.51              |
| 8:M:37:ILE:HG22   | 8:M:164:ALA:CB    | 2.41                     | 0.51              |
| 9:V:169:LEU:HD11  | 9:V:213:TYR:CD2   | 2.44                     | 0.51              |
| 9:V:201:ARG:NH1   | 9:V:204:ASP:OD2   | 2.44                     | 0.51              |
| 9:V:340:GLY:HA2   | 9:V:405:THR:OG1   | 2.09                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 9:V:486:ILE:HD13  | 9:V:489:MET:CE    | 2.41                     | 0.51              |
| 11:X:167:VAL:HG22 | 11:X:196:THR:HG23 | 1.91                     | 0.51              |
| 11:X:393:VAL:HG22 | 11:X:393:VAL:O    | 2.10                     | 0.51              |
| 14:a:8:LEU:HD11   | 14:a:26:GLU:CD    | 2.35                     | 0.51              |
| 15:b:17:ARG:HG2   | 15:b:80:PRO:CG    | 2.40                     | 0.51              |
| 18:f:45:LEU:HB2   | 18:f:50:LYS:CE    | 2.41                     | 0.51              |
| 18:f:135:GLY:O    | 18:f:139:CYS:N    | 2.36                     | 0.51              |
| 18:f:213:GLN:HE21 | 18:f:215:ASP:HB3  | 1.76                     | 0.51              |
| 19:g:126:TYR:CA   | 19:g:161:SER:HA   | 2.40                     | 0.51              |
| 22:A:79:ASP:OD1   | 23:B:137:SER:HB3  | 2.10                     | 0.51              |
| 23:B:184:TYR:CD1  | 23:B:238:ALA:HB1  | 2.45                     | 0.51              |
| 23:B:187:ILE:HD12 | 23:B:194:ILE:HD11 | 1.92                     | 0.51              |
| 23:B:202:GLU:OE2  | 23:B:242:GLN:NE2  | 2.43                     | 0.51              |
| 24:E:215:ILE:HD13 | 24:E:260:LEU:HB2  | 1.93                     | 0.51              |
| 25:F:188:ILE:CG1  | 25:F:235:LEU:HG   | 2.41                     | 0.51              |
| 25:F:285:ILE:O    | 25:F:330:ALA:HA   | 2.10                     | 0.51              |
| 27:U:108:TYR:CG   | 27:U:134:VAL:HG21 | 2.45                     | 0.51              |
| 27:U:228:ALA:HA   | 27:U:231:ASP:OD2  | 2.10                     | 0.51              |
| 27:U:352:ILE:CG2  | 27:U:376:MET:HE1  | 2.41                     | 0.51              |
| 27:U:393:LEU:O    | 27:U:393:LEU:HD12 | 2.10                     | 0.51              |
| 27:U:763:VAL:O    | 27:U:767:THR:HG23 | 2.10                     | 0.51              |
| 27:U:788:VAL:HG13 | 27:U:788:VAL:O    | 2.10                     | 0.51              |
| 27:U:899:ARG:NH2  | 27:U:918:SER:HB2  | 2.25                     | 0.51              |
| 1:C:71:SER:OG     | 2:D:112:TYR:HD2   | 1.94                     | 0.51              |
| 1:C:292:ILE:O     | 1:C:292:ILE:CG2   | 2.56                     | 0.51              |
| 1:C:307:ARG:HH12  | 1:C:309:GLY:HA3   | 1.75                     | 0.51              |
| 3:G:141:ILE:HD11  | 3:G:227:PHE:CE1   | 2.39                     | 0.51              |
| 3:G:200:THR:HA    | 3:G:203:SER:OG    | 2.11                     | 0.51              |
| 4:H:29:VAL:HG22   | 4:H:133:SER:H     | 1.75                     | 0.51              |
| 4:H:35:SER:HB2    | 4:H:163:MET:CE    | 2.38                     | 0.51              |
| 7:L:34:ALA:HB2    | 7:L:163:ALA:O     | 2.11                     | 0.51              |
| 10:W:24:VAL:HG21  | 10:W:65:ARG:HB2   | 1.92                     | 0.51              |
| 11:X:401:LEU:HD21 | 12:Y:369:THR:OG1  | 2.09                     | 0.51              |
| 13:Z:43:TRP:HE3   | 13:Z:44:GLN:H     | 1.59                     | 0.51              |
| 14:a:5:PRO:O      | 14:a:9:GLN:HG2    | 2.10                     | 0.51              |
| 14:a:162:TYR:CD1  | 14:a:165:THR:HG21 | 2.45                     | 0.51              |
| 18:f:169:GLU:HG3  | 18:f:184:LEU:HD11 | 1.93                     | 0.51              |
| 19:g:110:ARG:O    | 19:g:113:ARG:HD3  | 2.10                     | 0.51              |
| 22:A:103:ASN:HA   | 22:A:109:PRO:HA   | 1.92                     | 0.51              |
| 25:F:176:GLU:HG3  | 25:F:247:THR:CG2  | 2.40                     | 0.51              |
| 25:F:206:MET:HG3  | 25:F:325:GLN:NE2  | 2.23                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 27:U:136:LYS:NZ   | 27:U:140:ARG:HD2  | 2.26                     | 0.51              |
| 27:U:846:LYS:HA   | 27:U:849:LYS:HD2  | 1.92                     | 0.51              |
| 2:D:182:GLU:HG2   | 2:D:183:LEU:N     | 2.25                     | 0.51              |
| 8:M:39:ILE:HD11   | 8:M:176:ILE:HG23  | 1.93                     | 0.51              |
| 9:V:212:TYR:HB2   | 9:V:253:LEU:HD21  | 1.91                     | 0.51              |
| 10:W:323:ASP:HB3  | 10:W:324:TYR:CD1  | 2.44                     | 0.51              |
| 11:X:182:ASN:CG   | 11:X:185:LYS:HB2  | 2.35                     | 0.51              |
| 12:Y:187:TYR:O    | 12:Y:191:ILE:HG23 | 2.10                     | 0.51              |
| 13:Z:69:PHE:CE1   | 15:b:60:VAL:HG11  | 2.46                     | 0.51              |
| 13:Z:165:GLU:HG2  | 13:Z:166:GLU:N    | 2.24                     | 0.51              |
| 14:a:122:LYS:HZ2  | 14:a:131:THR:HB   | 1.75                     | 0.51              |
| 14:a:122:LYS:HA   | 14:a:125:ILE:O    | 2.10                     | 0.51              |
| 14:a:315:LEU:HD13 | 14:a:320:VAL:HG12 | 1.91                     | 0.51              |
| 18:f:60:VAL:O     | 18:f:105:LYS:NZ   | 2.38                     | 0.51              |
| 18:f:92:VAL:HG23  | 22:A:32:LEU:HB3   | 1.93                     | 0.51              |
| 18:f:186:THR:O    | 18:f:189:LYS:HB2  | 2.10                     | 0.51              |
| 18:f:367:SER:HB3  | 18:f:370:MET:HG2  | 1.91                     | 0.51              |
| 18:f:466:LEU:HD12 | 18:f:481:SER:CA   | 2.37                     | 0.51              |
| 19:g:137:GLN:HB2  | 19:g:145:GLN:HB2  | 1.92                     | 0.51              |
| 19:g:140:LYS:HE3  | 19:g:140:LYS:HA   | 1.93                     | 0.51              |
| 22:A:111:TYR:CE1  | 22:A:125:LEU:HD21 | 2.45                     | 0.51              |
| 22:A:364:VAL:HG22 | 22:A:368:ILE:HG13 | 1.91                     | 0.51              |
| 24:E:294:ARG:O    | 24:E:295:LEU:HB2  | 2.10                     | 0.51              |
| 24:E:322:LYS:CB   | 24:E:361:PHE:HD2  | 2.23                     | 0.51              |
| 26:K:190:THR:HG22 | 26:K:193:GLU:HB2  | 1.91                     | 0.51              |
| 26:K:206:MET:HE1  | 26:K:210:LEU:HD13 | 1.93                     | 0.51              |
| 27:U:533:VAL:O    | 27:U:536:ALA:N    | 2.43                     | 0.51              |
| 28:e:60:LEU:O     | 28:e:64:GLY:N     | 2.44                     | 0.51              |
| 2:D:60:TYR:HD1    | 27:U:607:VAL:HG21 | 1.74                     | 0.51              |
| 2:D:134:LYS:HE3   | 24:E:105:LEU:HD12 | 1.93                     | 0.51              |
| 2:D:225:ALA:HB1   | 2:D:260:ALA:HA    | 1.93                     | 0.51              |
| 4:H:196:LYS:CA    | 4:H:203:MET:HE1   | 2.38                     | 0.51              |
| 7:L:85:CYS:O      | 7:L:89:ARG:HG3    | 2.10                     | 0.51              |
| 7:L:193:ARG:HA    | 7:L:196:ARG:CG    | 2.41                     | 0.51              |
| 8:M:49:VAL:CG1    | 8:M:66:LEU:HD22   | 2.40                     | 0.51              |
| 9:V:182:LYS:O     | 9:V:186:LYS:N     | 2.35                     | 0.51              |
| 9:V:466:ILE:HG13  | 9:V:471:GLU:HB3   | 1.93                     | 0.51              |
| 12:Y:122:THR:HA   | 12:Y:125:ARG:NH1  | 2.26                     | 0.51              |
| 13:Z:201:LEU:HD13 | 16:c:225:TRP:CZ3  | 2.46                     | 0.51              |
| 13:Z:234:PHE:CZ   | 14:a:352:ARG:HB2  | 2.46                     | 0.51              |
| 14:a:160:SER:O    | 14:a:163:TYR:HD2  | 1.94                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 14:a:245:VAL:CG1  | 14:a:247:ARG:HD2  | 2.40                     | 0.51              |
| 14:a:374:ILE:O    | 14:a:376:THR:HG23 | 2.11                     | 0.51              |
| 15:b:48:ASN:HB2   | 15:b:64:LEU:CD2   | 2.40                     | 0.51              |
| 17:d:108:ASN:HB3  | 17:d:111:LYS:HB2  | 1.92                     | 0.51              |
| 18:f:314:TYR:O    | 18:f:318:THR:N    | 2.32                     | 0.51              |
| 23:B:114:GLU:OE1  | 23:B:115:ILE:C    | 2.53                     | 0.51              |
| 24:E:50:LEU:HD22  | 25:F:83:ASN:HB3   | 1.93                     | 0.51              |
| 24:E:81:VAL:HB    | 24:E:105:LEU:O    | 2.10                     | 0.51              |
| 24:E:92:LEU:HA    | 24:E:96:THR:HG21  | 1.92                     | 0.51              |
| 24:E:140:GLU:O    | 24:E:144:GLU:HG3  | 2.11                     | 0.51              |
| 24:E:175:PRO:HB2  | 24:E:303:LEU:HD13 | 1.93                     | 0.51              |
| 25:F:181:PRO:HG2  | 25:F:238:ARG:CZ   | 2.41                     | 0.51              |
| 26:K:109:VAL:HG22 | 26:K:154:PHE:CD2  | 2.45                     | 0.51              |
| 26:K:233:GLU:N    | 26:K:233:GLU:OE2  | 2.43                     | 0.51              |
| 1:C:96:VAL:HG21   | 23:B:151:LEU:HD21 | 1.92                     | 0.51              |
| 2:D:55:GLU:OE1    | 2:D:55:GLU:HA     | 2.10                     | 0.51              |
| 3:G:32:ILE:HD11   | 3:G:156:PRO:HD3   | 1.93                     | 0.51              |
| 3:G:49:VAL:HG21   | 3:G:195:VAL:CG2   | 2.40                     | 0.51              |
| 3:G:143:ILE:CD1   | 3:G:220:VAL:HG13  | 2.41                     | 0.51              |
| 3:G:173:THR:OG1   | 3:G:174:GLU:OE1   | 2.22                     | 0.51              |
| 5:I:34:CYS:O      | 5:I:163:CYS:HA    | 2.11                     | 0.51              |
| 8:M:98:PHE:CE2    | 8:M:102:PHE:HD2   | 2.29                     | 0.51              |
| 9:V:447:ILE:CG2   | 9:V:448:GLU:N     | 2.74                     | 0.51              |
| 11:X:417:LYS:O    | 13:Z:280:ILE:HD11 | 2.11                     | 0.51              |
| 13:Z:156:GLU:HG2  | 13:Z:157:HIS:N    | 2.25                     | 0.51              |
| 13:Z:175:LEU:O    | 13:Z:175:LEU:HD23 | 2.11                     | 0.51              |
| 15:b:73:SER:HA    | 25:F:61:ARG:CD    | 2.39                     | 0.51              |
| 18:f:379:GLY:HA3  | 18:f:416:MET:CE   | 2.38                     | 0.51              |
| 18:f:785:ARG:HD3  | 18:f:785:ARG:N    | 2.23                     | 0.51              |
| 23:B:54:PRO:HD3   | 23:B:60:LEU:HG    | 1.92                     | 0.51              |
| 23:B:223:ILE:CG2  | 23:B:347:ILE:HG21 | 2.41                     | 0.51              |
| 24:E:327:ASP:O    | 24:E:328:TYR:C    | 2.53                     | 0.51              |
| 24:E:349:GLU:CD   | 24:E:374:VAL:HG22 | 2.36                     | 0.51              |
| 24:E:364:GLN:C    | 24:E:366:ASP:N    | 2.68                     | 0.51              |
| 26:K:39:GLY:HA3   | 26:K:153:LEU:HD21 | 1.93                     | 0.51              |
| 27:U:95:GLU:O     | 27:U:99:THR:HG22  | 2.11                     | 0.51              |
| 2:D:358:VAL:HG13  | 2:D:358:VAL:O     | 2.11                     | 0.51              |
| 5:I:196:VAL:O     | 5:I:200:THR:OG1   | 2.27                     | 0.51              |
| 9:V:76:LYS:HE2    | 9:V:147:PHE:CE1   | 2.46                     | 0.51              |
| 9:V:214:HIS:HA    | 9:V:217:VAL:HG22  | 1.92                     | 0.51              |
| 9:V:479:ARG:HH22  | 12:Y:370:ILE:HD12 | 1.76                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 10:W:102:ALA:O    | 10:W:106:GLN:NE2  | 2.44                     | 0.51              |
| 11:X:57:LEU:HD22  | 11:X:66:LEU:CB    | 2.39                     | 0.51              |
| 11:X:384:VAL:HG23 | 11:X:386:ILE:HD11 | 1.93                     | 0.51              |
| 13:Z:41:GLY:HA3   | 13:Z:49:ASP:O     | 2.10                     | 0.51              |
| 13:Z:145:HIS:O    | 13:Z:146:ASP:C    | 2.53                     | 0.51              |
| 13:Z:177:ARG:HG2  | 13:Z:177:ARG:HH11 | 1.75                     | 0.51              |
| 13:Z:243:GLN:OE1  | 17:d:328:THR:HA   | 2.11                     | 0.51              |
| 14:a:94:LEU:HA    | 14:a:97:LEU:HD21  | 1.93                     | 0.51              |
| 14:a:109:GLU:HG3  | 14:a:112:ILE:HG21 | 1.91                     | 0.51              |
| 15:b:25:ARG:NH1   | 15:b:144:GLY:HA3  | 2.26                     | 0.51              |
| 15:b:25:ARG:O     | 15:b:28:ALA:HB3   | 2.09                     | 0.51              |
| 17:d:147:ILE:O    | 17:d:150:ILE:HB   | 2.09                     | 0.51              |
| 17:d:197:LEU:HD22 | 17:d:259:PHE:HB3  | 1.93                     | 0.51              |
| 18:f:110:TYR:CZ   | 18:f:119:LYS:HG3  | 2.46                     | 0.51              |
| 18:f:408:LEU:HD12 | 18:f:443:GLY:CA   | 2.41                     | 0.51              |
| 18:f:447:ALA:O    | 18:f:450:ILE:HG22 | 2.11                     | 0.51              |
| 18:f:499:THR:CA   | 18:f:502:LEU:HG   | 2.38                     | 0.51              |
| 22:A:182:GLU:O    | 22:A:185:GLU:HG2  | 2.11                     | 0.51              |
| 22:A:238:ILE:HB   | 22:A:272:ILE:HD12 | 1.92                     | 0.51              |
| 22:A:297:ARG:CD   | 25:F:257:VAL:HG21 | 2.41                     | 0.51              |
| 22:A:328:ASP:OD1  | 22:A:329:PRO:HD2  | 2.11                     | 0.51              |
| 22:A:368:ILE:HD13 | 22:A:406:GLU:HB2  | 1.92                     | 0.51              |
| 22:A:402:LYS:C    | 23:B:214:MET:HE1  | 2.35                     | 0.51              |
| 24:E:266:GLY:O    | 24:E:267:PHE:C    | 2.54                     | 0.51              |
| 25:F:232:GLY:H    | 29:F:501:ATP:PB   | 2.33                     | 0.51              |
| 25:F:341:ALA:HA   | 25:F:344:ARG:HG3  | 1.93                     | 0.51              |
| 26:K:33:LEU:H     | 26:K:33:LEU:HD12  | 1.75                     | 0.51              |
| 27:U:59:PHE:O     | 27:U:63:VAL:HG23  | 2.11                     | 0.51              |
| 27:U:513:GLY:HA3  | 27:U:548:LEU:HD22 | 1.93                     | 0.51              |
| 1:C:273:MET:HE2   | 1:C:302:ASP:OD2   | 2.11                     | 0.51              |
| 1:C:305:LEU:O     | 1:C:306:LEU:HD23  | 2.11                     | 0.51              |
| 2:D:85:ILE:HD11   | 24:E:68:LYS:HG2   | 1.93                     | 0.51              |
| 7:L:108:LEU:HD12  | 7:L:108:LEU:O     | 2.10                     | 0.51              |
| 7:L:155:ASP:H     | 8:M:62:SER:HB2    | 1.76                     | 0.51              |
| 8:M:46:VAL:CG1    | 8:M:193:VAL:HG21  | 2.41                     | 0.51              |
| 9:V:86:VAL:HG13   | 9:V:200:ARG:NH1   | 2.24                     | 0.51              |
| 9:V:196:SER:CB    | 9:V:234:ARG:HH22  | 2.24                     | 0.51              |
| 9:V:447:ILE:HG22  | 9:V:448:GLU:H     | 1.76                     | 0.51              |
| 10:W:199:TYR:O    | 10:W:203:GLN:HG3  | 2.11                     | 0.51              |
| 11:X:191:THR:O    | 11:X:195:THR:HB   | 2.11                     | 0.51              |
| 14:a:234:ILE:O    | 14:a:238:TYR:HB2  | 2.11                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 15:b:181:ASP:HA   | 15:b:184:ILE:HG12 | 1.92                     | 0.51              |
| 17:d:275:ILE:CD1  | 17:d:291:LEU:HG   | 2.40                     | 0.51              |
| 18:f:131:MET:HE1  | 22:A:36:TYR:HE1   | 1.75                     | 0.51              |
| 18:f:695:ALA:O    | 18:f:699:VAL:HG22 | 2.11                     | 0.51              |
| 18:f:814:SER:O    | 18:f:814:SER:OG   | 2.27                     | 0.51              |
| 25:F:168:TYR:CE2  | 25:F:274:LEU:HA   | 2.46                     | 0.51              |
| 25:F:180:ARG:O    | 25:F:182:THR:N    | 2.43                     | 0.51              |
| 27:U:151:ILE:O    | 27:U:154:ALA:HB3  | 2.11                     | 0.51              |
| 27:U:529:ILE:HD11 | 27:U:566:LEU:CD1  | 2.41                     | 0.51              |
| 27:U:646:PRO:CB   | 27:U:680:VAL:HG21 | 2.41                     | 0.51              |
| 27:U:698:GLN:HB3  | 27:U:702:THR:OG1  | 2.10                     | 0.51              |
| 27:U:797:MET:HE2  | 27:U:797:MET:CA   | 2.41                     | 0.51              |
| 27:U:803:LYS:O    | 27:U:893:THR:N    | 2.34                     | 0.51              |
| 27:U:807:LYS:HB2  | 27:U:808:PRO:CD   | 2.32                     | 0.51              |
| 1:C:43:ARG:NE     | 9:V:498:PRO:HB3   | 2.26                     | 0.50              |
| 2:D:355:SER:HB2   | 2:D:393:ILE:HG22  | 1.92                     | 0.50              |
| 4:H:203:MET:CG    | 4:H:208:ILE:HG13  | 2.42                     | 0.50              |
| 7:L:43:HIS:CG     | 7:L:184:LEU:HD13  | 2.46                     | 0.50              |
| 7:L:62:LYS:HE3    | 25:F:439:ALA:C    | 2.36                     | 0.50              |
| 8:M:55:SER:N      | 8:M:58:TYR:HE1    | 2.09                     | 0.50              |
| 8:M:141:SER:OG    | 8:M:144:ASP:HB2   | 2.10                     | 0.50              |
| 9:V:65:ARG:HB3    | 9:V:65:ARG:NH1    | 2.26                     | 0.50              |
| 10:W:407:ASP:CG   | 11:X:344:ARG:HD3  | 2.36                     | 0.50              |
| 11:X:306:LEU:HD21 | 11:X:314:ARG:HH21 | 1.75                     | 0.50              |
| 12:Y:15:PRO:HG3   | 12:Y:147:ILE:HD13 | 1.92                     | 0.50              |
| 12:Y:134:LEU:HD21 | 12:Y:171:GLY:O    | 2.11                     | 0.50              |
| 14:a:156:TYR:CD2  | 14:a:179:PHE:HB2  | 2.36                     | 0.50              |
| 14:a:185:ILE:HG22 | 14:a:187:ASP:HB3  | 1.93                     | 0.50              |
| 14:a:280:MET:HE1  | 14:a:299:SER:HB2  | 1.92                     | 0.50              |
| 15:b:36:VAL:CA    | 15:b:188:ILE:HD11 | 2.41                     | 0.50              |
| 17:d:152:ALA:HB1  | 17:d:191:LEU:HD22 | 1.92                     | 0.50              |
| 17:d:195:ASN:O    | 17:d:199:LEU:HG   | 2.11                     | 0.50              |
| 17:d:263:LEU:HD12 | 17:d:266:THR:HB   | 1.93                     | 0.50              |
| 18:f:191:ILE:HD13 | 18:f:207:LEU:CD2  | 2.40                     | 0.50              |
| 18:f:270:LEU:O    | 18:f:273:ASN:N    | 2.44                     | 0.50              |
| 18:f:701:ASN:HB2  | 18:f:876:HIS:ND1  | 2.26                     | 0.50              |
| 18:f:775:THR:O    | 18:f:776:LEU:HD23 | 2.11                     | 0.50              |
| 23:B:285:ASP:OD1  | 23:B:286:GLU:N    | 2.44                     | 0.50              |
| 24:E:108:MET:O    | 24:E:109:ARG:HB3  | 2.11                     | 0.50              |
| 24:E:328:TYR:HA   | 24:E:331:ILE:HD12 | 1.93                     | 0.50              |
| 24:E:352:MET:O    | 24:E:356:ARG:HG2  | 2.11                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 25:F:205:PRO:HB3  | 25:F:219:PRO:HB3  | 1.92                     | 0.50              |
| 25:F:398:ALA:O    | 25:F:402:GLU:HB2  | 2.11                     | 0.50              |
| 26:K:91:LYS:HZ3   | 26:K:95:GLU:CG    | 2.23                     | 0.50              |
| 27:U:542:GLU:HA   | 27:U:545:LEU:HD12 | 1.92                     | 0.50              |
| 27:U:665:ASN:C    | 27:U:667:GLU:H    | 2.19                     | 0.50              |
| 1:C:49:ARG:HB2    | 2:D:61:ILE:HD11   | 1.93                     | 0.50              |
| 4:H:222:THR:HG22  | 4:H:225:GLU:CD    | 2.36                     | 0.50              |
| 4:H:222:THR:HG22  | 4:H:225:GLU:OE1   | 2.10                     | 0.50              |
| 7:L:78:THR:HG22   | 25:F:439:ALA:HB3  | 1.93                     | 0.50              |
| 9:V:165:ALA:CB    | 9:V:191:LEU:HD11  | 2.42                     | 0.50              |
| 9:V:261:TYR:HB2   | 9:V:263:LEU:CD1   | 2.40                     | 0.50              |
| 9:V:488:ASN:O     | 9:V:492:LYS:N     | 2.36                     | 0.50              |
| 10:W:50:LEU:HA    | 10:W:53:GLN:CD    | 2.36                     | 0.50              |
| 10:W:55:ARG:HH11  | 10:W:93:ARG:HB3   | 1.75                     | 0.50              |
| 10:W:161:GLU:O    | 10:W:165:ILE:HG12 | 2.10                     | 0.50              |
| 13:Z:190:ARG:HE   | 16:c:297:VAL:HG11 | 1.77                     | 0.50              |
| 14:a:24:ARG:NH2   | 14:a:27:GLU:OE1   | 2.44                     | 0.50              |
| 14:a:149:THR:HA   | 14:a:152:HIS:CE1  | 2.45                     | 0.50              |
| 14:a:357:CYS:HA   | 14:a:360:VAL:HG12 | 1.93                     | 0.50              |
| 18:f:92:VAL:HG23  | 22:A:32:LEU:CB    | 2.41                     | 0.50              |
| 18:f:343:LYS:HG2  | 18:f:773:LYS:HE2  | 1.93                     | 0.50              |
| 18:f:659:LEU:O    | 18:f:662:MET:HG2  | 2.10                     | 0.50              |
| 18:f:679:LEU:CD2  | 18:f:687:ARG:HA   | 2.41                     | 0.50              |
| 18:f:806:VAL:O    | 18:f:811:LEU:N    | 2.43                     | 0.50              |
| 19:g:130:VAL:O    | 19:g:130:VAL:HG23 | 2.11                     | 0.50              |
| 22:A:249:TYR:HD2  | 22:A:252:GLU:OE1  | 1.93                     | 0.50              |
| 24:E:81:VAL:HG21  | 24:E:107:ILE:HG13 | 1.92                     | 0.50              |
| 25:F:310:MET:HE3  | 25:F:342:LEU:CG   | 2.41                     | 0.50              |
| 27:U:579:ARG:O    | 27:U:583:MET:HG2  | 2.10                     | 0.50              |
| 27:U:755:THR:HG23 | 27:U:755:THR:O    | 2.11                     | 0.50              |
| 27:U:902:PRO:CB   | 27:U:912:ILE:HD13 | 2.40                     | 0.50              |
| 3:G:191:PHE:HE1   | 3:G:219:VAL:CG1   | 2.25                     | 0.50              |
| 4:H:9:SER:HB3     | 4:H:12:THR:HG23   | 1.92                     | 0.50              |
| 5:I:21:VAL:HG11   | 5:I:153:SER:HB2   | 1.93                     | 0.50              |
| 10:W:115:ILE:O    | 10:W:121:LYS:HD2  | 2.10                     | 0.50              |
| 10:W:435:LEU:CD1  | 13:Z:237:LEU:HD23 | 2.42                     | 0.50              |
| 10:W:435:LEU:HD23 | 10:W:435:LEU:C    | 2.35                     | 0.50              |
| 11:X:126:ARG:NH2  | 11:X:127:GLN:HE21 | 2.10                     | 0.50              |
| 12:Y:189:VAL:HG13 | 12:Y:288:PHE:CE1  | 2.47                     | 0.50              |
| 12:Y:356:THR:HG21 | 12:Y:358:ARG:HH12 | 1.77                     | 0.50              |
| 13:Z:225:GLN:N    | 13:Z:227:ILE:HG22 | 2.25                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 14:a:97:LEU:HD13  | 14:a:114:CYS:CB   | 2.30                     | 0.50              |
| 15:b:10:VAL:HA    | 15:b:112:PHE:HB2  | 1.94                     | 0.50              |
| 17:d:130:PRO:HG3  | 27:U:3:THR:CG2    | 2.41                     | 0.50              |
| 18:f:96:LEU:HD23  | 18:f:129:LEU:HA   | 1.90                     | 0.50              |
| 18:f:846:VAL:HG22 | 18:f:880:ALA:CB   | 2.41                     | 0.50              |
| 18:f:850:VAL:HG21 | 18:f:863:THR:CG2  | 2.41                     | 0.50              |
| 19:g:165:ALA:O    | 19:g:169:PHE:HB3  | 2.11                     | 0.50              |
| 23:B:222:VAL:HG23 | 23:B:224:LEU:HD11 | 1.94                     | 0.50              |
| 23:B:223:ILE:HG22 | 23:B:350:LYS:HA   | 1.92                     | 0.50              |
| 26:K:91:LYS:O     | 26:K:91:LYS:CD    | 2.58                     | 0.50              |
| 27:U:96:TYR:O     | 27:U:100:ILE:HG12 | 2.10                     | 0.50              |
| 27:U:138:PHE:CD1  | 27:U:162:VAL:HG21 | 2.46                     | 0.50              |
| 27:U:206:MET:HA   | 27:U:206:MET:CE   | 2.29                     | 0.50              |
| 27:U:797:MET:O    | 27:U:925:VAL:HG23 | 2.11                     | 0.50              |
| 27:U:925:VAL:HG12 | 27:U:927:PRO:HD3  | 1.91                     | 0.50              |
| 1:C:271:ARG:HG2   | 23:B:253:SER:OG   | 2.11                     | 0.50              |
| 2:D:154:LEU:HD11  | 24:E:267:PHE:HE1  | 1.74                     | 0.50              |
| 2:D:341:LYS:HG2   | 2:D:375:ILE:HD11  | 1.94                     | 0.50              |
| 4:H:214:ASN:OD1   | 4:H:214:ASN:C     | 2.54                     | 0.50              |
| 7:L:41:LYS:HB2    | 7:L:180:MET:O     | 2.12                     | 0.50              |
| 7:L:200:PRO:HB2   | 7:L:202:GLU:CD    | 2.36                     | 0.50              |
| 8:M:73:VAL:HA     | 8:M:139:SER:HB2   | 1.93                     | 0.50              |
| 8:M:78:ALA:HB3    | 8:M:165:ILE:HG22  | 1.92                     | 0.50              |
| 9:V:101:LEU:N     | 9:V:102:PRO:HD2   | 2.27                     | 0.50              |
| 9:V:173:ILE:HG12  | 9:V:213:TYR:HE2   | 1.74                     | 0.50              |
| 9:V:264:TYR:HE2   | 17:d:213:GLU:HG3  | 1.75                     | 0.50              |
| 10:W:230:MET:CE   | 10:W:233:LEU:HB3  | 2.41                     | 0.50              |
| 10:W:235:GLN:CA   | 10:W:243:ILE:HD11 | 2.37                     | 0.50              |
| 11:X:173:GLU:O    | 11:X:176:THR:HG22 | 2.11                     | 0.50              |
| 11:X:190:LEU:HD21 | 11:X:214:SER:CB   | 2.37                     | 0.50              |
| 11:X:382:GLU:O    | 11:X:384:VAL:HG13 | 2.12                     | 0.50              |
| 11:X:394:ASP:OD2  | 12:Y:362:LYS:HE2  | 2.12                     | 0.50              |
| 12:Y:153:ASP:C    | 12:Y:153:ASP:OD1  | 2.54                     | 0.50              |
| 13:Z:223:ASN:C    | 13:Z:225:GLN:H    | 2.20                     | 0.50              |
| 14:a:101:ARG:HG3  | 14:a:111:VAL:HB   | 1.94                     | 0.50              |
| 14:a:164:GLN:CG   | 14:a:164:GLN:O    | 2.59                     | 0.50              |
| 18:f:217:LEU:HG   | 18:f:221:ILE:HD11 | 1.92                     | 0.50              |
| 18:f:439:TYR:CE2  | 18:f:476:THR:HG21 | 2.46                     | 0.50              |
| 18:f:535:THR:CG2  | 18:f:576:ILE:HD11 | 2.41                     | 0.50              |
| 18:f:711:SER:N    | 18:f:729:MET:HE3  | 2.26                     | 0.50              |
| 18:f:870:THR:HA   | 18:f:871:PRO:C    | 2.36                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 23:B:270:LEU:O    | 23:B:270:LEU:HD12 | 2.12                     | 0.50              |
| 23:B:434:THR:HB   | 23:B:435:PRO:CD   | 2.39                     | 0.50              |
| 25:F:365:ILE:HA   | 25:F:368:ILE:CD1  | 2.42                     | 0.50              |
| 27:U:7:GLY:O      | 27:U:10:SER:HB2   | 2.12                     | 0.50              |
| 27:U:41:SER:O     | 27:U:43:ASP:N     | 2.45                     | 0.50              |
| 27:U:138:PHE:CE1  | 27:U:154:ALA:HA   | 2.47                     | 0.50              |
| 27:U:228:ALA:O    | 27:U:232:ILE:HG12 | 2.11                     | 0.50              |
| 1:C:232:ARG:O     | 1:C:236:VAL:HG23  | 2.11                     | 0.50              |
| 3:G:93:ARG:HH12   | 3:G:97:GLU:HG2    | 1.77                     | 0.50              |
| 4:H:65:VAL:HB     | 4:H:209:GLU:OE1   | 2.12                     | 0.50              |
| 5:I:92:LEU:HD21   | 5:I:96:ARG:NH1    | 2.24                     | 0.50              |
| 5:I:198:ASN:HB3   | 5:I:199:LYS:NZ    | 2.25                     | 0.50              |
| 6:J:82:ILE:CG2    | 6:J:127:PHE:HE1   | 2.25                     | 0.50              |
| 7:L:174:ARG:HG2   | 7:L:175:HIS:CD2   | 2.46                     | 0.50              |
| 8:M:36:ALA:O      | 8:M:164:ALA:HA    | 2.11                     | 0.50              |
| 8:M:216:VAL:HG13  | 8:M:224:HIS:HD2   | 1.76                     | 0.50              |
| 10:W:249:ALA:O    | 10:W:253:THR:HG23 | 2.12                     | 0.50              |
| 10:W:317:TRP:CZ2  | 10:W:355:LYS:HB2  | 2.47                     | 0.50              |
| 10:W:340:VAL:O    | 10:W:350:ARG:HD2  | 2.12                     | 0.50              |
| 10:W:372:ARG:NH2  | 14:a:327:VAL:HB   | 2.27                     | 0.50              |
| 11:X:189:ALA:O    | 11:X:192:SER:HB2  | 2.12                     | 0.50              |
| 11:X:270:LEU:H    | 11:X:270:LEU:HD12 | 1.76                     | 0.50              |
| 11:X:290:VAL:O    | 11:X:293:ALA:HB3  | 2.10                     | 0.50              |
| 13:Z:177:ARG:HH22 | 16:c:153:GLY:CA   | 2.24                     | 0.50              |
| 14:a:281:THR:HA   | 14:a:284:ARG:CG   | 2.41                     | 0.50              |
| 15:b:7:MET:HE1    | 15:b:64:LEU:HG    | 1.93                     | 0.50              |
| 17:d:208:PHE:O    | 17:d:211:GLU:HB3  | 2.12                     | 0.50              |
| 17:d:284:PHE:HB3  | 17:d:314:ASN:OD1  | 2.11                     | 0.50              |
| 18:f:564:LEU:CD2  | 18:f:567:LEU:HD11 | 2.41                     | 0.50              |
| 18:f:720:GLU:OE2  | 18:f:806:VAL:HG22 | 2.11                     | 0.50              |
| 19:g:112:LEU:HD13 | 19:g:115:LYS:HE2  | 1.93                     | 0.50              |
| 19:g:131:ILE:HA   | 19:g:153:ALA:CB   | 2.39                     | 0.50              |
| 22:A:284:ARG:HA   | 22:A:296:GLN:NE2  | 2.26                     | 0.50              |
| 22:A:286:ASP:HB2  | 25:F:337:ILE:HD11 | 1.93                     | 0.50              |
| 22:A:372:LEU:HD11 | 22:A:376:LEU:HD11 | 1.92                     | 0.50              |
| 23:B:224:LEU:CD1  | 23:B:328:ILE:HG23 | 2.42                     | 0.50              |
| 24:E:326:ILE:HG23 | 24:E:364:GLN:OE1  | 2.12                     | 0.50              |
| 25:F:188:ILE:CD1  | 25:F:236:LEU:HA   | 2.36                     | 0.50              |
| 27:U:265:ILE:HG23 | 27:U:326:ILE:HG23 | 1.91                     | 0.50              |
| 27:U:453:HIS:ND1  | 27:U:453:HIS:O    | 2.44                     | 0.50              |
| 27:U:685:GLN:HE21 | 27:U:769:PHE:HZ   | 1.60                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 27:U:789:ILE:HA   | 27:U:880:ASN:O    | 2.12                     | 0.50              |
| 1:C:404:LEU:O     | 5:I:80:THR:HG22   | 2.12                     | 0.50              |
| 2:D:148:ASP:OD1   | 2:D:149:SER:N     | 2.43                     | 0.50              |
| 6:J:43:LEU:HD23   | 6:J:209:ALA:O     | 2.12                     | 0.50              |
| 7:L:70:ILE:HG21   | 7:L:108:LEU:HD23  | 1.94                     | 0.50              |
| 7:L:183:ASN:ND2   | 7:L:186:GLU:HB2   | 2.26                     | 0.50              |
| 9:V:334:VAL:HG13  | 9:V:395:ILE:HD13  | 1.91                     | 0.50              |
| 9:V:443:ARG:HD3   | 17:d:274:CYS:SG   | 2.51                     | 0.50              |
| 9:V:479:ARG:HG3   | 12:Y:377:LEU:CD1  | 2.42                     | 0.50              |
| 10:W:40:LEU:CD2   | 10:W:79:GLU:HG3   | 2.41                     | 0.50              |
| 10:W:196:VAL:HG12 | 10:W:196:VAL:O    | 2.12                     | 0.50              |
| 11:X:47:GLU:HG2   | 11:X:80:ILE:HG21  | 1.93                     | 0.50              |
| 11:X:412:ASP:O    | 11:X:415:TYR:HB2  | 2.11                     | 0.50              |
| 12:Y:104:MET:HE1  | 12:Y:130:LYS:HE3  | 1.93                     | 0.50              |
| 12:Y:186:LEU:CD2  | 12:Y:287:LEU:HD22 | 2.41                     | 0.50              |
| 12:Y:376:LEU:CD2  | 13:Z:265:LEU:HD11 | 2.41                     | 0.50              |
| 13:Z:55:ALA:HB3   | 16:c:102:THR:OG1  | 2.12                     | 0.50              |
| 13:Z:216:ALA:HB1  | 14:a:347:LYS:NZ   | 2.26                     | 0.50              |
| 14:a:132:LYS:HD2  | 14:a:132:LYS:N    | 2.27                     | 0.50              |
| 14:a:142:LEU:HD21 | 14:a:152:HIS:CD2  | 2.47                     | 0.50              |
| 14:a:279:GLU:O    | 14:a:283:THR:HG23 | 2.11                     | 0.50              |
| 15:b:6:THR:HG23   | 15:b:110:ILE:HD13 | 1.94                     | 0.50              |
| 17:d:127:ASN:HD22 | 17:d:136:LEU:CD1  | 2.20                     | 0.50              |
| 18:f:266:LEU:HD21 | 18:f:294:MET:O    | 2.11                     | 0.50              |
| 18:f:432:TYR:O    | 18:f:433:LEU:C    | 2.53                     | 0.50              |
| 20:u:118:ASP:O    | 20:u:119:ILE:O    | 2.30                     | 0.50              |
| 22:A:174:TYR:CD1  | 22:A:184:ILE:HD13 | 2.46                     | 0.50              |
| 22:A:355:PHE:CE2  | 22:A:385:ILE:HG23 | 2.46                     | 0.50              |
| 24:E:152:PRO:HG2  | 24:E:274:LYS:HE2  | 1.93                     | 0.50              |
| 24:E:235:ILE:CD1  | 24:E:277:MET:C    | 2.85                     | 0.50              |
| 25:F:168:TYR:O    | 25:F:172:VAL:HB   | 2.11                     | 0.50              |
| 25:F:226:TYR:HB2  | 25:F:335:VAL:CG2  | 2.42                     | 0.50              |
| 27:U:252:LEU:HD23 | 27:U:329:LEU:HD22 | 1.92                     | 0.50              |
| 27:U:624:PHE:CD1  | 27:U:658:ILE:HG21 | 2.46                     | 0.50              |
| 27:U:765:VAL:HG13 | 27:U:778:PHE:CB   | 2.41                     | 0.50              |
| 1:C:43:ARG:HD3    | 9:V:498:PRO:HA    | 1.94                     | 0.50              |
| 1:C:165:ILE:HD11  | 1:C:292:ILE:HG12  | 1.92                     | 0.50              |
| 1:C:298:ILE:O     | 1:C:298:ILE:HG12  | 2.10                     | 0.50              |
| 1:C:405:TRP:CZ3   | 5:I:78:GLY:HA2    | 2.47                     | 0.50              |
| 2:D:336:PRO:HB2   | 2:D:341:LYS:HG3   | 1.94                     | 0.50              |
| 4:H:48:THR:OG1    | 4:H:64:LYS:NZ     | 2.29                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:I:18:LEU:HD21   | 6:J:125:ARG:HD2   | 1.94                     | 0.50              |
| 5:I:122:THR:C     | 6:J:125:ARG:HH21  | 2.19                     | 0.50              |
| 5:I:179:TYR:CZ    | 5:I:181:GLU:HB2   | 2.47                     | 0.50              |
| 7:L:75:ALA:HB3    | 7:L:161:ILE:CD1   | 2.41                     | 0.50              |
| 7:L:154:PHE:CB    | 8:M:58:TYR:CD2    | 2.94                     | 0.50              |
| 9:V:176:MET:HE1   | 9:V:213:TYR:CA    | 2.41                     | 0.50              |
| 9:V:482:PHE:CD1   | 9:V:482:PHE:C     | 2.90                     | 0.50              |
| 10:W:280:ASP:OD1  | 10:W:282:GLU:N    | 2.43                     | 0.50              |
| 12:Y:382:LYS:O    | 12:Y:386:VAL:HG23 | 2.12                     | 0.50              |
| 12:Y:385:ARG:HA   | 12:Y:388:ASN:HD21 | 1.77                     | 0.50              |
| 13:Z:231:GLN:OE1  | 14:a:341:LEU:HD21 | 2.12                     | 0.50              |
| 13:Z:251:LEU:C    | 13:Z:251:LEU:HD23 | 2.37                     | 0.50              |
| 14:a:111:VAL:HG13 | 14:a:115:LYS:HZ2  | 1.77                     | 0.50              |
| 14:a:295:GLU:O    | 14:a:298:LYS:HG2  | 2.11                     | 0.50              |
| 18:f:52:LEU:O     | 18:f:56:LEU:HD23  | 2.12                     | 0.50              |
| 18:f:107:LYS:HE3  | 18:f:142:TYR:OH   | 2.12                     | 0.50              |
| 18:f:179:VAL:HA   | 18:f:182:GLU:OE1  | 2.12                     | 0.50              |
| 18:f:333:LEU:O    | 18:f:337:LEU:HD13 | 2.12                     | 0.50              |
| 18:f:882:LEU:CD1  | 18:f:889:PRO:HD3  | 2.41                     | 0.50              |
| 19:g:107:ILE:CG1  | 19:g:115:LYS:HZ2  | 2.24                     | 0.50              |
| 19:g:162:GLU:HG2  | 19:g:163:GLU:N    | 2.27                     | 0.50              |
| 24:E:40:TYR:HB2   | 25:F:73:ILE:HD11  | 1.92                     | 0.50              |
| 24:E:342:ASP:O    | 24:E:374:VAL:HG11 | 2.12                     | 0.50              |
| 25:F:282:ILE:HA   | 25:F:327:LYS:O    | 2.11                     | 0.50              |
| 25:F:334:ARG:HH11 | 25:F:334:ARG:HG3  | 1.76                     | 0.50              |
| 26:K:203:LYS:HG3  | 26:K:210:LEU:HB2  | 1.94                     | 0.50              |
| 27:U:243:LEU:O    | 27:U:913:ILE:HD13 | 2.11                     | 0.50              |
| 27:U:563:ALA:C    | 27:U:565:ALA:N    | 2.68                     | 0.50              |
| 27:U:813:TYR:CE1  | 27:U:883:ARG:HD2  | 2.46                     | 0.50              |
| 1:C:403:LYS:CB    | 4:H:156:PHE:HE1   | 2.23                     | 0.50              |
| 2:D:99:ASN:HA     | 2:D:115:ILE:HB    | 1.93                     | 0.50              |
| 2:D:218:ALA:O     | 2:D:219:VAL:C     | 2.54                     | 0.50              |
| 3:G:199:ILE:CD1   | 3:G:215:ILE:HD13  | 2.41                     | 0.50              |
| 3:G:206:LEU:HB2   | 3:G:208:ILE:HG12  | 1.93                     | 0.50              |
| 6:J:120:GLN:O     | 6:J:120:GLN:HG3   | 2.12                     | 0.50              |
| 6:J:212:ARG:HD2   | 6:J:215:GLN:CD    | 2.37                     | 0.50              |
| 7:L:23:GLU:O      | 7:L:26:MET:HB3    | 2.11                     | 0.50              |
| 8:M:41:CYS:HB2    | 8:M:186:CYS:N     | 2.27                     | 0.50              |
| 9:V:72:LEU:HD12   | 9:V:120:PHE:CE1   | 2.37                     | 0.50              |
| 10:W:18:VAL:O     | 10:W:19:ASP:HB2   | 2.12                     | 0.50              |
| 10:W:364:ARG:HB3  | 10:W:368:LYS:NZ   | 2.27                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 10:W:391:ALA:HA   | 10:W:394:SER:OG   | 2.12                     | 0.50              |
| 12:Y:219:PHE:CD1  | 12:Y:219:PHE:C    | 2.89                     | 0.50              |
| 13:Z:249:PHE:HZ   | 16:c:303:MET:SD   | 2.35                     | 0.50              |
| 14:a:293:PHE:CG   | 14:a:329:LYS:HG3  | 2.46                     | 0.50              |
| 14:a:313:LYS:O    | 14:a:316:SER:OG   | 2.24                     | 0.50              |
| 14:a:324:ILE:HG23 | 14:a:331:VAL:HG22 | 1.94                     | 0.50              |
| 15:b:36:VAL:N     | 15:b:188:ILE:HD11 | 2.27                     | 0.50              |
| 16:c:141:VAL:HG22 | 16:c:203:ILE:HD12 | 1.94                     | 0.50              |
| 18:f:267:ARG:NH2  | 18:f:893:ILE:HB   | 2.26                     | 0.50              |
| 18:f:307:LEU:HD11 | 18:f:311:VAL:HG21 | 1.93                     | 0.50              |
| 18:f:433:LEU:CG   | 19:g:173:GLU:HA   | 2.42                     | 0.50              |
| 22:A:206:ILE:HG21 | 25:F:404:GLY:HA3  | 1.94                     | 0.50              |
| 23:B:248:LEU:HD12 | 23:B:280:SER:OG   | 2.11                     | 0.50              |
| 23:B:430:LYS:HA   | 23:B:430:LYS:NZ   | 2.26                     | 0.50              |
| 24:E:255:ARG:O    | 24:E:258:MET:HG2  | 2.12                     | 0.50              |
| 24:E:318:GLY:N    | 24:E:319:PRO:HD2  | 2.26                     | 0.50              |
| 25:F:169:ASP:CG   | 25:F:170:SER:H    | 2.20                     | 0.50              |
| 25:F:283:ILE:HD13 | 25:F:283:ILE:N    | 2.27                     | 0.50              |
| 27:U:38:ILE:CG2   | 27:U:67:VAL:HG21  | 2.42                     | 0.50              |
| 27:U:630:PRO:O    | 27:U:634:PRO:HD3  | 2.12                     | 0.50              |
| 1:C:338:LEU:HD13  | 1:C:342:ILE:CG2   | 2.41                     | 0.50              |
| 2:D:41:TYR:CZ     | 27:U:155:LEU:HD11 | 2.47                     | 0.50              |
| 2:D:247:VAL:HB    | 2:D:291:GLU:HG3   | 1.93                     | 0.50              |
| 3:G:80:MET:CE     | 3:G:91:VAL:HG23   | 2.38                     | 0.50              |
| 6:J:26:VAL:CG2    | 6:J:130:SER:HB3   | 2.42                     | 0.50              |
| 8:M:236:GLU:O     | 8:M:240:LYS:HG3   | 2.11                     | 0.50              |
| 9:V:128:ARG:CA    | 9:V:132:LEU:HD23  | 2.42                     | 0.50              |
| 9:V:279:GLN:CG    | 9:V:279:GLN:O     | 2.60                     | 0.50              |
| 9:V:428:LEU:CD1   | 9:V:437:ILE:HG21  | 2.39                     | 0.50              |
| 10:W:109:CYS:HA   | 10:W:112:VAL:HB   | 1.93                     | 0.50              |
| 10:W:445:LEU:O    | 10:W:449:GLU:HG2  | 2.11                     | 0.50              |
| 12:Y:124:PHE:CD1  | 12:Y:140:ILE:HD12 | 2.47                     | 0.50              |
| 14:a:216:LEU:HD22 | 14:a:237:LEU:O    | 2.12                     | 0.50              |
| 15:b:17:ARG:HD3   | 15:b:81:LYS:HZ3   | 1.76                     | 0.50              |
| 15:b:121:GLU:OE1  | 15:b:152:LYS:HB3  | 2.12                     | 0.50              |
| 17:d:136:LEU:CB   | 17:d:141:LEU:HD21 | 2.42                     | 0.50              |
| 18:f:67:ASP:HB3   | 18:f:70:LEU:CG    | 2.42                     | 0.50              |
| 18:f:691:PRO:O    | 18:f:728:ALA:HB2  | 2.11                     | 0.50              |
| 22:A:391:GLU:OE1  | 22:A:391:GLU:HA   | 2.11                     | 0.50              |
| 25:F:126:THR:OG1  | 25:F:130:GLN:O    | 2.27                     | 0.50              |
| 25:F:314:LEU:O    | 25:F:347:ARG:NH1  | 2.41                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 25:F:388:THR:CG2  | 25:F:424:ILE:HG13 | 2.42                     | 0.50              |
| 27:U:633:CYS:HA   | 27:U:636:VAL:HG12 | 1.94                     | 0.50              |
| 27:U:890:LYS:HG3  | 27:U:891:VAL:N    | 2.27                     | 0.50              |
| 1:C:151:ILE:HG12  | 1:C:198:LEU:CG    | 2.41                     | 0.49              |
| 1:C:151:ILE:HG12  | 1:C:198:LEU:HG    | 1.94                     | 0.49              |
| 2:D:154:LEU:HD11  | 24:E:267:PHE:CZ   | 2.46                     | 0.49              |
| 2:D:391:ARG:HH22  | 2:D:395:LEU:HB2   | 1.77                     | 0.49              |
| 5:I:90:LEU:CD2    | 5:I:110:LEU:HD11  | 2.39                     | 0.49              |
| 6:J:210:VAL:CG1   | 6:J:220:LEU:HD21  | 2.42                     | 0.49              |
| 7:L:8:ASN:O       | 26:K:14:THR:HG22  | 2.12                     | 0.49              |
| 7:L:109:VAL:O     | 7:L:112:ILE:HG22  | 2.11                     | 0.49              |
| 7:L:126:ARG:CD    | 26:K:21:LEU:HD11  | 2.42                     | 0.49              |
| 7:L:164:ARG:HG2   | 7:L:164:ARG:O     | 2.12                     | 0.49              |
| 10:W:451:MET:CE   | 13:Z:100:LYS:HD3  | 2.42                     | 0.49              |
| 13:Z:106:ILE:HG21 | 13:Z:153:LYS:HG3  | 1.94                     | 0.49              |
| 13:Z:142:GLU:CD   | 13:Z:153:LYS:HA   | 2.35                     | 0.49              |
| 14:a:100:THR:HA   | 14:a:103:LYS:HE2  | 1.93                     | 0.49              |
| 14:a:230:ARG:HB3  | 14:a:232:TRP:NE1  | 2.27                     | 0.49              |
| 14:a:328:ASP:N    | 14:a:328:ASP:OD1  | 2.44                     | 0.49              |
| 15:b:12:ASN:O     | 15:b:80:PRO:HA    | 2.11                     | 0.49              |
| 17:d:129:LEU:HD11 | 27:U:8:ILE:HD11   | 1.94                     | 0.49              |
| 18:f:399:LEU:HD22 | 18:f:410:ALA:CB   | 2.42                     | 0.49              |
| 18:f:564:LEU:HD22 | 18:f:567:LEU:HD11 | 1.94                     | 0.49              |
| 22:A:58:LYS:HE3   | 23:B:76:GLU:OE2   | 2.12                     | 0.49              |
| 22:A:190:VAL:HG11 | 22:A:212:VAL:CG1  | 2.42                     | 0.49              |
| 23:B:186:ASP:O    | 23:B:367:ILE:HD13 | 2.12                     | 0.49              |
| 24:E:111:LEU:HD13 | 25:F:97:LEU:CD1   | 2.41                     | 0.49              |
| 24:E:122:MET:SD   | 25:F:344:ARG:CZ   | 3.00                     | 0.49              |
| 24:E:151:LEU:HB3  | 24:E:159:PHE:HE2  | 1.75                     | 0.49              |
| 24:E:168:LYS:HA   | 24:E:274:LYS:HE3  | 1.94                     | 0.49              |
| 25:F:145:LEU:HD11 | 25:F:151:VAL:CG1  | 2.42                     | 0.49              |
| 25:F:188:ILE:HD13 | 25:F:236:LEU:CA   | 2.37                     | 0.49              |
| 27:U:114:GLU:HA   | 27:U:114:GLU:OE2  | 2.12                     | 0.49              |
| 27:U:253:TYR:CE1  | 27:U:331:GLY:HA3  | 2.47                     | 0.49              |
| 27:U:332:GLU:O    | 27:U:336:GLU:HG2  | 2.12                     | 0.49              |
| 27:U:373:ASN:ND2  | 27:U:411:ILE:HD11 | 2.27                     | 0.49              |
| 27:U:410:VAL:HG22 | 27:U:448:LEU:HD12 | 1.94                     | 0.49              |
| 27:U:792:ASN:HD21 | 27:U:796:LYS:HE2  | 1.77                     | 0.49              |
| 27:U:900:TYR:OH   | 27:U:921:ILE:HA   | 2.12                     | 0.49              |
| 1:C:117:ARG:HG2   | 1:C:117:ARG:NH1   | 2.27                     | 0.49              |
| 1:C:197:THR:O     | 1:C:197:THR:HG22  | 2.12                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:368:MET:HE3   | 1:C:368:MET:HA    | 1.94                     | 0.49              |
| 2:D:277:ALA:HB3   | 2:D:283:ARG:HG2   | 1.92                     | 0.49              |
| 3:G:47:CYS:SG     | 3:G:191:PHE:HA    | 2.52                     | 0.49              |
| 3:G:73:THR:CG2    | 3:G:74:GLU:N      | 2.75                     | 0.49              |
| 3:G:123:GLN:C     | 3:G:123:GLN:OE1   | 2.55                     | 0.49              |
| 5:I:86:LEU:HD11   | 5:I:114:LEU:HD11  | 1.94                     | 0.49              |
| 5:I:212:GLU:C     | 5:I:213:ILE:HD12  | 2.37                     | 0.49              |
| 9:V:327:THR:O     | 9:V:330:LYS:HB2   | 2.12                     | 0.49              |
| 10:W:321:VAL:HG22 | 10:W:351:TRP:CZ2  | 2.47                     | 0.49              |
| 11:X:143:TYR:CE2  | 11:X:179:ALA:CB   | 2.95                     | 0.49              |
| 11:X:377:ILE:HD13 | 12:Y:310:SER:O    | 2.11                     | 0.49              |
| 11:X:407:MET:HE2  | 11:X:407:MET:CA   | 2.38                     | 0.49              |
| 12:Y:110:TYR:O    | 12:Y:114:ILE:HG23 | 2.12                     | 0.49              |
| 13:Z:230:LEU:C    | 13:Z:230:LEU:HD23 | 2.36                     | 0.49              |
| 14:a:18:GLN:HB2   | 14:a:19:PRO:CD    | 2.39                     | 0.49              |
| 14:a:25:LEU:HA    | 14:a:28:LEU:CD2   | 2.41                     | 0.49              |
| 14:a:284:ARG:HD3  | 14:a:288:HIS:O    | 2.11                     | 0.49              |
| 14:a:292:THR:O    | 14:a:295:GLU:HG2  | 2.12                     | 0.49              |
| 15:b:15:TYR:HD2   | 15:b:116:PRO:HD2  | 1.75                     | 0.49              |
| 16:c:26:ASP:OD1   | 16:c:27:THR:N     | 2.45                     | 0.49              |
| 16:c:27:THR:HG23  | 16:c:175:ARG:HB3  | 1.94                     | 0.49              |
| 17:d:160:ASP:O    | 17:d:163:SER:OG   | 2.23                     | 0.49              |
| 18:f:52:LEU:HB3   | 18:f:98:PHE:CE2   | 2.47                     | 0.49              |
| 18:f:297:MET:HE1  | 18:f:782:HIS:HD2  | 1.77                     | 0.49              |
| 18:f:650:GLN:O    | 18:f:653:ALA:HB3  | 2.12                     | 0.49              |
| 19:g:109:GLY:HA3  | 19:g:138:LEU:CA   | 2.38                     | 0.49              |
| 19:g:115:LYS:HE3  | 19:g:142:LEU:HD22 | 1.93                     | 0.49              |
| 19:g:122:LEU:HB2  | 19:g:127:ILE:HD13 | 1.93                     | 0.49              |
| 22:A:372:LEU:O    | 22:A:372:LEU:HD22 | 2.12                     | 0.49              |
| 24:E:345:ASN:O    | 24:E:346:VAL:C    | 2.54                     | 0.49              |
| 25:F:233:LYS:HG2  | 29:F:501:ATP:O2B  | 2.12                     | 0.49              |
| 25:F:276:LYS:CE   | 25:F:326:VAL:HG21 | 2.39                     | 0.49              |
| 25:F:321:GLN:OE1  | 25:F:321:GLN:N    | 2.44                     | 0.49              |
| 27:U:78:LEU:HD22  | 27:U:104:CYS:SG   | 2.52                     | 0.49              |
| 27:U:177:LEU:HD21 | 27:U:205:TYR:CE1  | 2.47                     | 0.49              |
| 27:U:177:LEU:C    | 27:U:177:LEU:HD23 | 2.37                     | 0.49              |
| 27:U:541:HIS:O    | 27:U:544:ILE:HG22 | 2.12                     | 0.49              |
| 27:U:799:LYS:HG3  | 27:U:925:VAL:HG22 | 1.94                     | 0.49              |
| 1:C:175:PHE:HD2   | 1:C:180:ILE:CD1   | 2.25                     | 0.49              |
| 1:C:219:LEU:HB2   | 1:C:254:ILE:CD1   | 2.41                     | 0.49              |
| 1:C:400:SER:HB3   | 4:H:26:LEU:CD2    | 2.41                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:D:391:ARG:CZ    | 2:D:395:LEU:HD12  | 2.42                     | 0.49              |
| 3:G:23:TYR:HA     | 3:G:26:GLU:HG3    | 1.92                     | 0.49              |
| 3:G:131:MET:HG2   | 8:M:125:TYR:CE1   | 2.46                     | 0.49              |
| 5:I:76:VAL:HG13   | 5:I:132:VAL:CG2   | 2.42                     | 0.49              |
| 5:I:82:ASP:HA     | 5:I:85:VAL:HG12   | 1.93                     | 0.49              |
| 7:L:70:ILE:HD13   | 7:L:108:LEU:HD23  | 1.93                     | 0.49              |
| 9:V:428:LEU:HD12  | 9:V:434:ALA:CB    | 2.41                     | 0.49              |
| 10:W:417:ARG:HB3  | 10:W:418:PRO:HD2  | 1.94                     | 0.49              |
| 10:W:424:LEU:HD11 | 13:Z:244:GLU:CD   | 2.36                     | 0.49              |
| 11:X:57:LEU:CD2   | 11:X:62:GLN:HB2   | 2.42                     | 0.49              |
| 11:X:132:ARG:NH2  | 11:X:135:SER:OG   | 2.45                     | 0.49              |
| 11:X:167:VAL:CG2  | 11:X:196:THR:HG23 | 2.42                     | 0.49              |
| 11:X:183:LEU:HB3  | 11:X:184:PRO:HD3  | 1.93                     | 0.49              |
| 13:Z:113:LYS:NZ   | 13:Z:117:PRO:O    | 2.45                     | 0.49              |
| 13:Z:176:LEU:C    | 13:Z:178:ASP:H    | 2.21                     | 0.49              |
| 14:a:122:LYS:O    | 14:a:127:ASP:HA   | 2.12                     | 0.49              |
| 15:b:147:GLU:HG2  | 15:b:150:THR:HG23 | 1.92                     | 0.49              |
| 18:f:45:LEU:CD2   | 18:f:50:LYS:HE2   | 2.37                     | 0.49              |
| 18:f:51:GLN:O     | 18:f:55:GLU:HG3   | 2.12                     | 0.49              |
| 18:f:226:TYR:HE2  | 18:f:261:ARG:HG3  | 1.71                     | 0.49              |
| 18:f:231:LEU:HD21 | 18:f:853:VAL:HA   | 1.93                     | 0.49              |
| 18:f:257:ARG:HA   | 18:f:257:ARG:NE   | 2.21                     | 0.49              |
| 18:f:369:ARG:HA   | 18:f:372:LEU:CD1  | 2.41                     | 0.49              |
| 18:f:380:PHE:HD1  | 18:f:771:LEU:HD21 | 1.77                     | 0.49              |
| 18:f:830:LEU:HD21 | 18:f:880:ALA:CB   | 2.43                     | 0.49              |
| 19:g:113:ARG:NE   | 19:g:138:LEU:HD13 | 2.27                     | 0.49              |
| 19:g:165:ALA:CA   | 19:g:169:PHE:H    | 2.26                     | 0.49              |
| 23:B:197:ILE:HB   | 23:B:351:ILE:CD1  | 2.42                     | 0.49              |
| 23:B:284:ILE:HG21 | 23:B:287:ILE:HD13 | 1.93                     | 0.49              |
| 24:E:147:GLU:O    | 24:E:151:LEU:HB2  | 2.12                     | 0.49              |
| 25:F:224:LEU:HD12 | 25:F:225:MET:H    | 1.76                     | 0.49              |
| 25:F:250:LYS:HA   | 25:F:284:PHE:O    | 2.12                     | 0.49              |
| 25:F:313:LEU:HD23 | 25:F:313:LEU:C    | 2.38                     | 0.49              |
| 25:F:368:ILE:O    | 25:F:371:ARG:HG3  | 2.13                     | 0.49              |
| 27:U:15:ASP:OD1   | 27:U:15:ASP:N     | 2.40                     | 0.49              |
| 27:U:46:GLU:HG3   | 27:U:80:TYR:CZ    | 2.47                     | 0.49              |
| 27:U:108:TYR:HE1  | 27:U:126:ILE:HG21 | 1.77                     | 0.49              |
| 27:U:588:MET:HA   | 27:U:588:MET:CE   | 2.42                     | 0.49              |
| 1:C:405:TRP:CH2   | 5:I:27:ALA:HB1    | 2.47                     | 0.49              |
| 2:D:147:ALA:HB1   | 2:D:253:LEU:CD1   | 2.42                     | 0.49              |
| 2:D:238:LYS:HE3   | 2:D:239:TYR:HE1   | 1.78                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:D:367:PRO:O     | 2:D:369:LYS:HD2   | 2.13                     | 0.49              |
| 3:G:191:PHE:CE1   | 3:G:219:VAL:HG11  | 2.46                     | 0.49              |
| 4:H:36:VAL:CG1    | 4:H:194:THR:HG22  | 2.40                     | 0.49              |
| 5:I:130:PHE:O     | 5:I:152:PRO:HB3   | 2.12                     | 0.49              |
| 7:L:46:LEU:CD1    | 7:L:63:ILE:HG12   | 2.42                     | 0.49              |
| 7:L:88:MET:HE2    | 7:L:108:LEU:HD21  | 1.93                     | 0.49              |
| 7:L:196:ARG:CZ    | 7:L:239:ARG:HG3   | 2.43                     | 0.49              |
| 10:W:301:LYS:HG3  | 10:W:327:GLU:HG3  | 1.93                     | 0.49              |
| 14:a:80:ILE:CG2   | 14:a:96:PHE:HZ    | 2.25                     | 0.49              |
| 14:a:134:THR:HA   | 14:a:137:ASP:OD2  | 2.12                     | 0.49              |
| 14:a:321:LYS:HD2  | 14:a:336:VAL:CG2  | 2.40                     | 0.49              |
| 15:b:11:ASP:CG    | 15:b:16:MET:HG3   | 2.37                     | 0.49              |
| 18:f:56:LEU:HB3   | 18:f:99:LEU:HD21  | 1.93                     | 0.49              |
| 18:f:130:ALA:HB1  | 18:f:139:CYS:HB2  | 1.93                     | 0.49              |
| 18:f:452:ASN:HB2  | 18:f:488:ALA:HB1  | 1.94                     | 0.49              |
| 18:f:494:ARG:HB3  | 18:f:496:ASP:OD1  | 2.12                     | 0.49              |
| 18:f:850:VAL:HG21 | 18:f:863:THR:HG21 | 1.94                     | 0.49              |
| 19:g:163:GLU:CA   | 19:g:166:ARG:HB2  | 2.31                     | 0.49              |
| 22:A:94:GLN:HB3   | 22:A:142:VAL:HG22 | 1.93                     | 0.49              |
| 22:A:220:THR:HG22 | 22:A:222:LYS:NZ   | 2.28                     | 0.49              |
| 23:B:56:THR:HG23  | 23:B:58:CYS:SG    | 2.52                     | 0.49              |
| 24:E:40:TYR:OH    | 25:F:72:LYS:HB3   | 2.13                     | 0.49              |
| 26:K:186:HIS:CD2  | 26:K:189:MET:CE   | 2.94                     | 0.49              |
| 27:U:265:ILE:HG22 | 27:U:326:ILE:HG23 | 1.91                     | 0.49              |
| 27:U:483:LEU:HD13 | 27:U:778:PHE:CE1  | 2.35                     | 0.49              |
| 27:U:588:MET:SD   | 27:U:764:LEU:HD22 | 2.52                     | 0.49              |
| 27:U:606:ALA:CB   | 27:U:619:VAL:HG23 | 2.40                     | 0.49              |
| 27:U:797:MET:HE2  | 27:U:797:MET:HA   | 1.93                     | 0.49              |
| 27:U:806:CYS:H    | 27:U:874:ASN:CB   | 2.26                     | 0.49              |
| 2:D:205:TYR:CG    | 2:D:314:ALA:HB2   | 2.47                     | 0.49              |
| 2:D:378:ILE:CD1   | 2:D:403:TYR:HD1   | 2.25                     | 0.49              |
| 3:G:38:THR:HG21   | 3:G:202:LEU:HD11  | 1.95                     | 0.49              |
| 6:J:4:ASP:OD1     | 6:J:4:ASP:C       | 2.55                     | 0.49              |
| 6:J:16:LEU:HD12   | 26:K:81:LEU:HD21  | 1.93                     | 0.49              |
| 7:L:22:ILE:CG2    | 7:L:150:SER:HB2   | 2.42                     | 0.49              |
| 8:M:184:MET:HB3   | 8:M:188:ASP:OD1   | 2.13                     | 0.49              |
| 8:M:211:LEU:CG    | 8:M:213:LEU:HD11  | 2.40                     | 0.49              |
| 9:V:67:LEU:HD12   | 9:V:107:ARG:NH1   | 2.24                     | 0.49              |
| 9:V:348:PHE:HB3   | 9:V:361:PHE:HD2   | 1.77                     | 0.49              |
| 10:W:210:ASN:CG   | 10:W:212:LYS:H    | 2.12                     | 0.49              |
| 13:Z:47:VAL:O     | 13:Z:47:VAL:CG2   | 2.60                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 13:Z:60:GLU:HG3   | 13:Z:68:TRP:HB3   | 1.93                     | 0.49              |
| 13:Z:144:VAL:HG21 | 14:a:178:ARG:HE   | 1.77                     | 0.49              |
| 13:Z:175:LEU:HD11 | 16:c:35:SER:CB    | 2.42                     | 0.49              |
| 14:a:68:GLU:HG3   | 14:a:69:HIS:H     | 1.74                     | 0.49              |
| 14:a:78:GLU:HA    | 14:a:81:LEU:HD21  | 1.93                     | 0.49              |
| 15:b:25:ARG:NH2   | 15:b:145:GLU:OE1  | 2.45                     | 0.49              |
| 15:b:26:LEU:CD2   | 15:b:80:PRO:HD3   | 2.43                     | 0.49              |
| 16:c:196:LEU:C    | 16:c:198:ARG:N    | 2.69                     | 0.49              |
| 17:d:248:LYS:O    | 17:d:251:ILE:HG23 | 2.11                     | 0.49              |
| 18:f:209:MET:HG2  | 18:f:248:LEU:HD21 | 1.94                     | 0.49              |
| 18:f:275:MET:SD   | 18:f:278:VAL:HB   | 2.53                     | 0.49              |
| 18:f:502:LEU:HB2  | 18:f:503:PRO:HD3  | 1.94                     | 0.49              |
| 18:f:531:ASN:H    | 18:f:565:ASN:HD21 | 1.60                     | 0.49              |
| 18:f:832:THR:O    | 18:f:840:LEU:N    | 2.45                     | 0.49              |
| 22:A:233:THR:C    | 22:A:235:ALA:H    | 2.20                     | 0.49              |
| 22:A:368:ILE:CD1  | 22:A:406:GLU:HA   | 2.43                     | 0.49              |
| 23:B:231:GLY:HA2  | 29:B:501:ATP:O2A  | 2.13                     | 0.49              |
| 24:E:36:LEU:HA    | 24:E:39:GLN:HE21  | 1.77                     | 0.49              |
| 27:U:147:TYR:HB2  | 27:U:176:MET:HE1  | 1.95                     | 0.49              |
| 27:U:341:PHE:CE1  | 27:U:345:ASN:HB3  | 2.47                     | 0.49              |
| 1:C:36:ASN:ND2    | 9:V:89:LYS:O      | 2.43                     | 0.49              |
| 1:C:329:LEU:HD11  | 1:C:347:ILE:CG2   | 2.43                     | 0.49              |
| 2:D:181:VAL:CG2   | 2:D:308:ILE:HD11  | 2.39                     | 0.49              |
| 2:D:346:SER:O     | 2:D:350:SER:HB3   | 2.13                     | 0.49              |
| 5:I:216:LEU:HD23  | 5:I:216:LEU:C     | 2.37                     | 0.49              |
| 7:L:135:ALA:HB2   | 7:L:144:ILE:CD1   | 2.42                     | 0.49              |
| 7:L:164:ARG:HB2   | 7:L:164:ARG:CZ    | 2.43                     | 0.49              |
| 9:V:248:ALA:HA    | 9:V:276:PHE:CE1   | 2.47                     | 0.49              |
| 11:X:414:LEU:CD1  | 13:Z:273:HIS:HB2  | 2.36                     | 0.49              |
| 13:Z:7:GLN:HG3    | 13:Z:47:VAL:HG12  | 1.92                     | 0.49              |
| 13:Z:32:GLN:CD    | 13:Z:33:LYS:H     | 2.16                     | 0.49              |
| 14:a:6:GLY:O      | 14:a:9:GLN:HB2    | 2.13                     | 0.49              |
| 14:a:173:TYR:CZ   | 14:a:177:LEU:HD11 | 2.48                     | 0.49              |
| 15:b:53:THR:HG22  | 15:b:61:LEU:HD11  | 1.94                     | 0.49              |
| 16:c:187:PRO:CB   | 16:c:192:LEU:HD21 | 2.40                     | 0.49              |
| 18:f:226:TYR:CD1  | 18:f:227:ALA:N    | 2.80                     | 0.49              |
| 18:f:449:GLY:HA3  | 18:f:484:GLY:C    | 2.38                     | 0.49              |
| 18:f:489:TYR:HD2  | 18:f:497:VAL:HG21 | 1.77                     | 0.49              |
| 18:f:801:VAL:O    | 18:f:804:LEU:HB2  | 2.13                     | 0.49              |
| 18:f:827:PRO:HB2  | 18:f:829:MET:CE   | 2.42                     | 0.49              |
| 24:E:311:ASP:HA   | 24:E:314:LYS:HB2  | 1.94                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 25:F:240:CYS:O    | 25:F:244:THR:OG1  | 2.17                     | 0.49              |
| 25:F:246:ALA:HA   | 25:F:280:PRO:O    | 2.12                     | 0.49              |
| 25:F:255:GLN:OE1  | 25:F:255:GLN:HA   | 2.12                     | 0.49              |
| 27:U:787:CYS:SG   | 27:U:789:ILE:CD1  | 3.01                     | 0.49              |
| 1:C:135:VAL:HG23  | 1:C:138:MET:HE3   | 1.93                     | 0.49              |
| 2:D:377:SER:O     | 2:D:379:CYS:N     | 2.46                     | 0.49              |
| 3:G:178:PHE:CE1   | 3:G:204:THR:HG21  | 2.48                     | 0.49              |
| 5:I:108:GLU:HA    | 5:I:148:TYR:HE2   | 1.77                     | 0.49              |
| 5:I:118:LYS:NZ    | 5:I:118:LYS:HB2   | 2.26                     | 0.49              |
| 5:I:134:LEU:N     | 5:I:134:LEU:HD23  | 2.28                     | 0.49              |
| 7:L:104:PRO:HG2   | 7:L:107:ARG:HB2   | 1.93                     | 0.49              |
| 9:V:134:PHE:CD2   | 9:V:187:ILE:HG13  | 2.48                     | 0.49              |
| 10:W:41:GLN:O     | 10:W:44:ILE:HG12  | 2.13                     | 0.49              |
| 10:W:230:MET:HG3  | 10:W:246:HIS:NE2  | 2.27                     | 0.49              |
| 11:X:137:TYR:CB   | 11:X:146:ALA:HB2  | 2.42                     | 0.49              |
| 12:Y:24:PHE:CZ    | 12:Y:289:ALA:HB2  | 2.48                     | 0.49              |
| 13:Z:132:GLY:HA3  | 16:c:222:LYS:HZ3  | 1.78                     | 0.49              |
| 13:Z:212:LEU:HB3  | 14:a:350:LYS:CB   | 2.43                     | 0.49              |
| 16:c:117:GLY:N    | 16:c:146:ASP:OD1  | 2.31                     | 0.49              |
| 17:d:197:LEU:CD1  | 17:d:256:TYR:HD1  | 2.26                     | 0.49              |
| 18:f:67:ASP:HB3   | 18:f:70:LEU:HG    | 1.94                     | 0.49              |
| 18:f:412:ALA:HB3  | 18:f:819:TYR:CE2  | 2.48                     | 0.49              |
| 19:g:116:ILE:HG22 | 19:g:127:ILE:HD12 | 1.93                     | 0.49              |
| 19:g:141:THR:HG22 | 19:g:144:GLU:CG   | 2.42                     | 0.49              |
| 20:u:215:THR:O    | 20:u:237:LYS:NZ   | 2.46                     | 0.49              |
| 24:E:150:GLU:C    | 24:E:150:GLU:OE1  | 2.56                     | 0.49              |
| 24:E:376:ASP:OD1  | 24:E:377:SER:N    | 2.46                     | 0.49              |
| 25:F:181:PRO:HB2  | 25:F:183:GLU:CD   | 2.37                     | 0.49              |
| 25:F:188:ILE:HG12 | 25:F:235:LEU:HG   | 1.94                     | 0.49              |
| 25:F:205:PRO:HB3  | 25:F:219:PRO:HB2  | 1.92                     | 0.49              |
| 25:F:375:VAL:HG22 | 25:F:379:VAL:HG21 | 1.95                     | 0.49              |
| 26:K:109:VAL:HG12 | 26:K:147:ASP:OD2  | 2.13                     | 0.49              |
| 27:U:110:LYS:O    | 27:U:114:GLU:HG2  | 2.13                     | 0.49              |
| 27:U:869:LYS:O    | 27:U:872:GLU:HG2  | 2.13                     | 0.49              |
| 1:C:94:LYS:CB     | 23:B:109:VAL:HB   | 2.36                     | 0.49              |
| 1:C:217:SER:OG    | 2:D:244:PRO:HB3   | 2.13                     | 0.49              |
| 1:C:300:ILE:HD13  | 2:D:276:ASP:OD2   | 2.13                     | 0.49              |
| 2:D:309:MET:HE1   | 2:D:321:LEU:HD11  | 1.94                     | 0.49              |
| 2:D:355:SER:OG    | 2:D:357:GLU:OE1   | 2.23                     | 0.49              |
| 2:D:403:TYR:CE1   | 2:D:407:ILE:HD12  | 2.47                     | 0.49              |
| 8:M:73:VAL:HG13   | 8:M:108:LEU:HD11  | 1.94                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 9:V:345:ARG:NH2   | 28:e:46:ASP:OD2   | 2.33                     | 0.49              |
| 9:V:492:LYS:HG3   | 9:V:493:ALA:N     | 2.27                     | 0.49              |
| 10:W:370:TYR:OH   | 14:a:308:GLU:CG   | 2.61                     | 0.49              |
| 10:W:423:ASN:C    | 10:W:423:ASN:OD1  | 2.55                     | 0.49              |
| 10:W:451:MET:HE2  | 13:Z:100:LYS:HD3  | 1.93                     | 0.49              |
| 13:Z:45:LYS:H     | 13:Z:45:LYS:CD    | 2.20                     | 0.49              |
| 13:Z:90:ARG:HB3   | 13:Z:90:ARG:NH1   | 2.27                     | 0.49              |
| 14:a:7:PHE:HE2    | 14:a:60:TYR:CA    | 2.20                     | 0.49              |
| 14:a:226:ARG:HA   | 14:a:229:ASP:OD1  | 2.12                     | 0.49              |
| 15:b:140:ILE:HG22 | 15:b:170:LEU:HD13 | 1.95                     | 0.49              |
| 17:d:109:LEU:HD23 | 17:d:154:TRP:CE2  | 2.48                     | 0.49              |
| 17:d:122:VAL:O    | 17:d:126:LEU:HG   | 2.13                     | 0.49              |
| 18:f:67:ASP:HB3   | 18:f:70:LEU:CD1   | 2.42                     | 0.49              |
| 18:f:209:MET:CE   | 23:B:59:ARG:HH11  | 2.26                     | 0.49              |
| 18:f:308:SER:HB2  | 18:f:310:ASP:OD1  | 2.13                     | 0.49              |
| 18:f:423:ASP:HA   | 19:g:156:LEU:HD13 | 1.95                     | 0.49              |
| 18:f:433:LEU:HD13 | 18:f:441:LYS:CA   | 2.39                     | 0.49              |
| 18:f:691:PRO:HB2  | 18:f:724:ASN:HB3  | 1.95                     | 0.49              |
| 18:f:799:VAL:HG21 | 18:f:821:LEU:CD2  | 2.42                     | 0.49              |
| 18:f:835:GLU:HG2  | 18:f:900:LEU:O    | 2.13                     | 0.49              |
| 18:f:852:VAL:HG22 | 18:f:852:VAL:O    | 2.12                     | 0.49              |
| 18:f:885:GLU:HG3  | 18:f:906:TYR:HD2  | 1.78                     | 0.49              |
| 22:A:119:ALA:CB   | 25:F:89:LEU:HD11  | 2.43                     | 0.49              |
| 22:A:433:ASN:HD21 | 26:K:66:LYS:HG2   | 1.78                     | 0.49              |
| 23:B:224:LEU:HD11 | 23:B:328:ILE:HG23 | 1.94                     | 0.49              |
| 23:B:272:ARG:NH1  | 23:B:276:GLU:OE2  | 2.46                     | 0.49              |
| 24:E:320:ILE:HA   | 25:F:215:LEU:O    | 2.12                     | 0.49              |
| 25:F:245:LYS:O    | 25:F:246:ALA:HB3  | 2.13                     | 0.49              |
| 25:F:251:LEU:CD2  | 25:F:256:LEU:HD11 | 2.42                     | 0.49              |
| 25:F:384:LEU:O    | 25:F:388:THR:HG23 | 2.12                     | 0.49              |
| 26:K:59:MET:SD    | 26:K:64:ILE:HD11  | 2.53                     | 0.49              |
| 26:K:199:LEU:CD1  | 26:K:238:ILE:HD11 | 2.42                     | 0.49              |
| 27:U:112:CYS:SG   | 27:U:158:ARG:HG2  | 2.53                     | 0.49              |
| 27:U:221:ILE:HD12 | 27:U:256:ALA:HB2  | 1.94                     | 0.49              |
| 27:U:883:ARG:HG3  | 27:U:883:ARG:O    | 2.12                     | 0.49              |
| 27:U:902:PRO:HB3  | 27:U:912:ILE:CD1  | 2.42                     | 0.49              |
| 1:C:246:ILE:HG21  | 1:C:248:MET:HE3   | 1.95                     | 0.49              |
| 3:G:54:LYS:HB2    | 3:G:216:GLU:OE1   | 2.13                     | 0.49              |
| 5:I:45:LEU:HD11   | 5:I:137:ILE:CG2   | 2.43                     | 0.49              |
| 6:J:37:GLY:O      | 6:J:142:PRO:HG3   | 2.13                     | 0.49              |
| 7:L:144:ILE:HG22  | 7:L:144:ILE:O     | 2.11                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:L:160:SER:O     | 7:L:160:SER:OG    | 2.27                     | 0.49              |
| 8:M:73:VAL:CG1    | 8:M:137:LEU:HD22  | 2.43                     | 0.49              |
| 9:V:85:ALA:HB2    | 9:V:93:PHE:HB2    | 1.95                     | 0.49              |
| 9:V:113:LEU:HD11  | 9:V:174:PHE:HB3   | 1.95                     | 0.49              |
| 9:V:289:LEU:HA    | 9:V:292:THR:CG2   | 2.42                     | 0.49              |
| 10:W:80:TRP:HA    | 10:W:80:TRP:HE3   | 1.78                     | 0.49              |
| 10:W:172:GLU:HG3  | 10:W:208:LYS:HD2  | 1.95                     | 0.49              |
| 11:X:109:LEU:HA   | 11:X:112:GLU:OE2  | 2.13                     | 0.49              |
| 13:Z:101:LEU:HD11 | 13:Z:138:TYR:CE2  | 2.48                     | 0.49              |
| 13:Z:208:ILE:HG23 | 13:Z:230:LEU:CD1  | 2.42                     | 0.49              |
| 14:a:113:LEU:H    | 14:a:113:LEU:HD12 | 1.78                     | 0.49              |
| 14:a:124:ASN:C    | 14:a:125:ILE:HD13 | 2.38                     | 0.49              |
| 14:a:189:PRO:O    | 14:a:192:GLU:N    | 2.46                     | 0.49              |
| 14:a:249:GLN:O    | 14:a:252:LYS:N    | 2.46                     | 0.49              |
| 15:b:2:VAL:HG13   | 15:b:2:VAL:O      | 2.13                     | 0.49              |
| 18:f:59:LEU:HD13  | 18:f:62:ARG:NH1   | 2.28                     | 0.49              |
| 18:f:67:ASP:CB    | 18:f:70:LEU:HD12  | 2.43                     | 0.49              |
| 18:f:160:ARG:O    | 18:f:163:ALA:HB3  | 2.13                     | 0.49              |
| 18:f:185:LEU:O    | 18:f:185:LEU:HD23 | 2.12                     | 0.49              |
| 18:f:459:CYS:SG   | 19:g:154:MET:N    | 2.86                     | 0.49              |
| 18:f:520:LEU:CD1  | 18:f:560:LEU:HD13 | 2.40                     | 0.49              |
| 18:f:610:GLN:OE1  | 27:U:830:THR:OG1  | 2.29                     | 0.49              |
| 19:g:112:LEU:HD22 | 19:g:145:GLN:OE1  | 2.13                     | 0.49              |
| 19:g:165:ALA:HA   | 19:g:168:ASN:CA   | 2.42                     | 0.49              |
| 19:g:165:ALA:HA   | 19:g:169:PHE:H    | 1.78                     | 0.49              |
| 23:B:364:ILE:HG12 | 29:B:501:ATP:N1   | 2.28                     | 0.49              |
| 24:E:40:TYR:CE2   | 25:F:72:LYS:HE2   | 2.42                     | 0.49              |
| 24:E:101:ASP:OD2  | 24:E:104:THR:HG23 | 2.13                     | 0.49              |
| 24:E:121:ASN:O    | 24:E:123:SER:N    | 2.46                     | 0.49              |
| 27:U:188:MET:HB3  | 27:U:194:ARG:HH21 | 1.78                     | 0.49              |
| 27:U:792:ASN:OD1  | 27:U:793:LYS:HG2  | 2.13                     | 0.49              |
| 1:C:165:ILE:HG12  | 1:C:292:ILE:HD11  | 1.92                     | 0.49              |
| 2:D:101:ALA:HB2   | 2:D:115:ILE:HD11  | 1.94                     | 0.49              |
| 2:D:309:MET:HE3   | 2:D:327:LEU:CG    | 2.43                     | 0.49              |
| 3:G:162:GLY:HA3   | 4:H:61:SER:HB2    | 1.93                     | 0.49              |
| 4:H:139:TRP:NE1   | 4:H:215:GLU:HA    | 2.28                     | 0.49              |
| 4:H:227:LYS:HE2   | 4:H:227:LYS:C     | 2.38                     | 0.49              |
| 8:M:213:LEU:O     | 8:M:226:ILE:HG13  | 2.12                     | 0.49              |
| 9:V:482:PHE:CE1   | 12:Y:377:LEU:HD22 | 2.47                     | 0.49              |
| 12:Y:181:LYS:HB3  | 12:Y:204:THR:HG21 | 1.95                     | 0.49              |
| 13:Z:40:LEU:HD11  | 13:Z:54:PHE:HE2   | 1.76                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 14:a:164:GLN:O    | 14:a:164:GLN:HG3  | 2.13                     | 0.49              |
| 14:a:329:LYS:HG3  | 14:a:329:LYS:O    | 2.12                     | 0.49              |
| 15:b:181:ASP:HA   | 15:b:184:ILE:CG1  | 2.43                     | 0.49              |
| 15:b:181:ASP:O    | 15:b:184:ILE:HG13 | 2.13                     | 0.49              |
| 17:d:95:TYR:HD2   | 17:d:143:LEU:HD22 | 1.78                     | 0.49              |
| 17:d:146:ASP:HA   | 17:d:149:GLU:CB   | 2.43                     | 0.49              |
| 17:d:204:ARG:NE   | 17:d:207:GLU:OE1  | 2.35                     | 0.49              |
| 18:f:240:VAL:O    | 18:f:245:ASN:HB3  | 2.11                     | 0.49              |
| 18:f:288:VAL:O    | 18:f:291:GLN:HB3  | 2.13                     | 0.49              |
| 18:f:556:ARG:CD   | 18:f:590:PHE:CZ   | 2.95                     | 0.49              |
| 18:f:812:GLY:C    | 18:f:813:LYS:HD3  | 2.38                     | 0.49              |
| 22:A:101:ILE:HD11 | 22:A:111:TYR:HE2  | 1.78                     | 0.49              |
| 24:E:147:GLU:O    | 24:E:151:LEU:HD13 | 2.13                     | 0.49              |
| 25:F:374:ASN:O    | 25:F:414:GLU:HA   | 2.12                     | 0.49              |
| 26:K:143:PHE:O    | 26:K:153:LEU:HD12 | 2.12                     | 0.49              |
| 27:U:246:TYR:HH   | 27:U:324:LYS:HG2  | 1.78                     | 0.49              |
| 2:D:133:HIS:ND1   | 2:D:136:SER:OG    | 2.35                     | 0.48              |
| 3:G:101:TRP:CH2   | 3:G:113:MET:HG3   | 2.48                     | 0.48              |
| 4:H:49:GLU:HG3    | 4:H:49:GLU:O      | 2.11                     | 0.48              |
| 4:H:74:LEU:HD13   | 4:H:134:LEU:CD1   | 2.43                     | 0.48              |
| 5:I:97:TYR:CE1    | 5:I:106:PRO:HD3   | 2.48                     | 0.48              |
| 6:J:26:VAL:O      | 6:J:162:GLY:HA2   | 2.13                     | 0.48              |
| 6:J:69:VAL:HG23   | 6:J:69:VAL:O      | 2.13                     | 0.48              |
| 7:L:55:GLU:OE1    | 7:L:55:GLU:N      | 2.32                     | 0.48              |
| 7:L:74:ILE:HG22   | 7:L:132:LEU:CD2   | 2.41                     | 0.48              |
| 7:L:130:VAL:O     | 7:L:130:VAL:HG13  | 2.13                     | 0.48              |
| 8:M:25:TYR:HA     | 8:M:28:LYS:CD     | 2.42                     | 0.48              |
| 8:M:25:TYR:HA     | 8:M:28:LYS:CG     | 2.41                     | 0.48              |
| 8:M:33:SER:HB2    | 8:M:79:GLY:CA     | 2.41                     | 0.48              |
| 8:M:98:PHE:CZ     | 8:M:106:ILE:HA    | 2.48                     | 0.48              |
| 9:V:128:ARG:O     | 9:V:132:LEU:HD23  | 2.13                     | 0.48              |
| 9:V:188:SER:O     | 9:V:192:MET:N     | 2.36                     | 0.48              |
| 9:V:209:LYS:HE3   | 9:V:213:TYR:OH    | 2.12                     | 0.48              |
| 10:W:188:GLU:O    | 10:W:192:LEU:HG   | 2.12                     | 0.48              |
| 10:W:360:GLU:O    | 10:W:363:ILE:HB   | 2.13                     | 0.48              |
| 12:Y:101:ARG:HH11 | 12:Y:101:ARG:HA   | 1.77                     | 0.48              |
| 12:Y:149:LEU:HA   | 12:Y:157:ILE:HD11 | 1.95                     | 0.48              |
| 14:a:112:ILE:HG23 | 14:a:113:LEU:H    | 1.77                     | 0.48              |
| 14:a:188:LEU:CD1  | 14:a:192:GLU:HB3  | 2.31                     | 0.48              |
| 14:a:287:ASN:OD1  | 14:a:288:HIS:ND1  | 2.46                     | 0.48              |
| 18:f:231:LEU:HD23 | 18:f:853:VAL:HA   | 1.95                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 18:f:337:LEU:HD21 | 18:f:873:LEU:HD11 | 1.95                     | 0.48              |
| 18:f:737:ASN:HD21 | 18:f:773:LYS:C    | 2.20                     | 0.48              |
| 19:g:109:GLY:HA2  | 19:g:112:LEU:HB2  | 1.95                     | 0.48              |
| 22:A:144:ARG:HH21 | 23:B:131:HIS:CD2  | 2.31                     | 0.48              |
| 23:B:283:PHE:CE2  | 23:B:285:ASP:HB2  | 2.48                     | 0.48              |
| 23:B:430:LYS:NZ   | 23:B:431:GLN:OE1  | 2.47                     | 0.48              |
| 24:E:121:ASN:C    | 24:E:123:SER:H    | 2.20                     | 0.48              |
| 25:F:180:ARG:HD3  | 25:F:242:ALA:HA   | 1.95                     | 0.48              |
| 26:K:173:ALA:HB1  | 26:K:205:VAL:CG2  | 2.43                     | 0.48              |
| 27:U:54:PHE:HB3   | 27:U:57:ARG:HG2   | 1.95                     | 0.48              |
| 27:U:98:GLU:C     | 27:U:98:GLU:OE1   | 2.56                     | 0.48              |
| 27:U:129:ARG:O    | 27:U:133:ILE:HG22 | 2.12                     | 0.48              |
| 27:U:377:HIS:C    | 27:U:380:THR:HG23 | 2.38                     | 0.48              |
| 27:U:609:ASP:CG   | 27:U:614:VAL:HG11 | 2.38                     | 0.48              |
| 27:U:770:TRP:O    | 27:U:770:TRP:HD1  | 1.96                     | 0.48              |
| 27:U:902:PRO:HG3  | 27:U:906:LEU:HB2  | 1.95                     | 0.48              |
| 2:D:46:LYS:NZ     | 27:U:187:LEU:HD11 | 2.28                     | 0.48              |
| 2:D:89:ILE:HD11   | 24:E:80:VAL:HG22  | 1.94                     | 0.48              |
| 5:I:43:VAL:HG13   | 5:I:137:ILE:HB    | 1.95                     | 0.48              |
| 8:M:50:GLU:CA     | 8:M:197:ILE:HD11  | 2.43                     | 0.48              |
| 8:M:215:TRP:CD2   | 8:M:227:VAL:HG22  | 2.48                     | 0.48              |
| 8:M:243:LEU:HD12  | 8:M:244:LYS:N     | 2.28                     | 0.48              |
| 10:W:147:LYS:HB2  | 10:W:185:PHE:HE1  | 1.77                     | 0.48              |
| 11:X:140:THR:HG22 | 11:X:140:THR:O    | 2.13                     | 0.48              |
| 11:X:254:MET:CE   | 11:X:270:LEU:HD23 | 2.44                     | 0.48              |
| 12:Y:192:ARG:HD3  | 12:Y:294:TYR:CG   | 2.48                     | 0.48              |
| 14:a:15:GLY:C     | 14:a:21:VAL:HG11  | 2.38                     | 0.48              |
| 14:a:215:GLU:O    | 14:a:219:HIS:HB2  | 2.12                     | 0.48              |
| 15:b:26:LEU:O     | 15:b:29:GLN:HG2   | 2.13                     | 0.48              |
| 15:b:103:LYS:HA   | 15:b:103:LYS:HE3  | 1.95                     | 0.48              |
| 15:b:140:ILE:CG2  | 15:b:170:LEU:HD13 | 2.43                     | 0.48              |
| 16:c:44:HIS:NE2   | 16:c:74:ALA:HB1   | 2.28                     | 0.48              |
| 17:d:101:GLU:O    | 17:d:107:PRO:HA   | 2.14                     | 0.48              |
| 18:f:267:ARG:NH1  | 18:f:783:SER:HA   | 2.28                     | 0.48              |
| 18:f:403:LYS:O    | 18:f:403:LYS:HG3  | 2.12                     | 0.48              |
| 18:f:498:LEU:HD22 | 18:f:534:VAL:HG21 | 1.95                     | 0.48              |
| 18:f:563:GLY:HA3  | 18:f:598:CYS:CB   | 2.42                     | 0.48              |
| 18:f:784:ASP:OD2  | 18:f:879:ARG:NE   | 2.46                     | 0.48              |
| 18:f:869:THR:HG23 | 18:f:869:THR:O    | 2.12                     | 0.48              |
| 22:A:177:VAL:HG22 | 22:A:224:LEU:HG   | 1.95                     | 0.48              |
| 23:B:103:ARG:HE   | 23:B:160:ILE:CG2  | 2.25                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 24:E:194:ASN:HD22 | 24:E:228:CYS:HB2  | 1.78                     | 0.48              |
| 24:E:309:ARG:O    | 24:E:313:LEU:HB2  | 2.14                     | 0.48              |
| 26:K:67:ILE:CD1   | 26:K:77:ALA:HA    | 2.42                     | 0.48              |
| 27:U:8:ILE:O      | 27:U:12:LEU:HD12  | 2.12                     | 0.48              |
| 27:U:357:LYS:HG3  | 27:U:358:ASP:N    | 2.27                     | 0.48              |
| 27:U:796:LYS:HZ3  | 27:U:921:ILE:HB   | 1.79                     | 0.48              |
| 1:C:188:LEU:HD23  | 1:C:315:ILE:HB    | 1.95                     | 0.48              |
| 1:C:222:LYS:HG3   | 1:C:223:PHE:H     | 1.77                     | 0.48              |
| 2:D:70:LYS:HE2    | 2:D:70:LYS:HB2    | 1.57                     | 0.48              |
| 2:D:71:GLU:HG3    | 27:U:644:TYR:CE2  | 2.49                     | 0.48              |
| 5:I:106:PRO:O     | 5:I:108:GLU:N     | 2.46                     | 0.48              |
| 6:J:35:VAL:CG2    | 6:J:191:VAL:HG23  | 2.43                     | 0.48              |
| 7:L:78:THR:HG23   | 25:F:437:TYR:O    | 2.14                     | 0.48              |
| 7:L:126:ARG:HD3   | 26:K:12:VAL:O     | 2.13                     | 0.48              |
| 7:L:224:TYR:CE1   | 7:L:232:PHE:HE1   | 2.32                     | 0.48              |
| 9:V:61:GLU:HG3    | 9:V:62:HIS:N      | 2.27                     | 0.48              |
| 9:V:323:GLY:O     | 9:V:326:GLN:HB2   | 2.12                     | 0.48              |
| 10:W:227:TYR:O    | 10:W:231:ILE:HG13 | 2.13                     | 0.48              |
| 11:X:339:ILE:HD11 | 11:X:350:ILE:HD13 | 1.95                     | 0.48              |
| 11:X:359:ALA:O    | 11:X:363:ARG:HG3  | 2.13                     | 0.48              |
| 12:Y:95:LEU:HB3   | 12:Y:99:GLU:CB    | 2.43                     | 0.48              |
| 12:Y:215:ASP:OD1  | 12:Y:215:ASP:N    | 2.47                     | 0.48              |
| 14:a:34:TRP:CG    | 14:a:70:ARG:HB2   | 2.48                     | 0.48              |
| 14:a:61:GLU:CA    | 14:a:64:ILE:HG22  | 2.40                     | 0.48              |
| 15:b:20:ASP:OD2   | 15:b:144:GLY:HA2  | 2.13                     | 0.48              |
| 17:d:297:LYS:O    | 17:d:300:THR:HB   | 2.12                     | 0.48              |
| 17:d:313:ASN:OD1  | 17:d:315:TYR:HB2  | 2.13                     | 0.48              |
| 18:f:300:ARG:HA   | 18:f:300:ARG:NE   | 2.28                     | 0.48              |
| 18:f:502:LEU:CD2  | 18:f:537:THR:HG21 | 2.42                     | 0.48              |
| 18:f:512:MET:HE2  | 18:f:512:MET:CA   | 2.41                     | 0.48              |
| 20:u:191:PRO:O    | 20:u:225:ILE:HD11 | 2.13                     | 0.48              |
| 22:A:146:LYS:O    | 22:A:147:TYR:HB2  | 2.12                     | 0.48              |
| 22:A:271:LEU:CD2  | 22:A:316:LYS:HB2  | 2.43                     | 0.48              |
| 22:A:433:ASN:O    | 26:K:35:SER:OG    | 2.18                     | 0.48              |
| 25:F:75:GLU:HA    | 25:F:78:GLU:OE1   | 2.13                     | 0.48              |
| 26:K:168:ARG:HG3  | 26:K:169:ALA:N    | 2.27                     | 0.48              |
| 26:K:212:ALA:CB   | 26:K:235:GLU:HG3  | 2.43                     | 0.48              |
| 27:U:422:LEU:HG   | 27:U:426:TYR:HE2  | 1.71                     | 0.48              |
| 2:D:51:LEU:HD12   | 2:D:51:LEU:O      | 2.12                     | 0.48              |
| 2:D:60:TYR:CZ     | 27:U:640:LEU:HD22 | 2.48                     | 0.48              |
| 2:D:73:LEU:CD1    | 13:Z:184:VAL:HG21 | 2.44                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:D:361:GLU:HA    | 2:D:364:VAL:CG2   | 2.39                     | 0.48              |
| 2:D:377:SER:HB3   | 2:D:406:VAL:HG11  | 1.95                     | 0.48              |
| 9:V:66:GLU:CA     | 9:V:69:THR:HG22   | 2.43                     | 0.48              |
| 9:V:358:MET:HE3   | 9:V:359:PRO:N     | 2.28                     | 0.48              |
| 10:W:346:GLU:H    | 10:W:346:GLU:CD   | 2.22                     | 0.48              |
| 11:X:211:ASP:O    | 11:X:214:SER:N    | 2.44                     | 0.48              |
| 11:X:254:MET:HE3  | 11:X:270:LEU:HD23 | 1.95                     | 0.48              |
| 14:a:5:PRO:O      | 14:a:8:LEU:HG     | 2.13                     | 0.48              |
| 14:a:202:LEU:HD21 | 14:a:257:GLN:NE2  | 2.27                     | 0.48              |
| 15:b:39:SER:CB    | 15:b:188:ILE:HG12 | 2.43                     | 0.48              |
| 15:b:143:PHE:HE1  | 15:b:183:LEU:HD21 | 1.77                     | 0.48              |
| 15:b:179:LEU:HG   | 15:b:180:ALA:H    | 1.78                     | 0.48              |
| 16:c:40:LYS:HD2   | 16:c:72:VAL:O     | 2.14                     | 0.48              |
| 16:c:68:ARG:HH12  | 27:U:540:GLN:HG3  | 1.77                     | 0.48              |
| 16:c:247:GLU:OE2  | 16:c:287:HIS:NE2  | 2.46                     | 0.48              |
| 16:c:292:MET:SD   | 17:d:346:LEU:HD13 | 2.53                     | 0.48              |
| 17:d:153:GLN:HA   | 17:d:156:ILE:HD11 | 1.95                     | 0.48              |
| 18:f:253:LEU:HD23 | 18:f:253:LEU:O    | 2.13                     | 0.48              |
| 18:f:339:ILE:HD12 | 18:f:385:PHE:HE1  | 1.79                     | 0.48              |
| 18:f:383:ALA:HA   | 18:f:417:ILE:HA   | 1.95                     | 0.48              |
| 18:f:426:LEU:HB3  | 19:g:156:LEU:HD22 | 1.95                     | 0.48              |
| 18:f:573:ILE:CG1  | 18:f:599:ALA:HB2  | 2.32                     | 0.48              |
| 20:u:166:LEU:HD11 | 20:u:204:MET:HB3  | 1.93                     | 0.48              |
| 23:B:294:ARG:CD   | 23:B:310:LEU:HD11 | 2.32                     | 0.48              |
| 23:B:365:PHE:C    | 23:B:369:THR:HG22 | 2.36                     | 0.48              |
| 23:B:374:LEU:HD12 | 23:B:414:VAL:CG1  | 2.43                     | 0.48              |
| 24:E:98:VAL:HB    | 24:E:107:ILE:CG2  | 2.44                     | 0.48              |
| 24:E:251:ARG:HG3  | 24:E:255:ARG:HH12 | 1.78                     | 0.48              |
| 25:F:382:GLU:O    | 25:F:386:ARG:HD2  | 2.14                     | 0.48              |
| 26:K:112:VAL:HG13 | 26:K:113:THR:N    | 2.28                     | 0.48              |
| 27:U:324:LYS:HZ1  | 27:U:333:MET:HE3  | 1.77                     | 0.48              |
| 27:U:560:MET:CE   | 27:U:593:SER:HB2  | 2.43                     | 0.48              |
| 27:U:628:ARG:HG2  | 27:U:628:ARG:HH11 | 1.76                     | 0.48              |
| 27:U:688:LEU:HD21 | 27:U:712:LEU:HD21 | 1.96                     | 0.48              |
| 27:U:717:ILE:HD12 | 27:U:717:ILE:O    | 2.13                     | 0.48              |
| 27:U:772:TRP:HB3  | 27:U:775:LEU:HG   | 1.95                     | 0.48              |
| 1:C:146:SER:OG    | 1:C:201:ARG:NH1   | 2.45                     | 0.48              |
| 3:G:50:ILE:HG23   | 3:G:141:ILE:HD13  | 1.94                     | 0.48              |
| 3:G:55:LYS:O      | 3:G:57:PRO:HD3    | 2.14                     | 0.48              |
| 3:G:155:ASP:HB2   | 3:G:156:PRO:CD    | 2.43                     | 0.48              |
| 7:L:74:ILE:CG2    | 7:L:132:LEU:HD21  | 2.40                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:L:196:ARG:HB3   | 7:L:205:LEU:HG    | 1.96                     | 0.48              |
| 8:M:149:TYR:HD1   | 8:M:159:GLY:CA    | 2.26                     | 0.48              |
| 9:V:66:GLU:HA     | 9:V:69:THR:CG2    | 2.44                     | 0.48              |
| 10:W:320:LEU:HD23 | 10:W:321:VAL:N    | 2.27                     | 0.48              |
| 11:X:395:LYS:H    | 11:X:395:LYS:HD3  | 1.77                     | 0.48              |
| 12:Y:58:CYS:HA    | 12:Y:63:TRP:HB2   | 1.96                     | 0.48              |
| 12:Y:187:TYR:CZ   | 12:Y:191:ILE:HG21 | 2.49                     | 0.48              |
| 13:Z:217:THR:CG2  | 13:Z:219:LYS:HG3  | 2.42                     | 0.48              |
| 14:a:12:GLN:HB2   | 14:a:23:HIS:HE1   | 1.79                     | 0.48              |
| 14:a:90:PRO:HA    | 14:a:121:LEU:CD2  | 2.43                     | 0.48              |
| 14:a:130:VAL:O    | 14:a:130:VAL:HG22 | 2.12                     | 0.48              |
| 16:c:114:SER:O    | 16:c:115:HIS:CD2  | 2.66                     | 0.48              |
| 16:c:233:ASP:OD1  | 16:c:233:ASP:C    | 2.56                     | 0.48              |
| 18:f:208:LEU:CD2  | 18:f:216:MET:HE2  | 2.43                     | 0.48              |
| 18:f:801:VAL:CA   | 18:f:804:LEU:HD12 | 2.41                     | 0.48              |
| 19:g:116:ILE:HG21 | 19:g:129:ILE:HG12 | 1.94                     | 0.48              |
| 20:u:137:CYS:O    | 20:u:138:LEU:HD23 | 2.14                     | 0.48              |
| 25:F:191:LEU:HD22 | 25:F:194:GLN:HG2  | 1.96                     | 0.48              |
| 25:F:251:LEU:HD21 | 25:F:256:LEU:HD11 | 1.96                     | 0.48              |
| 25:F:288:LEU:O    | 25:F:292:GLY:N    | 2.47                     | 0.48              |
| 25:F:314:LEU:CA   | 25:F:347:ARG:HH12 | 2.27                     | 0.48              |
| 25:F:360:GLU:C    | 25:F:360:GLU:OE1  | 2.56                     | 0.48              |
| 25:F:397:LYS:HD2  | 29:F:501:ATP:O3'  | 2.14                     | 0.48              |
| 27:U:120:GLU:OE1  | 27:U:120:GLU:N    | 2.39                     | 0.48              |
| 27:U:343:ILE:HD12 | 27:U:381:THR:OG1  | 2.13                     | 0.48              |
| 27:U:368:ALA:HB2  | 27:U:728:PHE:CD1  | 2.48                     | 0.48              |
| 27:U:518:LEU:CD2  | 27:U:554:LEU:HD13 | 2.43                     | 0.48              |
| 27:U:831:ALA:O    | 27:U:836:THR:HG21 | 2.13                     | 0.48              |
| 27:U:902:PRO:CG   | 27:U:906:LEU:HB2  | 2.42                     | 0.48              |
| 3:G:69:LEU:HB3    | 3:G:229:ILE:HD11  | 1.94                     | 0.48              |
| 3:G:131:MET:HE3   | 8:M:124:LEU:CD1   | 2.41                     | 0.48              |
| 4:H:203:MET:HG3   | 4:H:208:ILE:HG13  | 1.95                     | 0.48              |
| 5:I:138:GLY:HA2   | 5:I:216:LEU:HD11  | 1.93                     | 0.48              |
| 5:I:158:GLY:H     | 6:J:58:THR:CB     | 2.26                     | 0.48              |
| 6:J:10:PHE:H      | 26:K:23:GLN:NE2   | 2.11                     | 0.48              |
| 7:L:56:LEU:H      | 7:L:56:LEU:CD2    | 2.25                     | 0.48              |
| 7:L:172:LEU:HD21  | 7:L:194:ALA:HB2   | 1.95                     | 0.48              |
| 9:V:198:GLN:CB    | 9:V:203:LEU:HD22  | 2.44                     | 0.48              |
| 9:V:367:VAL:HG21  | 9:V:398:LEU:HD21  | 1.96                     | 0.48              |
| 10:W:34:LEU:HD12  | 10:W:43:VAL:HG22  | 1.95                     | 0.48              |
| 10:W:52:LYS:NZ    | 10:W:52:LYS:HB2   | 2.27                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 10:W:223:LYS:CE   | 10:W:253:THR:HG22 | 2.43                     | 0.48              |
| 10:W:278:PRO:HA   | 10:W:357:ARG:NE   | 2.28                     | 0.48              |
| 10:W:405:LYS:HB3  | 11:X:343:SER:HB2  | 1.95                     | 0.48              |
| 11:X:219:ALA:HB1  | 11:X:322:HIS:CE1  | 2.48                     | 0.48              |
| 11:X:395:LYS:HD3  | 11:X:395:LYS:N    | 2.28                     | 0.48              |
| 13:Z:144:VAL:HG21 | 14:a:178:ARG:NE   | 2.29                     | 0.48              |
| 16:c:136:LEU:HD12 | 20:u:275:MET:HE1  | 1.96                     | 0.48              |
| 16:c:144:VAL:O    | 16:c:145:VAL:HB   | 2.13                     | 0.48              |
| 18:f:117:GLU:OE1  | 18:f:117:GLU:HA   | 2.12                     | 0.48              |
| 18:f:140:LEU:HD23 | 18:f:140:LEU:C    | 2.39                     | 0.48              |
| 18:f:323:ASN:OD1  | 18:f:326:LEU:HD13 | 2.13                     | 0.48              |
| 18:f:852:VAL:HG23 | 18:f:859:PRO:CB   | 2.42                     | 0.48              |
| 19:g:158:LEU:HD23 | 19:g:169:PHE:HB3  | 1.95                     | 0.48              |
| 20:u:196:ILE:C    | 20:u:197:PHE:HD1  | 2.22                     | 0.48              |
| 22:A:55:LEU:HD11  | 23:B:76:GLU:OE1   | 2.13                     | 0.48              |
| 22:A:325:ASP:C    | 22:A:325:ASP:OD1  | 2.56                     | 0.48              |
| 23:B:433:GLY:O    | 23:B:434:THR:HG23 | 2.13                     | 0.48              |
| 24:E:168:LYS:O    | 24:E:168:LYS:HG2  | 2.13                     | 0.48              |
| 25:F:61:ARG:O     | 25:F:65:GLU:HG3   | 2.12                     | 0.48              |
| 25:F:120:LYS:HD3  | 25:F:120:LYS:N    | 2.29                     | 0.48              |
| 25:F:375:VAL:CG2  | 25:F:420:TYR:HE2  | 2.25                     | 0.48              |
| 27:U:357:LYS:HZ2  | 27:U:389:ASN:HD22 | 1.60                     | 0.48              |
| 27:U:399:TRP:CZ3  | 27:U:472:ILE:HG23 | 2.49                     | 0.48              |
| 27:U:633:CYS:O    | 27:U:636:VAL:HG12 | 2.14                     | 0.48              |
| 27:U:842:LYS:HG3  | 27:U:846:LYS:CE   | 2.43                     | 0.48              |
| 27:U:902:PRO:HG3  | 27:U:906:LEU:CB   | 2.44                     | 0.48              |
| 1:C:347:ILE:HG12  | 1:C:383:PHE:HB3   | 1.95                     | 0.48              |
| 1:C:362:VAL:HG23  | 1:C:390:VAL:CG1   | 2.43                     | 0.48              |
| 3:G:97:GLU:OE1    | 3:G:97:GLU:HA     | 2.14                     | 0.48              |
| 6:J:41:VAL:HB     | 6:J:134:VAL:CG2   | 2.44                     | 0.48              |
| 6:J:104:VAL:HG21  | 6:J:135:GLY:O     | 2.14                     | 0.48              |
| 6:J:144:LEU:C     | 6:J:144:LEU:HD12  | 2.39                     | 0.48              |
| 9:V:101:LEU:HA    | 9:V:104:THR:HG22  | 1.95                     | 0.48              |
| 9:V:281:ASN:OD1   | 9:V:282:ASN:N     | 2.47                     | 0.48              |
| 10:W:315:MET:HE2  | 10:W:358:VAL:CG2  | 2.36                     | 0.48              |
| 11:X:109:LEU:HA   | 11:X:112:GLU:HG2  | 1.94                     | 0.48              |
| 11:X:282:ARG:HA   | 11:X:285:GLU:CD   | 2.39                     | 0.48              |
| 12:Y:117:LYS:HB2  | 12:Y:151:TYR:CE2  | 2.48                     | 0.48              |
| 13:Z:78:MET:CE    | 16:c:98:MET:HE3   | 2.43                     | 0.48              |
| 14:a:44:PHE:O     | 14:a:47:ASP:HB3   | 2.14                     | 0.48              |
| 14:a:303:THR:HG22 | 14:a:306:GLU:CD   | 2.39                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 14:a:325:ASP:OD2  | 14:a:328:ASP:HB2  | 2.13                     | 0.48              |
| 16:c:249:LEU:HD11 | 16:c:253:LYS:NZ   | 2.29                     | 0.48              |
| 17:d:251:ILE:O    | 17:d:251:ILE:HG13 | 2.13                     | 0.48              |
| 18:f:89:MET:O     | 18:f:91:SER:N     | 2.46                     | 0.48              |
| 18:f:90:THR:CG2   | 23:B:412:MET:H    | 2.26                     | 0.48              |
| 18:f:223:GLU:OE1  | 18:f:223:GLU:N    | 2.42                     | 0.48              |
| 18:f:237:VAL:HB   | 18:f:249:LEU:CD2  | 2.44                     | 0.48              |
| 18:f:829:MET:SD   | 18:f:829:MET:N    | 2.86                     | 0.48              |
| 22:A:83:ASP:CB    | 23:B:136:LEU:HD12 | 2.43                     | 0.48              |
| 22:A:135:GLU:HG3  | 22:A:138:MET:SD   | 2.53                     | 0.48              |
| 23:B:216:ILE:HG22 | 23:B:217:LYS:N    | 2.29                     | 0.48              |
| 24:E:361:PHE:HE1  | 24:E:366:ASP:CB   | 2.27                     | 0.48              |
| 25:F:81:LYS:HB2   | 25:F:81:LYS:HE2   | 1.44                     | 0.48              |
| 25:F:188:ILE:HG12 | 25:F:235:LEU:HD23 | 1.94                     | 0.48              |
| 26:K:38:ILE:HD11  | 26:K:202:LEU:HD13 | 1.96                     | 0.48              |
| 26:K:190:THR:HG23 | 26:K:192:LYS:N    | 2.29                     | 0.48              |
| 1:C:151:ILE:HG12  | 1:C:198:LEU:HD21  | 1.95                     | 0.48              |
| 1:C:250:GLU:OE1   | 1:C:250:GLU:HA    | 2.14                     | 0.48              |
| 1:C:351:MET:HE3   | 1:C:354:ALA:HB1   | 1.94                     | 0.48              |
| 3:G:52:THR:HG22   | 3:G:216:GLU:O     | 2.13                     | 0.48              |
| 3:G:178:PHE:HD2   | 3:G:201:CYS:HG    | 1.62                     | 0.48              |
| 4:H:35:SER:O      | 4:H:162:ALA:HA    | 2.14                     | 0.48              |
| 4:H:46:LEU:HD13   | 4:H:75:VAL:HG22   | 1.95                     | 0.48              |
| 4:H:77:SER:OG     | 4:H:163:MET:HB2   | 2.14                     | 0.48              |
| 4:H:79:MET:O      | 4:H:132:VAL:HG11  | 2.13                     | 0.48              |
| 7:L:184:LEU:HD11  | 7:L:214:ILE:CG2   | 2.38                     | 0.48              |
| 7:L:196:ARG:HH12  | 7:L:239:ARG:HA    | 1.79                     | 0.48              |
| 8:M:194:ALA:HB2   | 8:M:213:LEU:HD21  | 1.96                     | 0.48              |
| 9:V:111:TYR:CE1   | 9:V:141:THR:HG21  | 2.49                     | 0.48              |
| 9:V:236:ARG:HA    | 9:V:236:ARG:NE    | 2.28                     | 0.48              |
| 9:V:309:MET:HE1   | 9:V:331:LEU:HB3   | 1.96                     | 0.48              |
| 9:V:443:ARG:HG2   | 17:d:277:LYS:HE2  | 1.96                     | 0.48              |
| 10:W:289:ARG:NE   | 10:W:289:ARG:HA   | 2.28                     | 0.48              |
| 10:W:416:GLN:O    | 10:W:416:GLN:HG2  | 2.13                     | 0.48              |
| 11:X:57:LEU:HD22  | 11:X:66:LEU:CG    | 2.44                     | 0.48              |
| 11:X:70:LEU:CA    | 11:X:73:VAL:HG22  | 2.44                     | 0.48              |
| 11:X:187:ARG:NH1  | 11:X:190:LEU:HD23 | 2.28                     | 0.48              |
| 12:Y:22:LEU:HD11  | 12:Y:40:GLU:CB    | 2.33                     | 0.48              |
| 13:Z:53:SER:OG    | 13:Z:54:PHE:N     | 2.46                     | 0.48              |
| 14:a:77:VAL:O     | 14:a:81:LEU:N     | 2.36                     | 0.48              |
| 14:a:329:LYS:CG   | 14:a:329:LYS:O    | 2.61                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 16:c:176:GLN:NE2  | 27:U:398:ASN:HD22 | 2.11                     | 0.48              |
| 18:f:78:LEU:CD1   | 18:f:125:ILE:HG21 | 2.43                     | 0.48              |
| 18:f:128:VAL:HG21 | 18:f:154:TRP:CE3  | 2.49                     | 0.48              |
| 18:f:300:ARG:HH22 | 18:f:897:PHE:HE2  | 1.61                     | 0.48              |
| 18:f:315:GLU:O    | 18:f:319:GLU:N    | 2.28                     | 0.48              |
| 18:f:332:ALA:HA   | 18:f:335:ARG:NE   | 2.22                     | 0.48              |
| 18:f:398:TRP:HD1  | 18:f:401:LYS:HE3  | 1.78                     | 0.48              |
| 18:f:402:ASN:HB3  | 18:f:406:GLY:CA   | 2.41                     | 0.48              |
| 18:f:718:ASP:CB   | 18:f:721:VAL:HG12 | 2.42                     | 0.48              |
| 18:f:734:SER:HA   | 18:f:768:LEU:O    | 2.13                     | 0.48              |
| 18:f:803:PHE:CD1  | 18:f:810:ILE:HG13 | 2.48                     | 0.48              |
| 18:f:844:VAL:CG2  | 18:f:870:THR:HG23 | 2.44                     | 0.48              |
| 22:A:409:PHE:O    | 22:A:412:ALA:N    | 2.47                     | 0.48              |
| 22:A:433:ASN:HB3  | 26:K:82:ILE:HD11  | 1.96                     | 0.48              |
| 23:B:275:GLU:OE1  | 23:B:275:GLU:HA   | 2.14                     | 0.48              |
| 26:K:228:MET:N    | 26:K:228:MET:SD   | 2.86                     | 0.48              |
| 27:U:408:LEU:HD11 | 27:U:426:TYR:CD2  | 2.48                     | 0.48              |
| 27:U:533:VAL:O    | 27:U:537:GLN:OE1  | 2.32                     | 0.48              |
| 27:U:847:GLU:O    | 27:U:851:GLU:HG2  | 2.14                     | 0.48              |
| 1:C:278:ASN:OD1   | 1:C:282:GLY:HA3   | 2.14                     | 0.48              |
| 1:C:281:ASP:CG    | 1:C:307:ARG:HH22  | 2.21                     | 0.48              |
| 2:D:239:TYR:O     | 2:D:240:LEU:C     | 2.57                     | 0.48              |
| 3:G:10:ASP:OD2    | 3:G:24:GLN:NE2    | 2.47                     | 0.48              |
| 3:G:207:SER:O     | 3:G:207:SER:OG    | 2.30                     | 0.48              |
| 6:J:26:VAL:HG21   | 6:J:130:SER:CB    | 2.44                     | 0.48              |
| 6:J:221:ASN:C     | 6:J:223:GLU:H     | 2.22                     | 0.48              |
| 7:L:49:LEU:HB2    | 7:L:195:LEU:HD22  | 1.94                     | 0.48              |
| 7:L:150:SER:O     | 7:L:150:SER:OG    | 2.28                     | 0.48              |
| 8:M:110:HIS:NE2   | 8:M:114:ARG:HD2   | 2.28                     | 0.48              |
| 9:V:75:ILE:C      | 9:V:79:VAL:HG23   | 2.39                     | 0.48              |
| 9:V:318:GLN:HG3   | 9:V:319:HIS:N     | 2.29                     | 0.48              |
| 9:V:452:ASN:C     | 9:V:452:ASN:OD1   | 2.57                     | 0.48              |
| 10:W:31:CYS:HA    | 10:W:43:VAL:HG22  | 1.95                     | 0.48              |
| 10:W:214:PHE:C    | 10:W:219:THR:HG21 | 2.38                     | 0.48              |
| 10:W:424:LEU:HD13 | 13:Z:248:ALA:CB   | 2.44                     | 0.48              |
| 11:X:57:LEU:HD13  | 11:X:66:LEU:HD13  | 1.96                     | 0.48              |
| 11:X:354:ILE:HG22 | 11:X:356:LEU:HB2  | 1.95                     | 0.48              |
| 12:Y:190:ALA:HB2  | 12:Y:287:LEU:CD1  | 2.44                     | 0.48              |
| 13:Z:23:PHE:CD2   | 13:Z:126:VAL:CG1  | 2.97                     | 0.48              |
| 14:a:44:PHE:HA    | 14:a:47:ASP:CB    | 2.43                     | 0.48              |
| 14:a:135:ILE:HG21 | 14:a:155:PHE:CE1  | 2.49                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 17:d:131:THR:OG1  | 27:U:26:LYS:HE2   | 2.13                     | 0.48              |
| 17:d:148:LEU:O    | 17:d:152:ALA:N    | 2.37                     | 0.48              |
| 18:f:173:LEU:CD2  | 18:f:181:ARG:HG3  | 2.44                     | 0.48              |
| 18:f:189:LYS:HZ2  | 18:f:216:MET:HE3  | 1.79                     | 0.48              |
| 18:f:205:CYS:SG   | 18:f:217:LEU:HD21 | 2.54                     | 0.48              |
| 18:f:433:LEU:HD23 | 19:g:173:GLU:HA   | 1.96                     | 0.48              |
| 18:f:447:ALA:CA   | 18:f:450:ILE:HG22 | 2.40                     | 0.48              |
| 18:f:482:ILE:HG21 | 18:f:504:VAL:HG11 | 1.95                     | 0.48              |
| 18:f:592:ASN:O    | 18:f:596:ASP:HB2  | 2.13                     | 0.48              |
| 18:f:832:THR:OG1  | 18:f:840:LEU:O    | 2.32                     | 0.48              |
| 18:f:844:VAL:HG21 | 18:f:870:THR:CG2  | 2.44                     | 0.48              |
| 21:v:11:ALA:O     | 21:v:12:UNK:C     | 2.62                     | 0.48              |
| 22:A:186:LYS:HE3  | 22:A:341:ILE:HG23 | 1.95                     | 0.48              |
| 22:A:426:THR:CG2  | 22:A:430:MET:HE3  | 2.41                     | 0.48              |
| 23:B:184:TYR:HD1  | 23:B:238:ALA:HB1  | 1.79                     | 0.48              |
| 23:B:380:LEU:O    | 23:B:384:ILE:HG13 | 2.14                     | 0.48              |
| 24:E:56:ILE:HB    | 24:E:100:LEU:CD1  | 2.44                     | 0.48              |
| 24:E:335:SER:HB3  | 24:E:338:PHE:CD2  | 2.49                     | 0.48              |
| 25:F:280:PRO:HB3  | 25:F:325:GLN:HB3  | 1.96                     | 0.48              |
| 26:K:113:THR:HG23 | 26:K:143:PHE:HD2  | 1.79                     | 0.48              |
| 27:U:35:TRP:CD1   | 27:U:70:HIS:HD2   | 2.32                     | 0.48              |
| 27:U:352:ILE:HG21 | 27:U:376:MET:HE1  | 1.96                     | 0.48              |
| 1:C:222:LYS:HG3   | 1:C:223:PHE:N     | 2.29                     | 0.48              |
| 2:D:231:VAL:HG11  | 24:E:262:ASN:CG   | 2.39                     | 0.48              |
| 2:D:282:ASP:HA    | 2:D:285:VAL:CG1   | 2.43                     | 0.48              |
| 4:H:69:THR:CG2    | 4:H:94:ALA:HB1    | 2.43                     | 0.48              |
| 6:J:9:VAL:HA      | 26:K:23:GLN:NE2   | 2.28                     | 0.48              |
| 6:J:127:PHE:O     | 6:J:149:PRO:HB3   | 2.14                     | 0.48              |
| 8:M:69:VAL:CG2    | 8:M:75:MET:HE2    | 2.44                     | 0.48              |
| 10:W:275:ILE:HD11 | 10:W:306:LEU:HA   | 1.95                     | 0.48              |
| 11:X:96:PHE:CZ    | 11:X:109:LEU:HD13 | 2.49                     | 0.48              |
| 12:Y:26:LEU:O     | 12:Y:32:ARG:HA    | 2.13                     | 0.48              |
| 12:Y:70:LEU:O     | 12:Y:74:LYS:N     | 2.26                     | 0.48              |
| 12:Y:104:MET:HE2  | 12:Y:104:MET:HB2  | 1.74                     | 0.48              |
| 13:Z:5:ALA:HB3    | 13:Z:46:LYS:NZ    | 2.29                     | 0.48              |
| 13:Z:223:ASN:HB3  | 13:Z:225:GLN:O    | 2.13                     | 0.48              |
| 13:Z:251:LEU:O    | 13:Z:255:ASP:HB2  | 2.13                     | 0.48              |
| 14:a:100:THR:HB   | 14:a:103:LYS:HE2  | 1.95                     | 0.48              |
| 16:c:279:ASP:O    | 16:c:280:PRO:C    | 2.55                     | 0.48              |
| 16:c:299:CYS:SG   | 17:d:339:VAL:HG21 | 2.54                     | 0.48              |
| 17:d:98:LEU:HB2   | 17:d:115:GLU:CG   | 2.44                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 18:f:426:LEU:HD12 | 19:g:169:PHE:HZ   | 1.71                     | 0.48              |
| 18:f:646:MET:HE3  | 18:f:650:GLN:HG3  | 1.95                     | 0.48              |
| 18:f:658:ALA:CA   | 18:f:697:ILE:HD11 | 2.43                     | 0.48              |
| 19:g:89:LEU:HD22  | 19:g:155:VAL:HG11 | 1.96                     | 0.48              |
| 19:g:131:ILE:CG2  | 19:g:147:VAL:HG22 | 2.35                     | 0.48              |
| 23:B:246:THR:CG2  | 23:B:280:SER:HB2  | 2.44                     | 0.48              |
| 25:F:266:LYS:CE   | 25:F:267:LEU:HD22 | 2.44                     | 0.48              |
| 26:K:31:ILE:CD1   | 26:K:140:ALA:CB   | 2.89                     | 0.48              |
| 27:U:78:LEU:HD23  | 27:U:100:ILE:HG23 | 1.95                     | 0.48              |
| 27:U:422:LEU:HG   | 27:U:426:TYR:CZ   | 2.48                     | 0.48              |
| 27:U:458:ILE:HD12 | 27:U:481:LEU:HD12 | 1.95                     | 0.48              |
| 27:U:471:ASP:O    | 27:U:474:ARG:N    | 2.46                     | 0.48              |
| 27:U:670:ASN:O    | 27:U:674:PRO:HD3  | 2.14                     | 0.48              |
| 1:C:72:TYR:CD1    | 2:D:111:TYR:HE1   | 2.32                     | 0.47              |
| 1:C:187:LEU:HD11  | 1:C:295:THR:HG22  | 1.95                     | 0.47              |
| 1:C:308:PRO:O     | 23:B:393:ALA:HB1  | 2.14                     | 0.47              |
| 3:G:143:ILE:CG2   | 3:G:222:VAL:HG22  | 2.44                     | 0.47              |
| 5:I:135:LEU:CG    | 5:I:164:ILE:HD11  | 2.44                     | 0.47              |
| 6:J:144:LEU:HG    | 6:J:156:TRP:O     | 2.14                     | 0.47              |
| 8:M:186:CYS:HA    | 8:M:189:ILE:CB    | 2.27                     | 0.47              |
| 8:M:194:ALA:O     | 8:M:197:ILE:HG22  | 2.14                     | 0.47              |
| 9:V:75:ILE:HG22   | 9:V:79:VAL:CG2    | 2.43                     | 0.47              |
| 9:V:497:PRO:HG3   | 13:Z:282:ASN:CB   | 2.44                     | 0.47              |
| 10:W:136:ILE:HA   | 10:W:139:GLU:OE2  | 2.13                     | 0.47              |
| 10:W:201:ARG:O    | 10:W:204:ILE:N    | 2.47                     | 0.47              |
| 11:X:362:GLU:OE2  | 11:X:378:LEU:HD13 | 2.14                     | 0.47              |
| 13:Z:136:GLU:HG3  | 13:Z:138:TYR:CZ   | 2.49                     | 0.47              |
| 14:a:61:GLU:HG3   | 14:a:79:ILE:CD1   | 2.44                     | 0.47              |
| 14:a:313:LYS:HE2  | 14:a:317:VAL:CG2  | 2.45                     | 0.47              |
| 14:a:319:LEU:HD12 | 14:a:319:LEU:H    | 1.79                     | 0.47              |
| 15:b:79:GLN:CD    | 15:b:81:LYS:HE3   | 2.39                     | 0.47              |
| 18:f:90:THR:HG21  | 23:B:413:LYS:N    | 2.29                     | 0.47              |
| 18:f:416:MET:HB2  | 18:f:450:ILE:CD1  | 2.44                     | 0.47              |
| 19:g:83:ALA:HB3   | 19:g:149:HIS:HB2  | 1.96                     | 0.47              |
| 19:g:89:LEU:HD12  | 19:g:99:ASN:CG    | 2.39                     | 0.47              |
| 22:A:39:SER:O     | 22:A:41:TYR:N     | 2.47                     | 0.47              |
| 22:A:83:ASP:OD1   | 23:B:137:SER:HB3  | 2.14                     | 0.47              |
| 23:B:250:VAL:HG21 | 23:B:284:ILE:HG12 | 1.96                     | 0.47              |
| 23:B:313:LEU:HD23 | 23:B:313:LEU:C    | 2.38                     | 0.47              |
| 25:F:198:LEU:HD23 | 25:F:198:LEU:O    | 2.14                     | 0.47              |
| 26:K:67:ILE:HG12  | 26:K:216:GLU:OE1  | 2.13                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 26:K:197:SER:O    | 26:K:201:ILE:HG13 | 2.15                     | 0.47              |
| 27:U:351:MET:CE   | 27:U:354:LYS:HD3  | 2.44                     | 0.47              |
| 27:U:498:LYS:NZ   | 27:U:531:ASP:OD2  | 2.40                     | 0.47              |
| 27:U:665:ASN:O    | 27:U:666:LYS:HB3  | 2.13                     | 0.47              |
| 27:U:885:MET:HB3  | 27:U:886:PRO:HD2  | 1.96                     | 0.47              |
| 1:C:31:LEU:HD12   | 1:C:35:VAL:HG13   | 1.95                     | 0.47              |
| 1:C:368:MET:CB    | 2:D:329:ARG:HH22  | 2.25                     | 0.47              |
| 1:C:368:MET:HE2   | 2:D:179:GLU:OE1   | 2.14                     | 0.47              |
| 2:D:269:ALA:HB2   | 24:E:258:MET:SD   | 2.54                     | 0.47              |
| 3:G:143:ILE:CD1   | 3:G:220:VAL:HG22  | 2.43                     | 0.47              |
| 4:H:177:ARG:HG2   | 4:H:177:ARG:O     | 2.14                     | 0.47              |
| 6:J:70:CYS:SG     | 6:J:134:VAL:HG13  | 2.54                     | 0.47              |
| 10:W:370:TYR:CE2  | 10:W:373:ILE:HD12 | 2.49                     | 0.47              |
| 11:X:84:LYS:O     | 11:X:88:LEU:HG    | 2.14                     | 0.47              |
| 11:X:93:LEU:CD1   | 11:X:132:ARG:HG2  | 2.44                     | 0.47              |
| 11:X:253:TYR:CD1  | 11:X:253:TYR:N    | 2.81                     | 0.47              |
| 11:X:339:ILE:CG2  | 11:X:387:ILE:HG13 | 2.43                     | 0.47              |
| 12:Y:41:LEU:HD21  | 12:Y:57:LEU:HD11  | 1.95                     | 0.47              |
| 12:Y:57:LEU:HD23  | 12:Y:57:LEU:C     | 2.40                     | 0.47              |
| 12:Y:282:MET:HB3  | 12:Y:292:TYR:HB2  | 1.96                     | 0.47              |
| 12:Y:376:LEU:HD12 | 12:Y:376:LEU:C    | 2.39                     | 0.47              |
| 14:a:262:ALA:HA   | 14:a:265:GLU:HG2  | 1.96                     | 0.47              |
| 17:d:102:TRP:CD2  | 17:d:150:ILE:HG12 | 2.49                     | 0.47              |
| 18:f:136:GLU:HA   | 18:f:139:CYS:HB3  | 1.96                     | 0.47              |
| 18:f:254:GLY:O    | 18:f:257:ARG:HB2  | 2.14                     | 0.47              |
| 18:f:452:ASN:CB   | 18:f:488:ALA:HB1  | 2.44                     | 0.47              |
| 18:f:550:LEU:O    | 18:f:555:ALA:HB3  | 2.15                     | 0.47              |
| 18:f:560:LEU:HD12 | 18:f:801:VAL:HG21 | 1.96                     | 0.47              |
| 18:f:613:LEU:C    | 18:f:613:LEU:HD23 | 2.39                     | 0.47              |
| 18:f:726:ILE:HG21 | 18:f:762:VAL:CA   | 2.45                     | 0.47              |
| 18:f:846:VAL:HB   | 18:f:868:HIS:HD2  | 1.79                     | 0.47              |
| 19:g:165:ALA:C    | 19:g:167:LYS:N    | 2.66                     | 0.47              |
| 23:B:271:PHE:HE2  | 23:B:312:LEU:HD12 | 1.78                     | 0.47              |
| 24:E:353:PHE:CE2  | 24:E:373:LYS:HD3  | 2.49                     | 0.47              |
| 25:F:134:LEU:CD1  | 25:F:160:ILE:HG12 | 2.44                     | 0.47              |
| 25:F:226:TYR:CB   | 25:F:335:VAL:HG21 | 2.44                     | 0.47              |
| 27:U:328:ILE:CG2  | 27:U:333:MET:HE3  | 2.44                     | 0.47              |
| 27:U:490:ARG:HB2  | 27:U:493:VAL:CG1  | 2.44                     | 0.47              |
| 27:U:521:LEU:HD12 | 27:U:522:GLY:H    | 1.76                     | 0.47              |
| 27:U:772:TRP:HA   | 27:U:772:TRP:CE3  | 2.49                     | 0.47              |
| 2:D:184:PRO:CG    | 2:D:306:LYS:HZ1   | 2.26                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:D:284:GLU:O     | 2:D:284:GLU:HG3   | 2.14                     | 0.47              |
| 3:G:155:ASP:HB2   | 3:G:156:PRO:HD2   | 1.97                     | 0.47              |
| 4:H:105:ILE:CD1   | 4:H:113:ARG:HH12  | 2.27                     | 0.47              |
| 5:I:198:ASN:HB3   | 5:I:199:LYS:HZ3   | 1.79                     | 0.47              |
| 7:L:24:TYR:O      | 7:L:27:GLU:N      | 2.45                     | 0.47              |
| 7:L:192:LEU:O     | 7:L:205:LEU:HD11  | 2.13                     | 0.47              |
| 8:M:95:ALA:O      | 8:M:98:PHE:N      | 2.47                     | 0.47              |
| 9:V:405:THR:O     | 9:V:408:ARG:N     | 2.47                     | 0.47              |
| 10:W:382:LEU:O    | 10:W:383:ASP:HB2  | 2.14                     | 0.47              |
| 13:Z:106:ILE:HD12 | 13:Z:153:LYS:HB3  | 1.96                     | 0.47              |
| 13:Z:121:LEU:CD1  | 13:Z:123:ILE:HG13 | 2.44                     | 0.47              |
| 13:Z:139:ILE:HG22 | 13:Z:140:SER:N    | 2.27                     | 0.47              |
| 14:a:374:ILE:HD13 | 17:d:347:GLU:CG   | 2.44                     | 0.47              |
| 16:c:22:ALA:O     | 27:U:398:ASN:ND2  | 2.48                     | 0.47              |
| 18:f:56:LEU:HB3   | 18:f:99:LEU:CD2   | 2.44                     | 0.47              |
| 18:f:188:VAL:HA   | 18:f:191:ILE:CG2  | 2.44                     | 0.47              |
| 18:f:231:LEU:HD21 | 18:f:853:VAL:CA   | 2.44                     | 0.47              |
| 18:f:263:PRO:HG2  | 18:f:890:VAL:O    | 2.14                     | 0.47              |
| 18:f:376:PHE:O    | 18:f:379:GLY:N    | 2.36                     | 0.47              |
| 18:f:422:VAL:CA   | 18:f:426:LEU:HD23 | 2.42                     | 0.47              |
| 18:f:735:GLY:CA   | 18:f:774:GLY:HA2  | 2.41                     | 0.47              |
| 18:f:828:ARG:HG2  | 18:f:874:LEU:O    | 2.15                     | 0.47              |
| 19:g:96:ASP:O     | 19:g:97:ARG:C     | 2.57                     | 0.47              |
| 19:g:112:LEU:HD23 | 19:g:136:LEU:HD13 | 1.95                     | 0.47              |
| 22:A:284:ARG:CZ   | 22:A:284:ARG:HB2  | 2.43                     | 0.47              |
| 22:A:287:ASP:CG   | 22:A:287:ASP:O    | 2.58                     | 0.47              |
| 22:A:306:LEU:CD2  | 22:A:317:VAL:HG21 | 2.44                     | 0.47              |
| 22:A:348:LEU:HD13 | 26:K:175:GLU:HB2  | 1.96                     | 0.47              |
| 23:B:187:ILE:HG22 | 23:B:234:LEU:CG   | 2.43                     | 0.47              |
| 24:E:262:ASN:O    | 24:E:266:GLY:HA3  | 2.14                     | 0.47              |
| 26:K:119:LEU:O    | 26:K:119:LEU:HD12 | 2.14                     | 0.47              |
| 27:U:444:TYR:CE1  | 27:U:448:LEU:HD21 | 2.48                     | 0.47              |
| 27:U:664:GLY:HA3  | 27:U:698:GLN:OE1  | 2.15                     | 0.47              |
| 27:U:699:THR:HG21 | 27:U:812:ALA:N    | 2.29                     | 0.47              |
| 1:C:213:ARG:NE    | 2:D:300:ASP:OD2   | 2.47                     | 0.47              |
| 1:C:316:GLU:OE2   | 1:C:316:GLU:N     | 2.39                     | 0.47              |
| 1:C:330:LYS:HB2   | 1:C:330:LYS:NZ    | 2.29                     | 0.47              |
| 1:C:362:VAL:CG2   | 1:C:390:VAL:HG11  | 2.41                     | 0.47              |
| 2:D:412:GLN:NE2   | 24:E:283:ASP:HA   | 2.28                     | 0.47              |
| 4:H:74:LEU:HB3    | 4:H:134:LEU:HD21  | 1.95                     | 0.47              |
| 5:I:35:LEU:HD23   | 5:I:197:LEU:HD21  | 1.97                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:I:211:VAL:HG22  | 5:I:212:GLU:N     | 2.29                     | 0.47              |
| 6:J:65:LEU:CD2    | 6:J:84:ILE:HG13   | 2.44                     | 0.47              |
| 7:L:46:LEU:HD13   | 7:L:73:SER:HB2    | 1.96                     | 0.47              |
| 8:M:72:HIS:HE2    | 8:M:105:ASN:HB3   | 1.78                     | 0.47              |
| 9:V:65:ARG:HB3    | 9:V:65:ARG:CZ     | 2.44                     | 0.47              |
| 9:V:254:LEU:O     | 9:V:257:ASN:HB3   | 2.15                     | 0.47              |
| 9:V:425:LYS:O     | 9:V:426:LEU:HD12  | 2.14                     | 0.47              |
| 10:W:60:MET:HE3   | 10:W:60:MET:N     | 2.15                     | 0.47              |
| 10:W:169:LEU:HD23 | 10:W:171:VAL:CG1  | 2.45                     | 0.47              |
| 10:W:296:LEU:CD2  | 10:W:303:LYS:HD2  | 2.44                     | 0.47              |
| 11:X:57:LEU:HD21  | 11:X:62:GLN:HB2   | 1.97                     | 0.47              |
| 11:X:57:LEU:HD11  | 11:X:65:GLU:CB    | 2.44                     | 0.47              |
| 11:X:224:ASP:C    | 11:X:224:ASP:OD1  | 2.57                     | 0.47              |
| 13:Z:34:ARG:NH1   | 13:Z:102:HIS:HB2  | 2.28                     | 0.47              |
| 13:Z:149:THR:HG23 | 13:Z:150:PRO:CD   | 2.38                     | 0.47              |
| 14:a:161:LYS:O    | 14:a:164:GLN:CG   | 2.63                     | 0.47              |
| 15:b:75:LEU:HD23  | 15:b:75:LEU:HA    | 1.77                     | 0.47              |
| 15:b:115:SER:OG   | 15:b:116:PRO:HD2  | 2.15                     | 0.47              |
| 16:c:211:GLU:OE2  | 16:c:215:LYS:NZ   | 2.40                     | 0.47              |
| 18:f:426:LEU:HB3  | 19:g:156:LEU:HD21 | 1.96                     | 0.47              |
| 19:g:105:LEU:HG   | 19:g:149:HIS:ND1  | 2.29                     | 0.47              |
| 22:A:190:VAL:HG13 | 22:A:209:PRO:O    | 2.14                     | 0.47              |
| 22:A:399:ALA:O    | 22:A:401:ARG:N    | 2.40                     | 0.47              |
| 23:B:201:VAL:CG2  | 23:B:239:VAL:HG21 | 2.44                     | 0.47              |
| 23:B:333:ARG:HG2  | 23:B:333:ARG:HH11 | 1.78                     | 0.47              |
| 24:E:277:MET:HE1  | 24:E:295:LEU:HD12 | 1.96                     | 0.47              |
| 25:F:294:LYS:HE2  | 25:F:337:ILE:O    | 2.14                     | 0.47              |
| 26:K:108:THR:HG22 | 26:K:110:GLU:H    | 1.79                     | 0.47              |
| 27:U:337:LEU:HD12 | 27:U:789:ILE:HG21 | 1.96                     | 0.47              |
| 27:U:342:LEU:O    | 27:U:346:ASN:HB2  | 2.14                     | 0.47              |
| 27:U:481:LEU:HD11 | 27:U:493:VAL:HG23 | 1.97                     | 0.47              |
| 1:C:287:LYS:HB2   | 1:C:287:LYS:HE2   | 1.60                     | 0.47              |
| 1:C:328:ILE:HG22  | 1:C:359:VAL:CG1   | 2.45                     | 0.47              |
| 1:C:329:LEU:HD22  | 1:C:344:LEU:HD22  | 1.97                     | 0.47              |
| 2:D:97:ASP:OD1    | 2:D:97:ASP:C      | 2.57                     | 0.47              |
| 2:D:355:SER:CB    | 2:D:395:LEU:HD23  | 2.45                     | 0.47              |
| 3:G:78:CYS:HA     | 3:G:139:ILE:O     | 2.14                     | 0.47              |
| 5:I:82:ASP:CG     | 5:I:128:ARG:HH12  | 2.19                     | 0.47              |
| 6:J:34:GLY:O      | 6:J:158:ALA:HA    | 2.14                     | 0.47              |
| 7:L:13:TRP:HZ3    | 7:L:17:GLY:O      | 1.97                     | 0.47              |
| 7:L:116:THR:C     | 7:L:119:PRO:HD2   | 2.40                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 9:V:449:ALA:HB1   | 9:V:459:GLN:O     | 2.15                     | 0.47              |
| 10:W:267:LEU:HD23 | 10:W:270:VAL:CG1  | 2.43                     | 0.47              |
| 10:W:296:LEU:HD23 | 10:W:303:LYS:CD   | 2.43                     | 0.47              |
| 11:X:173:GLU:C    | 11:X:176:THR:HG22 | 2.40                     | 0.47              |
| 12:Y:297:ARG:CB   | 12:Y:297:ARG:NH1  | 2.77                     | 0.47              |
| 14:a:280:MET:CE   | 14:a:299:SER:HB2  | 2.44                     | 0.47              |
| 14:a:295:GLU:HA   | 14:a:298:LYS:HE3  | 1.95                     | 0.47              |
| 15:b:80:PRO:CD    | 15:b:81:LYS:HE2   | 2.44                     | 0.47              |
| 15:b:119:ASP:H    | 15:b:152:LYS:NZ   | 2.13                     | 0.47              |
| 16:c:143:VAL:HG12 | 16:c:144:VAL:H    | 1.79                     | 0.47              |
| 18:f:350:LYS:HD3  | 18:f:353:LEU:HB2  | 1.96                     | 0.47              |
| 18:f:398:TRP:HA   | 18:f:401:LYS:HE3  | 1.95                     | 0.47              |
| 18:f:496:ASP:OD1  | 18:f:496:ASP:N    | 2.47                     | 0.47              |
| 18:f:560:LEU:CD1  | 18:f:801:VAL:HG21 | 2.44                     | 0.47              |
| 22:A:158:ASP:HB2  | 22:A:259:GLU:OE1  | 2.14                     | 0.47              |
| 22:A:366:ARG:O    | 22:A:367:ASP:CB   | 2.62                     | 0.47              |
| 22:A:398:ARG:NH2  | 23:B:349:ARG:HH22 | 2.11                     | 0.47              |
| 23:B:133:VAL:CG1  | 23:B:157:HIS:HB3  | 2.45                     | 0.47              |
| 24:E:152:PRO:HG3  | 24:E:274:LYS:HE2  | 1.95                     | 0.47              |
| 24:E:182:LEU:O    | 24:E:182:LEU:HD12 | 2.15                     | 0.47              |
| 27:U:69:TYR:CE2   | 27:U:96:TYR:HB2   | 2.49                     | 0.47              |
| 27:U:815:ALA:HB1  | 27:U:816:PRO:HD2  | 1.94                     | 0.47              |
| 1:C:58:LEU:HD12   | 1:C:58:LEU:O      | 2.14                     | 0.47              |
| 1:C:207:THR:HG23  | 1:C:209:CYS:N     | 2.25                     | 0.47              |
| 2:D:192:LYS:HG2   | 2:D:192:LYS:O     | 2.15                     | 0.47              |
| 3:G:31:ALA:HA     | 8:M:18:GLY:O      | 2.15                     | 0.47              |
| 3:G:152:TYR:HE2   | 4:H:61:SER:HG     | 1.61                     | 0.47              |
| 3:G:240:VAL:CG2   | 10:W:94:ARG:HD3   | 2.45                     | 0.47              |
| 4:H:135:LEU:HD22  | 4:H:146:LEU:CD2   | 2.41                     | 0.47              |
| 5:I:108:GLU:HA    | 5:I:148:TYR:CE2   | 2.49                     | 0.47              |
| 7:L:88:MET:HE1    | 7:L:134:ILE:HG12  | 1.96                     | 0.47              |
| 9:V:90:GLU:CG     | 9:V:92:ARG:HB2    | 2.45                     | 0.47              |
| 9:V:99:ARG:O      | 9:V:102:PRO:HD2   | 2.14                     | 0.47              |
| 9:V:264:TYR:HD1   | 9:V:295:ILE:CD1   | 2.27                     | 0.47              |
| 10:W:270:VAL:HG22 | 10:W:290:ILE:CD1  | 2.43                     | 0.47              |
| 11:X:74:ARG:HG2   | 11:X:74:ARG:HH11  | 1.79                     | 0.47              |
| 11:X:90:ARG:NH1   | 11:X:128:ALA:HB1  | 2.29                     | 0.47              |
| 11:X:419:LYS:HE3  | 11:X:419:LYS:CA   | 2.31                     | 0.47              |
| 12:Y:97:GLU:CA    | 12:Y:100:ILE:HG12 | 2.44                     | 0.47              |
| 12:Y:348:ASP:OD2  | 12:Y:351:ASN:HB2  | 2.14                     | 0.47              |
| 13:Z:34:ARG:HH21  | 13:Z:96:HIS:CD2   | 2.33                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 13:Z:152:SER:OG   | 13:Z:153:LYS:N    | 2.48                     | 0.47              |
| 13:Z:179:ILE:HD12 | 16:c:218:LEU:HD11 | 1.96                     | 0.47              |
| 13:Z:227:ILE:HD11 | 14:a:346:ILE:CD1  | 2.44                     | 0.47              |
| 14:a:137:ASP:HA   | 14:a:140:GLU:OE1  | 2.14                     | 0.47              |
| 15:b:173:VAL:HG21 | 15:b:183:LEU:HD11 | 1.97                     | 0.47              |
| 16:c:196:LEU:HD23 | 16:c:197:ASN:N    | 2.30                     | 0.47              |
| 17:d:129:LEU:HD12 | 27:U:26:LYS:HG2   | 1.96                     | 0.47              |
| 17:d:150:ILE:O    | 17:d:154:TRP:N    | 2.43                     | 0.47              |
| 18:f:275:MET:HA   | 18:f:275:MET:CE   | 2.37                     | 0.47              |
| 18:f:398:TRP:CD1  | 18:f:401:LYS:HE3  | 2.50                     | 0.47              |
| 18:f:423:ASP:HA   | 19:g:156:LEU:HD12 | 1.96                     | 0.47              |
| 18:f:524:MET:HA   | 18:f:527:VAL:HG13 | 1.95                     | 0.47              |
| 18:f:830:LEU:HB3  | 18:f:872:VAL:H    | 1.80                     | 0.47              |
| 19:g:91:PRO:O     | 19:g:94:LYS:HD3   | 2.14                     | 0.47              |
| 23:B:383:LEU:HD21 | 23:B:419:PHE:CB   | 2.33                     | 0.47              |
| 24:E:121:ASN:C    | 24:E:123:SER:N    | 2.72                     | 0.47              |
| 25:F:245:LYS:HD3  | 25:F:245:LYS:N    | 2.28                     | 0.47              |
| 26:K:94:VAL:HG12  | 26:K:98:ASN:ND2   | 2.30                     | 0.47              |
| 27:U:44:LYS:O     | 27:U:48:LEU:HD13  | 2.14                     | 0.47              |
| 27:U:117:ASP:HB2  | 27:U:118:LEU:HD22 | 1.95                     | 0.47              |
| 27:U:405:THR:HG22 | 27:U:427:LEU:HG   | 1.96                     | 0.47              |
| 27:U:615:ARG:NE   | 27:U:645:ASN:HD21 | 2.11                     | 0.47              |
| 1:C:57:ARG:O      | 1:C:61:GLU:HB2    | 2.13                     | 0.47              |
| 1:C:140:VAL:HB    | 1:C:211:PHE:O     | 2.14                     | 0.47              |
| 1:C:277:LEU:HD22  | 1:C:310:ARG:CZ    | 2.44                     | 0.47              |
| 1:C:347:ILE:HD11  | 1:C:380:GLN:OE1   | 2.14                     | 0.47              |
| 2:D:266:GLU:OE2   | 24:E:262:ASN:HB2  | 2.15                     | 0.47              |
| 3:G:22:LEU:HB3    | 3:G:25:VAL:HG23   | 1.97                     | 0.47              |
| 3:G:54:LYS:HE2    | 3:G:56:VAL:CG2    | 2.45                     | 0.47              |
| 3:G:80:MET:CB     | 3:G:87:SER:HB2    | 2.44                     | 0.47              |
| 4:H:44:VAL:O      | 4:H:213:CYS:N     | 2.32                     | 0.47              |
| 4:H:87:VAL:O      | 4:H:90:ALA:HB3    | 2.15                     | 0.47              |
| 4:H:219:ARG:NH2   | 4:H:225:GLU:OE1   | 2.47                     | 0.47              |
| 5:I:10:THR:HG21   | 5:I:125:GLY:CA    | 2.44                     | 0.47              |
| 5:I:143:TYR:HB2   | 5:I:146:GLN:NE2   | 2.28                     | 0.47              |
| 6:J:45:VAL:CG2    | 6:J:62:ILE:HD11   | 2.45                     | 0.47              |
| 6:J:68:ASN:HB2    | 6:J:137:ASP:CG    | 2.39                     | 0.47              |
| 6:J:79:ASP:CG     | 6:J:125:ARG:HH12  | 2.22                     | 0.47              |
| 7:L:166:GLN:NE2   | 25:F:380:ASN:HD22 | 2.13                     | 0.47              |
| 8:M:122:TYR:CD2   | 8:M:131:PHE:HE1   | 2.32                     | 0.47              |
| 9:V:73:GLU:O      | 9:V:77:GLU:N      | 2.33                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 9:V:109:ASN:H     | 9:V:112:VAL:HG23  | 1.79                     | 0.47              |
| 9:V:110:HIS:CG    | 9:V:136:GLU:HB2   | 2.49                     | 0.47              |
| 9:V:151:THR:H     | 9:V:154:ALA:HB3   | 1.80                     | 0.47              |
| 9:V:176:MET:HG2   | 9:V:217:VAL:HG12  | 1.95                     | 0.47              |
| 9:V:216:ARG:O     | 9:V:219:GLU:HB3   | 2.15                     | 0.47              |
| 9:V:300:LEU:CD1   | 17:d:205:VAL:HG13 | 2.45                     | 0.47              |
| 9:V:324:PHE:CE1   | 9:V:328:VAL:HG23  | 2.50                     | 0.47              |
| 9:V:490:SER:OG    | 13:Z:271:ALA:HB1  | 2.15                     | 0.47              |
| 10:W:136:ILE:HG23 | 10:W:139:GLU:OE2  | 2.14                     | 0.47              |
| 10:W:151:THR:O    | 10:W:155:GLN:HG3  | 2.15                     | 0.47              |
| 10:W:166:LEU:HG   | 10:W:189:GLN:HG2  | 1.97                     | 0.47              |
| 11:X:57:LEU:HD23  | 11:X:57:LEU:C     | 2.40                     | 0.47              |
| 11:X:70:LEU:HD13  | 11:X:92:LEU:HB3   | 1.96                     | 0.47              |
| 11:X:253:TYR:N    | 11:X:253:TYR:HD1  | 2.13                     | 0.47              |
| 11:X:397:TYR:CZ   | 13:Z:258:VAL:HG11 | 2.50                     | 0.47              |
| 12:Y:95:LEU:HD12  | 12:Y:99:GLU:HG3   | 1.95                     | 0.47              |
| 12:Y:138:LEU:CD2  | 12:Y:167:LEU:HG   | 2.44                     | 0.47              |
| 12:Y:146:ARG:CZ   | 12:Y:146:ARG:HB2  | 2.44                     | 0.47              |
| 12:Y:148:GLY:O    | 12:Y:152:MET:N    | 2.48                     | 0.47              |
| 12:Y:271:PHE:CE2  | 12:Y:303:ALA:HB2  | 2.50                     | 0.47              |
| 13:Z:9:VAL:HG21   | 13:Z:120:VAL:HG21 | 1.95                     | 0.47              |
| 13:Z:193:ASN:O    | 13:Z:193:ASN:ND2  | 2.44                     | 0.47              |
| 13:Z:200:GLY:O    | 13:Z:203:SER:N    | 2.48                     | 0.47              |
| 14:a:100:THR:HA   | 14:a:103:LYS:HD3  | 1.96                     | 0.47              |
| 14:a:274:LEU:HD21 | 14:a:278:MET:HE1  | 1.97                     | 0.47              |
| 14:a:291:LEU:HA   | 14:a:295:GLU:OE2  | 2.14                     | 0.47              |
| 14:a:360:VAL:HA   | 16:c:308:VAL:HG22 | 1.96                     | 0.47              |
| 15:b:35:ILE:CG2   | 15:b:184:ILE:HG22 | 2.38                     | 0.47              |
| 15:b:109:ILE:O    | 15:b:139:ASP:N    | 2.34                     | 0.47              |
| 16:c:227:GLU:HA   | 16:c:227:GLU:OE2  | 2.15                     | 0.47              |
| 17:d:275:ILE:HA   | 17:d:279:TYR:CD2  | 2.50                     | 0.47              |
| 18:f:202:HIS:NE2  | 18:f:854:GLY:HA2  | 2.30                     | 0.47              |
| 18:f:264:GLU:CG   | 18:f:892:PRO:HG3  | 2.44                     | 0.47              |
| 18:f:319:GLU:OE2  | 18:f:320:ILE:HG13 | 2.13                     | 0.47              |
| 18:f:342:PRO:HG2  | 18:f:389:LYS:HG3  | 1.96                     | 0.47              |
| 18:f:376:PHE:HE1  | 18:f:409:SER:HB3  | 1.78                     | 0.47              |
| 18:f:399:LEU:HD22 | 18:f:410:ALA:HB1  | 1.97                     | 0.47              |
| 18:f:463:LEU:HD23 | 18:f:463:LEU:C    | 2.40                     | 0.47              |
| 18:f:562:LEU:HD23 | 18:f:566:HIS:HD2  | 1.80                     | 0.47              |
| 18:f:573:ILE:O    | 18:f:577:LEU:HG   | 2.15                     | 0.47              |
| 18:f:796:LEU:O    | 18:f:800:LEU:HD23 | 2.15                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 18:f:803:PHE:CD1  | 18:f:806:VAL:HG12 | 2.50                     | 0.47              |
| 22:A:194:PRO:HG3  | 22:A:201:PHE:CE2  | 2.50                     | 0.47              |
| 22:A:333:ARG:HH21 | 22:A:336:ARG:CZ   | 2.28                     | 0.47              |
| 23:B:204:PRO:HB3  | 23:B:218:PRO:HB3  | 1.96                     | 0.47              |
| 24:E:42:LYS:HA    | 24:E:45:ASN:ND2   | 2.30                     | 0.47              |
| 24:E:169:GLY:HA2  | 24:E:275:MET:O    | 2.13                     | 0.47              |
| 25:F:226:TYR:CE1  | 25:F:353:GLU:HB2  | 2.49                     | 0.47              |
| 25:F:276:LYS:HD2  | 25:F:276:LYS:HA   | 1.65                     | 0.47              |
| 27:U:142:LEU:HD21 | 27:U:166:THR:CG2  | 2.44                     | 0.47              |
| 27:U:330:SER:O    | 27:U:453:HIS:NE2  | 2.46                     | 0.47              |
| 27:U:792:ASN:OD1  | 27:U:796:LYS:HG2  | 2.15                     | 0.47              |
| 27:U:842:LYS:C    | 27:U:846:LYS:HE3  | 2.39                     | 0.47              |
| 1:C:220:VAL:HG21  | 2:D:287:ARG:HD3   | 1.97                     | 0.47              |
| 1:C:222:LYS:HE3   | 1:C:222:LYS:HB2   | 1.77                     | 0.47              |
| 1:C:368:MET:HB3   | 2:D:329:ARG:NH2   | 2.28                     | 0.47              |
| 2:D:282:ASP:OD1   | 24:E:248:SER:HB2  | 2.15                     | 0.47              |
| 3:G:107:TYR:HE2   | 3:G:110:PRO:HD3   | 1.79                     | 0.47              |
| 4:H:84:ARG:O      | 4:H:87:VAL:HG12   | 2.15                     | 0.47              |
| 6:J:2:SER:HA      | 6:J:5:ARG:NH2     | 2.30                     | 0.47              |
| 7:L:196:ARG:HH22  | 7:L:239:ARG:H     | 1.61                     | 0.47              |
| 8:M:227:VAL:CB    | 8:M:232:ARG:HH12  | 2.27                     | 0.47              |
| 9:V:151:THR:N     | 9:V:154:ALA:HB3   | 2.29                     | 0.47              |
| 9:V:224:LEU:CD2   | 9:V:257:ASN:HA    | 2.41                     | 0.47              |
| 11:X:46:LYS:HG2   | 11:X:76:PHE:CD1   | 2.49                     | 0.47              |
| 13:Z:6:VAL:CG2    | 13:Z:139:ILE:HD11 | 2.44                     | 0.47              |
| 13:Z:106:ILE:HG13 | 13:Z:153:LYS:HB2  | 1.97                     | 0.47              |
| 13:Z:260:VAL:HG13 | 16:c:292:MET:HG3  | 1.95                     | 0.47              |
| 14:a:118:ILE:HG12 | 14:a:122:LYS:CD   | 2.42                     | 0.47              |
| 14:a:132:LYS:HD3  | 14:a:162:TYR:CE1  | 2.49                     | 0.47              |
| 14:a:138:VAL:O    | 14:a:142:LEU:N    | 2.44                     | 0.47              |
| 14:a:281:THR:CG2  | 14:a:335:TRP:CZ3  | 2.97                     | 0.47              |
| 14:a:304:VAL:O    | 14:a:307:VAL:HG12 | 2.14                     | 0.47              |
| 15:b:179:LEU:HG   | 15:b:180:ALA:N    | 2.30                     | 0.47              |
| 16:c:118:PHE:C    | 16:c:121:TRP:HE1  | 2.23                     | 0.47              |
| 18:f:92:VAL:HG12  | 23:B:410:ARG:HB3  | 1.97                     | 0.47              |
| 18:f:105:LYS:O    | 18:f:109:ILE:HG22 | 2.15                     | 0.47              |
| 18:f:502:LEU:HD22 | 18:f:537:THR:CG2  | 2.44                     | 0.47              |
| 18:f:558:LEU:HB2  | 18:f:559:PRO:HD3  | 1.95                     | 0.47              |
| 18:f:607:LEU:CD1  | 27:U:835:ILE:HG13 | 2.45                     | 0.47              |
| 22:A:186:LYS:HB3  | 22:A:186:LYS:NZ   | 2.29                     | 0.47              |
| 22:A:240:VAL:HG11 | 22:A:274:PHE:CD1  | 2.50                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 23:B:292:THR:O    | 23:B:309:MET:HE1  | 2.15                     | 0.47              |
| 24:E:322:LYS:HB2  | 24:E:361:PHE:HD2  | 1.79                     | 0.47              |
| 25:F:202:ILE:C    | 25:F:205:PRO:HD2  | 2.40                     | 0.47              |
| 25:F:384:LEU:HD11 | 25:F:420:TYR:CG   | 2.49                     | 0.47              |
| 26:K:151:PRO:C    | 26:K:152:GLN:HG2  | 2.39                     | 0.47              |
| 26:K:172:SER:O    | 26:K:173:ALA:HB3  | 2.15                     | 0.47              |
| 27:U:160:LEU:HD13 | 27:U:196:LYS:HG2  | 1.96                     | 0.47              |
| 27:U:174:PRO:O    | 27:U:177:LEU:HB3  | 2.15                     | 0.47              |
| 27:U:398:ASN:O    | 27:U:401:LYS:HB3  | 2.15                     | 0.47              |
| 27:U:700:GLU:HA   | 27:U:706:VAL:CG1  | 2.44                     | 0.47              |
| 1:C:205:HIS:HD2   | 1:C:206:HIS:CD2   | 2.33                     | 0.47              |
| 3:G:72:ILE:CD1    | 3:G:78:CYS:HB3    | 2.40                     | 0.47              |
| 4:H:128:ARG:HG3   | 4:H:129:PRO:HD2   | 1.97                     | 0.47              |
| 4:H:155:TYR:HE1   | 5:I:60:PHE:CZ     | 2.33                     | 0.47              |
| 5:I:218:ARG:NH2   | 5:I:221:GLY:HA2   | 2.30                     | 0.47              |
| 6:J:227:LYS:O     | 6:J:231:GLU:N     | 2.29                     | 0.47              |
| 7:L:233:LEU:HD23  | 7:L:233:LEU:HA    | 1.75                     | 0.47              |
| 8:M:49:VAL:HG12   | 8:M:66:LEU:HD22   | 1.97                     | 0.47              |
| 9:V:161:PRO:HA    | 9:V:164:GLU:CG    | 2.45                     | 0.47              |
| 9:V:252:ASN:ND2   | 9:V:284:GLU:OE1   | 2.46                     | 0.47              |
| 9:V:438:VAL:HG11  | 9:V:458:VAL:CG2   | 2.43                     | 0.47              |
| 10:W:369:TYR:HB3  | 14:a:324:ILE:CD1  | 2.45                     | 0.47              |
| 10:W:370:TYR:HE1  | 14:a:312:MET:CE   | 2.28                     | 0.47              |
| 12:Y:81:LEU:HG    | 12:Y:110:TYR:CE2  | 2.50                     | 0.47              |
| 12:Y:229:ILE:HA   | 12:Y:299:MET:CE   | 2.45                     | 0.47              |
| 12:Y:387:ILE:O    | 12:Y:389:MET:HG2  | 2.15                     | 0.47              |
| 14:a:24:ARG:NE    | 14:a:24:ARG:O     | 2.48                     | 0.47              |
| 14:a:108:ASP:C    | 14:a:108:ASP:OD1  | 2.56                     | 0.47              |
| 14:a:111:VAL:HG13 | 14:a:115:LYS:NZ   | 2.30                     | 0.47              |
| 15:b:41:THR:CG2   | 15:b:42:ARG:HH11  | 2.27                     | 0.47              |
| 15:b:161:ASN:HD21 | 15:b:168:SER:N    | 2.08                     | 0.47              |
| 16:c:195:GLY:HA3  | 16:c:199:HIS:NE2  | 2.30                     | 0.47              |
| 18:f:211:ILE:O    | 18:f:211:ILE:HG22 | 2.15                     | 0.47              |
| 18:f:379:GLY:O    | 18:f:383:ALA:N    | 2.47                     | 0.47              |
| 18:f:698:SER:HB2  | 18:f:706:ILE:HD13 | 1.96                     | 0.47              |
| 19:g:103:THR:OG1  | 19:g:115:LYS:HD2  | 2.15                     | 0.47              |
| 19:g:112:LEU:CD1  | 19:g:116:ILE:HG13 | 2.45                     | 0.47              |
| 19:g:112:LEU:HD22 | 19:g:142:LEU:CG   | 2.45                     | 0.47              |
| 26:K:53:ARG:HG2   | 26:K:53:ARG:O     | 2.15                     | 0.47              |
| 26:K:99:HIS:CD2   | 26:K:107:MET:HE3  | 2.50                     | 0.47              |
| 27:U:514:LEU:HD21 | 27:U:765:VAL:HG23 | 1.97                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 27:U:680:VAL:HG11 | 27:U:682:TYR:CE1  | 2.50                     | 0.47              |
| 27:U:748:LEU:HD23 | 27:U:760:VAL:HA   | 1.97                     | 0.47              |
| 28:e:59:GLU:OE1   | 28:e:62:LYS:NZ    | 2.31                     | 0.47              |
| 1:C:401:ILE:HD12  | 4:H:23:GLU:HG2    | 1.97                     | 0.47              |
| 2:D:355:SER:HB3   | 2:D:395:LEU:HD23  | 1.97                     | 0.47              |
| 3:G:123:GLN:NE2   | 3:G:127:GLN:HE21  | 2.08                     | 0.47              |
| 4:H:34:PRO:HD2    | 4:H:49:GLU:HG2    | 1.97                     | 0.47              |
| 5:I:232:GLU:O     | 5:I:235:GLN:NE2   | 2.48                     | 0.47              |
| 6:J:173:GLU:HG3   | 26:K:58:LEU:CD1   | 2.44                     | 0.47              |
| 7:L:75:ALA:HB3    | 7:L:161:ILE:HD12  | 1.95                     | 0.47              |
| 8:M:17:ASP:OD2    | 8:M:19:ARG:NE     | 2.47                     | 0.47              |
| 8:M:39:ILE:HD11   | 8:M:176:ILE:CG2   | 2.45                     | 0.47              |
| 8:M:39:ILE:HD13   | 8:M:162:GLY:HA3   | 1.96                     | 0.47              |
| 8:M:150:MET:C     | 8:M:150:MET:SD    | 2.98                     | 0.47              |
| 8:M:188:ASP:O     | 8:M:192:GLU:HG2   | 2.14                     | 0.47              |
| 9:V:111:TYR:CE1   | 9:V:115:LYS:HG3   | 2.50                     | 0.47              |
| 9:V:264:TYR:CD2   | 17:d:213:GLU:HG3  | 2.48                     | 0.47              |
| 9:V:407:VAL:HG11  | 9:V:441:ALA:HB3   | 1.97                     | 0.47              |
| 10:W:396:LEU:HD22 | 10:W:401:THR:CG2  | 2.45                     | 0.47              |
| 11:X:299:LEU:HD22 | 11:X:354:ILE:HG23 | 1.97                     | 0.47              |
| 12:Y:41:LEU:CD2   | 12:Y:57:LEU:HD11  | 2.44                     | 0.47              |
| 12:Y:194:PHE:CE1  | 12:Y:288:PHE:HE1  | 2.34                     | 0.47              |
| 14:a:123:LEU:HD12 | 14:a:123:LEU:O    | 2.14                     | 0.47              |
| 14:a:248:PHE:CZ   | 14:a:249:GLN:HG3  | 2.50                     | 0.47              |
| 15:b:26:LEU:O     | 15:b:30:GLN:N     | 2.30                     | 0.47              |
| 15:b:55:ALA:O     | 15:b:56:ASN:HB3   | 2.14                     | 0.47              |
| 16:c:115:HIS:O    | 16:c:116:PRO:C    | 2.58                     | 0.47              |
| 17:d:99:LYS:HG2   | 17:d:103:ASN:CG   | 2.40                     | 0.47              |
| 17:d:153:GLN:CA   | 17:d:156:ILE:HG12 | 2.45                     | 0.47              |
| 17:d:254:GLU:O    | 17:d:257:THR:N    | 2.39                     | 0.47              |
| 18:f:106:LEU:O    | 18:f:110:TYR:HB2  | 2.14                     | 0.47              |
| 18:f:149:GLU:HG3  | 18:f:150:GLU:N    | 2.30                     | 0.47              |
| 18:f:157:GLU:OE2  | 22:A:36:TYR:OH    | 2.25                     | 0.47              |
| 18:f:333:LEU:HD12 | 18:f:337:LEU:CD1  | 2.45                     | 0.47              |
| 18:f:646:MET:O    | 18:f:646:MET:HG3  | 2.15                     | 0.47              |
| 18:f:828:ARG:C    | 18:f:828:ARG:HD3  | 2.40                     | 0.47              |
| 18:f:840:LEU:HG   | 18:f:840:LEU:O    | 2.14                     | 0.47              |
| 20:u:189:GLN:OE1  | 20:u:259:ARG:NE   | 2.48                     | 0.47              |
| 25:F:366:MET:HE2  | 25:F:366:MET:HB2  | 1.71                     | 0.47              |
| 27:U:115:ASN:HB3  | 27:U:123:LYS:CG   | 2.45                     | 0.47              |
| 27:U:401:LYS:HE3  | 27:U:437:TYR:CB   | 2.36                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 27:U:415:HIS:H    | 27:U:449:ILE:HG23 | 1.80                     | 0.47              |
| 1:C:49:ARG:HH12   | 27:U:639:LEU:C    | 2.24                     | 0.46              |
| 1:C:315:ILE:HG22  | 1:C:317:PHE:CE1   | 2.50                     | 0.46              |
| 1:C:387:VAL:O     | 1:C:391:MET:HB3   | 2.16                     | 0.46              |
| 2:D:212:LYS:HB2   | 31:D:501:ADP:O3B  | 2.15                     | 0.46              |
| 4:H:65:VAL:HG12   | 4:H:218:PHE:CZ    | 2.47                     | 0.46              |
| 5:I:17:ARG:HG2    | 6:J:28:LYS:NZ     | 2.29                     | 0.46              |
| 5:I:174:MET:HE1   | 5:I:196:VAL:HA    | 1.97                     | 0.46              |
| 6:J:198:VAL:O     | 6:J:201:SER:N     | 2.47                     | 0.46              |
| 9:V:208:ALA:HB2   | 9:V:246:GLY:HA2   | 1.97                     | 0.46              |
| 9:V:429:ASP:OD1   | 9:V:430:SER:N     | 2.48                     | 0.46              |
| 10:W:105:VAL:CG1  | 10:W:106:GLN:N    | 2.78                     | 0.46              |
| 10:W:128:LEU:O    | 10:W:132:THR:HG23 | 2.15                     | 0.46              |
| 10:W:223:LYS:HD3  | 10:W:253:THR:HG22 | 1.96                     | 0.46              |
| 11:X:171:LEU:HD23 | 11:X:209:THR:HG22 | 1.96                     | 0.46              |
| 11:X:180:LEU:O    | 11:X:181:SER:HB2  | 2.14                     | 0.46              |
| 12:Y:161:THR:HG23 | 12:Y:184:GLN:OE1  | 2.15                     | 0.46              |
| 12:Y:334:LEU:O    | 12:Y:338:ILE:HG13 | 2.15                     | 0.46              |
| 13:Z:6:VAL:O      | 13:Z:158:VAL:HG23 | 2.14                     | 0.46              |
| 14:a:42:LEU:HD11  | 14:a:78:GLU:HB3   | 1.97                     | 0.46              |
| 14:a:309:LEU:HD12 | 14:a:312:MET:CB   | 2.45                     | 0.46              |
| 15:b:140:ILE:HG21 | 15:b:153:LEU:CD2  | 2.44                     | 0.46              |
| 16:c:299:CYS:O    | 16:c:303:MET:HG2  | 2.15                     | 0.46              |
| 17:d:201:SER:HA   | 17:d:263:LEU:HD13 | 1.96                     | 0.46              |
| 17:d:331:PRO:HB2  | 17:d:334:GLU:HB3  | 1.97                     | 0.46              |
| 18:f:280:ASP:O    | 18:f:284:SER:N    | 2.35                     | 0.46              |
| 18:f:381:VAL:HG22 | 18:f:770:HIS:HB2  | 1.97                     | 0.46              |
| 19:g:136:LEU:CD2  | 19:g:147:VAL:HG21 | 2.42                     | 0.46              |
| 23:B:266:LEU:C    | 23:B:266:LEU:HD23 | 2.40                     | 0.46              |
| 23:B:317:ASP:C    | 23:B:317:ASP:OD1  | 2.58                     | 0.46              |
| 23:B:375:ALA:HA   | 23:B:413:LYS:HD2  | 1.97                     | 0.46              |
| 23:B:396:LYS:O    | 23:B:396:LYS:HG2  | 2.14                     | 0.46              |
| 24:E:65:THR:CG2   | 24:E:68:LYS:HB2   | 2.44                     | 0.46              |
| 25:F:248:PHE:HD1  | 25:F:282:ILE:CD1  | 2.25                     | 0.46              |
| 25:F:257:VAL:O    | 25:F:257:VAL:CG1  | 2.63                     | 0.46              |
| 25:F:266:LYS:HE3  | 25:F:267:LEU:HD22 | 1.96                     | 0.46              |
| 25:F:383:GLU:HA   | 25:F:386:ARG:HD3  | 1.97                     | 0.46              |
| 26:K:39:GLY:HA3   | 26:K:153:LEU:CD2  | 2.45                     | 0.46              |
| 27:U:108:TYR:HB2  | 27:U:134:VAL:HG21 | 1.97                     | 0.46              |
| 27:U:159:ARG:HB3  | 27:U:162:VAL:CG1  | 2.45                     | 0.46              |
| 27:U:348:THR:HG22 | 27:U:741:GLY:HA2  | 1.97                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 27:U:490:ARG:HB2  | 27:U:493:VAL:HG12 | 1.95                     | 0.46              |
| 27:U:678:ASP:HB3  | 27:U:683:VAL:CG1  | 2.44                     | 0.46              |
| 27:U:792:ASN:CB   | 27:U:914:LEU:HB3  | 2.39                     | 0.46              |
| 2:D:122:GLU:OE1   | 2:D:122:GLU:N     | 2.41                     | 0.46              |
| 4:H:227:LYS:HD2   | 4:H:227:LYS:O     | 2.16                     | 0.46              |
| 6:J:58:THR:HA     | 6:J:60:ARG:HH21   | 1.80                     | 0.46              |
| 7:L:6:TYR:HE1     | 8:M:9:LEU:CD1     | 2.28                     | 0.46              |
| 7:L:113:GLY:HA2   | 7:L:116:THR:OG1   | 2.15                     | 0.46              |
| 8:M:84:ALA:HA     | 8:M:133:CYS:SG    | 2.55                     | 0.46              |
| 8:M:227:VAL:HB    | 8:M:232:ARG:NH1   | 2.30                     | 0.46              |
| 9:V:232:HIS:CE1   | 9:V:258:TYR:OH    | 2.68                     | 0.46              |
| 10:W:44:ILE:HG13  | 10:W:45:GLU:OE1   | 2.15                     | 0.46              |
| 10:W:50:LEU:O     | 10:W:53:GLN:HB2   | 2.16                     | 0.46              |
| 11:X:86:ALA:O     | 11:X:90:ARG:HB2   | 2.15                     | 0.46              |
| 11:X:224:ASP:OD1  | 11:X:227:THR:HB   | 2.16                     | 0.46              |
| 11:X:272:SER:HA   | 11:X:277:LEU:CD2  | 2.45                     | 0.46              |
| 12:Y:190:ALA:HA   | 12:Y:291:HIS:NE2  | 2.29                     | 0.46              |
| 13:Z:10:VAL:HG23  | 13:Z:10:VAL:O     | 2.15                     | 0.46              |
| 13:Z:48:LEU:HD12  | 13:Z:49:ASP:N     | 2.31                     | 0.46              |
| 13:Z:102:HIS:N    | 13:Z:105:ASP:OD2  | 2.47                     | 0.46              |
| 13:Z:133:LEU:HA   | 13:Z:133:LEU:HD12 | 1.75                     | 0.46              |
| 14:a:38:THR:O     | 14:a:41:VAL:N     | 2.48                     | 0.46              |
| 14:a:39:LEU:O     | 14:a:43:ASP:HB2   | 2.14                     | 0.46              |
| 14:a:94:LEU:HD21  | 14:a:118:ILE:CA   | 2.24                     | 0.46              |
| 14:a:277:LEU:HA   | 14:a:280:MET:CG   | 2.46                     | 0.46              |
| 15:b:16:MET:O     | 15:b:25:ARG:HD3   | 2.15                     | 0.46              |
| 15:b:153:LEU:O    | 15:b:156:PHE:HB3  | 2.15                     | 0.46              |
| 16:c:87:VAL:HG11  | 20:u:278:PHE:HE2  | 1.80                     | 0.46              |
| 17:d:302:TYR:CD1  | 17:d:306:ARG:HG3  | 2.46                     | 0.46              |
| 18:f:188:VAL:HG11 | 18:f:211:ILE:CD1  | 2.45                     | 0.46              |
| 18:f:261:ARG:HA   | 18:f:261:ARG:NE   | 2.29                     | 0.46              |
| 18:f:379:GLY:O    | 18:f:383:ALA:HB2  | 2.16                     | 0.46              |
| 18:f:439:TYR:C    | 18:f:439:TYR:CD1  | 2.93                     | 0.46              |
| 18:f:536:SER:O    | 18:f:540:GLN:HG2  | 2.14                     | 0.46              |
| 18:f:612:LEU:HD22 | 18:f:660:ILE:CD1  | 2.40                     | 0.46              |
| 18:f:726:ILE:HG13 | 18:f:762:VAL:CG2  | 2.35                     | 0.46              |
| 22:A:105:ASP:OD1  | 22:A:105:ASP:N    | 2.47                     | 0.46              |
| 23:B:125:THR:HG22 | 23:B:126:SER:N    | 2.30                     | 0.46              |
| 24:E:320:ILE:HD12 | 24:E:347:CYS:SG   | 2.54                     | 0.46              |
| 26:K:68:VAL:O     | 26:K:76:CYS:N     | 2.45                     | 0.46              |
| 26:K:70:ILE:HB    | 26:K:74:ILE:O     | 2.15                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 26:K:91:LYS:HG2   | 26:K:119:LEU:CD2  | 2.46                     | 0.46              |
| 26:K:239:LYS:HG3  | 26:K:240:ASP:OD1  | 2.15                     | 0.46              |
| 27:U:427:LEU:HD12 | 27:U:438:GLN:HG2  | 1.96                     | 0.46              |
| 27:U:450:HIS:CG   | 27:U:457:ILE:HG13 | 2.50                     | 0.46              |
| 27:U:465:LEU:HD12 | 27:U:477:GLY:C    | 2.40                     | 0.46              |
| 27:U:625:ILE:HG13 | 27:U:626:LEU:CD2  | 2.45                     | 0.46              |
| 27:U:699:THR:HG1  | 27:U:701:ILE:HG22 | 1.80                     | 0.46              |
| 1:C:100:ASP:OD1   | 1:C:101:LYS:HD3   | 2.15                     | 0.46              |
| 1:C:277:LEU:HD21  | 1:C:304:ALA:C     | 2.40                     | 0.46              |
| 3:G:10:ASP:C      | 3:G:12:HIS:H      | 2.24                     | 0.46              |
| 3:G:49:VAL:CG2    | 3:G:195:VAL:HG22  | 2.43                     | 0.46              |
| 5:I:217:THR:O     | 5:I:223:THR:HA    | 2.16                     | 0.46              |
| 7:L:49:LEU:HD12   | 7:L:49:LEU:C      | 2.39                     | 0.46              |
| 7:L:193:ARG:CA    | 7:L:196:ARG:HG2   | 2.45                     | 0.46              |
| 8:M:161:TRP:CZ2   | 8:M:182:LYS:HE3   | 2.51                     | 0.46              |
| 9:V:215:ALA:O     | 9:V:219:GLU:N     | 2.46                     | 0.46              |
| 9:V:215:ALA:O     | 9:V:219:GLU:HB2   | 2.15                     | 0.46              |
| 9:V:338:LEU:O     | 9:V:404:LYS:NZ    | 2.40                     | 0.46              |
| 10:W:105:VAL:HG13 | 10:W:106:GLN:N    | 2.30                     | 0.46              |
| 10:W:139:GLU:O    | 10:W:142:ARG:HB3  | 2.15                     | 0.46              |
| 10:W:183:VAL:CG1  | 10:W:222:LEU:HD13 | 2.38                     | 0.46              |
| 10:W:187:LEU:HD11 | 10:W:226:TYR:HA   | 1.97                     | 0.46              |
| 10:W:271:VAL:CG1  | 10:W:302:TYR:HD2  | 2.28                     | 0.46              |
| 13:Z:5:ALA:O      | 13:Z:46:LYS:HD2   | 2.14                     | 0.46              |
| 14:a:156:TYR:N    | 14:a:156:TYR:CD1  | 2.83                     | 0.46              |
| 14:a:360:VAL:HG23 | 16:c:308:VAL:HG22 | 1.98                     | 0.46              |
| 15:b:27:GLN:HA    | 15:b:30:GLN:HB3   | 1.96                     | 0.46              |
| 17:d:126:LEU:O    | 17:d:127:ASN:HB2  | 2.15                     | 0.46              |
| 17:d:141:LEU:CD1  | 17:d:182:LEU:HD11 | 2.44                     | 0.46              |
| 18:f:267:ARG:CD   | 18:f:893:ILE:HD13 | 2.45                     | 0.46              |
| 18:f:452:ASN:HB2  | 18:f:488:ALA:CB   | 2.45                     | 0.46              |
| 19:g:83:ALA:N     | 19:g:149:HIS:HB3  | 2.30                     | 0.46              |
| 19:g:140:LYS:HD2  | 19:g:140:LYS:N    | 2.29                     | 0.46              |
| 19:g:166:ARG:HA   | 19:g:170:GLN:CG   | 2.45                     | 0.46              |
| 22:A:263:MET:O    | 22:A:263:MET:HG2  | 2.15                     | 0.46              |
| 22:A:286:ASP:N    | 25:F:337:ILE:HD11 | 2.29                     | 0.46              |
| 23:B:167:THR:HG22 | 23:B:172:THR:OG1  | 2.14                     | 0.46              |
| 25:F:436:GLN:OE1  | 25:F:437:TYR:N    | 2.48                     | 0.46              |
| 27:U:137:MET:CE   | 27:U:137:MET:HA   | 2.45                     | 0.46              |
| 27:U:481:LEU:HD11 | 27:U:493:VAL:HG21 | 1.97                     | 0.46              |
| 1:C:114:VAL:HB    | 1:C:123:LEU:CD2   | 2.44                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:165:ILE:HD11  | 1:C:292:ILE:HD11  | 1.97                     | 0.46              |
| 1:C:173:GLU:HB2   | 22:A:34:LYS:HD3   | 1.98                     | 0.46              |
| 1:C:369:TYR:HB2   | 1:C:382:ASP:OD1   | 2.15                     | 0.46              |
| 2:D:94:GLU:HB2    | 2:D:102:ILE:HG21  | 1.97                     | 0.46              |
| 2:D:313:ARG:O     | 2:D:314:ALA:HB3   | 2.16                     | 0.46              |
| 3:G:38:THR:HG22   | 3:G:53:GLN:OE1    | 2.16                     | 0.46              |
| 4:H:38:ILE:CD1    | 4:H:191:ALA:HA    | 2.46                     | 0.46              |
| 5:I:98:LEU:HD12   | 5:I:98:LEU:C      | 2.39                     | 0.46              |
| 5:I:190:LEU:HD12  | 5:I:236:LEU:CD2   | 2.35                     | 0.46              |
| 9:V:284:GLU:OE1   | 9:V:284:GLU:HA    | 2.16                     | 0.46              |
| 10:W:34:LEU:HA    | 10:W:37:GLU:OE1   | 2.15                     | 0.46              |
| 10:W:132:THR:O    | 10:W:135:LYS:HB2  | 2.16                     | 0.46              |
| 10:W:186:ILE:HG23 | 10:W:205:ILE:HG23 | 1.96                     | 0.46              |
| 11:X:50:ILE:HD12  | 11:X:76:PHE:CZ    | 2.50                     | 0.46              |
| 12:Y:24:PHE:CZ    | 12:Y:289:ALA:CB   | 2.98                     | 0.46              |
| 12:Y:121:LEU:HD13 | 12:Y:144:LEU:HD22 | 1.97                     | 0.46              |
| 14:a:39:LEU:O     | 14:a:43:ASP:N     | 2.36                     | 0.46              |
| 14:a:123:LEU:HD21 | 14:a:161:LYS:CG   | 2.44                     | 0.46              |
| 14:a:189:PRO:HD2  | 14:a:192:GLU:HB2  | 1.96                     | 0.46              |
| 14:a:274:LEU:HD23 | 14:a:275:LEU:N    | 2.31                     | 0.46              |
| 15:b:130:ARG:NE   | 15:b:131:LEU:HD22 | 2.19                     | 0.46              |
| 16:c:82:VAL:HG11  | 16:c:113:HIS:HB2  | 1.98                     | 0.46              |
| 16:c:125:VAL:HG21 | 20:u:289:HIS:HA   | 1.96                     | 0.46              |
| 16:c:163:ILE:HG22 | 16:c:199:HIS:O    | 2.15                     | 0.46              |
| 18:f:188:VAL:HG11 | 18:f:211:ILE:HD13 | 1.97                     | 0.46              |
| 18:f:307:LEU:HB3  | 18:f:314:TYR:CD1  | 2.50                     | 0.46              |
| 18:f:319:GLU:HA   | 18:f:322:SER:OG   | 2.15                     | 0.46              |
| 18:f:433:LEU:N    | 19:g:172:GLU:HA   | 2.30                     | 0.46              |
| 18:f:482:ILE:HD12 | 18:f:518:THR:N    | 2.30                     | 0.46              |
| 18:f:543:MET:HE2  | 18:f:543:MET:CA   | 2.39                     | 0.46              |
| 18:f:591:ALA:O    | 18:f:595:VAL:HG13 | 2.16                     | 0.46              |
| 18:f:680:ARG:HH12 | 22:A:66:LYS:HA    | 1.80                     | 0.46              |
| 18:f:852:VAL:HG23 | 18:f:859:PRO:CG   | 2.45                     | 0.46              |
| 19:g:87:VAL:HA    | 19:g:153:ALA:H    | 1.81                     | 0.46              |
| 22:A:55:LEU:HD23  | 23:B:72:LEU:HB3   | 1.97                     | 0.46              |
| 25:F:120:LYS:C    | 25:F:137:ILE:HG23 | 2.40                     | 0.46              |
| 25:F:198:LEU:O    | 25:F:202:ILE:N    | 2.45                     | 0.46              |
| 26:K:42:THR:HG21  | 26:K:194:ALA:HB2  | 1.96                     | 0.46              |
| 27:U:493:VAL:CG1  | 27:U:519:VAL:HG21 | 2.44                     | 0.46              |
| 27:U:536:ALA:O    | 27:U:545:LEU:HD21 | 2.16                     | 0.46              |
| 27:U:712:LEU:C    | 27:U:712:LEU:HD23 | 2.40                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:57:ARG:HH21   | 27:U:649:ARG:CZ   | 2.28                     | 0.46              |
| 1:C:76:VAL:HG22   | 1:C:87:VAL:CG1    | 2.45                     | 0.46              |
| 1:C:315:ILE:HG22  | 1:C:317:PHE:HE1   | 1.80                     | 0.46              |
| 1:C:320:PRO:HD3   | 1:C:355:SER:O     | 2.15                     | 0.46              |
| 3:G:212:PRO:HG3   | 3:G:236:ASP:CG    | 2.41                     | 0.46              |
| 5:I:82:ASP:HB3    | 5:I:130:PHE:CD1   | 2.50                     | 0.46              |
| 5:I:122:THR:O     | 6:J:125:ARG:NE    | 2.48                     | 0.46              |
| 6:J:109:ARG:HG3   | 6:J:109:ARG:NH1   | 2.30                     | 0.46              |
| 7:L:158:ALA:O     | 8:M:57:LEU:HD13   | 2.14                     | 0.46              |
| 9:V:123:SER:HB2   | 9:V:125:ASN:ND2   | 2.30                     | 0.46              |
| 9:V:188:SER:HA    | 9:V:191:LEU:HB3   | 1.98                     | 0.46              |
| 10:W:179:LYS:HB3  | 10:W:213:PHE:CE2  | 2.51                     | 0.46              |
| 10:W:274:VAL:HG22 | 10:W:287:VAL:HG22 | 1.98                     | 0.46              |
| 10:W:425:LEU:HD12 | 13:Z:252:LYS:HG3  | 1.98                     | 0.46              |
| 11:X:90:ARG:HA    | 11:X:93:LEU:HG    | 1.97                     | 0.46              |
| 12:Y:57:LEU:HD23  | 12:Y:57:LEU:O     | 2.15                     | 0.46              |
| 12:Y:134:LEU:HD12 | 12:Y:134:LEU:C    | 2.39                     | 0.46              |
| 13:Z:195:VAL:HG23 | 14:a:367:VAL:CG1  | 2.45                     | 0.46              |
| 14:a:109:GLU:HG3  | 14:a:151:VAL:HG11 | 1.98                     | 0.46              |
| 14:a:221:VAL:CA   | 14:a:225:LEU:HD12 | 2.45                     | 0.46              |
| 15:b:7:MET:HB2    | 15:b:97:LEU:CD1   | 2.45                     | 0.46              |
| 18:f:275:MET:HE2  | 18:f:275:MET:CA   | 2.44                     | 0.46              |
| 18:f:692:LEU:HD21 | 18:f:724:ASN:CG   | 2.41                     | 0.46              |
| 19:g:125:ASN:O    | 19:g:161:SER:HB2  | 2.15                     | 0.46              |
| 22:A:138:MET:O    | 22:A:140:VAL:HG13 | 2.16                     | 0.46              |
| 24:E:130:VAL:HG13 | 24:E:186:ALA:HA   | 1.97                     | 0.46              |
| 25:F:270:ASP:O    | 25:F:273:ALA:N    | 2.49                     | 0.46              |
| 25:F:310:MET:CE   | 25:F:342:LEU:HG   | 2.46                     | 0.46              |
| 27:U:169:GLU:O    | 27:U:170:SER:C    | 2.59                     | 0.46              |
| 27:U:367:THR:HG21 | 27:U:773:PHE:CD2  | 2.51                     | 0.46              |
| 27:U:588:MET:HE1  | 27:U:760:VAL:HG11 | 1.95                     | 0.46              |
| 27:U:836:THR:CG2  | 27:U:837:ALA:N    | 2.78                     | 0.46              |
| 1:C:63:LEU:HD11   | 2:D:78:GLU:HB3    | 1.97                     | 0.46              |
| 2:D:102:ILE:O     | 2:D:102:ILE:CG2   | 2.63                     | 0.46              |
| 2:D:161:ASP:OD1   | 2:D:161:ASP:C     | 2.58                     | 0.46              |
| 2:D:186:THR:OG1   | 2:D:187:HIS:ND1   | 2.41                     | 0.46              |
| 5:I:50:ARG:HH11   | 5:I:50:ARG:HB2    | 1.81                     | 0.46              |
| 6:J:86:ARG:HG3    | 6:J:110:TYR:OH    | 2.16                     | 0.46              |
| 7:L:222:THR:HG1   | 7:L:224:TYR:HE2   | 1.63                     | 0.46              |
| 8:M:27:MET:HG2    | 8:M:153:PRO:CG    | 2.45                     | 0.46              |
| 8:M:73:VAL:HG12   | 8:M:74:GLY:N      | 2.31                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 8:M:195:LYS:HA    | 8:M:239:ALA:CB    | 2.46                     | 0.46              |
| 9:V:195:ILE:HB    | 9:V:203:LEU:HD21  | 1.96                     | 0.46              |
| 9:V:275:VAL:O     | 9:V:275:VAL:HG13  | 2.14                     | 0.46              |
| 9:V:330:LYS:HG2   | 9:V:360:TYR:CE1   | 2.51                     | 0.46              |
| 10:W:449:GLU:OE2  | 10:W:449:GLU:HA   | 2.15                     | 0.46              |
| 13:Z:6:VAL:HG12   | 13:Z:43:TRP:HH2   | 1.81                     | 0.46              |
| 13:Z:67:VAL:HG11  | 15:b:91:ARG:CB    | 2.46                     | 0.46              |
| 14:a:57:ILE:O     | 14:a:61:GLU:HG2   | 2.16                     | 0.46              |
| 14:a:112:ILE:CD1  | 14:a:138:VAL:HG11 | 2.44                     | 0.46              |
| 14:a:172:TYR:O    | 14:a:176:ALA:N    | 2.38                     | 0.46              |
| 18:f:89:MET:C     | 18:f:91:SER:N     | 2.74                     | 0.46              |
| 18:f:110:TYR:HE2  | 18:f:123:ALA:HB2  | 1.80                     | 0.46              |
| 18:f:253:LEU:HD23 | 18:f:253:LEU:C    | 2.41                     | 0.46              |
| 18:f:272:LEU:HD23 | 18:f:272:LEU:O    | 2.16                     | 0.46              |
| 18:f:433:LEU:HD12 | 18:f:433:LEU:C    | 2.41                     | 0.46              |
| 18:f:460:ASP:OD1  | 18:f:460:ASP:O    | 2.34                     | 0.46              |
| 18:f:701:ASN:ND2  | 18:f:876:HIS:CE1  | 2.83                     | 0.46              |
| 18:f:830:LEU:HD21 | 18:f:880:ALA:HB1  | 1.97                     | 0.46              |
| 18:f:886:GLU:HB3  | 18:f:887:PHE:CE1  | 2.50                     | 0.46              |
| 19:g:160:GLN:HB3  | 19:g:164:ASP:HB3  | 1.96                     | 0.46              |
| 22:A:212:VAL:HG22 | 22:A:318:LEU:CD2  | 2.39                     | 0.46              |
| 22:A:256:MET:HE2  | 22:A:256:MET:HB2  | 1.83                     | 0.46              |
| 23:B:139:VAL:HG21 | 23:B:159:VAL:CG1  | 2.43                     | 0.46              |
| 23:B:224:LEU:N    | 23:B:224:LEU:HD12 | 2.30                     | 0.46              |
| 27:U:25:HIS:HA    | 27:U:59:PHE:CE1   | 2.50                     | 0.46              |
| 27:U:32:ASN:HA    | 27:U:70:HIS:NE2   | 2.31                     | 0.46              |
| 27:U:253:TYR:HA   | 27:U:261:LEU:HD21 | 1.98                     | 0.46              |
| 27:U:368:ALA:HB2  | 27:U:728:PHE:HD1  | 1.79                     | 0.46              |
| 27:U:488:THR:CG2  | 27:U:490:ARG:H    | 2.19                     | 0.46              |
| 27:U:772:TRP:CG   | 27:U:774:PRO:HD2  | 2.51                     | 0.46              |
| 1:C:119:ASP:HB2   | 16:c:193:ILE:HD12 | 1.96                     | 0.46              |
| 2:D:122:GLU:N     | 2:D:122:GLU:CD    | 2.74                     | 0.46              |
| 2:D:329:ARG:HH11  | 2:D:329:ARG:CG    | 2.28                     | 0.46              |
| 3:G:10:ASP:C      | 3:G:12:HIS:N      | 2.74                     | 0.46              |
| 3:G:98:ALA:CB     | 3:G:109:ILE:HG21  | 2.45                     | 0.46              |
| 3:G:128:ASN:O     | 3:G:130:GLU:N     | 2.46                     | 0.46              |
| 4:H:97:TYR:CE2    | 4:H:105:ILE:HA    | 2.51                     | 0.46              |
| 5:I:105:ILE:CD1   | 5:I:110:LEU:HB2   | 2.45                     | 0.46              |
| 7:L:148:CYS:HB2   | 7:L:149:PRO:HD2   | 1.98                     | 0.46              |
| 9:V:118:GLN:OE1   | 9:V:128:ARG:NH2   | 2.48                     | 0.46              |
| 9:V:134:PHE:HD2   | 9:V:187:ILE:HG13  | 1.80                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 9:V:191:LEU:O     | 9:V:195:ILE:N     | 2.37                     | 0.46              |
| 9:V:379:LEU:HD22  | 9:V:395:ILE:HG21  | 1.97                     | 0.46              |
| 9:V:414:TYR:HA    | 12:Y:347:ILE:O    | 2.16                     | 0.46              |
| 10:W:40:LEU:O     | 10:W:41:GLN:C     | 2.58                     | 0.46              |
| 10:W:54:THR:CG2   | 10:W:63:THR:HG23  | 2.46                     | 0.46              |
| 10:W:71:VAL:CG1   | 10:W:104:MET:HE3  | 2.46                     | 0.46              |
| 11:X:153:LEU:CD1  | 11:X:169:VAL:HG21 | 2.36                     | 0.46              |
| 11:X:160:MET:HG2  | 11:X:161:ASP:N    | 2.24                     | 0.46              |
| 11:X:379:ASP:OD1  | 11:X:379:ASP:C    | 2.57                     | 0.46              |
| 12:Y:121:LEU:HD21 | 12:Y:156:LEU:CD2  | 2.45                     | 0.46              |
| 14:a:308:GLU:HB2  | 14:a:329:LYS:NZ   | 2.31                     | 0.46              |
| 14:a:342:ASP:OD1  | 14:a:342:ASP:C    | 2.59                     | 0.46              |
| 17:d:236:LEU:HD22 | 17:d:267:ILE:HD11 | 1.98                     | 0.46              |
| 18:f:62:ARG:HH21  | 18:f:70:LEU:HD23  | 1.80                     | 0.46              |
| 18:f:482:ILE:HG13 | 18:f:483:PHE:N    | 2.31                     | 0.46              |
| 18:f:882:LEU:HD13 | 18:f:889:PRO:HD3  | 1.97                     | 0.46              |
| 19:g:168:ASN:O    | 19:g:171:LEU:HB2  | 2.15                     | 0.46              |
| 22:A:429:TYR:HH   | 26:K:33:LEU:HB3   | 1.77                     | 0.46              |
| 23:B:99:VAL:O     | 23:B:103:ARG:HG3  | 2.16                     | 0.46              |
| 23:B:256:ILE:HD11 | 23:B:305:ILE:HG23 | 1.97                     | 0.46              |
| 24:E:100:LEU:HD12 | 24:E:100:LEU:O    | 2.16                     | 0.46              |
| 24:E:146:ARG:O    | 24:E:150:GLU:HB3  | 2.16                     | 0.46              |
| 25:F:180:ARG:C    | 25:F:182:THR:H    | 2.24                     | 0.46              |
| 25:F:209:LYS:H    | 25:F:209:LYS:HG3  | 1.52                     | 0.46              |
| 25:F:399:VAL:HB   | 25:F:424:ILE:HD13 | 1.98                     | 0.46              |
| 26:K:157:ASP:HB2  | 26:K:158:PRO:CD   | 2.37                     | 0.46              |
| 27:U:105:ILE:HG22 | 27:U:134:VAL:HG22 | 1.97                     | 0.46              |
| 27:U:344:ARG:HE   | 27:U:927:PRO:CG   | 2.29                     | 0.46              |
| 27:U:397:THR:O    | 27:U:398:ASN:HB2  | 2.15                     | 0.46              |
| 27:U:796:LYS:CG   | 27:U:798:PRO:HD3  | 2.44                     | 0.46              |
| 27:U:810:THR:HG23 | 27:U:872:GLU:CD   | 2.40                     | 0.46              |
| 1:C:142:LYS:HD2   | 1:C:142:LYS:O     | 2.16                     | 0.46              |
| 1:C:162:LYS:HD3   | 1:C:166:GLU:OE1   | 2.16                     | 0.46              |
| 1:C:383:PHE:O     | 1:C:386:ALA:N     | 2.45                     | 0.46              |
| 6:J:59:VAL:O      | 6:J:60:ARG:C      | 2.59                     | 0.46              |
| 7:L:97:PHE:CD1    | 7:L:97:PHE:C      | 2.93                     | 0.46              |
| 8:M:215:TRP:CE3   | 8:M:227:VAL:HG22  | 2.51                     | 0.46              |
| 9:V:117:VAL:CG2   | 9:V:132:LEU:HD11  | 2.45                     | 0.46              |
| 10:W:108:CYS:O    | 10:W:112:VAL:N    | 2.49                     | 0.46              |
| 10:W:393:LEU:O    | 10:W:393:LEU:HD12 | 2.14                     | 0.46              |
| 11:X:161:ASP:CG   | 11:X:162:ASP:H    | 2.24                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 12:Y:122:THR:HG23 | 12:Y:123:ALA:N    | 2.30                     | 0.46              |
| 12:Y:197:ALA:HB3  | 12:Y:226:VAL:HG11 | 1.97                     | 0.46              |
| 13:Z:48:LEU:HD21  | 13:Z:92:VAL:CG2   | 2.46                     | 0.46              |
| 13:Z:137:ALA:HB3  | 13:Z:158:VAL:HG13 | 1.98                     | 0.46              |
| 14:a:100:THR:HA   | 14:a:103:LYS:CE   | 2.45                     | 0.46              |
| 14:a:118:ILE:HG13 | 14:a:122:LYS:HB3  | 1.98                     | 0.46              |
| 14:a:122:LYS:HE2  | 14:a:130:VAL:HG13 | 1.97                     | 0.46              |
| 14:a:172:TYR:HE2  | 14:a:199:THR:O    | 1.98                     | 0.46              |
| 15:b:150:THR:HG21 | 15:b:152:LYS:HD3  | 1.97                     | 0.46              |
| 18:f:250:ARG:O    | 18:f:254:GLY:N    | 2.44                     | 0.46              |
| 18:f:329:ASN:HA   | 18:f:332:ALA:HB3  | 1.97                     | 0.46              |
| 18:f:453:SER:N    | 18:f:488:ALA:HA   | 2.31                     | 0.46              |
| 19:g:131:ILE:CG1  | 19:g:151:VAL:CG1  | 2.92                     | 0.46              |
| 22:A:79:ASP:O     | 22:A:82:ALA:N     | 2.48                     | 0.46              |
| 25:F:294:LYS:HB3  | 25:F:295:ARG:CZ   | 2.46                     | 0.46              |
| 27:U:2:ILE:O      | 27:U:3:THR:OG1    | 2.31                     | 0.46              |
| 27:U:12:LEU:HD22  | 27:U:45:ILE:HD11  | 1.96                     | 0.46              |
| 27:U:122:GLU:HG3  | 27:U:122:GLU:O    | 2.15                     | 0.46              |
| 27:U:213:PHE:CA   | 27:U:216:VAL:HG12 | 2.43                     | 0.46              |
| 27:U:258:GLN:OE1  | 27:U:488:THR:HA   | 2.16                     | 0.46              |
| 1:C:33:LEU:HD12   | 9:V:201:ARG:CG    | 2.41                     | 0.46              |
| 1:C:96:VAL:HG12   | 1:C:96:VAL:O      | 2.15                     | 0.46              |
| 1:C:161:ILE:HD12  | 1:C:186:VAL:HG11  | 1.97                     | 0.46              |
| 2:D:236:VAL:O     | 2:D:236:VAL:CG1   | 2.61                     | 0.46              |
| 2:D:238:LYS:HZ3   | 24:E:207:TYR:HB2  | 1.81                     | 0.46              |
| 2:D:382:SER:HA    | 2:D:402:ALA:HB2   | 1.97                     | 0.46              |
| 2:D:392:TYR:CE2   | 10:W:200:ILE:HG21 | 2.51                     | 0.46              |
| 3:G:199:ILE:HG21  | 3:G:242:LEU:HG    | 1.97                     | 0.46              |
| 4:H:38:ILE:HD13   | 4:H:191:ALA:CA    | 2.46                     | 0.46              |
| 5:I:82:ASP:HB3    | 5:I:130:PHE:HD1   | 1.80                     | 0.46              |
| 5:I:174:MET:CE    | 5:I:195:LYS:HG3   | 2.45                     | 0.46              |
| 6:J:36:ARG:HG3    | 6:J:36:ARG:NH1    | 2.29                     | 0.46              |
| 6:J:71:MET:HE1    | 6:J:111:ILE:HD13  | 1.98                     | 0.46              |
| 7:L:166:GLN:HB3   | 25:F:417:HIS:CD2  | 2.51                     | 0.46              |
| 8:M:178:LYS:O     | 8:M:179:LEU:HD12  | 2.16                     | 0.46              |
| 9:V:113:LEU:HD13  | 9:V:171:VAL:HA    | 1.97                     | 0.46              |
| 9:V:114:TYR:O     | 9:V:118:GLN:N     | 2.34                     | 0.46              |
| 9:V:150:ARG:HB3   | 9:V:154:ALA:C     | 2.41                     | 0.46              |
| 11:X:97:LEU:HD12  | 11:X:136:LEU:HG   | 1.98                     | 0.46              |
| 13:Z:44:GLN:OE1   | 13:Z:44:GLN:HA    | 2.16                     | 0.46              |
| 13:Z:288:LYS:O    | 13:Z:288:LYS:HG2  | 2.15                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 14:a:7:PHE:HZ     | 14:a:59:LEU:HB3   | 1.81                     | 0.46              |
| 14:a:61:GLU:O     | 14:a:64:ILE:HG22  | 2.15                     | 0.46              |
| 14:a:131:THR:HG23 | 14:a:132:LYS:N    | 2.30                     | 0.46              |
| 16:c:117:GLY:HA2  | 16:c:146:ASP:OD2  | 2.15                     | 0.46              |
| 18:f:180:GLN:C    | 18:f:183:PRO:HD2  | 2.40                     | 0.46              |
| 18:f:745:LEU:HD13 | 18:f:766:GLN:CA   | 2.45                     | 0.46              |
| 22:A:187:LEU:HD21 | 22:A:229:VAL:CG2  | 2.41                     | 0.46              |
| 22:A:433:ASN:CB   | 26:K:82:ILE:HD11  | 2.46                     | 0.46              |
| 24:E:35:GLU:HA    | 24:E:38:LYS:HE2   | 1.97                     | 0.46              |
| 25:F:85:THR:O     | 25:F:86:LEU:HG    | 2.16                     | 0.46              |
| 25:F:231:THR:HG22 | 25:F:354:PHE:HD2  | 1.81                     | 0.46              |
| 25:F:388:THR:HG22 | 25:F:424:ILE:HG13 | 1.98                     | 0.46              |
| 27:U:167:ILE:HD12 | 27:U:176:MET:HG3  | 1.98                     | 0.46              |
| 27:U:554:LEU:CD2  | 27:U:588:MET:HG3  | 2.42                     | 0.46              |
| 1:C:336:MET:HE3   | 1:C:378:VAL:CG2   | 2.43                     | 0.46              |
| 3:G:51:VAL:HG13   | 3:G:198:ALA:HB1   | 1.98                     | 0.46              |
| 4:H:118:MET:CE    | 4:H:151:PRO:HA    | 2.44                     | 0.46              |
| 4:H:188:ILE:O     | 4:H:192:ILE:HD12  | 2.16                     | 0.46              |
| 7:L:26:MET:HA     | 7:L:26:MET:CE     | 2.41                     | 0.46              |
| 8:M:209:PHE:CD1   | 8:M:210:GLU:N     | 2.84                     | 0.46              |
| 9:V:105:SER:O     | 9:V:108:LEU:HD21  | 2.16                     | 0.46              |
| 9:V:160:LEU:O     | 9:V:164:GLU:HG2   | 2.15                     | 0.46              |
| 9:V:261:TYR:HB2   | 9:V:263:LEU:HD13  | 1.98                     | 0.46              |
| 9:V:287:ARG:NH2   | 28:e:21:GLU:HG2   | 2.30                     | 0.46              |
| 9:V:384:GLU:C     | 9:V:384:GLU:CD    | 2.84                     | 0.46              |
| 10:W:326:MET:SD   | 10:W:330:LYS:HB2  | 2.55                     | 0.46              |
| 11:X:268:GLN:CD   | 11:X:288:LYS:HZ1  | 2.24                     | 0.46              |
| 12:Y:19:ILE:HD11  | 12:Y:44:ALA:CB    | 2.34                     | 0.46              |
| 13:Z:74:TYR:HD1   | 13:Z:74:TYR:C     | 2.24                     | 0.46              |
| 15:b:172:THR:HG23 | 15:b:172:THR:O    | 2.16                     | 0.46              |
| 16:c:46:ARG:O     | 16:c:46:ARG:HD3   | 2.16                     | 0.46              |
| 16:c:157:ILE:HG23 | 16:c:157:ILE:O    | 2.16                     | 0.46              |
| 17:d:88:LEU:HD12  | 17:d:88:LEU:O     | 2.16                     | 0.46              |
| 18:f:612:LEU:HD23 | 18:f:656:GLY:C    | 2.41                     | 0.46              |
| 18:f:782:HIS:CE1  | 18:f:895:GLU:HB3  | 2.51                     | 0.46              |
| 19:g:110:ARG:HE   | 19:g:110:ARG:HB2  | 1.64                     | 0.46              |
| 22:A:177:VAL:HG11 | 22:A:184:ILE:HD11 | 1.96                     | 0.46              |
| 23:B:287:ILE:HD12 | 23:B:290:ILE:HG23 | 1.98                     | 0.46              |
| 24:E:279:THR:OG1  | 24:E:280:ASN:N    | 2.47                     | 0.46              |
| 25:F:177:VAL:HG12 | 25:F:179:GLU:H    | 1.81                     | 0.46              |
| 25:F:244:THR:HA   | 25:F:245:LYS:HZ3  | 1.81                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 26:K:42:THR:N     | 26:K:45:GLY:O     | 2.45                     | 0.46              |
| 27:U:346:ASN:OD1  | 27:U:347:ASN:N    | 2.49                     | 0.46              |
| 27:U:497:LEU:HD11 | 27:U:515:ALA:HB1  | 1.98                     | 0.46              |
| 28:e:24:ALA:O     | 28:e:25:GLU:C     | 2.59                     | 0.46              |
| 1:C:113:ARG:NE    | 1:C:130:LYS:HB2   | 2.30                     | 0.45              |
| 1:C:357:ALA:HB3   | 2:D:323:ARG:HD2   | 1.96                     | 0.45              |
| 3:G:51:VAL:HG23   | 3:G:202:LEU:HD22  | 1.99                     | 0.45              |
| 3:G:101:TRP:CD1   | 3:G:109:ILE:HA    | 2.51                     | 0.45              |
| 3:G:143:ILE:HG12  | 3:G:220:VAL:CG2   | 2.42                     | 0.45              |
| 4:H:71:HIS:CE1    | 4:H:104:PRO:CB    | 3.00                     | 0.45              |
| 5:I:38:LEU:HD13   | 5:I:180:LYS:O     | 2.15                     | 0.45              |
| 6:J:136:PHE:HZ    | 6:J:213:ARG:HH21  | 1.62                     | 0.45              |
| 6:J:156:TRP:CD2   | 6:J:159:ASN:OD1   | 2.69                     | 0.45              |
| 7:L:24:TYR:CZ     | 26:K:17:PRO:HB3   | 2.50                     | 0.45              |
| 8:M:63:ASN:HA     | 8:M:85:ARG:HH21   | 1.81                     | 0.45              |
| 8:M:184:MET:HB3   | 8:M:188:ASP:CG    | 2.41                     | 0.45              |
| 9:V:292:THR:HG23  | 9:V:308:THR:HG21  | 1.97                     | 0.45              |
| 9:V:463:MET:SD    | 9:V:464:ILE:O     | 2.75                     | 0.45              |
| 10:W:55:ARG:HH12  | 10:W:93:ARG:HD3   | 1.81                     | 0.45              |
| 10:W:361:HIS:HB2  | 10:W:364:ARG:HH22 | 1.82                     | 0.45              |
| 11:X:54:GLY:O     | 11:X:58:ALA:N     | 2.32                     | 0.45              |
| 12:Y:168:ILE:HG13 | 12:Y:172:GLY:HA3  | 1.98                     | 0.45              |
| 14:a:365:MET:HA   | 14:a:368:GLU:HG2  | 1.98                     | 0.45              |
| 15:b:147:GLU:H    | 15:b:147:GLU:CD   | 2.24                     | 0.45              |
| 18:f:399:LEU:O    | 18:f:402:ASN:N    | 2.44                     | 0.45              |
| 18:f:665:GLU:H    | 18:f:665:GLU:CD   | 2.25                     | 0.45              |
| 18:f:830:LEU:HB3  | 18:f:872:VAL:CA   | 2.47                     | 0.45              |
| 18:f:875:ALA:O    | 18:f:878:GLU:HG2  | 2.16                     | 0.45              |
| 19:g:116:ILE:O    | 19:g:122:LEU:HD13 | 2.16                     | 0.45              |
| 20:u:136:GLU:O    | 20:u:168:THR:HG22 | 2.16                     | 0.45              |
| 22:A:124:ASP:O    | 22:A:148:GLN:HG2  | 2.16                     | 0.45              |
| 22:A:165:GLN:HA   | 22:A:238:ILE:HA   | 1.98                     | 0.45              |
| 22:A:214:LEU:HD23 | 22:A:343:PHE:CE1  | 2.51                     | 0.45              |
| 22:A:423:PHE:O    | 22:A:424:SER:C    | 2.59                     | 0.45              |
| 24:E:232:MET:SD   | 24:E:277:MET:SD   | 3.14                     | 0.45              |
| 24:E:276:ILE:O    | 24:E:277:MET:C    | 2.58                     | 0.45              |
| 25:F:168:TYR:HD2  | 25:F:274:LEU:HD13 | 1.81                     | 0.45              |
| 26:K:33:LEU:HD12  | 26:K:33:LEU:N     | 2.31                     | 0.45              |
| 27:U:140:ARG:HB3  | 27:U:140:ARG:CZ   | 2.46                     | 0.45              |
| 27:U:324:LYS:NZ   | 27:U:333:MET:HE3  | 2.31                     | 0.45              |
| 27:U:489:ALA:C    | 27:U:520:MET:HE1  | 2.41                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 27:U:524:LYS:HD2  | 27:U:556:MET:SD   | 2.56                     | 0.45              |
| 1:C:158:ILE:HA    | 1:C:161:ILE:HG22  | 1.99                     | 0.45              |
| 2:D:175:GLN:O     | 2:D:179:GLU:HB2   | 2.16                     | 0.45              |
| 2:D:342:ARG:HB2   | 2:D:342:ARG:CZ    | 2.46                     | 0.45              |
| 3:G:16:PHE:CE2    | 4:H:128:ARG:HD2   | 2.51                     | 0.45              |
| 3:G:172:GLN:HA    | 3:G:175:SER:HG    | 1.81                     | 0.45              |
| 5:I:45:LEU:CD2    | 5:I:75:SER:HB2    | 2.46                     | 0.45              |
| 7:L:193:ARG:HA    | 7:L:196:ARG:CD    | 2.47                     | 0.45              |
| 8:M:39:ILE:O      | 8:M:46:VAL:N      | 2.34                     | 0.45              |
| 8:M:213:LEU:HD12  | 8:M:213:LEU:N     | 2.32                     | 0.45              |
| 9:V:79:VAL:CG1    | 9:V:163:VAL:HG11  | 2.46                     | 0.45              |
| 9:V:364:THR:HG21  | 28:e:43:TRP:HH2   | 1.81                     | 0.45              |
| 10:W:193:CYS:HB2  | 10:W:202:THR:OG1  | 2.15                     | 0.45              |
| 11:X:125:LEU:O    | 11:X:128:ALA:N    | 2.48                     | 0.45              |
| 11:X:323:LEU:HD23 | 11:X:323:LEU:HA   | 1.76                     | 0.45              |
| 11:X:339:ILE:HG23 | 11:X:387:ILE:HG13 | 1.98                     | 0.45              |
| 11:X:406:ASN:HD21 | 16:c:253:LYS:HD3  | 1.80                     | 0.45              |
| 13:Z:74:TYR:C     | 13:Z:74:TYR:CD1   | 2.95                     | 0.45              |
| 13:Z:126:VAL:CG1  | 13:Z:127:LYS:N    | 2.79                     | 0.45              |
| 13:Z:265:LEU:C    | 13:Z:265:LEU:HD23 | 2.41                     | 0.45              |
| 14:a:89:ASP:C     | 14:a:89:ASP:OD1   | 2.58                     | 0.45              |
| 14:a:148:VAL:HG11 | 14:a:151:VAL:CG1  | 2.46                     | 0.45              |
| 15:b:113:VAL:CG2  | 15:b:140:ILE:HD12 | 2.46                     | 0.45              |
| 17:d:225:TYR:HB3  | 17:d:256:TYR:OH   | 2.16                     | 0.45              |
| 18:f:191:ILE:O    | 18:f:194:TYR:HB3  | 2.16                     | 0.45              |
| 19:g:122:LEU:HB3  | 19:g:127:ILE:HG21 | 1.98                     | 0.45              |
| 22:A:321:THR:HG23 | 22:A:321:THR:O    | 2.16                     | 0.45              |
| 22:A:375:ARG:HD3  | 26:K:173:ALA:CB   | 2.28                     | 0.45              |
| 23:B:93:GLU:O     | 23:B:97:SER:OG    | 2.27                     | 0.45              |
| 24:E:149:ILE:CD1  | 24:E:276:ILE:CG1  | 2.94                     | 0.45              |
| 24:E:334:LEU:CD1  | 24:E:368:MET:HG2  | 2.47                     | 0.45              |
| 25:F:274:LEU:HD12 | 25:F:278:LYS:NZ   | 2.31                     | 0.45              |
| 27:U:161:ASP:OD1  | 27:U:162:VAL:N    | 2.46                     | 0.45              |
| 27:U:842:LYS:HG3  | 27:U:846:LYS:HE3  | 1.96                     | 0.45              |
| 27:U:887:ALA:HB3  | 27:U:888:GLN:OE1  | 2.15                     | 0.45              |
| 1:C:187:LEU:HD11  | 1:C:295:THR:CG2   | 2.47                     | 0.45              |
| 1:C:238:ALA:O     | 1:C:289:ILE:HD12  | 2.16                     | 0.45              |
| 1:C:266:ASP:OD2   | 2:D:283:ARG:HD2   | 2.15                     | 0.45              |
| 1:C:308:PRO:HG2   | 23:B:394:ASP:OD1  | 2.15                     | 0.45              |
| 2:D:97:ASP:OD1    | 2:D:100:THR:CG2   | 2.63                     | 0.45              |
| 2:D:143:LEU:HD11  | 24:E:64:LEU:CD1   | 2.47                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:D:160:PRO:HB3   | 2:D:217:LYS:HG2   | 1.99                     | 0.45              |
| 3:G:183:VAL:HG13  | 3:G:183:VAL:O     | 2.17                     | 0.45              |
| 5:I:21:VAL:CG1    | 5:I:153:SER:HB2   | 2.46                     | 0.45              |
| 5:I:42:GLY:HA2    | 5:I:145:PHE:CE2   | 2.51                     | 0.45              |
| 5:I:69:ASN:HB3    | 5:I:72:MET:HB2    | 1.97                     | 0.45              |
| 6:J:9:VAL:HG23    | 6:J:9:VAL:O       | 2.16                     | 0.45              |
| 9:V:470:ARG:NH1   | 9:V:474:LEU:HD22  | 2.31                     | 0.45              |
| 10:W:263:TRP:CZ3  | 10:W:267:LEU:HD12 | 2.40                     | 0.45              |
| 11:X:407:MET:SD   | 13:Z:266:ILE:HD13 | 2.57                     | 0.45              |
| 14:a:235:ASP:O    | 14:a:239:ALA:N    | 2.47                     | 0.45              |
| 14:a:247:ARG:HD3  | 14:a:301:LYS:HZ3  | 1.80                     | 0.45              |
| 15:b:151:GLU:CA   | 15:b:154:THR:HG22 | 2.46                     | 0.45              |
| 16:c:196:LEU:C    | 16:c:198:ARG:H    | 2.23                     | 0.45              |
| 18:f:307:LEU:HB3  | 18:f:314:TYR:CE1  | 2.51                     | 0.45              |
| 18:f:473:ASN:O    | 18:f:509:LYS:NZ   | 2.45                     | 0.45              |
| 18:f:567:LEU:O    | 18:f:790:GLN:NE2  | 2.50                     | 0.45              |
| 18:f:701:ASN:ND2  | 18:f:876:HIS:HE1  | 2.14                     | 0.45              |
| 18:f:888:LEU:HD11 | 18:f:903:ASN:OD1  | 2.15                     | 0.45              |
| 19:g:131:ILE:HG21 | 19:g:147:VAL:HG13 | 1.97                     | 0.45              |
| 19:g:141:THR:HG22 | 19:g:144:GLU:CD   | 2.40                     | 0.45              |
| 22:A:190:VAL:CG2  | 22:A:339:ARG:HE   | 2.30                     | 0.45              |
| 22:A:213:LEU:CD1  | 22:A:321:THR:HG22 | 2.46                     | 0.45              |
| 22:A:214:LEU:HD23 | 22:A:343:PHE:CZ   | 2.51                     | 0.45              |
| 25:F:375:VAL:HG21 | 25:F:420:TYR:HE2  | 1.81                     | 0.45              |
| 27:U:199:ARG:HA   | 27:U:202:VAL:CG1  | 2.45                     | 0.45              |
| 27:U:514:LEU:CD1  | 27:U:547:GLY:HA2  | 2.46                     | 0.45              |
| 27:U:646:PRO:HG3  | 27:U:649:ARG:NH2  | 2.32                     | 0.45              |
| 27:U:792:ASN:HA   | 27:U:914:LEU:H    | 1.81                     | 0.45              |
| 1:C:37:ASP:OD1    | 1:C:37:ASP:C      | 2.59                     | 0.45              |
| 3:G:180:GLU:OE1   | 4:H:55:ILE:HG22   | 2.17                     | 0.45              |
| 3:G:215:ILE:HD11  | 3:G:217:VAL:HG23  | 1.97                     | 0.45              |
| 4:H:34:PRO:HD2    | 4:H:49:GLU:CG     | 2.46                     | 0.45              |
| 4:H:203:MET:HB3   | 4:H:230:LEU:HD22  | 1.98                     | 0.45              |
| 5:I:33:THR:HA     | 5:I:164:ILE:O     | 2.16                     | 0.45              |
| 5:I:65:ILE:HD13   | 5:I:75:SER:HB2    | 1.98                     | 0.45              |
| 7:L:33:SER:O      | 7:L:62:LYS:NZ     | 2.41                     | 0.45              |
| 8:M:97:ASN:O      | 8:M:101:ASN:ND2   | 2.50                     | 0.45              |
| 8:M:232:ARG:O     | 8:M:236:GLU:HG3   | 2.17                     | 0.45              |
| 9:V:358:MET:SD    | 9:V:358:MET:C     | 3.00                     | 0.45              |
| 10:W:63:THR:HA    | 10:W:66:ILE:HB    | 1.98                     | 0.45              |
| 10:W:267:LEU:HB3  | 10:W:299:ILE:CD1  | 2.46                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 10:W:440:ASN:ND2  | 16:c:226:MET:HE3  | 2.30                     | 0.45              |
| 10:W:453:HIS:CE1  | 13:Z:221:PRO:HG3  | 2.52                     | 0.45              |
| 11:X:265:GLU:H    | 11:X:265:GLU:HG2  | 1.56                     | 0.45              |
| 13:Z:16:LEU:HD13  | 16:c:216:MET:HG2  | 1.98                     | 0.45              |
| 13:Z:110:GLU:OE1  | 13:Z:110:GLU:HA   | 2.16                     | 0.45              |
| 16:c:25:VAL:O     | 16:c:25:VAL:HG12  | 2.16                     | 0.45              |
| 17:d:89:GLN:HA    | 17:d:92:THR:OG1   | 2.17                     | 0.45              |
| 17:d:164:PHE:O    | 17:d:168:MET:HB2  | 2.16                     | 0.45              |
| 17:d:226:ILE:O    | 17:d:229:PRO:HD2  | 2.17                     | 0.45              |
| 18:f:59:LEU:HD12  | 18:f:74:ALA:HA    | 1.99                     | 0.45              |
| 18:f:326:LEU:HD21 | 18:f:420:TRP:CD2  | 2.51                     | 0.45              |
| 18:f:456:ARG:HH21 | 18:f:492:SER:HA   | 1.78                     | 0.45              |
| 18:f:700:SER:HB3  | 18:f:779:CYS:SG   | 2.57                     | 0.45              |
| 20:u:182:PHE:HE2  | 20:u:248:VAL:HG22 | 1.80                     | 0.45              |
| 22:A:173:THR:HG22 | 22:A:174:TYR:H    | 1.81                     | 0.45              |
| 22:A:227:ARG:HA   | 23:B:319:PHE:CE1  | 2.51                     | 0.45              |
| 24:E:112:PRO:CG   | 25:F:97:LEU:HD22  | 2.46                     | 0.45              |
| 25:F:228:PRO:HG2  | 25:F:356:MET:HG3  | 1.97                     | 0.45              |
| 25:F:292:GLY:HA3  | 25:F:338:LEU:CD2  | 2.46                     | 0.45              |
| 25:F:371:ARG:HG2  | 25:F:371:ARG:HH11 | 1.81                     | 0.45              |
| 27:U:9:ILE:HA     | 27:U:12:LEU:CD1   | 2.46                     | 0.45              |
| 27:U:179:TYR:O    | 27:U:183:LEU:HD23 | 2.17                     | 0.45              |
| 27:U:789:ILE:HD13 | 27:U:911:ILE:HG12 | 1.98                     | 0.45              |
| 1:C:88:LYS:HE2    | 1:C:94:LYS:HZ2    | 1.75                     | 0.45              |
| 1:C:371:LEU:HD23  | 1:C:371:LEU:C     | 2.41                     | 0.45              |
| 3:G:164:LYS:N     | 4:H:56:LEU:O      | 2.48                     | 0.45              |
| 5:I:107:CYS:O     | 5:I:110:LEU:HB3   | 2.16                     | 0.45              |
| 5:I:136:TYR:CE1   | 5:I:150:SER:HB2   | 2.48                     | 0.45              |
| 5:I:214:ALA:HA    | 5:I:226:ARG:O     | 2.16                     | 0.45              |
| 7:L:133:LEU:HD13  | 7:L:146:GLN:HB2   | 1.98                     | 0.45              |
| 7:L:156:CYS:HA    | 8:M:58:TYR:HA     | 1.99                     | 0.45              |
| 9:V:176:MET:CE    | 9:V:216:ARG:HB3   | 2.46                     | 0.45              |
| 9:V:190:ASP:CA    | 9:V:193:GLN:HB2   | 2.30                     | 0.45              |
| 10:W:20:TYR:N     | 10:W:59:ASP:OD2   | 2.49                     | 0.45              |
| 10:W:105:VAL:HG21 | 10:W:132:THR:CG2  | 2.46                     | 0.45              |
| 10:W:235:GLN:HA   | 10:W:235:GLN:OE1  | 2.17                     | 0.45              |
| 10:W:272:LEU:HD11 | 10:W:341:PHE:HE2  | 1.80                     | 0.45              |
| 10:W:363:ILE:CD1  | 10:W:378:MET:CE   | 2.95                     | 0.45              |
| 11:X:68:GLY:CA    | 11:X:71:LYS:HG2   | 2.46                     | 0.45              |
| 11:X:138:PHE:HE2  | 11:X:175:LYS:HE2  | 1.82                     | 0.45              |
| 11:X:167:VAL:HG13 | 11:X:210:LEU:HD21 | 1.98                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 11:X:400:ALA:HA   | 13:Z:262:LEU:HD22 | 1.98                     | 0.45              |
| 12:Y:24:PHE:CD2   | 12:Y:286:TRP:HA   | 2.51                     | 0.45              |
| 12:Y:88:LEU:O     | 12:Y:92:GLU:HG3   | 2.16                     | 0.45              |
| 13:Z:38:VAL:HG13  | 13:Z:91:ILE:HG23  | 1.98                     | 0.45              |
| 14:a:65:SER:HA    | 14:a:68:GLU:HB3   | 1.99                     | 0.45              |
| 14:a:245:VAL:HG12 | 14:a:247:ARG:H    | 1.81                     | 0.45              |
| 14:a:255:TRP:O    | 14:a:258:GLN:NE2  | 2.50                     | 0.45              |
| 15:b:7:MET:HE2    | 15:b:7:MET:CA     | 2.46                     | 0.45              |
| 15:b:91:ARG:HG2   | 15:b:127:LEU:CD2  | 2.46                     | 0.45              |
| 15:b:130:ARG:HA   | 15:b:133:LYS:HE3  | 1.98                     | 0.45              |
| 17:d:91:ALA:HA    | 17:d:119:LEU:CD2  | 2.46                     | 0.45              |
| 17:d:197:LEU:HD12 | 17:d:256:TYR:CD1  | 2.50                     | 0.45              |
| 17:d:319:ALA:HA   | 17:d:322:GLN:OE1  | 2.16                     | 0.45              |
| 18:f:63:LEU:HB3   | 18:f:106:LEU:HD21 | 1.98                     | 0.45              |
| 18:f:218:GLU:O    | 18:f:258:LYS:HD3  | 2.15                     | 0.45              |
| 18:f:233:LEU:HD12 | 18:f:252:ALA:HB2  | 1.99                     | 0.45              |
| 18:f:404:ASP:O    | 18:f:407:MET:N    | 2.49                     | 0.45              |
| 22:A:23:ARG:HB3   | 22:A:23:ARG:CZ    | 2.45                     | 0.45              |
| 22:A:54:GLN:OE1   | 22:A:54:GLN:C     | 2.59                     | 0.45              |
| 22:A:417:ILE:HG22 | 22:A:418:LYS:N    | 2.32                     | 0.45              |
| 23:B:266:LEU:HD23 | 23:B:266:LEU:O    | 2.16                     | 0.45              |
| 24:E:235:ILE:O    | 24:E:235:ILE:CG2  | 2.65                     | 0.45              |
| 25:F:250:LYS:HD2  | 25:F:250:LYS:O    | 2.17                     | 0.45              |
| 25:F:254:PRO:HD3  | 25:F:287:GLU:O    | 2.16                     | 0.45              |
| 25:F:312:GLU:HA   | 25:F:312:GLU:OE1  | 2.17                     | 0.45              |
| 27:U:85:GLY:HA2   | 27:U:88:PHE:CD1   | 2.52                     | 0.45              |
| 27:U:528:ALA:O    | 27:U:532:MET:HB2  | 2.17                     | 0.45              |
| 1:C:155:ASP:O     | 1:C:159:LYS:HG3   | 2.17                     | 0.45              |
| 2:D:111:TYR:CD2   | 2:D:137:ASN:ND2   | 2.85                     | 0.45              |
| 3:G:18:PRO:HA     | 4:H:24:TYR:CD2    | 2.52                     | 0.45              |
| 3:G:178:PHE:CE2   | 3:G:201:CYS:HA    | 2.52                     | 0.45              |
| 4:H:4:ARG:H       | 4:H:4:ARG:HG2     | 1.48                     | 0.45              |
| 5:I:105:ILE:HD13  | 5:I:110:LEU:HD13  | 1.97                     | 0.45              |
| 7:L:22:ILE:HD11   | 7:L:120:THR:OG1   | 2.16                     | 0.45              |
| 7:L:166:GLN:OE1   | 7:L:166:GLN:HA    | 2.17                     | 0.45              |
| 9:V:108:LEU:HD11  | 9:V:177:ASN:ND2   | 2.24                     | 0.45              |
| 9:V:169:LEU:HB2   | 9:V:210:CYS:SG    | 2.56                     | 0.45              |
| 9:V:365:GLN:HE21  | 28:e:46:ASP:HB3   | 1.81                     | 0.45              |
| 11:X:374:PHE:CE2  | 11:X:387:ILE:HD12 | 2.51                     | 0.45              |
| 12:Y:83:ARG:HG3   | 12:Y:87:GLU:OE1   | 2.16                     | 0.45              |
| 14:a:61:GLU:HA    | 14:a:64:ILE:CG2   | 2.40                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 14:a:99:LYS:O     | 14:a:102:GLU:HG2  | 2.15                     | 0.45              |
| 14:a:114:CYS:O    | 14:a:118:ILE:HG22 | 2.17                     | 0.45              |
| 15:b:37:CYS:SG    | 15:b:38:HIS:ND1   | 2.84                     | 0.45              |
| 15:b:71:ILE:H     | 15:b:71:ILE:CD1   | 2.30                     | 0.45              |
| 15:b:80:PRO:HD2   | 15:b:81:LYS:HE2   | 1.98                     | 0.45              |
| 17:d:141:LEU:HB3  | 17:d:182:LEU:HD13 | 1.98                     | 0.45              |
| 18:f:237:VAL:HG12 | 18:f:248:LEU:HB2  | 1.98                     | 0.45              |
| 18:f:343:LYS:O    | 18:f:382:ASN:ND2  | 2.26                     | 0.45              |
| 18:f:562:LEU:CD1  | 18:f:580:LEU:HD21 | 2.46                     | 0.45              |
| 18:f:674:THR:O    | 18:f:678:LEU:HD13 | 2.16                     | 0.45              |
| 18:f:891:THR:HG23 | 18:f:892:PRO:HD2  | 1.99                     | 0.45              |
| 19:g:90:PRO:HB2   | 19:g:157:GLU:HB2  | 1.98                     | 0.45              |
| 19:g:103:THR:CG2  | 19:g:115:LYS:HD2  | 2.46                     | 0.45              |
| 22:A:34:LYS:HE2   | 22:A:34:LYS:HB2   | 1.49                     | 0.45              |
| 22:A:395:PHE:CD2  | 22:A:411:GLU:HB3  | 2.51                     | 0.45              |
| 24:E:235:ILE:HD13 | 24:E:277:MET:HE3  | 1.97                     | 0.45              |
| 25:F:203:VAL:HG22 | 25:F:244:THR:HB   | 1.98                     | 0.45              |
| 25:F:352:ILE:HD12 | 25:F:352:ILE:HA   | 1.83                     | 0.45              |
| 27:U:46:GLU:HG3   | 27:U:80:TYR:CE2   | 2.51                     | 0.45              |
| 27:U:233:LEU:HD23 | 27:U:233:LEU:HA   | 1.77                     | 0.45              |
| 27:U:250:PHE:HD2  | 27:U:911:ILE:HB   | 1.81                     | 0.45              |
| 27:U:375:PHE:O    | 27:U:739:ALA:HA   | 2.17                     | 0.45              |
| 27:U:458:ILE:HG13 | 27:U:485:ALA:HB2  | 1.99                     | 0.45              |
| 27:U:661:ALA:HB2  | 27:U:748:LEU:HD12 | 1.98                     | 0.45              |
| 27:U:889:LEU:HD12 | 27:U:908:ILE:HA   | 1.99                     | 0.45              |
| 1:C:273:MET:CE    | 1:C:274:LEU:HD23  | 2.47                     | 0.45              |
| 2:D:106:THR:HG21  | 24:E:78:ARG:H     | 1.82                     | 0.45              |
| 2:D:119:ILE:HD11  | 2:D:140:VAL:C     | 2.41                     | 0.45              |
| 2:D:162:VAL:O     | 2:D:162:VAL:HG12  | 2.17                     | 0.45              |
| 5:I:135:LEU:HD21  | 5:I:162:THR:CG2   | 2.44                     | 0.45              |
| 6:J:71:MET:HG2    | 6:J:84:ILE:HD11   | 1.99                     | 0.45              |
| 7:L:40:SER:HG     | 7:L:187:LEU:HD22  | 1.82                     | 0.45              |
| 7:L:49:LEU:HD12   | 7:L:209:ASN:O     | 2.17                     | 0.45              |
| 7:L:168:ALA:HB2   | 7:L:198:THR:HG22  | 1.97                     | 0.45              |
| 9:V:101:LEU:O     | 9:V:105:SER:HB3   | 2.16                     | 0.45              |
| 9:V:101:LEU:HD21  | 9:V:169:LEU:HD23  | 1.98                     | 0.45              |
| 9:V:147:PHE:O     | 9:V:149:PRO:HD3   | 2.17                     | 0.45              |
| 9:V:208:ALA:HA    | 9:V:211:TYR:CD2   | 2.52                     | 0.45              |
| 9:V:256:ARG:NH2   | 28:e:21:GLU:O     | 2.50                     | 0.45              |
| 9:V:264:TYR:CD1   | 9:V:295:ILE:HD13  | 2.51                     | 0.45              |
| 10:W:203:GLN:HG2  | 10:W:233:LEU:HD11 | 1.98                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 12:Y:81:LEU:HG    | 12:Y:110:TYR:HE2  | 1.82                     | 0.45              |
| 12:Y:148:GLY:C    | 12:Y:157:ILE:HD11 | 2.41                     | 0.45              |
| 12:Y:193:ASP:C    | 12:Y:193:ASP:OD1  | 2.59                     | 0.45              |
| 12:Y:272:PHE:HB3  | 28:e:56:LEU:HD11  | 1.97                     | 0.45              |
| 15:b:25:ARG:NH2   | 15:b:144:GLY:HA3  | 2.32                     | 0.45              |
| 16:c:49:VAL:O     | 16:c:116:PRO:HG3  | 2.17                     | 0.45              |
| 17:d:127:ASN:HD22 | 17:d:136:LEU:HD21 | 1.80                     | 0.45              |
| 17:d:152:ALA:HB3  | 17:d:191:LEU:HD22 | 1.99                     | 0.45              |
| 17:d:199:LEU:HD11 | 17:d:211:GLU:HG2  | 1.99                     | 0.45              |
| 18:f:210:GLU:O    | 18:f:212:GLU:OE2  | 2.35                     | 0.45              |
| 18:f:264:GLU:OE2  | 18:f:892:PRO:HG3  | 2.16                     | 0.45              |
| 19:g:79:THR:O     | 19:g:82:ILE:HG13  | 2.16                     | 0.45              |
| 19:g:100:LEU:H    | 19:g:100:LEU:CD2  | 2.26                     | 0.45              |
| 19:g:126:TYR:HA   | 19:g:161:SER:HA   | 1.97                     | 0.45              |
| 19:g:159:LYS:HB2  | 19:g:168:ASN:HD21 | 1.81                     | 0.45              |
| 22:A:227:ARG:HA   | 23:B:319:PHE:HE1  | 1.81                     | 0.45              |
| 22:A:307:ASP:HB3  | 22:A:336:ARG:HG3  | 1.98                     | 0.45              |
| 22:A:423:PHE:HB3  | 22:A:428:ARG:HH12 | 1.81                     | 0.45              |
| 23:B:64:LYS:O     | 23:B:68:ILE:HG13  | 2.16                     | 0.45              |
| 24:E:151:LEU:N    | 24:E:152:PRO:HD2  | 2.32                     | 0.45              |
| 25:F:134:LEU:HD12 | 25:F:160:ILE:CD1  | 2.47                     | 0.45              |
| 25:F:177:VAL:HG12 | 25:F:179:GLU:HG3  | 1.96                     | 0.45              |
| 25:F:393:GLY:O    | 25:F:396:CYS:HB2  | 2.16                     | 0.45              |
| 26:K:20:ARG:HH21  | 26:K:25:GLU:CD    | 2.25                     | 0.45              |
| 27:U:236:LEU:HG   | 27:U:241:ASN:HB3  | 1.99                     | 0.45              |
| 27:U:832:VAL:O    | 27:U:834:SER:N    | 2.50                     | 0.45              |
| 1:C:49:ARG:CZ     | 27:U:639:LEU:HG   | 2.47                     | 0.45              |
| 1:C:80:MET:HE3    | 1:C:80:MET:HB2    | 1.67                     | 0.45              |
| 1:C:157:GLN:O     | 1:C:161:ILE:HG22  | 2.16                     | 0.45              |
| 2:D:406:VAL:HG12  | 2:D:406:VAL:O     | 2.17                     | 0.45              |
| 4:H:74:LEU:HD13   | 4:H:134:LEU:HD22  | 1.99                     | 0.45              |
| 5:I:90:LEU:HA     | 5:I:90:LEU:HD23   | 1.79                     | 0.45              |
| 5:I:122:THR:O     | 6:J:125:ARG:NH2   | 2.50                     | 0.45              |
| 5:I:158:GLY:H     | 6:J:58:THR:HG21   | 1.82                     | 0.45              |
| 6:J:32:ALA:HB3    | 6:J:161:ILE:HG13  | 1.99                     | 0.45              |
| 6:J:150:SER:O     | 26:K:83:LYS:HD2   | 2.16                     | 0.45              |
| 8:M:220:THR:HG22  | 8:M:220:THR:O     | 2.15                     | 0.45              |
| 8:M:243:LEU:HD12  | 8:M:244:LYS:HG2   | 1.98                     | 0.45              |
| 9:V:76:LYS:HE2    | 9:V:147:PHE:CZ    | 2.52                     | 0.45              |
| 9:V:212:TYR:CD1   | 9:V:253:LEU:HD11  | 2.36                     | 0.45              |
| 9:V:227:VAL:O     | 9:V:231:LEU:HG    | 2.17                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 9:V:243:ASP:OD1   | 9:V:244:ALA:N     | 2.49                     | 0.45              |
| 9:V:281:ASN:OD1   | 9:V:283:ASN:HB2   | 2.17                     | 0.45              |
| 9:V:309:MET:SD    | 9:V:331:LEU:HB3   | 2.57                     | 0.45              |
| 9:V:421:ASP:OD2   | 12:Y:349:LYS:HE3  | 2.16                     | 0.45              |
| 9:V:462:GLU:HG2   | 9:V:462:GLU:O     | 2.17                     | 0.45              |
| 10:W:82:LEU:C     | 10:W:86:ASN:HD22  | 2.18                     | 0.45              |
| 10:W:206:SER:HA   | 10:W:209:ILE:CG2  | 2.47                     | 0.45              |
| 10:W:280:ASP:O    | 10:W:284:SER:HB3  | 2.17                     | 0.45              |
| 11:X:80:ILE:CD1   | 11:X:85:ALA:HB2   | 2.47                     | 0.45              |
| 12:Y:95:LEU:HD12  | 12:Y:99:GLU:CG    | 2.46                     | 0.45              |
| 13:Z:20:VAL:HG22  | 13:Z:126:VAL:HG22 | 1.98                     | 0.45              |
| 14:a:109:GLU:CD   | 14:a:112:ILE:HG22 | 2.41                     | 0.45              |
| 15:b:138:VAL:O    | 15:b:160:LEU:HD11 | 2.16                     | 0.45              |
| 15:b:142:ASN:O    | 15:b:142:ASN:OD1  | 2.35                     | 0.45              |
| 17:d:95:TYR:CE1   | 17:d:99:LYS:HD2   | 2.52                     | 0.45              |
| 17:d:214:ARG:HA   | 17:d:214:ARG:HD2  | 1.81                     | 0.45              |
| 17:d:282:ILE:HG23 | 17:d:287:ALA:HB2  | 1.99                     | 0.45              |
| 18:f:237:VAL:HG11 | 18:f:249:LEU:HD23 | 1.99                     | 0.45              |
| 18:f:323:ASN:OD1  | 18:f:455:VAL:HG12 | 2.17                     | 0.45              |
| 18:f:478:ARG:HD2  | 18:f:514:VAL:CG1  | 2.46                     | 0.45              |
| 18:f:608:LYS:HD3  | 18:f:608:LYS:HA   | 1.63                     | 0.45              |
| 19:g:83:ALA:H     | 19:g:149:HIS:HB3  | 1.82                     | 0.45              |
| 22:A:93:LEU:HD12  | 23:B:132:TYR:HD2  | 1.81                     | 0.45              |
| 22:A:287:ASP:O    | 22:A:287:ASP:OD1  | 2.34                     | 0.45              |
| 23:B:417:GLU:OE1  | 23:B:417:GLU:N    | 2.50                     | 0.45              |
| 24:E:149:ILE:HD11 | 24:E:276:ILE:CG1  | 2.45                     | 0.45              |
| 25:F:129:ARG:HB2  | 25:F:129:ARG:CZ   | 2.45                     | 0.45              |
| 26:K:41:GLN:NE2   | 26:K:151:PRO:O    | 2.49                     | 0.45              |
| 27:U:191:LYS:HA   | 27:U:194:ARG:HB3  | 1.99                     | 0.45              |
| 27:U:351:MET:HE1  | 27:U:354:LYS:CE   | 2.47                     | 0.45              |
| 1:C:246:ILE:N     | 1:C:246:ILE:HD12  | 2.32                     | 0.45              |
| 2:D:219:VAL:O     | 2:D:223:THR:HG22  | 2.17                     | 0.45              |
| 2:D:384:MET:HE1   | 24:E:159:PHE:CE1  | 2.34                     | 0.45              |
| 4:H:74:LEU:HA     | 4:H:135:LEU:O     | 2.16                     | 0.45              |
| 5:I:14:PRO:O      | 6:J:24:GLU:HG3    | 2.16                     | 0.45              |
| 5:I:238:LYS:HA    | 5:I:241:GLU:HB2   | 1.99                     | 0.45              |
| 7:L:81:ALA:CB     | 7:L:130:VAL:HG21  | 2.46                     | 0.45              |
| 8:M:210:GLU:HG2   | 8:M:211:LEU:N     | 2.32                     | 0.45              |
| 9:V:218:TYR:CD2   | 9:V:227:VAL:HG13  | 2.52                     | 0.45              |
| 9:V:273:LYS:HE3   | 9:V:273:LYS:CA    | 2.47                     | 0.45              |
| 10:W:425:LEU:HD23 | 13:Z:245:PHE:CE2  | 2.52                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 12:Y:26:LEU:HG    | 12:Y:37:VAL:HG12  | 1.98                     | 0.45              |
| 13:Z:40:LEU:HB3   | 13:Z:89:GLU:HB3   | 1.99                     | 0.45              |
| 15:b:118:GLU:CD   | 15:b:118:GLU:H    | 2.25                     | 0.45              |
| 16:c:144:VAL:HG12 | 16:c:145:VAL:N    | 2.30                     | 0.45              |
| 16:c:189:ILE:C    | 16:c:191:ALA:H    | 2.24                     | 0.45              |
| 17:d:163:SER:O    | 17:d:166:ARG:HG2  | 2.17                     | 0.45              |
| 19:g:141:THR:O    | 19:g:145:GLN:HG2  | 2.17                     | 0.45              |
| 22:A:123:VAL:HB   | 22:A:147:TYR:O    | 2.17                     | 0.45              |
| 27:U:145:HIS:O    | 27:U:146:LYS:C    | 2.59                     | 0.45              |
| 27:U:402:PHE:CE1  | 27:U:441:GLY:HA2  | 2.51                     | 0.45              |
| 27:U:878:LEU:HB2  | 27:U:882:ALA:HB2  | 1.99                     | 0.45              |
| 1:C:72:TYR:CE1    | 2:D:111:TYR:HE1   | 2.35                     | 0.45              |
| 1:C:164:VAL:HG21  | 1:C:313:ARG:HG3   | 1.99                     | 0.45              |
| 1:C:217:SER:O     | 2:D:248:ARG:NH2   | 2.50                     | 0.45              |
| 1:C:237:MET:HE2   | 1:C:237:MET:HB3   | 1.79                     | 0.45              |
| 2:D:45:LYS:HB3    | 27:U:187:LEU:CD1  | 2.42                     | 0.45              |
| 3:G:143:ILE:HG13  | 3:G:221:THR:C     | 2.42                     | 0.45              |
| 4:H:36:VAL:CG2    | 4:H:47:ALA:HB3    | 2.46                     | 0.45              |
| 7:L:24:TYR:O      | 7:L:27:GLU:HB2    | 2.17                     | 0.45              |
| 8:M:224:HIS:O     | 8:M:224:HIS:CG    | 2.69                     | 0.45              |
| 9:V:117:VAL:HG21  | 9:V:132:LEU:CD1   | 2.47                     | 0.45              |
| 9:V:279:GLN:O     | 9:V:279:GLN:HG2   | 2.17                     | 0.45              |
| 9:V:324:PHE:CD2   | 28:e:19:PHE:CE2   | 3.04                     | 0.45              |
| 11:X:46:LYS:HG2   | 11:X:76:PHE:HE1   | 1.81                     | 0.45              |
| 11:X:74:ARG:HD3   | 11:X:116:TRP:CD1  | 2.52                     | 0.45              |
| 11:X:374:PHE:HE2  | 11:X:387:ILE:CD1  | 2.30                     | 0.45              |
| 12:Y:257:ARG:HG2  | 12:Y:257:ARG:NH1  | 2.32                     | 0.45              |
| 13:Z:44:GLN:HB2   | 13:Z:47:VAL:O     | 2.17                     | 0.45              |
| 13:Z:225:GLN:O    | 13:Z:226:ILE:HB   | 2.16                     | 0.45              |
| 14:a:111:VAL:HG22 | 14:a:115:LYS:HG2  | 1.99                     | 0.45              |
| 14:a:111:VAL:C    | 14:a:115:LYS:HG3  | 2.41                     | 0.45              |
| 14:a:158:LEU:HA   | 14:a:161:LYS:HB2  | 1.98                     | 0.45              |
| 17:d:129:LEU:HD12 | 27:U:26:LYS:CG    | 2.47                     | 0.45              |
| 19:g:89:LEU:CD2   | 19:g:155:VAL:HG11 | 2.47                     | 0.45              |
| 22:A:217:PRO:HG2  | 22:A:345:LEU:CD2  | 2.47                     | 0.45              |
| 23:B:256:ILE:HD12 | 23:B:305:ILE:HG23 | 1.99                     | 0.45              |
| 23:B:428:TYR:O    | 23:B:429:LYS:HB3  | 2.16                     | 0.45              |
| 25:F:177:VAL:HG13 | 25:F:179:GLU:HG3  | 1.99                     | 0.45              |
| 25:F:191:LEU:HD22 | 25:F:194:GLN:CG   | 2.46                     | 0.45              |
| 25:F:252:ALA:HA   | 25:F:286:ASP:N    | 2.31                     | 0.45              |
| 25:F:304:ARG:O    | 25:F:308:ARG:HG2  | 2.17                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 26:K:67:ILE:HD13  | 26:K:67:ILE:HA    | 1.79                     | 0.45              |
| 27:U:122:GLU:O    | 27:U:124:LYS:NZ   | 2.34                     | 0.45              |
| 27:U:498:LYS:NZ   | 27:U:531:ASP:HB3  | 2.32                     | 0.45              |
| 27:U:633:CYS:N    | 27:U:634:PRO:HD2  | 2.31                     | 0.45              |
| 2:D:144:PRO:HG2   | 24:E:64:LEU:HD22  | 1.99                     | 0.44              |
| 4:H:65:VAL:CG1    | 4:H:218:PHE:HZ    | 2.26                     | 0.44              |
| 6:J:28:LYS:HE3    | 23:B:439:TYR:CD1  | 2.53                     | 0.44              |
| 6:J:43:LEU:HD13   | 6:J:134:VAL:HG11  | 1.98                     | 0.44              |
| 6:J:45:VAL:HG21   | 6:J:61:LYS:HD3    | 1.95                     | 0.44              |
| 7:L:35:THR:O      | 7:L:160:SER:HA    | 2.16                     | 0.44              |
| 8:M:47:PHE:CE2    | 8:M:138:GLY:HA3   | 2.52                     | 0.44              |
| 9:V:64:GLN:HA     | 9:V:67:LEU:HB2    | 1.99                     | 0.44              |
| 9:V:64:GLN:CG     | 9:V:109:ASN:HD21  | 2.20                     | 0.44              |
| 9:V:172:VAL:O     | 9:V:175:MET:HB2   | 2.17                     | 0.44              |
| 9:V:371:ASN:ND2   | 9:V:374:LYS:HG3   | 2.32                     | 0.44              |
| 9:V:451:ILE:HG22  | 17:d:279:TYR:HD1  | 1.82                     | 0.44              |
| 10:W:172:GLU:HG2  | 10:W:208:LYS:HD2  | 1.99                     | 0.44              |
| 10:W:235:GLN:HA   | 10:W:243:ILE:CD1  | 2.41                     | 0.44              |
| 10:W:409:LEU:HB3  | 11:X:344:ARG:HH12 | 1.81                     | 0.44              |
| 11:X:151:SER:O    | 11:X:155:ARG:HG3  | 2.17                     | 0.44              |
| 11:X:224:ASP:CG   | 11:X:227:THR:HB   | 2.42                     | 0.44              |
| 12:Y:95:LEU:HG    | 12:Y:99:GLU:HG3   | 2.00                     | 0.44              |
| 12:Y:350:VAL:HG12 | 12:Y:351:ASN:ND2  | 2.32                     | 0.44              |
| 13:Z:16:LEU:HD23  | 13:Z:162:ILE:HD12 | 1.98                     | 0.44              |
| 13:Z:142:GLU:CD   | 13:Z:153:LYS:HD2  | 2.41                     | 0.44              |
| 13:Z:170:VAL:HG21 | 16:c:150:SER:O    | 2.17                     | 0.44              |
| 14:a:33:LEU:HD13  | 14:a:36:GLN:OE1   | 2.16                     | 0.44              |
| 14:a:160:SER:O    | 14:a:163:TYR:CD2  | 2.70                     | 0.44              |
| 15:b:141:ILE:HG13 | 15:b:143:PHE:CE1  | 2.53                     | 0.44              |
| 16:c:191:ALA:C    | 16:c:193:ILE:N    | 2.74                     | 0.44              |
| 16:c:195:GLY:HA3  | 16:c:199:HIS:CD2  | 2.52                     | 0.44              |
| 17:d:160:ASP:HB3  | 17:d:163:SER:OG   | 2.17                     | 0.44              |
| 18:f:613:LEU:HD13 | 23:B:74:MET:HE3   | 1.99                     | 0.44              |
| 18:f:680:ARG:HH11 | 22:A:66:LYS:HG3   | 1.76                     | 0.44              |
| 18:f:716:ASP:OD1  | 18:f:717:ALA:N    | 2.49                     | 0.44              |
| 18:f:761:MET:HA   | 18:f:764:LEU:HB3  | 1.98                     | 0.44              |
| 22:A:332:MET:C    | 22:A:340:LYS:HZ3  | 2.24                     | 0.44              |
| 22:A:363:SER:O    | 22:A:363:SER:OG   | 2.34                     | 0.44              |
| 23:B:220:LYS:HG3  | 23:B:326:LYS:HD3  | 1.99                     | 0.44              |
| 24:E:303:LEU:O    | 24:E:304:PRO:C    | 2.60                     | 0.44              |
| 25:F:341:ALA:HA   | 25:F:344:ARG:NH1  | 2.32                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 25:F:358:ASN:C    | 25:F:358:ASN:OD1  | 2.60                     | 0.44              |
| 27:U:24:LEU:HD11  | 27:U:48:LEU:HD23  | 1.98                     | 0.44              |
| 27:U:136:LYS:HD2  | 27:U:140:ARG:HG3  | 1.97                     | 0.44              |
| 27:U:831:ALA:O    | 27:U:836:THR:HB   | 2.17                     | 0.44              |
| 27:U:902:PRO:HB3  | 27:U:912:ILE:HD13 | 1.98                     | 0.44              |
| 1:C:23:TYR:CD1    | 27:U:105:ILE:HD11 | 2.51                     | 0.44              |
| 1:C:25:LEU:O      | 1:C:25:LEU:HD23   | 2.16                     | 0.44              |
| 1:C:91:PRO:HG2    | 1:C:92:GLU:CD     | 2.42                     | 0.44              |
| 1:C:121:TYR:HB2   | 23:B:106:PRO:HD3  | 2.00                     | 0.44              |
| 2:D:45:LYS:CG     | 27:U:187:LEU:HB3  | 2.42                     | 0.44              |
| 2:D:164:TYR:O     | 2:D:167:ILE:HG12  | 2.16                     | 0.44              |
| 3:G:40:VAL:O      | 3:G:50:ILE:HA     | 2.17                     | 0.44              |
| 3:G:131:MET:HE2   | 3:G:131:MET:HB3   | 1.91                     | 0.44              |
| 3:G:189:TRP:CZ3   | 3:G:197:THR:HG21  | 2.52                     | 0.44              |
| 3:G:199:ILE:CG2   | 3:G:242:LEU:HG    | 2.47                     | 0.44              |
| 4:H:95:GLN:HA     | 4:H:95:GLN:OE1    | 2.18                     | 0.44              |
| 7:L:84:LEU:HD23   | 7:L:84:LEU:HA     | 1.86                     | 0.44              |
| 7:L:154:PHE:HB3   | 8:M:58:TYR:HD2    | 1.80                     | 0.44              |
| 7:L:160:SER:HB2   | 7:L:168:ALA:HB3   | 1.99                     | 0.44              |
| 7:L:204:ASP:HA    | 7:L:239:ARG:HH21  | 1.81                     | 0.44              |
| 9:V:493:ALA:C     | 9:V:495:ARG:N     | 2.67                     | 0.44              |
| 10:W:230:MET:HE3  | 10:W:233:LEU:HB3  | 1.99                     | 0.44              |
| 11:X:299:LEU:HD11 | 11:X:334:ASN:ND2  | 2.30                     | 0.44              |
| 12:Y:39:ASP:O     | 12:Y:43:ALA:N     | 2.38                     | 0.44              |
| 13:Z:29:VAL:HG23  | 13:Z:30:GLY:N     | 2.32                     | 0.44              |
| 14:a:257:GLN:HG3  | 14:a:257:GLN:O    | 2.17                     | 0.44              |
| 18:f:62:ARG:HH12  | 18:f:74:ALA:CB    | 2.27                     | 0.44              |
| 18:f:234:THR:C    | 18:f:237:VAL:HG22 | 2.43                     | 0.44              |
| 18:f:240:VAL:HG11 | 18:f:248:LEU:CD1  | 2.48                     | 0.44              |
| 18:f:460:ASP:N    | 18:f:461:PRO:HD3  | 2.33                     | 0.44              |
| 18:f:500:LEU:HD23 | 18:f:500:LEU:C    | 2.42                     | 0.44              |
| 19:g:85:ILE:HD12  | 19:g:131:ILE:HD11 | 1.99                     | 0.44              |
| 24:E:36:LEU:HA    | 24:E:39:GLN:NE2   | 2.32                     | 0.44              |
| 24:E:121:ASN:HB2  | 24:E:221:TYR:CZ   | 2.52                     | 0.44              |
| 24:E:157:GLU:O    | 24:E:161:ARG:N    | 2.48                     | 0.44              |
| 24:E:253:ILE:HA   | 24:E:256:THR:CG2  | 2.48                     | 0.44              |
| 25:F:384:LEU:HD23 | 25:F:384:LEU:HA   | 1.74                     | 0.44              |
| 26:K:88:LEU:HA    | 26:K:88:LEU:HD23  | 1.73                     | 0.44              |
| 26:K:107:MET:HG2  | 26:K:111:SER:CB   | 2.47                     | 0.44              |
| 26:K:205:VAL:O    | 26:K:205:VAL:CG2  | 2.65                     | 0.44              |
| 27:U:806:CYS:HB2  | 27:U:872:GLU:OE2  | 2.17                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 27:U:880:ASN:N    | 27:U:881:PRO:CD   | 2.80                     | 0.44              |
| 27:U:894:MET:CG   | 27:U:895:PRO:HD2  | 2.47                     | 0.44              |
| 27:U:901:GLN:O    | 27:U:915:LYS:HB3  | 2.17                     | 0.44              |
| 1:C:97:VAL:HG23   | 1:C:98:ASP:O      | 2.18                     | 0.44              |
| 1:C:161:ILE:HD13  | 1:C:188:LEU:HD21  | 1.98                     | 0.44              |
| 1:C:212:ILE:HG21  | 1:C:237:MET:HE1   | 2.00                     | 0.44              |
| 2:D:203:LEU:HA    | 2:D:309:MET:O     | 2.17                     | 0.44              |
| 4:H:36:VAL:HG11   | 4:H:194:THR:CG2   | 2.42                     | 0.44              |
| 5:I:6:ASP:OD1     | 5:I:6:ASP:O       | 2.35                     | 0.44              |
| 5:I:133:SER:HB2   | 5:I:150:SER:O     | 2.16                     | 0.44              |
| 6:J:51:ALA:H      | 6:J:54:GLN:HE21   | 1.64                     | 0.44              |
| 8:M:81:LEU:O      | 8:M:84:ALA:N      | 2.50                     | 0.44              |
| 8:M:220:THR:HG21  | 8:M:223:ARG:C     | 2.42                     | 0.44              |
| 9:V:185:GLN:OE1   | 9:V:221:LEU:HD11  | 2.16                     | 0.44              |
| 9:V:391:THR:O     | 9:V:391:THR:HG22  | 2.18                     | 0.44              |
| 13:Z:187:LEU:O    | 13:Z:191:ILE:HG12 | 2.17                     | 0.44              |
| 15:b:29:GLN:HG2   | 15:b:30:GLN:N     | 2.32                     | 0.44              |
| 15:b:154:THR:HA   | 15:b:170:LEU:HD23 | 2.00                     | 0.44              |
| 16:c:173:GLU:O    | 16:c:175:ARG:N    | 2.47                     | 0.44              |
| 16:c:249:LEU:HD11 | 16:c:253:LYS:HE3  | 1.99                     | 0.44              |
| 18:f:107:LYS:HA   | 18:f:107:LYS:CE   | 2.44                     | 0.44              |
| 18:f:267:ARG:HH11 | 18:f:783:SER:CB   | 2.29                     | 0.44              |
| 18:f:496:ASP:O    | 18:f:499:THR:OG1  | 2.21                     | 0.44              |
| 18:f:563:GLY:HA3  | 18:f:598:CYS:HB2  | 2.00                     | 0.44              |
| 18:f:803:PHE:HD1  | 18:f:806:VAL:HG12 | 1.83                     | 0.44              |
| 19:g:111:GLU:O    | 19:g:114:SER:HB2  | 2.17                     | 0.44              |
| 19:g:125:ASN:C    | 19:g:161:SER:CB   | 2.90                     | 0.44              |
| 23:B:203:LEU:HB3  | 23:B:211:TYR:OH   | 2.17                     | 0.44              |
| 23:B:205:LEU:CD2  | 23:B:279:PRO:HB3  | 2.47                     | 0.44              |
| 23:B:384:ILE:HG13 | 23:B:384:ILE:H    | 1.61                     | 0.44              |
| 24:E:351:GLY:O    | 24:E:355:ILE:N    | 2.47                     | 0.44              |
| 25:F:76:ASN:HD21  | 25:F:80:ILE:HD11  | 1.83                     | 0.44              |
| 27:U:137:MET:O    | 27:U:140:ARG:N    | 2.51                     | 0.44              |
| 27:U:458:ILE:CD1  | 27:U:485:ALA:HB2  | 2.47                     | 0.44              |
| 27:U:559:ARG:O    | 27:U:560:MET:HB3  | 2.17                     | 0.44              |
| 27:U:838:LYS:O    | 27:U:838:LYS:HD3  | 2.17                     | 0.44              |
| 1:C:338:LEU:HA    | 1:C:338:LEU:HD23  | 1.72                     | 0.44              |
| 1:C:368:MET:SD    | 2:D:191:TYR:HE1   | 2.41                     | 0.44              |
| 3:G:165:ALA:HB1   | 3:G:179:LEU:CD1   | 2.37                     | 0.44              |
| 5:I:65:ILE:HD11   | 5:I:75:SER:HB2    | 2.00                     | 0.44              |
| 7:L:195:LEU:HD23  | 7:L:195:LEU:HA    | 1.86                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 8:M:164:ALA:HB3   | 8:M:172:ALA:HB3   | 1.99                     | 0.44              |
| 9:V:162:GLU:OE1   | 9:V:203:LEU:N     | 2.50                     | 0.44              |
| 9:V:247:GLN:NE2   | 9:V:277:PRO:HD3   | 2.32                     | 0.44              |
| 9:V:447:ILE:HG22  | 9:V:449:ALA:N     | 2.32                     | 0.44              |
| 10:W:52:LYS:HG3   | 10:W:55:ARG:NH2   | 2.31                     | 0.44              |
| 10:W:276:LEU:HD11 | 10:W:341:PHE:CE1  | 2.53                     | 0.44              |
| 10:W:406:VAL:HG23 | 11:X:342:PHE:HA   | 1.98                     | 0.44              |
| 11:X:331:LEU:HD21 | 11:X:364:LYS:HG2  | 1.95                     | 0.44              |
| 11:X:368:MET:HG2  | 11:X:373:LYS:CB   | 2.46                     | 0.44              |
| 12:Y:294:TYR:O    | 12:Y:298:GLU:HG2  | 2.17                     | 0.44              |
| 12:Y:308:LEU:HD23 | 12:Y:314:LEU:HD21 | 2.00                     | 0.44              |
| 14:a:197:ALA:HB3  | 14:a:226:ARG:CD   | 2.48                     | 0.44              |
| 14:a:208:GLU:OE1  | 14:a:208:GLU:O    | 2.36                     | 0.44              |
| 17:d:163:SER:HA   | 17:d:166:ARG:CD   | 2.46                     | 0.44              |
| 17:d:197:LEU:HD23 | 17:d:197:LEU:C    | 2.42                     | 0.44              |
| 18:f:298:LEU:HD11 | 18:f:305:LEU:CD2  | 2.47                     | 0.44              |
| 18:f:450:ILE:CG1  | 18:f:822:VAL:HG11 | 2.48                     | 0.44              |
| 19:g:131:ILE:CD1  | 19:g:153:ALA:HB2  | 2.37                     | 0.44              |
| 22:A:304:ASN:OD1  | 22:A:304:ASN:C    | 2.59                     | 0.44              |
| 22:A:372:LEU:HD13 | 22:A:376:LEU:HD11 | 1.99                     | 0.44              |
| 23:B:287:ILE:HG21 | 23:B:329:MET:HE3  | 1.99                     | 0.44              |
| 24:E:132:TYR:OH   | 24:E:187:VAL:HA   | 2.17                     | 0.44              |
| 26:K:186:HIS:NE2  | 26:K:189:MET:SD   | 2.91                     | 0.44              |
| 27:U:96:TYR:HA    | 27:U:99:THR:CG2   | 2.48                     | 0.44              |
| 27:U:672:LEU:HD11 | 27:U:690:ALA:HB3  | 2.00                     | 0.44              |
| 1:C:21:ARG:CA     | 1:C:24:TYR:CD2    | 2.98                     | 0.44              |
| 1:C:75:GLU:HA     | 1:C:112:CYS:O     | 2.17                     | 0.44              |
| 2:D:229:ARG:HG2   | 2:D:229:ARG:HH11  | 1.82                     | 0.44              |
| 4:H:180:GLU:OE2   | 4:H:181:ASP:HB2   | 2.18                     | 0.44              |
| 6:J:43:LEU:O      | 6:J:43:LEU:HG     | 2.17                     | 0.44              |
| 7:L:81:ALA:CA     | 7:L:130:VAL:HG21  | 2.45                     | 0.44              |
| 9:V:248:ALA:CA    | 9:V:276:PHE:HE1   | 2.29                     | 0.44              |
| 9:V:285:TRP:HZ3   | 9:V:289:LEU:HD21  | 1.83                     | 0.44              |
| 9:V:375:PHE:CE1   | 9:V:379:LEU:HD21  | 2.52                     | 0.44              |
| 9:V:375:PHE:CD1   | 9:V:379:LEU:HD11  | 2.53                     | 0.44              |
| 10:W:67:LEU:HD23  | 10:W:67:LEU:HA    | 1.78                     | 0.44              |
| 10:W:87:ILE:HG23  | 10:W:104:MET:HE2  | 2.00                     | 0.44              |
| 10:W:140:ILE:HD12 | 10:W:140:ILE:N    | 2.30                     | 0.44              |
| 10:W:167:GLN:HA   | 10:W:189:GLN:NE2  | 2.32                     | 0.44              |
| 10:W:210:ASN:OD1  | 10:W:210:ASN:C    | 2.60                     | 0.44              |
| 10:W:310:THR:O    | 10:W:310:THR:HG22 | 2.17                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 10:W:315:MET:O    | 10:W:315:MET:CG   | 2.66                     | 0.44              |
| 10:W:367:ALA:HA   | 10:W:415:PHE:CD2  | 2.52                     | 0.44              |
| 11:X:211:ASP:OD2  | 11:X:234:GLU:HG3  | 2.18                     | 0.44              |
| 11:X:289:CYS:SG   | 11:X:305:ALA:HB1  | 2.57                     | 0.44              |
| 13:Z:57:PRO:CD    | 13:Z:74:TYR:CD2   | 3.01                     | 0.44              |
| 13:Z:62:ASP:OD2   | 13:Z:63:LYS:HD3   | 2.17                     | 0.44              |
| 14:a:16:PRO:HD2   | 14:a:47:ASP:OD2   | 2.17                     | 0.44              |
| 14:a:51:ALA:O     | 14:a:54:ASP:N     | 2.45                     | 0.44              |
| 14:a:80:ILE:HA    | 14:a:83:VAL:CB    | 2.30                     | 0.44              |
| 14:a:216:LEU:HD11 | 14:a:234:ILE:HD12 | 1.99                     | 0.44              |
| 15:b:11:ASP:OD1   | 15:b:13:SER:N     | 2.34                     | 0.44              |
| 15:b:33:VAL:CA    | 15:b:36:VAL:HG22  | 2.41                     | 0.44              |
| 15:b:121:GLU:HA   | 15:b:124:LEU:HD23 | 1.97                     | 0.44              |
| 16:c:52:GLU:HG2   | 16:c:116:PRO:HD2  | 1.98                     | 0.44              |
| 18:f:95:PRO:O     | 18:f:99:LEU:HB2   | 2.18                     | 0.44              |
| 18:f:177:GLU:OE2  | 18:f:180:GLN:NE2  | 2.50                     | 0.44              |
| 18:f:398:TRP:CD1  | 18:f:401:LYS:HZ1  | 2.35                     | 0.44              |
| 22:A:125:LEU:N    | 22:A:125:LEU:HD23 | 2.32                     | 0.44              |
| 22:A:233:THR:O    | 22:A:234:ASP:HB2  | 2.18                     | 0.44              |
| 22:A:414:ASN:O    | 22:A:419:SER:HB2  | 2.17                     | 0.44              |
| 23:B:303:ARG:HG2  | 23:B:307:ARG:HH22 | 1.83                     | 0.44              |
| 24:E:361:PHE:HE1  | 24:E:366:ASP:HB3  | 1.75                     | 0.44              |
| 25:F:95:GLU:C     | 25:F:96:LEU:HD12  | 2.42                     | 0.44              |
| 25:F:134:LEU:CD1  | 25:F:160:ILE:H    | 2.30                     | 0.44              |
| 25:F:332:THR:CG2  | 25:F:334:ARG:H    | 2.30                     | 0.44              |
| 25:F:341:ALA:HA   | 25:F:344:ARG:HH11 | 1.81                     | 0.44              |
| 25:F:382:GLU:O    | 25:F:386:ARG:NH1  | 2.48                     | 0.44              |
| 26:K:165:CYS:CB   | 26:K:168:ARG:HB2  | 2.48                     | 0.44              |
| 27:U:200:VAL:O    | 27:U:204:ILE:HG22 | 2.17                     | 0.44              |
| 27:U:792:ASN:OD1  | 27:U:796:LYS:HB3  | 2.18                     | 0.44              |
| 27:U:902:PRO:HB2  | 27:U:912:ILE:HD13 | 1.98                     | 0.44              |
| 1:C:219:LEU:HB2   | 1:C:254:ILE:HD13  | 1.99                     | 0.44              |
| 1:C:328:ILE:HG21  | 1:C:359:VAL:HB    | 2.00                     | 0.44              |
| 2:D:116:LEU:HD23  | 2:D:119:ILE:CG1   | 2.48                     | 0.44              |
| 2:D:272:THR:O     | 2:D:273:LYS:C     | 2.60                     | 0.44              |
| 4:H:87:VAL:CG1    | 4:H:88:HIS:N      | 2.80                     | 0.44              |
| 4:H:230:LEU:O     | 4:H:233:ILE:HG22  | 2.18                     | 0.44              |
| 5:I:4:ARG:HA      | 5:I:4:ARG:HD2     | 1.71                     | 0.44              |
| 6:J:10:PHE:HE1    | 6:J:16:LEU:CG     | 2.21                     | 0.44              |
| 6:J:23:GLN:HG3    | 6:J:149:PRO:HG2   | 1.99                     | 0.44              |
| 7:L:7:ASP:OD1     | 7:L:24:TYR:CE2    | 2.71                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:L:88:MET:HG2    | 7:L:112:ILE:HD13  | 1.99                     | 0.44              |
| 7:L:199:LEU:HD12  | 7:L:205:LEU:HD23  | 1.99                     | 0.44              |
| 9:V:72:LEU:O      | 9:V:76:LYS:HB3    | 2.18                     | 0.44              |
| 9:V:81:GLN:CA     | 9:V:84:LYS:HB3    | 2.44                     | 0.44              |
| 9:V:162:GLU:CD    | 9:V:203:LEU:HA    | 2.42                     | 0.44              |
| 9:V:364:THR:HG21  | 28:e:43:TRP:CH2   | 2.53                     | 0.44              |
| 9:V:400:HIS:CG    | 17:d:234:GLN:HB3  | 2.53                     | 0.44              |
| 11:X:74:ARG:HG2   | 11:X:74:ARG:NH1   | 2.33                     | 0.44              |
| 11:X:225:TRP:O    | 11:X:226:LYS:C    | 2.60                     | 0.44              |
| 11:X:339:ILE:HD11 | 11:X:345:VAL:HG11 | 1.98                     | 0.44              |
| 12:Y:11:LEU:HB3   | 12:Y:12:PRO:HD2   | 1.99                     | 0.44              |
| 12:Y:220:VAL:CB   | 12:Y:249:VAL:HG11 | 2.47                     | 0.44              |
| 12:Y:325:VAL:HG21 | 12:Y:329:PHE:HD2  | 1.82                     | 0.44              |
| 13:Z:250:TYR:O    | 13:Z:254:ASN:HB2  | 2.18                     | 0.44              |
| 13:Z:263:ALA:HB1  | 16:c:288:VAL:HG13 | 2.00                     | 0.44              |
| 14:a:296:ILE:HG21 | 14:a:307:VAL:CG2  | 2.42                     | 0.44              |
| 16:c:26:ASP:OD1   | 16:c:26:ASP:C     | 2.60                     | 0.44              |
| 16:c:279:ASP:OD1  | 16:c:279:ASP:C    | 2.60                     | 0.44              |
| 17:d:197:LEU:CD2  | 17:d:259:PHE:HB3  | 2.48                     | 0.44              |
| 18:f:44:GLU:O     | 22:A:23:ARG:NH2   | 2.51                     | 0.44              |
| 18:f:431:LYS:HA   | 19:g:171:LEU:CB   | 2.43                     | 0.44              |
| 18:f:479:LEU:HD21 | 18:f:513:GLU:CG   | 2.44                     | 0.44              |
| 18:f:726:ILE:HG21 | 18:f:762:VAL:N    | 2.33                     | 0.44              |
| 19:g:129:ILE:HG23 | 19:g:153:ALA:CB   | 2.46                     | 0.44              |
| 22:A:92:PRO:HG3   | 22:A:144:ARG:NH1  | 2.33                     | 0.44              |
| 22:A:233:THR:C    | 22:A:235:ALA:N    | 2.75                     | 0.44              |
| 23:B:250:VAL:HG23 | 23:B:252:GLY:H    | 1.83                     | 0.44              |
| 24:E:77:PRO:HD2   | 24:E:79:TYR:OH    | 2.18                     | 0.44              |
| 24:E:253:ILE:HA   | 24:E:256:THR:HG22 | 1.99                     | 0.44              |
| 24:E:304:PRO:HB2  | 24:E:309:ARG:HD2  | 1.99                     | 0.44              |
| 25:F:244:THR:HA   | 25:F:245:LYS:NZ   | 2.33                     | 0.44              |
| 27:U:353:LEU:HD11 | 27:U:373:ASN:HB2  | 1.99                     | 0.44              |
| 27:U:661:ALA:C    | 27:U:746:ILE:HD11 | 2.42                     | 0.44              |
| 1:C:214:VAL:HG11  | 1:C:219:LEU:CD2   | 2.41                     | 0.44              |
| 1:C:276:LEU:CD2   | 1:C:305:LEU:HD11  | 2.48                     | 0.44              |
| 2:D:67:ASN:ND2    | 27:U:607:VAL:O    | 2.50                     | 0.44              |
| 2:D:369:LYS:HA    | 2:D:369:LYS:CE    | 2.10                     | 0.44              |
| 3:G:98:ALA:HA     | 3:G:109:ILE:HG21  | 1.99                     | 0.44              |
| 3:G:143:ILE:HD13  | 3:G:143:ILE:N     | 2.32                     | 0.44              |
| 3:G:171:LYS:CE    | 3:G:171:LYS:CA    | 2.90                     | 0.44              |
| 4:H:74:LEU:HD13   | 4:H:134:LEU:CD2   | 2.48                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:I:119:GLN:CG    | 6:J:78:ALA:HB1    | 2.47                     | 0.44              |
| 7:L:224:TYR:CD1   | 7:L:232:PHE:HE1   | 2.36                     | 0.44              |
| 9:V:82:LEU:HD22   | 9:V:162:GLU:CG    | 2.48                     | 0.44              |
| 9:V:113:LEU:HD11  | 9:V:171:VAL:HA    | 1.99                     | 0.44              |
| 10:W:135:LYS:CB   | 10:W:138:VAL:HG12 | 2.46                     | 0.44              |
| 10:W:331:GLY:HA3  | 10:W:337:ALA:CB   | 2.34                     | 0.44              |
| 10:W:409:LEU:HD23 | 11:X:344:ARG:HH22 | 1.83                     | 0.44              |
| 11:X:192:SER:O    | 11:X:196:THR:HG22 | 2.18                     | 0.44              |
| 11:X:270:LEU:HD12 | 11:X:270:LEU:N    | 2.33                     | 0.44              |
| 11:X:318:ILE:N    | 11:X:318:ILE:HD12 | 2.32                     | 0.44              |
| 11:X:378:LEU:HD23 | 11:X:378:LEU:HA   | 1.87                     | 0.44              |
| 11:X:407:MET:CE   | 11:X:410:VAL:HG11 | 2.48                     | 0.44              |
| 12:Y:214:MET:HE3  | 12:Y:219:PHE:CD2  | 2.53                     | 0.44              |
| 13:Z:205:LEU:HD11 | 14:a:356:TRP:CD2  | 2.52                     | 0.44              |
| 14:a:122:LYS:HG3  | 14:a:126:GLY:O    | 2.17                     | 0.44              |
| 14:a:317:VAL:CG1  | 14:a:319:LEU:HD11 | 2.47                     | 0.44              |
| 14:a:364:GLU:O    | 14:a:368:GLU:HG2  | 2.18                     | 0.44              |
| 15:b:5:SER:HB2    | 15:b:64:LEU:HD11  | 2.00                     | 0.44              |
| 15:b:11:ASP:HB2   | 15:b:112:PHE:O    | 2.18                     | 0.44              |
| 15:b:51:LEU:HD23  | 15:b:71:ILE:CG2   | 2.30                     | 0.44              |
| 15:b:79:GLN:O     | 15:b:81:LYS:HG2   | 2.17                     | 0.44              |
| 15:b:86:PHE:CE1   | 15:b:140:ILE:HD11 | 2.53                     | 0.44              |
| 17:d:127:ASN:ND2  | 17:d:129:LEU:O    | 2.51                     | 0.44              |
| 17:d:341:GLU:OE1  | 17:d:341:GLU:HA   | 2.18                     | 0.44              |
| 18:f:182:GLU:N    | 18:f:183:PRO:HD2  | 2.33                     | 0.44              |
| 18:f:246:SER:HA   | 18:f:249:LEU:CD1  | 2.47                     | 0.44              |
| 18:f:799:VAL:HG21 | 18:f:821:LEU:HD23 | 1.98                     | 0.44              |
| 19:g:128:LYS:HB3  | 19:g:158:LEU:CD2  | 2.48                     | 0.44              |
| 20:u:216:GLN:OE1  | 20:u:216:GLN:O    | 2.36                     | 0.44              |
| 23:B:260:LEU:HD12 | 23:B:304:GLU:CG   | 2.47                     | 0.44              |
| 24:E:206:LYS:HB2  | 24:E:206:LYS:HE2  | 1.59                     | 0.44              |
| 24:E:303:LEU:HD12 | 24:E:303:LEU:HA   | 1.77                     | 0.44              |
| 26:K:236:GLU:O    | 26:K:239:LYS:HG2  | 2.18                     | 0.44              |
| 27:U:41:SER:O     | 27:U:42:VAL:C     | 2.61                     | 0.44              |
| 27:U:110:LYS:O    | 27:U:110:LYS:HD3  | 2.18                     | 0.44              |
| 27:U:873:PRO:CB   | 27:U:876:GLN:HG3  | 2.47                     | 0.44              |
| 27:U:878:LEU:HD12 | 27:U:882:ALA:HB1  | 1.98                     | 0.44              |
| 1:C:149:GLU:HA    | 1:C:149:GLU:OE2   | 2.18                     | 0.44              |
| 3:G:72:ILE:HG21   | 3:G:114:LEU:CD2   | 2.45                     | 0.44              |
| 3:G:80:MET:HE1    | 3:G:138:MET:CG    | 2.42                     | 0.44              |
| 3:G:191:PHE:O     | 3:G:195:VAL:HG23  | 2.18                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:H:100:VAL:HG12  | 4:H:101:TYR:CE1   | 2.53                     | 0.44              |
| 4:H:160:ALA:O     | 5:I:55:LEU:HD13   | 2.18                     | 0.44              |
| 5:I:206:LEU:HD23  | 5:I:211:VAL:HG11  | 1.99                     | 0.44              |
| 6:J:36:ARG:HG3    | 6:J:36:ARG:HH11   | 1.82                     | 0.44              |
| 6:J:198:VAL:O     | 6:J:199:VAL:C     | 2.61                     | 0.44              |
| 7:L:72:ILE:C      | 7:L:72:ILE:CD1    | 2.91                     | 0.44              |
| 7:L:81:ALA:HB2    | 7:L:130:VAL:CG2   | 2.48                     | 0.44              |
| 7:L:183:ASN:ND2   | 7:L:186:GLU:OE1   | 2.51                     | 0.44              |
| 7:L:228:ASP:C     | 7:L:231:PRO:HD2   | 2.42                     | 0.44              |
| 8:M:148:LEU:O     | 8:M:159:GLY:HA2   | 2.17                     | 0.44              |
| 9:V:114:TYR:CD1   | 9:V:132:LEU:HD12  | 2.53                     | 0.44              |
| 11:X:311:ALA:HA   | 11:X:315:ASP:CG   | 2.42                     | 0.44              |
| 14:a:118:ILE:CG1  | 14:a:122:LYS:HB3  | 2.48                     | 0.44              |
| 14:a:292:THR:HG22 | 14:a:294:GLU:N    | 2.33                     | 0.44              |
| 15:b:98:LYS:HG2   | 20:u:203:SER:HB2  | 1.99                     | 0.44              |
| 15:b:109:ILE:O    | 15:b:138:VAL:HA   | 2.18                     | 0.44              |
| 16:c:68:ARG:NE    | 16:c:208:ARG:HH12 | 2.16                     | 0.44              |
| 16:c:161:ARG:NH2  | 16:c:203:ILE:HD13 | 2.33                     | 0.44              |
| 17:d:190:GLN:O    | 17:d:193:GLY:N    | 2.51                     | 0.44              |
| 18:f:124:ASP:HB3  | 18:f:154:TRP:CZ2  | 2.52                     | 0.44              |
| 19:g:112:LEU:HD11 | 19:g:116:ILE:CG1  | 2.46                     | 0.44              |
| 20:u:238:PHE:N    | 20:u:238:PHE:CD1  | 2.86                     | 0.44              |
| 23:B:120:HIS:HD2  | 23:B:132:TYR:CZ   | 2.36                     | 0.44              |
| 23:B:225:TYR:CD2  | 23:B:334:ILE:HG21 | 2.53                     | 0.44              |
| 24:E:56:ILE:CD1   | 24:E:102:MET:HA   | 2.47                     | 0.44              |
| 24:E:153:LEU:CD1  | 24:E:191:LEU:HD23 | 2.48                     | 0.44              |
| 25:F:139:LEU:N    | 25:F:139:LEU:HD23 | 2.33                     | 0.44              |
| 26:K:190:THR:HG22 | 26:K:193:GLU:H    | 1.82                     | 0.44              |
| 27:U:31:VAL:HG22  | 27:U:38:ILE:CD1   | 2.48                     | 0.44              |
| 27:U:247:GLN:HG3  | 27:U:904:LYS:HB2  | 2.00                     | 0.44              |
| 27:U:616:ARG:HD3  | 27:U:770:TRP:CZ3  | 2.53                     | 0.44              |
| 27:U:624:PHE:CZ   | 27:U:658:ILE:HD13 | 2.52                     | 0.44              |
| 27:U:877:LEU:O    | 27:U:877:LEU:HD23 | 2.18                     | 0.44              |
| 1:C:198:LEU:HD12  | 1:C:198:LEU:O     | 2.18                     | 0.44              |
| 1:C:307:ARG:NH1   | 1:C:309:GLY:HA3   | 2.32                     | 0.44              |
| 2:D:265:ASP:OD1   | 2:D:266:GLU:N     | 2.51                     | 0.44              |
| 2:D:274:ARG:HB3   | 2:D:286:GLN:OE1   | 2.18                     | 0.44              |
| 3:G:139:ILE:HG12  | 3:G:153:LYS:HG3   | 1.99                     | 0.44              |
| 4:H:98:TYR:O      | 4:H:102:GLN:N     | 2.45                     | 0.44              |
| 4:H:158:TRP:CD1   | 4:H:161:THR:HG21  | 2.53                     | 0.44              |
| 7:L:188:VAL:HG21  | 7:L:212:ILE:HG21  | 1.99                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 9:V:96:ARG:HG2    | 9:V:97:ALA:N      | 2.32                     | 0.44              |
| 9:V:150:ARG:HA    | 9:V:154:ALA:CB    | 2.48                     | 0.44              |
| 9:V:313:LEU:HD21  | 9:V:329:HIS:CE1   | 2.50                     | 0.44              |
| 11:X:157:LEU:HA   | 11:X:157:LEU:HD23 | 1.76                     | 0.44              |
| 11:X:349:HIS:NE2  | 11:X:353:LEU:CD1  | 2.81                     | 0.44              |
| 11:X:390:GLU:O    | 11:X:390:GLU:CG   | 2.66                     | 0.44              |
| 13:Z:70:LEU:HD23  | 13:Z:70:LEU:C     | 2.43                     | 0.44              |
| 13:Z:84:LYS:HD3   | 25:F:79:LYS:HE3   | 2.00                     | 0.44              |
| 13:Z:109:ASN:HD22 | 13:Z:140:SER:HB2  | 1.83                     | 0.44              |
| 14:a:54:ASP:CB    | 14:a:86:GLN:HG3   | 2.48                     | 0.44              |
| 14:a:54:ASP:HB3   | 14:a:86:GLN:HG3   | 1.99                     | 0.44              |
| 14:a:112:ILE:CA   | 14:a:115:LYS:HG3  | 2.47                     | 0.44              |
| 14:a:243:GLY:HA3  | 14:a:279:GLU:HG3  | 1.98                     | 0.44              |
| 14:a:325:ASP:OD1  | 14:a:325:ASP:C    | 2.60                     | 0.44              |
| 18:f:440:ILE:O    | 18:f:443:GLY:N    | 2.49                     | 0.44              |
| 18:f:533:ASP:O    | 18:f:536:SER:OG   | 2.33                     | 0.44              |
| 19:g:110:ARG:O    | 19:g:114:SER:OG   | 2.32                     | 0.44              |
| 19:g:130:VAL:CG1  | 19:g:135:GLN:HE21 | 2.31                     | 0.44              |
| 20:u:233:LEU:HD13 | 20:u:238:PHE:HE2  | 1.82                     | 0.44              |
| 22:A:376:LEU:C    | 22:A:378:PRO:HD3  | 2.43                     | 0.44              |
| 23:B:77:GLU:HG2   | 23:B:81:ASN:ND2   | 2.33                     | 0.44              |
| 23:B:123:VAL:HG21 | 23:B:152:LEU:CD2  | 2.47                     | 0.44              |
| 23:B:371:ARG:HG3  | 23:B:371:ARG:NH1  | 2.33                     | 0.44              |
| 24:E:36:LEU:O     | 24:E:39:GLN:HG3   | 2.18                     | 0.44              |
| 24:E:56:ILE:H     | 24:E:56:ILE:HG13  | 1.68                     | 0.44              |
| 24:E:139:SER:O    | 24:E:143:ARG:HB2  | 2.18                     | 0.44              |
| 25:F:133:PHE:CD1  | 25:F:133:PHE:C    | 2.95                     | 0.44              |
| 27:U:117:ASP:CB   | 27:U:118:LEU:HD22 | 2.48                     | 0.44              |
| 27:U:536:ALA:HB1  | 27:U:578:LEU:CD2  | 2.17                     | 0.44              |
| 27:U:624:PHE:CE1  | 27:U:658:ILE:HD13 | 2.53                     | 0.44              |
| 1:C:63:LEU:O      | 1:C:67:GLN:HG2    | 2.18                     | 0.43              |
| 2:D:116:LEU:HB3   | 2:D:119:ILE:HD11  | 1.99                     | 0.43              |
| 5:I:44:LEU:C      | 5:I:44:LEU:HD12   | 2.42                     | 0.43              |
| 7:L:63:ILE:C      | 7:L:64:LEU:HD23   | 2.42                     | 0.43              |
| 7:L:227:ASP:OD1   | 7:L:227:ASP:N     | 2.51                     | 0.43              |
| 9:V:90:GLU:O      | 9:V:90:GLU:HG2    | 2.17                     | 0.43              |
| 9:V:198:GLN:HB2   | 9:V:203:LEU:HD22  | 1.98                     | 0.43              |
| 10:W:28:LEU:HB2   | 10:W:29:PRO:HD3   | 2.00                     | 0.43              |
| 12:Y:167:LEU:HD12 | 12:Y:170:GLU:OE1  | 2.18                     | 0.43              |
| 12:Y:263:LEU:O    | 12:Y:306:GLN:NE2  | 2.51                     | 0.43              |
| 12:Y:304:TYR:CE1  | 12:Y:330:ILE:HD11 | 2.53                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 13:Z:16:LEU:HD23  | 13:Z:162:ILE:CD1  | 2.48                     | 0.43              |
| 14:a:360:VAL:HG23 | 16:c:308:VAL:CG2  | 2.47                     | 0.43              |
| 16:c:219:ASN:HA   | 16:c:222:LYS:HB2  | 1.99                     | 0.43              |
| 17:d:129:LEU:HD11 | 27:U:8:ILE:CD1    | 2.48                     | 0.43              |
| 17:d:197:LEU:HD22 | 17:d:259:PHE:CB   | 2.48                     | 0.43              |
| 18:f:229:VAL:HG13 | 18:f:230:CYS:N    | 2.32                     | 0.43              |
| 18:f:237:VAL:HG12 | 18:f:248:LEU:CB   | 2.47                     | 0.43              |
| 18:f:378:ASN:O    | 18:f:417:ILE:HD11 | 2.18                     | 0.43              |
| 18:f:460:ASP:HB3  | 19:g:133:LYS:HD2  | 2.00                     | 0.43              |
| 18:f:479:LEU:HD12 | 18:f:514:VAL:HG22 | 2.00                     | 0.43              |
| 18:f:538:ILE:HG21 | 18:f:562:LEU:HA   | 2.00                     | 0.43              |
| 18:f:716:ASP:HB3  | 18:f:721:VAL:HG13 | 2.00                     | 0.43              |
| 18:f:723:TYR:HB3  | 18:f:761:MET:CE   | 2.48                     | 0.43              |
| 18:f:802:SER:HB2  | 18:f:809:ILE:HG21 | 2.00                     | 0.43              |
| 18:f:832:THR:HG23 | 18:f:870:THR:CG2  | 2.45                     | 0.43              |
| 19:g:161:SER:O    | 19:g:165:ALA:CB   | 2.66                     | 0.43              |
| 22:A:219:GLY:O    | 22:A:381:THR:HB   | 2.18                     | 0.43              |
| 23:B:232:LYS:HB2  | 23:B:232:LYS:NZ   | 2.33                     | 0.43              |
| 25:F:203:VAL:O    | 25:F:207:ASN:HB2  | 2.18                     | 0.43              |
| 25:F:289:ASP:CG   | 25:F:332:THR:HG23 | 2.43                     | 0.43              |
| 26:K:220:VAL:CA   | 26:K:228:MET:HE1  | 2.47                     | 0.43              |
| 27:U:92:ASP:HA    | 27:U:97:VAL:HG11  | 2.00                     | 0.43              |
| 27:U:265:ILE:HG13 | 27:U:265:ILE:H    | 1.58                     | 0.43              |
| 27:U:420:LEU:HD12 | 27:U:420:LEU:O    | 2.18                     | 0.43              |
| 27:U:587:ALA:CB   | 27:U:624:PHE:HD2  | 2.28                     | 0.43              |
| 27:U:797:MET:HB3  | 27:U:925:VAL:O    | 2.17                     | 0.43              |
| 27:U:869:LYS:O    | 27:U:872:GLU:CG   | 2.66                     | 0.43              |
| 27:U:895:PRO:CG   | 27:U:902:PRO:HD3  | 2.48                     | 0.43              |
| 1:C:301:LEU:HD13  | 1:C:305:LEU:HD23  | 1.98                     | 0.43              |
| 4:H:34:PRO:CD     | 4:H:49:GLU:OE1    | 2.66                     | 0.43              |
| 5:I:88:ASN:OD1    | 5:I:88:ASN:C      | 2.61                     | 0.43              |
| 9:V:121:PHE:CZ    | 9:V:159:LEU:HD12  | 2.52                     | 0.43              |
| 9:V:175:MET:CG    | 9:V:184:ALA:HB2   | 2.47                     | 0.43              |
| 9:V:186:LYS:N     | 9:V:186:LYS:HD3   | 2.33                     | 0.43              |
| 9:V:334:VAL:HG21  | 9:V:391:THR:HG21  | 2.00                     | 0.43              |
| 10:W:413:ILE:O    | 10:W:414:ASN:C    | 2.61                     | 0.43              |
| 11:X:394:ASP:CG   | 12:Y:362:LYS:HE2  | 2.44                     | 0.43              |
| 13:Z:75:LEU:HD23  | 13:Z:75:LEU:C     | 2.43                     | 0.43              |
| 13:Z:224:HIS:H    | 13:Z:227:ILE:HG21 | 1.83                     | 0.43              |
| 14:a:54:ASP:HB3   | 14:a:86:GLN:CG    | 2.48                     | 0.43              |
| 15:b:79:GLN:HG3   | 15:b:81:LYS:CG    | 2.47                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 16:c:293:THR:O    | 16:c:297:VAL:HG23 | 2.18                     | 0.43              |
| 17:d:262:ILE:HG13 | 17:d:262:ILE:H    | 1.63                     | 0.43              |
| 18:f:659:LEU:O    | 18:f:659:LEU:HD12 | 2.19                     | 0.43              |
| 18:f:831:VAL:HG22 | 18:f:871:PRO:CB   | 2.20                     | 0.43              |
| 19:g:105:LEU:HD13 | 19:g:142:LEU:CD2  | 2.48                     | 0.43              |
| 19:g:109:GLY:C    | 19:g:112:LEU:H    | 2.27                     | 0.43              |
| 19:g:126:TYR:HA   | 19:g:160:GLN:C    | 2.42                     | 0.43              |
| 20:u:137:CYS:C    | 20:u:138:LEU:HD23 | 2.43                     | 0.43              |
| 24:E:367:PHE:HA   | 24:E:370:ALA:HB3  | 1.98                     | 0.43              |
| 25:F:167:GLU:OE1  | 25:F:167:GLU:HA   | 2.18                     | 0.43              |
| 25:F:188:ILE:HD11 | 25:F:235:LEU:HG   | 2.00                     | 0.43              |
| 25:F:233:LYS:N    | 29:F:501:ATP:O2B  | 2.51                     | 0.43              |
| 27:U:8:ILE:O      | 27:U:11:LEU:N     | 2.51                     | 0.43              |
| 27:U:35:TRP:CD1   | 27:U:35:TRP:H     | 2.36                     | 0.43              |
| 27:U:804:SER:OG   | 27:U:805:ASN:N    | 2.51                     | 0.43              |
| 1:C:306:LEU:O     | 1:C:314:LYS:HE2   | 2.18                     | 0.43              |
| 1:C:364:THR:O     | 1:C:368:MET:HG2   | 2.17                     | 0.43              |
| 2:D:238:LYS:NZ    | 24:E:207:TYR:HB2  | 2.34                     | 0.43              |
| 2:D:303:VAL:O     | 2:D:303:VAL:CG1   | 2.65                     | 0.43              |
| 2:D:360:LEU:HD23  | 2:D:360:LEU:HA    | 1.75                     | 0.43              |
| 2:D:377:SER:O     | 2:D:378:ILE:C     | 2.61                     | 0.43              |
| 3:G:58:ASP:OD1    | 3:G:59:LYS:N      | 2.51                     | 0.43              |
| 4:H:174:LEU:C     | 4:H:176:LYS:N     | 2.76                     | 0.43              |
| 4:H:179:ASN:H     | 4:H:182:LEU:HD21  | 1.82                     | 0.43              |
| 5:I:205:LYS:O     | 5:I:206:LEU:C     | 2.61                     | 0.43              |
| 7:L:56:LEU:HD12   | 26:K:185:TYR:CD2  | 2.52                     | 0.43              |
| 7:L:79:ALA:HB2    | 26:K:121:LEU:HD22 | 1.98                     | 0.43              |
| 9:V:324:PHE:CE1   | 9:V:328:VAL:HG21  | 2.54                     | 0.43              |
| 10:W:19:ASP:HA    | 10:W:59:ASP:OD2   | 2.17                     | 0.43              |
| 10:W:357:ARG:HD3  | 10:W:357:ARG:HA   | 1.70                     | 0.43              |
| 11:X:115:GLU:O    | 11:X:118:LYS:HB2  | 2.18                     | 0.43              |
| 11:X:334:ASN:ND2  | 11:X:354:ILE:HD13 | 2.32                     | 0.43              |
| 12:Y:169:GLU:OE1  | 12:Y:169:GLU:C    | 2.62                     | 0.43              |
| 12:Y:293:ARG:HG2  | 12:Y:293:ARG:NH1  | 2.32                     | 0.43              |
| 12:Y:387:ILE:CG2  | 13:Z:275:LEU:HD23 | 2.47                     | 0.43              |
| 13:Z:38:VAL:HG21  | 13:Z:75:LEU:CD1   | 2.49                     | 0.43              |
| 13:Z:67:VAL:HG11  | 15:b:91:ARG:HB2   | 1.99                     | 0.43              |
| 14:a:9:GLN:O      | 14:a:12:GLN:HB3   | 2.18                     | 0.43              |
| 14:a:59:LEU:HD12  | 14:a:59:LEU:HA    | 1.88                     | 0.43              |
| 14:a:96:PHE:O     | 14:a:100:THR:HG23 | 2.18                     | 0.43              |
| 14:a:297:ALA:HB1  | 14:a:302:ILE:O    | 2.19                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 17:d:243:LYS:O    | 17:d:246:LEU:HG   | 2.19                     | 0.43              |
| 18:f:388:ASP:CB   | 18:f:417:ILE:HD13 | 2.48                     | 0.43              |
| 18:f:701:ASN:ND2  | 18:f:703:ARG:HH12 | 2.04                     | 0.43              |
| 18:f:893:ILE:HD12 | 18:f:893:ILE:N    | 2.34                     | 0.43              |
| 19:g:142:LEU:HA   | 19:g:145:GLN:OE1  | 2.18                     | 0.43              |
| 19:g:165:ALA:C    | 19:g:167:LYS:H    | 2.22                     | 0.43              |
| 22:A:140:VAL:HG21 | 22:A:149:ILE:HD13 | 1.99                     | 0.43              |
| 22:A:161:VAL:HG12 | 22:A:263:MET:SD   | 2.58                     | 0.43              |
| 22:A:170:PRO:CG   | 22:A:230:ALA:HB3  | 2.49                     | 0.43              |
| 23:B:380:LEU:H    | 23:B:380:LEU:HD12 | 1.83                     | 0.43              |
| 24:E:36:LEU:HB3   | 25:F:69:MET:HG2   | 2.01                     | 0.43              |
| 25:F:201:ALA:C    | 25:F:202:ILE:HG12 | 2.43                     | 0.43              |
| 25:F:413:THR:OG1  | 25:F:414:GLU:N    | 2.51                     | 0.43              |
| 25:F:425:LEU:CD1  | 25:F:432:LYS:HB2  | 2.48                     | 0.43              |
| 25:F:428:GLN:O    | 25:F:429:ALA:HB3  | 2.19                     | 0.43              |
| 26:K:91:LYS:HE2   | 26:K:95:GLU:HG3   | 2.00                     | 0.43              |
| 27:U:38:ILE:H     | 27:U:38:ILE:HG13  | 1.56                     | 0.43              |
| 27:U:812:ALA:O    | 27:U:813:TYR:C    | 2.62                     | 0.43              |
| 1:C:274:LEU:HD12  | 23:B:289:ALA:HB2  | 2.00                     | 0.43              |
| 1:C:289:ILE:HD13  | 1:C:289:ILE:N     | 2.33                     | 0.43              |
| 2:D:235:PHE:O     | 2:D:288:ILE:HD11  | 2.19                     | 0.43              |
| 2:D:337:ASP:OD1   | 2:D:338:ARG:N     | 2.52                     | 0.43              |
| 4:H:13:PHE:HE2    | 5:I:129:PRO:O     | 2.02                     | 0.43              |
| 4:H:100:VAL:HG12  | 4:H:101:TYR:HD1   | 1.83                     | 0.43              |
| 5:I:90:LEU:HD11   | 5:I:136:TYR:CE2   | 2.34                     | 0.43              |
| 5:I:99:LEU:C      | 5:I:99:LEU:HD23   | 2.43                     | 0.43              |
| 5:I:139:TRP:CD1   | 5:I:218:ARG:HG3   | 2.54                     | 0.43              |
| 5:I:192:LEU:O     | 5:I:196:VAL:HG12  | 2.18                     | 0.43              |
| 6:J:7:ILE:HD11    | 6:J:126:PRO:HD3   | 2.00                     | 0.43              |
| 6:J:98:VAL:HG12   | 6:J:100:ASP:OD1   | 2.19                     | 0.43              |
| 7:L:38:LEU:HD23   | 7:L:38:LEU:O      | 2.19                     | 0.43              |
| 7:L:125:ARG:HH22  | 26:K:125:GLU:CG   | 2.18                     | 0.43              |
| 8:M:63:ASN:HB2    | 8:M:81:LEU:HD23   | 2.00                     | 0.43              |
| 8:M:66:LEU:HD12   | 8:M:66:LEU:HA     | 1.46                     | 0.43              |
| 8:M:216:VAL:CG1   | 8:M:224:HIS:HA    | 2.49                     | 0.43              |
| 9:V:175:MET:HE1   | 9:V:180:ARG:HH21  | 1.82                     | 0.43              |
| 9:V:212:TYR:CD2   | 9:V:213:TYR:CD1   | 3.06                     | 0.43              |
| 9:V:248:ALA:CB    | 9:V:276:PHE:HE1   | 2.31                     | 0.43              |
| 9:V:258:TYR:HD2   | 9:V:267:ALA:CA    | 2.32                     | 0.43              |
| 9:V:287:ARG:NH2   | 28:e:21:GLU:CG    | 2.81                     | 0.43              |
| 9:V:338:LEU:HG    | 9:V:398:LEU:HD13  | 2.01                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 9:V:348:PHE:H     | 9:V:348:PHE:HD1   | 1.67                     | 0.43              |
| 9:V:353:LEU:HA    | 9:V:356:SER:OG    | 2.19                     | 0.43              |
| 9:V:394:LEU:HD23  | 9:V:397:ARG:NH1   | 2.33                     | 0.43              |
| 10:W:108:CYS:CB   | 10:W:128:LEU:HD11 | 2.38                     | 0.43              |
| 10:W:381:LEU:HD23 | 10:W:381:LEU:N    | 2.33                     | 0.43              |
| 11:X:76:PHE:CE2   | 11:X:80:ILE:HD13  | 2.53                     | 0.43              |
| 11:X:232:PHE:CE2  | 11:X:253:TYR:HB3  | 2.54                     | 0.43              |
| 12:Y:101:ARG:HA   | 12:Y:101:ARG:NH1  | 2.34                     | 0.43              |
| 12:Y:152:MET:HA   | 12:Y:152:MET:CE   | 2.43                     | 0.43              |
| 13:Z:8:LYS:HB2    | 13:Z:8:LYS:HE2    | 1.76                     | 0.43              |
| 14:a:70:ARG:HH12  | 15:b:17:ARG:NE    | 2.16                     | 0.43              |
| 14:a:80:ILE:HG21  | 14:a:96:PHE:HZ    | 1.82                     | 0.43              |
| 14:a:226:ARG:HH22 | 14:a:233:LEU:HB3  | 1.83                     | 0.43              |
| 14:a:269:LEU:HA   | 14:a:272:ILE:HG22 | 2.00                     | 0.43              |
| 15:b:37:CYS:SG    | 15:b:38:HIS:N     | 2.91                     | 0.43              |
| 17:d:238:GLU:O    | 17:d:238:GLU:CG   | 2.67                     | 0.43              |
| 17:d:347:GLU:OE1  | 17:d:347:GLU:HA   | 2.18                     | 0.43              |
| 18:f:233:LEU:CB   | 18:f:252:ALA:HB2  | 2.48                     | 0.43              |
| 18:f:692:LEU:HB3  | 18:f:800:LEU:CD1  | 2.45                     | 0.43              |
| 18:f:723:TYR:C    | 18:f:761:MET:HE1  | 2.43                     | 0.43              |
| 18:f:731:MET:O    | 18:f:734:SER:OG   | 2.19                     | 0.43              |
| 19:g:83:ALA:HB1   | 19:g:150:ASN:CG   | 2.43                     | 0.43              |
| 22:A:139:ARG:CZ   | 22:A:156:LYS:HG3  | 2.49                     | 0.43              |
| 23:B:138:PHE:HE2  | 23:B:160:ILE:HG23 | 1.83                     | 0.43              |
| 23:B:144:LEU:HD12 | 23:B:144:LEU:HA   | 1.72                     | 0.43              |
| 23:B:162:VAL:HG13 | 23:B:162:VAL:O    | 2.19                     | 0.43              |
| 24:E:35:GLU:O     | 24:E:38:LYS:HD2   | 2.19                     | 0.43              |
| 24:E:38:LYS:H     | 24:E:38:LYS:HG3   | 1.41                     | 0.43              |
| 24:E:49:ALA:HB1   | 25:F:138:GLY:HA2  | 2.01                     | 0.43              |
| 24:E:145:LEU:CD1  | 24:E:172:LEU:HD21 | 2.48                     | 0.43              |
| 24:E:172:LEU:CD1  | 24:E:276:ILE:HG23 | 2.49                     | 0.43              |
| 26:K:28:ILE:HG13  | 26:K:158:PRO:CG   | 2.43                     | 0.43              |
| 26:K:34:GLY:O     | 26:K:53:ARG:NH2   | 2.51                     | 0.43              |
| 26:K:88:LEU:HD22  | 26:K:116:VAL:CG1  | 2.39                     | 0.43              |
| 27:U:177:LEU:HD11 | 27:U:205:TYR:CE1  | 2.52                     | 0.43              |
| 27:U:538:GLU:O    | 27:U:538:GLU:CG   | 2.64                     | 0.43              |
| 27:U:617:ALA:O    | 27:U:621:SER:HB2  | 2.17                     | 0.43              |
| 27:U:873:PRO:O    | 27:U:874:ASN:CB   | 2.66                     | 0.43              |
| 27:U:900:TYR:HB3  | 27:U:914:LEU:CD2  | 2.40                     | 0.43              |
| 1:C:311:ILE:HD13  | 1:C:311:ILE:HA    | 1.79                     | 0.43              |
| 2:D:100:THR:C     | 2:D:115:ILE:HG13  | 2.43                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:D:220:ALA:O     | 2:D:223:THR:HG22  | 2.19                     | 0.43              |
| 3:G:17:SER:HB2    | 3:G:18:PRO:HD2    | 1.99                     | 0.43              |
| 3:G:67:THR:HA     | 3:G:216:GLU:OE2   | 2.18                     | 0.43              |
| 4:H:72:ILE:HA     | 4:H:137:CYS:O     | 2.19                     | 0.43              |
| 4:H:119:GLN:CG    | 5:I:81:SER:HB2    | 2.49                     | 0.43              |
| 5:I:45:LEU:HD22   | 5:I:65:ILE:HD11   | 1.98                     | 0.43              |
| 5:I:211:VAL:CG2   | 5:I:212:GLU:N     | 2.82                     | 0.43              |
| 6:J:51:ALA:HB3    | 6:J:54:GLN:CG     | 2.46                     | 0.43              |
| 7:L:50:LYS:N      | 7:L:209:ASN:O     | 2.51                     | 0.43              |
| 7:L:211:SER:HB2   | 7:L:225:ASP:OD1   | 2.18                     | 0.43              |
| 8:M:123:THR:O     | 8:M:123:THR:OG1   | 2.36                     | 0.43              |
| 8:M:169:ARG:H     | 8:M:169:ARG:HG3   | 1.60                     | 0.43              |
| 9:V:236:ARG:NH1   | 27:U:70:HIS:HA    | 2.33                     | 0.43              |
| 9:V:400:HIS:ND1   | 17:d:234:GLN:HB3  | 2.34                     | 0.43              |
| 9:V:428:LEU:HD13  | 9:V:434:ALA:HA    | 2.01                     | 0.43              |
| 9:V:447:ILE:CG2   | 9:V:448:GLU:H     | 2.30                     | 0.43              |
| 10:W:166:LEU:HD23 | 10:W:192:LEU:HD11 | 2.00                     | 0.43              |
| 10:W:347:GLY:HA2  | 10:W:350:ARG:HD2  | 2.01                     | 0.43              |
| 11:X:393:VAL:O    | 11:X:394:ASP:OD1  | 2.36                     | 0.43              |
| 12:Y:41:LEU:O     | 12:Y:41:LEU:HD12  | 2.18                     | 0.43              |
| 12:Y:282:MET:HE3  | 12:Y:295:TYR:CG   | 2.53                     | 0.43              |
| 13:Z:124:ILE:HA   | 13:Z:134:PRO:O    | 2.18                     | 0.43              |
| 14:a:54:ASP:O     | 14:a:58:LYS:CB    | 2.66                     | 0.43              |
| 14:a:57:ILE:HG13  | 14:a:61:GLU:HG2   | 2.01                     | 0.43              |
| 14:a:61:GLU:O     | 14:a:65:SER:HB3   | 2.18                     | 0.43              |
| 14:a:115:LYS:HD2  | 14:a:137:ASP:OD1  | 2.19                     | 0.43              |
| 14:a:357:CYS:O    | 14:a:360:VAL:HG12 | 2.19                     | 0.43              |
| 15:b:63:THR:HG22  | 15:b:64:LEU:N     | 2.34                     | 0.43              |
| 15:b:171:VAL:HG11 | 15:b:187:PRO:HG3  | 1.99                     | 0.43              |
| 16:c:168:MET:HE1  | 16:c:169:VAL:CG1  | 2.49                     | 0.43              |
| 17:d:193:GLY:HA3  | 17:d:225:TYR:HB3  | 2.00                     | 0.43              |
| 17:d:349:ILE:HD13 | 17:d:349:ILE:N    | 2.34                     | 0.43              |
| 18:f:185:LEU:CD2  | 18:f:189:LYS:HE2  | 2.48                     | 0.43              |
| 20:u:215:THR:HG21 | 20:u:238:PHE:CE1  | 2.53                     | 0.43              |
| 22:A:94:GLN:HG2   | 22:A:115:VAL:HG13 | 2.00                     | 0.43              |
| 22:A:191:VAL:HG13 | 22:A:271:LEU:HD11 | 2.00                     | 0.43              |
| 22:A:333:ARG:HH21 | 22:A:336:ARG:NH1  | 2.16                     | 0.43              |
| 23:B:52:VAL:HG11  | 23:B:65:LEU:HD21  | 1.99                     | 0.43              |
| 23:B:329:MET:SD   | 23:B:347:ILE:HD11 | 2.58                     | 0.43              |
| 24:E:93:LYS:O     | 24:E:94:PRO:C     | 2.60                     | 0.43              |
| 24:E:168:LYS:HA   | 24:E:274:LYS:CE   | 2.48                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 24:E:270:LEU:O    | 24:E:271:HIS:CG   | 2.71                     | 0.43              |
| 24:E:309:ARG:NH2  | 24:E:332:VAL:O    | 2.51                     | 0.43              |
| 25:F:90:VAL:CG1   | 25:F:90:VAL:O     | 2.67                     | 0.43              |
| 26:K:199:LEU:HD12 | 26:K:210:LEU:HD21 | 2.00                     | 0.43              |
| 27:U:236:LEU:HD23 | 27:U:245:ALA:HA   | 1.99                     | 0.43              |
| 27:U:257:SER:O    | 27:U:261:LEU:HD12 | 2.18                     | 0.43              |
| 27:U:616:ARG:CD   | 27:U:770:TRP:CZ3  | 3.02                     | 0.43              |
| 1:C:234:LEU:HD12  | 1:C:237:MET:CE    | 2.49                     | 0.43              |
| 2:D:194:ILE:O     | 2:D:194:ILE:HG22  | 2.19                     | 0.43              |
| 2:D:377:SER:C     | 2:D:379:CYS:H     | 2.25                     | 0.43              |
| 2:D:378:ILE:HG13  | 2:D:406:VAL:HB    | 1.98                     | 0.43              |
| 3:G:22:LEU:HD23   | 3:G:22:LEU:HA     | 1.85                     | 0.43              |
| 3:G:54:LYS:HE2    | 3:G:56:VAL:HG21   | 2.01                     | 0.43              |
| 4:H:34:PRO:HD2    | 4:H:49:GLU:OE1    | 2.19                     | 0.43              |
| 6:J:34:GLY:HA3    | 6:J:132:LEU:HD13  | 2.00                     | 0.43              |
| 6:J:93:SER:O      | 6:J:97:THR:HG23   | 2.19                     | 0.43              |
| 8:M:44:GLY:HA3    | 8:M:216:VAL:O     | 2.19                     | 0.43              |
| 9:V:102:PRO:O     | 9:V:106:ARG:NH2   | 2.51                     | 0.43              |
| 9:V:212:TYR:OH    | 28:e:21:GLU:OE2   | 2.25                     | 0.43              |
| 10:W:60:MET:N     | 10:W:97:LEU:HD12  | 2.34                     | 0.43              |
| 10:W:88:MET:HE1   | 10:W:130:MET:SD   | 2.58                     | 0.43              |
| 10:W:346:GLU:HB2  | 10:W:350:ARG:CZ   | 2.48                     | 0.43              |
| 10:W:392:PHE:O    | 10:W:392:PHE:HD1  | 2.01                     | 0.43              |
| 11:X:118:LYS:HB3  | 11:X:118:LYS:HE3  | 1.89                     | 0.43              |
| 11:X:407:MET:HA   | 11:X:407:MET:CE   | 2.35                     | 0.43              |
| 12:Y:82:LYS:HD2   | 12:Y:82:LYS:O     | 2.18                     | 0.43              |
| 13:Z:28:LYS:HB3   | 13:Z:28:LYS:HE2   | 1.72                     | 0.43              |
| 15:b:6:THR:HB     | 15:b:49:VAL:HG12  | 2.00                     | 0.43              |
| 15:b:103:LYS:HB2  | 20:u:134:GLY:O    | 2.18                     | 0.43              |
| 16:c:121:TRP:HZ3  | 16:c:123:SER:OG   | 2.01                     | 0.43              |
| 17:d:127:ASN:ND2  | 17:d:136:LEU:HD21 | 2.34                     | 0.43              |
| 17:d:129:LEU:HB3  | 17:d:130:PRO:CD   | 2.41                     | 0.43              |
| 17:d:130:PRO:HD3  | 17:d:177:ASP:OD2  | 2.17                     | 0.43              |
| 17:d:165:GLU:HG2  | 17:d:198:PHE:CZ   | 2.54                     | 0.43              |
| 17:d:300:THR:HA   | 17:d:303:ALA:CB   | 2.34                     | 0.43              |
| 18:f:124:ASP:CG   | 18:f:147:SER:HB3  | 2.44                     | 0.43              |
| 18:f:446:LEU:O    | 18:f:450:ILE:HB   | 2.19                     | 0.43              |
| 18:f:833:PHE:HA   | 18:f:840:LEU:N    | 2.32                     | 0.43              |
| 18:f:846:VAL:HB   | 18:f:868:HIS:CD2  | 2.53                     | 0.43              |
| 19:g:113:ARG:O    | 19:g:124:GLU:HA   | 2.19                     | 0.43              |
| 19:g:127:ILE:O    | 19:g:127:ILE:HG13 | 2.18                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 20:u:221:THR:HG22 | 20:u:224:ASP:OD2  | 2.18                     | 0.43              |
| 22:A:115:VAL:HB   | 22:A:118:PHE:HB3  | 2.00                     | 0.43              |
| 22:A:384:GLU:OE1  | 22:A:417:ILE:HD13 | 2.19                     | 0.43              |
| 23:B:187:ILE:HG22 | 23:B:234:LEU:HD21 | 1.99                     | 0.43              |
| 23:B:294:ARG:HG3  | 23:B:294:ARG:HH11 | 1.83                     | 0.43              |
| 24:E:363:VAL:HG13 | 24:E:365:GLU:HB2  | 1.99                     | 0.43              |
| 27:U:347:ASN:CB   | 27:U:813:TYR:HE2  | 2.27                     | 0.43              |
| 27:U:736:ILE:HD13 | 27:U:783:TYR:OH   | 2.18                     | 0.43              |
| 1:C:43:ARG:HD3    | 9:V:498:PRO:CA    | 2.48                     | 0.43              |
| 1:C:46:GLN:OE1    | 27:U:639:LEU:HB2  | 2.19                     | 0.43              |
| 1:C:165:ILE:HG21  | 1:C:203:VAL:HG11  | 2.00                     | 0.43              |
| 1:C:338:LEU:O     | 12:Y:174:TRP:HB3  | 2.19                     | 0.43              |
| 2:D:45:LYS:CG     | 27:U:187:LEU:HD13 | 2.48                     | 0.43              |
| 2:D:391:ARG:NH2   | 2:D:398:ASP:OD2   | 2.52                     | 0.43              |
| 3:G:52:THR:CG2    | 3:G:216:GLU:HB2   | 2.49                     | 0.43              |
| 3:G:240:VAL:HG22  | 10:W:94:ARG:HD3   | 2.01                     | 0.43              |
| 6:J:102:VAL:HG13  | 6:J:106:TYR:CD2   | 2.53                     | 0.43              |
| 6:J:108:THR:OG1   | 6:J:133:ILE:HG21  | 2.19                     | 0.43              |
| 6:J:118:TYR:CD2   | 6:J:127:PHE:HE2   | 2.35                     | 0.43              |
| 7:L:56:LEU:HD12   | 26:K:167:ALA:HB3  | 2.01                     | 0.43              |
| 7:L:121:GLN:HG3   | 8:M:129:ARG:NH2   | 2.34                     | 0.43              |
| 7:L:125:ARG:CZ    | 26:K:125:GLU:HA   | 2.49                     | 0.43              |
| 9:V:192:MET:CE    | 9:V:214:HIS:HB2   | 2.46                     | 0.43              |
| 9:V:324:PHE:CD2   | 28:e:19:PHE:HE2   | 2.35                     | 0.43              |
| 10:W:102:ALA:C    | 10:W:106:GLN:NE2  | 2.77                     | 0.43              |
| 10:W:230:MET:HE1  | 10:W:233:LEU:CG   | 2.48                     | 0.43              |
| 11:X:68:GLY:O     | 11:X:71:LYS:HG3   | 2.19                     | 0.43              |
| 11:X:225:TRP:HA   | 11:X:228:ALA:HB3  | 2.00                     | 0.43              |
| 11:X:244:SER:HG   | 11:X:246:LYS:NZ   | 2.13                     | 0.43              |
| 12:Y:16:ASP:HB3   | 12:Y:19:ILE:HD12  | 1.99                     | 0.43              |
| 14:a:153:SER:OG   | 14:a:157:ASP:OD2  | 2.37                     | 0.43              |
| 14:a:221:VAL:CB   | 14:a:225:LEU:HD12 | 2.49                     | 0.43              |
| 14:a:247:ARG:O    | 14:a:251:LEU:HD13 | 2.18                     | 0.43              |
| 15:b:7:MET:CE     | 15:b:7:MET:HA     | 2.49                     | 0.43              |
| 17:d:295:THR:HB   | 17:d:298:LYS:CG   | 2.32                     | 0.43              |
| 18:f:304:PHE:HE1  | 18:f:321:MET:C    | 2.27                     | 0.43              |
| 18:f:446:LEU:CD2  | 18:f:483:PHE:HB3  | 2.48                     | 0.43              |
| 18:f:720:GLU:CD   | 18:f:806:VAL:HG22 | 2.44                     | 0.43              |
| 18:f:785:ARG:NH2  | 18:f:877:GLY:H    | 2.15                     | 0.43              |
| 19:g:137:GLN:O    | 19:g:145:GLN:NE2  | 2.46                     | 0.43              |
| 22:A:190:VAL:HG21 | 22:A:209:PRO:HB2  | 1.99                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:A:190:VAL:HG23 | 22:A:339:ARG:HE   | 1.82                     | 0.43              |
| 22:A:300:LEU:HA   | 22:A:300:LEU:HD23 | 1.84                     | 0.43              |
| 22:A:433:ASN:O    | 26:K:66:LYS:HD3   | 2.18                     | 0.43              |
| 23:B:98:LYS:HA    | 23:B:98:LYS:HD3   | 1.87                     | 0.43              |
| 23:B:401:GLU:HB3  | 23:B:422:SER:OG   | 2.19                     | 0.43              |
| 25:F:134:LEU:HG   | 25:F:158:TYR:O    | 2.19                     | 0.43              |
| 25:F:265:ALA:O    | 25:F:269:ARG:HG2  | 2.19                     | 0.43              |
| 27:U:655:ALA:O    | 27:U:659:CYS:CB   | 2.66                     | 0.43              |
| 27:U:764:LEU:HD12 | 27:U:764:LEU:O    | 2.17                     | 0.43              |
| 27:U:809:SER:HA   | 27:U:872:GLU:OE1  | 2.17                     | 0.43              |
| 2:D:89:ILE:HD11   | 24:E:80:VAL:CG2   | 2.48                     | 0.43              |
| 2:D:103:VAL:HG11  | 2:D:132:LEU:HD22  | 1.98                     | 0.43              |
| 2:D:282:ASP:CA    | 2:D:285:VAL:HG12  | 2.46                     | 0.43              |
| 2:D:345:PHE:CD2   | 2:D:364:VAL:HG12  | 2.53                     | 0.43              |
| 4:H:157:ALA:O     | 5:I:57:ASP:HB3    | 2.17                     | 0.43              |
| 5:I:97:TYR:CD1    | 5:I:105:ILE:HA    | 2.54                     | 0.43              |
| 5:I:111:VAL:HG21  | 5:I:148:TYR:HD2   | 1.83                     | 0.43              |
| 5:I:134:LEU:HD23  | 5:I:150:SER:HB3   | 1.99                     | 0.43              |
| 8:M:69:VAL:CG1    | 8:M:111:LEU:HD21  | 2.43                     | 0.43              |
| 9:V:183:GLU:O     | 9:V:187:ILE:HG13  | 2.19                     | 0.43              |
| 9:V:236:ARG:CZ    | 9:V:236:ARG:HB2   | 2.48                     | 0.43              |
| 9:V:330:LYS:HB3   | 9:V:360:TYR:CZ    | 2.54                     | 0.43              |
| 10:W:259:GLU:H    | 10:W:259:GLU:HG2  | 1.54                     | 0.43              |
| 10:W:354:LEU:HD12 | 10:W:354:LEU:HA   | 1.81                     | 0.43              |
| 10:W:438:LEU:HD11 | 13:Z:229:GLN:HG3  | 1.99                     | 0.43              |
| 11:X:80:ILE:CG1   | 11:X:85:ALA:HB2   | 2.49                     | 0.43              |
| 11:X:178:HIS:NE2  | 11:X:220:ALA:HB2  | 2.34                     | 0.43              |
| 13:Z:209:ARG:HG2  | 13:Z:209:ARG:HH11 | 1.84                     | 0.43              |
| 13:Z:227:ILE:CD1  | 14:a:346:ILE:HD11 | 2.48                     | 0.43              |
| 13:Z:250:TYR:OH   | 17:d:330:ILE:HA   | 2.18                     | 0.43              |
| 14:a:8:LEU:O      | 14:a:12:GLN:HB2   | 2.17                     | 0.43              |
| 14:a:92:VAL:C     | 14:a:95:THR:HG1   | 2.22                     | 0.43              |
| 14:a:93:ALA:O     | 14:a:97:LEU:HG    | 2.18                     | 0.43              |
| 14:a:123:LEU:HD21 | 14:a:158:LEU:HA   | 2.01                     | 0.43              |
| 14:a:123:LEU:CD2  | 14:a:161:LYS:HG3  | 2.49                     | 0.43              |
| 14:a:236:THR:O    | 14:a:239:ALA:HB3  | 2.19                     | 0.43              |
| 15:b:179:LEU:CG   | 15:b:180:ALA:H    | 2.31                     | 0.43              |
| 16:c:282:ARG:O    | 16:c:286:GLU:HB3  | 2.18                     | 0.43              |
| 17:d:198:PHE:O    | 17:d:201:SER:OG   | 2.36                     | 0.43              |
| 19:g:112:LEU:HD22 | 19:g:142:LEU:CD1  | 2.49                     | 0.43              |
| 20:u:126:LEU:CD1  | 20:u:175:VAL:HG21 | 2.48                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 25:F:93:VAL:HG21  | 25:F:145:LEU:HD12 | 1.99                     | 0.43              |
| 25:F:134:LEU:HD11 | 25:F:160:ILE:H    | 1.84                     | 0.43              |
| 25:F:203:VAL:CG2  | 25:F:244:THR:HG21 | 2.49                     | 0.43              |
| 25:F:415:LEU:N    | 25:F:415:LEU:HD23 | 2.32                     | 0.43              |
| 26:K:202:LEU:HD12 | 26:K:202:LEU:HA   | 1.81                     | 0.43              |
| 27:U:151:ILE:O    | 27:U:155:LEU:HG   | 2.19                     | 0.43              |
| 27:U:888:GLN:HA   | 27:U:891:VAL:HG22 | 2.00                     | 0.43              |
| 28:e:50:ASP:N     | 28:e:50:ASP:OD1   | 2.50                     | 0.43              |
| 1:C:73:VAL:O      | 1:C:73:VAL:HG13   | 2.19                     | 0.43              |
| 1:C:97:VAL:HG11   | 1:C:116:LEU:HD13  | 2.01                     | 0.43              |
| 1:C:141:GLU:OE1   | 1:C:141:GLU:HA    | 2.19                     | 0.43              |
| 1:C:332:HIS:CD2   | 1:C:360:LYS:HB2   | 2.54                     | 0.43              |
| 2:D:235:PHE:HD2   | 2:D:270:ILE:CD1   | 2.31                     | 0.43              |
| 2:D:238:LYS:HE3   | 2:D:239:TYR:CE1   | 2.53                     | 0.43              |
| 2:D:239:TYR:OH    | 22:A:289:ALA:CB   | 2.67                     | 0.43              |
| 2:D:329:ARG:NH1   | 2:D:329:ARG:CG    | 2.82                     | 0.43              |
| 2:D:410:ASP:O     | 2:D:412:GLN:N     | 2.52                     | 0.43              |
| 3:G:202:LEU:HB3   | 3:G:210:PHE:CE2   | 2.52                     | 0.43              |
| 4:H:33:ALA:HB3    | 4:H:64:LYS:HZ1    | 1.82                     | 0.43              |
| 4:H:101:TYR:O     | 4:H:102:GLN:HB2   | 2.19                     | 0.43              |
| 5:I:10:THR:CG2    | 5:I:125:GLY:HA2   | 2.49                     | 0.43              |
| 5:I:41:ASP:C      | 5:I:41:ASP:OD1    | 2.62                     | 0.43              |
| 5:I:114:LEU:HD23  | 5:I:136:TYR:OH    | 2.19                     | 0.43              |
| 6:J:67:ASP:O      | 6:J:211:MET:HE1   | 2.19                     | 0.43              |
| 7:L:148:CYS:SG    | 7:L:150:SER:HB3   | 2.59                     | 0.43              |
| 8:M:184:MET:HB3   | 8:M:188:ASP:OD2   | 2.18                     | 0.43              |
| 8:M:201:HIS:CD2   | 8:M:209:PHE:CD2   | 3.06                     | 0.43              |
| 9:V:61:GLU:HA     | 9:V:64:GLN:CB     | 2.44                     | 0.43              |
| 9:V:207:ALA:HB1   | 9:V:211:TYR:CZ    | 2.54                     | 0.43              |
| 9:V:434:ALA:CA    | 9:V:437:ILE:HG22  | 2.45                     | 0.43              |
| 9:V:498:PRO:O     | 9:V:499:LYS:C     | 2.62                     | 0.43              |
| 10:W:105:VAL:HG21 | 10:W:132:THR:HG22 | 2.01                     | 0.43              |
| 10:W:169:LEU:HD23 | 10:W:171:VAL:HG12 | 2.01                     | 0.43              |
| 10:W:171:VAL:HG11 | 10:W:185:PHE:CG   | 2.54                     | 0.43              |
| 10:W:302:TYR:HE1  | 10:W:327:GLU:OE1  | 2.01                     | 0.43              |
| 11:X:70:LEU:HA    | 11:X:73:VAL:CG2   | 2.46                     | 0.43              |
| 11:X:258:LYS:HD3  | 11:X:258:LYS:HA   | 1.87                     | 0.43              |
| 12:Y:128:TYR:CZ   | 12:Y:163:LYS:HE2  | 2.54                     | 0.43              |
| 13:Z:59:ASP:OD2   | 20:u:202:ARG:NH1  | 2.51                     | 0.43              |
| 14:a:52:GLN:C     | 14:a:54:ASP:H     | 2.27                     | 0.43              |
| 14:a:74:LEU:HA    | 14:a:77:VAL:CG1   | 2.48                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 14:a:84:VAL:CG2   | 14:a:93:ALA:CB    | 2.97                     | 0.43              |
| 14:a:293:PHE:CD1  | 14:a:329:LYS:HG3  | 2.54                     | 0.43              |
| 15:b:111:ALA:HB3  | 15:b:140:ILE:CD1  | 2.36                     | 0.43              |
| 16:c:49:VAL:HG21  | 24:E:103:THR:HG21 | 2.01                     | 0.43              |
| 16:c:179:SER:HA   | 27:U:725:MET:HE1  | 2.01                     | 0.43              |
| 17:d:89:GLN:HA    | 17:d:92:THR:HG1   | 1.83                     | 0.43              |
| 17:d:109:LEU:CD1  | 17:d:158:ARG:HA   | 2.49                     | 0.43              |
| 18:f:188:VAL:O    | 18:f:192:VAL:HG23 | 2.19                     | 0.43              |
| 18:f:690:VAL:HB   | 18:f:691:PRO:HD3  | 2.01                     | 0.43              |
| 18:f:738:ASN:OD1  | 18:f:740:ARG:N    | 2.52                     | 0.43              |
| 18:f:792:ALA:CA   | 18:f:824:ALA:HB2  | 2.49                     | 0.43              |
| 23:B:112:LEU:HB2  | 23:B:150:VAL:HG11 | 2.00                     | 0.43              |
| 23:B:204:PRO:HB3  | 23:B:218:PRO:CB   | 2.49                     | 0.43              |
| 23:B:222:VAL:HG23 | 23:B:224:LEU:HD12 | 2.00                     | 0.43              |
| 24:E:33:LEU:CD2   | 25:F:66:LEU:HD22  | 2.48                     | 0.43              |
| 24:E:335:SER:HB3  | 24:E:338:PHE:CG   | 2.54                     | 0.43              |
| 25:F:93:VAL:HA    | 25:F:124:ILE:HD13 | 2.01                     | 0.43              |
| 25:F:202:ILE:HD13 | 25:F:327:LYS:HG3  | 2.01                     | 0.43              |
| 25:F:311:LEU:HA   | 25:F:314:LEU:HB2  | 2.01                     | 0.43              |
| 26:K:164:GLN:HG3  | 26:K:164:GLN:O    | 2.18                     | 0.43              |
| 26:K:211:ASN:OD1  | 26:K:213:THR:N    | 2.48                     | 0.43              |
| 27:U:641:SER:OG   | 27:U:675:MET:HE1  | 2.18                     | 0.43              |
| 1:C:82:LYS:HE2    | 1:C:105:ILE:HG22  | 2.00                     | 0.43              |
| 1:C:152:GLY:O     | 29:C:501:ATP:N6   | 2.48                     | 0.43              |
| 1:C:273:MET:SD    | 1:C:273:MET:C     | 3.02                     | 0.43              |
| 2:D:75:ALA:O      | 2:D:79:VAL:HG23   | 2.19                     | 0.43              |
| 2:D:274:ARG:HH11  | 2:D:290:LEU:HD21  | 1.83                     | 0.43              |
| 2:D:275:PHE:O     | 2:D:276:ASP:C     | 2.60                     | 0.43              |
| 5:I:158:GLY:H     | 6:J:58:THR:CG2    | 2.32                     | 0.43              |
| 5:I:206:LEU:O     | 5:I:237:ILE:HD12  | 2.19                     | 0.43              |
| 7:L:55:GLU:HB2    | 26:K:182:GLN:CG   | 2.49                     | 0.43              |
| 7:L:64:LEU:HD23   | 7:L:64:LEU:N      | 2.33                     | 0.43              |
| 7:L:72:ILE:HG22   | 7:L:134:ILE:HG12  | 2.01                     | 0.43              |
| 7:L:199:LEU:HA    | 7:L:199:LEU:HD23  | 1.80                     | 0.43              |
| 9:V:225:ASP:HA    | 9:V:228:ARG:HB2   | 2.00                     | 0.43              |
| 10:W:19:ASP:HA    | 10:W:59:ASP:CG    | 2.44                     | 0.43              |
| 10:W:369:TYR:HB3  | 14:a:324:ILE:HD13 | 2.01                     | 0.43              |
| 10:W:422:ASN:OD1  | 16:c:235:SER:HA   | 2.19                     | 0.43              |
| 11:X:247:ALA:O    | 11:X:250:SER:HB2  | 2.18                     | 0.43              |
| 12:Y:34:ASP:CG    | 12:Y:37:VAL:HG23  | 2.44                     | 0.43              |
| 13:Z:6:VAL:HG22   | 13:Z:139:ILE:CD1  | 2.49                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 13:Z:37:GLY:HA3   | 13:Z:95:TYR:CZ    | 2.54                     | 0.43              |
| 14:a:12:GLN:HB2   | 14:a:23:HIS:CE1   | 2.53                     | 0.43              |
| 14:a:12:GLN:CG    | 14:a:18:GLN:HB3   | 2.41                     | 0.43              |
| 14:a:114:CYS:C    | 14:a:117:ALA:H    | 2.27                     | 0.43              |
| 14:a:160:SER:HA   | 14:a:163:TYR:CB   | 2.42                     | 0.43              |
| 14:a:226:ARG:NH2  | 14:a:233:LEU:HB3  | 2.34                     | 0.43              |
| 14:a:277:LEU:HD23 | 14:a:277:LEU:C    | 2.44                     | 0.43              |
| 15:b:1:MET:HE2    | 15:b:1:MET:HB2    | 1.86                     | 0.43              |
| 15:b:8:VAL:N      | 15:b:50:GLY:O     | 2.52                     | 0.43              |
| 15:b:15:TYR:CD2   | 15:b:116:PRO:HD2  | 2.52                     | 0.43              |
| 15:b:23:PRO:CG    | 15:b:27:GLN:CD    | 2.81                     | 0.43              |
| 15:b:89:GLY:O     | 15:b:92:VAL:HG12  | 2.18                     | 0.43              |
| 17:d:117:GLY:CA   | 17:d:120:LYS:HE3  | 2.33                     | 0.43              |
| 18:f:234:THR:HG23 | 18:f:786:GLN:OE1  | 2.19                     | 0.43              |
| 18:f:237:VAL:HB   | 18:f:249:LEU:HD23 | 2.01                     | 0.43              |
| 18:f:344:VAL:HG12 | 18:f:345:PRO:CD   | 2.48                     | 0.43              |
| 18:f:808:ASN:OD1  | 18:f:808:ASN:N    | 2.51                     | 0.43              |
| 18:f:878:GLU:OE1  | 18:f:878:GLU:CA   | 2.62                     | 0.43              |
| 19:g:109:GLY:O    | 19:g:138:LEU:HD22 | 2.19                     | 0.43              |
| 19:g:158:LEU:HB3  | 19:g:165:ALA:HB2  | 1.96                     | 0.43              |
| 20:u:167:ILE:O    | 20:u:167:ILE:CG2  | 2.67                     | 0.43              |
| 22:A:48:VAL:HG21  | 23:B:62:LEU:HD13  | 2.00                     | 0.43              |
| 22:A:99:THR:O     | 22:A:99:THR:HG22  | 2.19                     | 0.43              |
| 22:A:196:LEU:O    | 22:A:197:HIS:HD2  | 2.02                     | 0.43              |
| 22:A:268:LYS:HG3  | 22:A:268:LYS:O    | 2.18                     | 0.43              |
| 23:B:164:MET:H    | 23:B:164:MET:HG3  | 1.71                     | 0.43              |
| 23:B:383:LEU:CD2  | 23:B:398:ILE:HD11 | 2.47                     | 0.43              |
| 25:F:224:LEU:O    | 25:F:352:ILE:N    | 2.45                     | 0.43              |
| 25:F:353:GLU:OE1  | 25:F:355:PRO:HD3  | 2.19                     | 0.43              |
| 26:K:28:ILE:O     | 26:K:31:ILE:HG22  | 2.19                     | 0.43              |
| 26:K:78:MET:CE    | 26:K:85:ALA:HB1   | 2.47                     | 0.43              |
| 27:U:199:ARG:HA   | 27:U:202:VAL:HG12 | 2.01                     | 0.43              |
| 27:U:399:TRP:HZ2  | 27:U:507:VAL:HG11 | 1.84                     | 0.43              |
| 27:U:452:ASN:HD21 | 27:U:758:PRO:HG3  | 1.84                     | 0.43              |
| 27:U:545:LEU:HB3  | 27:U:577:ILE:CG2  | 2.45                     | 0.43              |
| 1:C:165:ILE:CD1   | 1:C:292:ILE:HD11  | 2.49                     | 0.42              |
| 1:C:174:LEU:HD11  | 22:A:30:ILE:HD11  | 2.02                     | 0.42              |
| 1:C:254:ILE:HA    | 1:C:269:VAL:CG2   | 2.48                     | 0.42              |
| 2:D:89:ILE:HG13   | 24:E:80:VAL:HG23  | 1.99                     | 0.42              |
| 2:D:251:PHE:O     | 2:D:255:LYS:HB2   | 2.19                     | 0.42              |
| 2:D:343:LEU:HD21  | 11:X:226:LYS:O    | 2.18                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:I:17:ARG:NH2    | 5:I:19:TYR:HE1    | 2.16                     | 0.42              |
| 6:J:104:VAL:HG13  | 6:J:133:ILE:HG22  | 2.01                     | 0.42              |
| 7:L:126:ARG:HD2   | 26:K:15:PHE:CE1   | 2.54                     | 0.42              |
| 9:V:63:SER:O      | 9:V:67:LEU:HD23   | 2.19                     | 0.42              |
| 9:V:132:LEU:N     | 9:V:133:PRO:HD2   | 2.34                     | 0.42              |
| 9:V:223:LYS:O     | 9:V:225:ASP:OD1   | 2.37                     | 0.42              |
| 10:W:355:LYS:O    | 10:W:355:LYS:HD2  | 2.19                     | 0.42              |
| 11:X:364:LYS:HD2  | 11:X:364:LYS:HA   | 1.79                     | 0.42              |
| 11:X:407:MET:O    | 11:X:410:VAL:HG12 | 2.18                     | 0.42              |
| 12:Y:155:ASP:OD1  | 12:Y:156:LEU:N    | 2.52                     | 0.42              |
| 12:Y:218:THR:HA   | 12:Y:221:THR:HG22 | 2.01                     | 0.42              |
| 12:Y:282:MET:HE3  | 12:Y:295:TYR:CD1  | 2.53                     | 0.42              |
| 12:Y:387:ILE:HG23 | 13:Z:275:LEU:HD23 | 2.00                     | 0.42              |
| 13:Z:96:HIS:NE2   | 13:Z:123:ILE:HG12 | 2.34                     | 0.42              |
| 13:Z:212:LEU:CD1  | 14:a:346:ILE:HD12 | 2.49                     | 0.42              |
| 14:a:28:LEU:CB    | 14:a:33:LEU:HD11  | 2.38                     | 0.42              |
| 14:a:74:LEU:CA    | 14:a:77:VAL:HG12  | 2.48                     | 0.42              |
| 14:a:97:LEU:HD12  | 14:a:98:GLU:OE1   | 2.18                     | 0.42              |
| 14:a:112:ILE:HD13 | 14:a:138:VAL:CG1  | 2.48                     | 0.42              |
| 14:a:119:GLY:O    | 14:a:123:LEU:HB3  | 2.19                     | 0.42              |
| 16:c:179:SER:O    | 16:c:179:SER:OG   | 2.26                     | 0.42              |
| 17:d:128:PHE:HE1  | 17:d:148:LEU:HD11 | 1.84                     | 0.42              |
| 17:d:283:LEU:HB2  | 17:d:315:TYR:CE1  | 2.53                     | 0.42              |
| 18:f:114:ALA:C    | 18:f:116:GLY:N    | 2.77                     | 0.42              |
| 18:f:135:GLY:O    | 18:f:136:GLU:C    | 2.62                     | 0.42              |
| 18:f:385:PHE:CE2  | 18:f:772:GLY:HA2  | 2.53                     | 0.42              |
| 18:f:586:PRO:HG3  | 18:f:645:ASP:OD1  | 2.18                     | 0.42              |
| 18:f:679:LEU:CG   | 18:f:690:VAL:HG11 | 2.42                     | 0.42              |
| 19:g:118:GLU:HG3  | 19:g:119:THR:N    | 2.34                     | 0.42              |
| 20:u:119:ILE:C    | 20:u:119:ILE:HD12 | 2.44                     | 0.42              |
| 20:u:182:PHE:CD2  | 20:u:194:VAL:HG21 | 2.54                     | 0.42              |
| 22:A:87:LEU:HD12  | 22:A:87:LEU:O     | 2.19                     | 0.42              |
| 22:A:96:ALA:CB    | 22:A:114:ASN:O    | 2.67                     | 0.42              |
| 22:A:286:ASP:CG   | 25:F:293:THR:HG22 | 2.44                     | 0.42              |
| 23:B:307:ARG:CZ   | 23:B:307:ARG:HB2  | 2.47                     | 0.42              |
| 25:F:321:GLN:O    | 25:F:324:THR:HG22 | 2.19                     | 0.42              |
| 25:F:407:ALA:CB   | 25:F:415:LEU:HD22 | 2.49                     | 0.42              |
| 27:U:71:LEU:O     | 27:U:71:LEU:HD23  | 2.18                     | 0.42              |
| 27:U:117:ASP:C    | 27:U:118:LEU:HD22 | 2.43                     | 0.42              |
| 27:U:141:CYS:SG   | 27:U:150:ALA:HB1  | 2.59                     | 0.42              |
| 27:U:164:GLU:O    | 27:U:168:LEU:HB2  | 2.19                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 27:U:387:ARG:HH22 | 27:U:426:TYR:HD1  | 1.65                     | 0.42              |
| 1:C:73:VAL:HG23   | 1:C:127:LEU:HD23  | 2.01                     | 0.42              |
| 1:C:226:GLU:OE2   | 1:C:226:GLU:HA    | 2.19                     | 0.42              |
| 1:C:251:ILE:HG22  | 1:C:295:THR:HB    | 2.01                     | 0.42              |
| 1:C:273:MET:HE1   | 1:C:274:LEU:HD23  | 2.01                     | 0.42              |
| 1:C:315:ILE:CG2   | 1:C:317:PHE:HE1   | 2.32                     | 0.42              |
| 1:C:336:MET:CE    | 1:C:378:VAL:HG21  | 2.45                     | 0.42              |
| 2:D:377:SER:HA    | 24:E:292:PRO:HG3  | 2.02                     | 0.42              |
| 3:G:57:PRO:O      | 3:G:58:ASP:HB2    | 2.19                     | 0.42              |
| 4:H:44:VAL:HB     | 4:H:137:CYS:HB2   | 2.01                     | 0.42              |
| 5:I:99:LEU:HD23   | 5:I:100:GLN:N     | 2.34                     | 0.42              |
| 5:I:232:GLU:HA    | 5:I:235:GLN:HG3   | 2.01                     | 0.42              |
| 6:J:35:VAL:HG22   | 6:J:191:VAL:HG23  | 2.01                     | 0.42              |
| 8:M:175:GLU:HB3   | 8:M:196:ILE:HD13  | 2.01                     | 0.42              |
| 9:V:165:ALA:HB1   | 9:V:191:LEU:HD11  | 2.01                     | 0.42              |
| 9:V:236:ARG:HD3   | 9:V:240:LEU:HD21  | 2.02                     | 0.42              |
| 9:V:303:SER:HA    | 9:V:339:LEU:HD21  | 2.01                     | 0.42              |
| 10:W:24:VAL:O     | 10:W:28:LEU:HG    | 2.19                     | 0.42              |
| 10:W:40:LEU:O     | 10:W:42:GLU:N     | 2.53                     | 0.42              |
| 10:W:214:PHE:HB3  | 10:W:223:LYS:CG   | 2.49                     | 0.42              |
| 11:X:239:TYR:O    | 11:X:242:ILE:HG12 | 2.20                     | 0.42              |
| 11:X:362:GLU:OE1  | 11:X:380:GLN:NE2  | 2.49                     | 0.42              |
| 12:Y:43:ALA:HA    | 12:Y:46:ARG:HH11  | 1.83                     | 0.42              |
| 13:Z:44:GLN:O     | 13:Z:45:LYS:C     | 2.63                     | 0.42              |
| 13:Z:111:LEU:O    | 13:Z:114:ARG:HB3  | 2.19                     | 0.42              |
| 13:Z:172:VAL:HG11 | 16:c:220:LEU:CD1  | 2.48                     | 0.42              |
| 13:Z:205:LEU:HD21 | 14:a:356:TRP:CZ3  | 2.54                     | 0.42              |
| 14:a:41:VAL:CG1   | 14:a:79:ILE:CD1   | 2.97                     | 0.42              |
| 15:b:25:ARG:NH1   | 15:b:145:GLU:H    | 2.09                     | 0.42              |
| 15:b:33:VAL:CG1   | 15:b:75:LEU:CD1   | 2.94                     | 0.42              |
| 15:b:121:GLU:OE2  | 15:b:152:LYS:HB3  | 2.18                     | 0.42              |
| 16:c:142:ALA:O    | 16:c:160:PHE:N    | 2.49                     | 0.42              |
| 16:c:200:TYR:O    | 16:c:200:TYR:CD1  | 2.72                     | 0.42              |
| 16:c:292:MET:SD   | 17:d:346:LEU:CD2  | 3.07                     | 0.42              |
| 17:d:146:ASP:HA   | 17:d:149:GLU:HB3  | 1.99                     | 0.42              |
| 18:f:51:GLN:HB3   | 18:f:55:GLU:OE2   | 2.18                     | 0.42              |
| 18:f:405:HIS:NE2  | 18:f:813:LYS:HB3  | 2.33                     | 0.42              |
| 18:f:672:LEU:HD22 | 18:f:694:LEU:CD2  | 2.49                     | 0.42              |
| 19:g:94:LYS:C     | 19:g:95:LYS:HG2   | 2.44                     | 0.42              |
| 19:g:161:SER:HB3  | 19:g:164:ASP:CB   | 2.49                     | 0.42              |
| 22:A:223:THR:O    | 22:A:223:THR:HG22 | 2.18                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:A:395:PHE:HE2  | 22:A:411:GLU:HG2  | 1.84                     | 0.42              |
| 23:B:137:SER:HA   | 23:B:141:LYS:NZ   | 2.34                     | 0.42              |
| 25:F:180:ARG:HB2  | 25:F:242:ALA:HB2  | 2.01                     | 0.42              |
| 26:K:24:VAL:HA    | 26:K:136:PRO:HG3  | 2.01                     | 0.42              |
| 26:K:91:LYS:CE    | 26:K:95:GLU:HG3   | 2.49                     | 0.42              |
| 26:K:196:LYS:NZ   | 26:K:196:LYS:HB3  | 2.34                     | 0.42              |
| 27:U:112:CYS:HB3  | 27:U:158:ARG:HG2  | 2.02                     | 0.42              |
| 27:U:580:ARG:HG3  | 27:U:614:VAL:HA   | 2.00                     | 0.42              |
| 27:U:622:LEU:O    | 27:U:625:ILE:HG12 | 2.19                     | 0.42              |
| 27:U:803:LYS:HG3  | 27:U:893:THR:CB   | 2.19                     | 0.42              |
| 27:U:803:LYS:HB2  | 27:U:875:PHE:CD1  | 2.51                     | 0.42              |
| 1:C:170:LYS:HE2   | 1:C:208:ASP:CG    | 2.44                     | 0.42              |
| 1:C:314:LYS:NZ    | 23:B:428:TYR:O    | 2.49                     | 0.42              |
| 1:C:375:ARG:NH2   | 1:C:382:ASP:OD2   | 2.52                     | 0.42              |
| 2:D:53:PHE:HZ     | 27:U:636:VAL:HB   | 1.83                     | 0.42              |
| 2:D:339:ARG:NH2   | 11:X:231:TYR:OH   | 2.52                     | 0.42              |
| 6:J:79:ASP:O      | 6:J:82:ILE:HG22   | 2.19                     | 0.42              |
| 6:J:146:GLN:HG2   | 6:J:147:THR:O     | 2.19                     | 0.42              |
| 7:L:19:ILE:HD13   | 8:M:129:ARG:NE    | 2.34                     | 0.42              |
| 7:L:134:ILE:HB    | 7:L:145:PHE:HB2   | 2.00                     | 0.42              |
| 9:V:65:ARG:HA     | 9:V:68:ASP:CB     | 2.49                     | 0.42              |
| 9:V:216:ARG:HA    | 9:V:219:GLU:HB3   | 2.02                     | 0.42              |
| 9:V:455:LYS:HG3   | 9:V:457:TYR:HD2   | 1.84                     | 0.42              |
| 9:V:472:PRO:HA    | 12:Y:366:TYR:OH   | 2.19                     | 0.42              |
| 10:W:115:ILE:HG13 | 10:W:124:LEU:CD2  | 2.50                     | 0.42              |
| 10:W:206:SER:O    | 10:W:209:ILE:HG23 | 2.18                     | 0.42              |
| 10:W:248:ARG:HG2  | 10:W:270:VAL:CG2  | 2.48                     | 0.42              |
| 11:X:183:LEU:HD21 | 11:X:220:ALA:C    | 2.45                     | 0.42              |
| 11:X:194:ARG:HH11 | 11:X:194:ARG:CG   | 2.31                     | 0.42              |
| 11:X:217:ILE:N    | 11:X:217:ILE:HD13 | 2.33                     | 0.42              |
| 11:X:326:LEU:O    | 11:X:329:ASN:N    | 2.51                     | 0.42              |
| 12:Y:70:LEU:HG    | 12:Y:74:LYS:HD2   | 2.01                     | 0.42              |
| 12:Y:165:LYS:NZ   | 12:Y:165:LYS:HB2  | 2.33                     | 0.42              |
| 12:Y:260:LEU:HD12 | 12:Y:260:LEU:O    | 2.20                     | 0.42              |
| 12:Y:338:ILE:HD12 | 12:Y:347:ILE:HG13 | 2.01                     | 0.42              |
| 13:Z:272:LEU:HD23 | 13:Z:272:LEU:HA   | 1.80                     | 0.42              |
| 14:a:45:VAL:CG2   | 14:a:79:ILE:HD11  | 2.45                     | 0.42              |
| 14:a:74:LEU:O     | 14:a:78:GLU:CB    | 2.66                     | 0.42              |
| 14:a:112:ILE:HG23 | 14:a:113:LEU:N    | 2.34                     | 0.42              |
| 14:a:116:THR:CG2  | 14:a:154:ARG:CB   | 2.96                     | 0.42              |
| 14:a:123:LEU:HD21 | 14:a:161:LYS:HG3  | 2.01                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 14:a:231:GLN:HG2  | 14:a:234:ILE:HG22 | 2.00                     | 0.42              |
| 16:c:177:THR:CG2  | 27:U:774:PRO:HD3  | 2.49                     | 0.42              |
| 16:c:259:VAL:O    | 16:c:262:GLU:N    | 2.53                     | 0.42              |
| 17:d:172:LYS:HE3  | 17:d:195:ASN:HD22 | 1.81                     | 0.42              |
| 18:f:123:ALA:O    | 18:f:127:SER:HB3  | 2.19                     | 0.42              |
| 18:f:180:GLN:O    | 18:f:184:LEU:HG   | 2.19                     | 0.42              |
| 18:f:203:GLU:HA   | 18:f:206:ASP:HB2  | 2.01                     | 0.42              |
| 18:f:307:LEU:HD11 | 18:f:311:VAL:CB   | 2.49                     | 0.42              |
| 18:f:327:ASN:HB2  | 18:f:420:TRP:O    | 2.18                     | 0.42              |
| 18:f:407:MET:HB3  | 18:f:440:ILE:HG22 | 2.01                     | 0.42              |
| 18:f:574:GLU:O    | 18:f:577:LEU:HG   | 2.19                     | 0.42              |
| 18:f:655:LEU:HD12 | 18:f:693:ALA:HA   | 2.00                     | 0.42              |
| 18:f:764:LEU:HD11 | 18:f:818:LEU:HD23 | 2.01                     | 0.42              |
| 18:f:783:SER:O    | 18:f:786:GLN:HB2  | 2.19                     | 0.42              |
| 18:f:872:VAL:HG12 | 18:f:873:LEU:H    | 1.84                     | 0.42              |
| 22:A:271:LEU:O    | 22:A:272:ILE:HD13 | 2.18                     | 0.42              |
| 23:B:251:VAL:C    | 23:B:253:SER:H    | 2.27                     | 0.42              |
| 24:E:169:GLY:HA3  | 24:E:295:LEU:HD23 | 2.00                     | 0.42              |
| 24:E:323:HIS:CE1  | 24:E:360:ASP:HB2  | 2.54                     | 0.42              |
| 25:F:224:LEU:HD21 | 25:F:338:LEU:HD12 | 2.00                     | 0.42              |
| 27:U:16:GLU:HB2   | 27:U:19:LEU:HB3   | 2.01                     | 0.42              |
| 27:U:82:LEU:HD11  | 27:U:129:ARG:C    | 2.45                     | 0.42              |
| 27:U:98:GLU:HA    | 27:U:101:ILE:HG12 | 2.02                     | 0.42              |
| 27:U:134:VAL:HG12 | 27:U:138:PHE:CD2  | 2.55                     | 0.42              |
| 27:U:181:LEU:CD1  | 27:U:219:CYS:SG   | 3.07                     | 0.42              |
| 27:U:423:MET:HA   | 27:U:423:MET:CE   | 2.45                     | 0.42              |
| 27:U:461:LEU:HD23 | 27:U:461:LEU:HA   | 1.64                     | 0.42              |
| 27:U:563:ALA:O    | 27:U:565:ALA:N    | 2.52                     | 0.42              |
| 27:U:719:ASP:O    | 27:U:727:LYS:HE2  | 2.19                     | 0.42              |
| 1:C:142:LYS:HE3   | 1:C:142:LYS:HB3   | 1.63                     | 0.42              |
| 1:C:251:ILE:CG2   | 1:C:301:LEU:HD11  | 2.49                     | 0.42              |
| 1:C:262:GLY:CA    | 23:B:295:TYR:CD2  | 3.02                     | 0.42              |
| 1:C:328:ILE:HG22  | 1:C:359:VAL:HG11  | 2.01                     | 0.42              |
| 2:D:58:GLU:HA     | 2:D:61:ILE:CG2    | 2.49                     | 0.42              |
| 2:D:205:TYR:CD1   | 2:D:205:TYR:C     | 2.97                     | 0.42              |
| 4:H:29:VAL:CG2    | 4:H:133:SER:H     | 2.32                     | 0.42              |
| 5:I:118:LYS:HD2   | 5:I:151:ASP:O     | 2.18                     | 0.42              |
| 6:J:9:VAL:HA      | 26:K:23:GLN:HE21  | 1.84                     | 0.42              |
| 6:J:20:GLU:HB3    | 22:A:428:ARG:HE   | 1.85                     | 0.42              |
| 7:L:204:ASP:HA    | 7:L:239:ARG:NH2   | 2.34                     | 0.42              |
| 8:M:25:TYR:CA     | 8:M:28:LYS:HG2    | 2.46                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 8:M:175:GLU:C     | 8:M:196:ILE:HD11  | 2.44                     | 0.42              |
| 9:V:111:TYR:CD1   | 9:V:138:PRO:HG3   | 2.54                     | 0.42              |
| 9:V:361:PHE:CD1   | 9:V:361:PHE:C     | 2.97                     | 0.42              |
| 9:V:404:LYS:HZ3   | 9:V:404:LYS:HB3   | 1.83                     | 0.42              |
| 9:V:455:LYS:CG    | 9:V:457:TYR:HD2   | 2.32                     | 0.42              |
| 9:V:470:ARG:HH12  | 9:V:474:LEU:CD1   | 2.31                     | 0.42              |
| 10:W:41:GLN:OE1   | 10:W:41:GLN:N     | 2.52                     | 0.42              |
| 10:W:320:LEU:HD23 | 10:W:320:LEU:C    | 2.44                     | 0.42              |
| 11:X:71:LYS:O     | 11:X:74:ARG:HB2   | 2.20                     | 0.42              |
| 11:X:140:THR:O    | 11:X:141:LYS:HB2  | 2.19                     | 0.42              |
| 11:X:171:LEU:CD2  | 11:X:209:THR:HG22 | 2.48                     | 0.42              |
| 11:X:363:ARG:HH22 | 12:Y:266:CYS:HB3  | 1.83                     | 0.42              |
| 12:Y:145:LEU:HD21 | 12:Y:160:ASN:HB2  | 1.99                     | 0.42              |
| 13:Z:177:ARG:HG2  | 13:Z:177:ARG:NH1  | 2.35                     | 0.42              |
| 14:a:76:LEU:HD12  | 14:a:80:ILE:CG2   | 2.49                     | 0.42              |
| 14:a:155:PHE:CD1  | 14:a:155:PHE:C    | 2.97                     | 0.42              |
| 15:b:52:ILE:HD12  | 15:b:60:VAL:HA    | 2.02                     | 0.42              |
| 15:b:60:VAL:O     | 15:b:61:LEU:C     | 2.62                     | 0.42              |
| 17:d:124:LEU:HD12 | 27:U:18:GLN:OE1   | 2.20                     | 0.42              |
| 17:d:129:LEU:CB   | 17:d:130:PRO:CD   | 2.98                     | 0.42              |
| 18:f:115:PRO:HA   | 18:f:119:LYS:CB   | 2.49                     | 0.42              |
| 18:f:143:ARG:CZ   | 18:f:148:GLN:O    | 2.68                     | 0.42              |
| 18:f:160:ARG:CB   | 18:f:160:ARG:HH11 | 2.32                     | 0.42              |
| 18:f:173:LEU:HD11 | 18:f:177:GLU:O    | 2.18                     | 0.42              |
| 18:f:419:LEU:CD2  | 18:f:822:VAL:HG13 | 2.49                     | 0.42              |
| 18:f:433:LEU:O    | 18:f:441:LYS:HG2  | 2.20                     | 0.42              |
| 18:f:517:VAL:CG2  | 18:f:557:TRP:HZ3  | 2.32                     | 0.42              |
| 18:f:517:VAL:HG23 | 18:f:557:TRP:HZ3  | 1.85                     | 0.42              |
| 18:f:560:LEU:O    | 18:f:560:LEU:HD23 | 2.20                     | 0.42              |
| 18:f:845:ARG:HB2  | 18:f:845:ARG:HH11 | 1.85                     | 0.42              |
| 22:A:95:VAL:HG11  | 22:A:139:ARG:HD2  | 2.02                     | 0.42              |
| 22:A:139:ARG:NH1  | 22:A:156:LYS:HG3  | 2.34                     | 0.42              |
| 22:A:271:LEU:HD23 | 22:A:316:LYS:HB2  | 2.02                     | 0.42              |
| 23:B:165:ASP:OD1  | 23:B:165:ASP:C    | 2.62                     | 0.42              |
| 24:E:57:VAL:HB    | 25:F:131:THR:OG1  | 2.19                     | 0.42              |
| 24:E:294:ARG:O    | 24:E:295:LEU:CB   | 2.67                     | 0.42              |
| 24:E:361:PHE:HZ   | 24:E:364:GLN:HA   | 1.84                     | 0.42              |
| 25:F:218:GLN:HE21 | 25:F:218:GLN:HB3  | 1.62                     | 0.42              |
| 25:F:232:GLY:HA3  | 29:F:501:ATP:C8   | 2.55                     | 0.42              |
| 25:F:370:SER:HB3  | 25:F:400:CYS:SG   | 2.59                     | 0.42              |
| 27:U:221:ILE:HD13 | 27:U:260:PHE:CE2  | 2.54                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 27:U:351:MET:HE1  | 27:U:354:LYS:CD   | 2.48                     | 0.42              |
| 27:U:422:LEU:C    | 27:U:422:LEU:HD23 | 2.44                     | 0.42              |
| 27:U:553:ALA:HA   | 27:U:585:THR:OG1  | 2.19                     | 0.42              |
| 1:C:150:MET:HA    | 1:C:331:ILE:HG21  | 2.01                     | 0.42              |
| 1:C:273:MET:SD    | 1:C:277:LEU:HG    | 2.59                     | 0.42              |
| 2:D:167:ILE:CG1   | 2:D:174:LYS:HD2   | 2.48                     | 0.42              |
| 3:G:32:ILE:HD11   | 3:G:156:PRO:CD    | 2.50                     | 0.42              |
| 3:G:76:ILE:HG21   | 3:G:140:LEU:HD22  | 2.01                     | 0.42              |
| 5:I:186:LEU:HD12  | 5:I:186:LEU:HA    | 1.73                     | 0.42              |
| 5:I:237:ILE:HG12  | 5:I:237:ILE:H     | 1.66                     | 0.42              |
| 8:M:40:ARG:HG3    | 8:M:40:ARG:O      | 2.20                     | 0.42              |
| 9:V:92:ARG:HA     | 9:V:95:LEU:HD12   | 2.01                     | 0.42              |
| 9:V:178:SER:HB3   | 9:V:180:ARG:NH1   | 2.34                     | 0.42              |
| 9:V:255:LEU:CD2   | 9:V:270:LEU:HD23  | 2.50                     | 0.42              |
| 10:W:289:ARG:CZ   | 10:W:289:ARG:CB   | 2.97                     | 0.42              |
| 11:X:192:SER:O    | 11:X:195:THR:HG22 | 2.18                     | 0.42              |
| 11:X:420:LYS:O    | 11:X:421:LEU:HB2  | 2.18                     | 0.42              |
| 14:a:12:GLN:HE21  | 14:a:18:GLN:HB2   | 1.83                     | 0.42              |
| 14:a:157:ASP:C    | 14:a:160:SER:HG   | 2.18                     | 0.42              |
| 15:b:161:ASN:ND2  | 15:b:168:SER:H    | 2.11                     | 0.42              |
| 16:c:51:MET:O     | 16:c:116:PRO:HG3  | 2.20                     | 0.42              |
| 18:f:319:GLU:HB2  | 18:f:324:VAL:CG2  | 2.49                     | 0.42              |
| 18:f:573:ILE:O    | 18:f:573:ILE:CG2  | 2.67                     | 0.42              |
| 18:f:590:PHE:CZ   | 18:f:652:VAL:HG11 | 2.55                     | 0.42              |
| 18:f:745:LEU:HB3  | 18:f:766:GLN:HG2  | 2.01                     | 0.42              |
| 19:g:125:ASN:C    | 19:g:161:SER:HB2  | 2.45                     | 0.42              |
| 20:u:126:LEU:HD22 | 20:u:175:VAL:HG21 | 2.02                     | 0.42              |
| 22:A:151:ILE:HG12 | 22:A:152:PRO:O    | 2.19                     | 0.42              |
| 22:A:222:LYS:HE2  | 29:A:501:ATP:O2B  | 2.19                     | 0.42              |
| 23:B:41:LYS:HE3   | 23:B:41:LYS:HB3   | 1.91                     | 0.42              |
| 23:B:295:TYR:CD1  | 23:B:295:TYR:C    | 2.98                     | 0.42              |
| 23:B:355:LEU:CD1  | 23:B:389:ASP:HB3  | 2.49                     | 0.42              |
| 23:B:409:GLU:HB3  | 23:B:411:ARG:NH1  | 2.35                     | 0.42              |
| 25:F:231:THR:N    | 29:F:501:ATP:O1B  | 2.52                     | 0.42              |
| 26:K:12:VAL:HG11  | 26:K:136:PRO:HD3  | 2.00                     | 0.42              |
| 26:K:21:LEU:HD23  | 26:K:21:LEU:HA    | 1.85                     | 0.42              |
| 27:U:188:MET:HB3  | 27:U:194:ARG:NH2  | 2.35                     | 0.42              |
| 27:U:242:LEU:HD21 | 27:U:321:GLN:CD   | 2.45                     | 0.42              |
| 27:U:363:SER:OG   | 27:U:724:VAL:HG22 | 2.20                     | 0.42              |
| 27:U:641:SER:HB3  | 27:U:652:ALA:HB1  | 2.01                     | 0.42              |
| 27:U:792:ASN:HD21 | 27:U:796:LYS:HG2  | 1.85                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:322:GLU:HA    | 1:C:325:ARG:NH2   | 2.34                     | 0.42              |
| 2:D:203:LEU:HD22  | 2:D:322:LEU:CD2   | 2.49                     | 0.42              |
| 2:D:252:ARG:HG2   | 2:D:252:ARG:NH1   | 2.34                     | 0.42              |
| 2:D:291:GLU:OE1   | 2:D:291:GLU:CA    | 2.67                     | 0.42              |
| 2:D:321:LEU:HG    | 2:D:321:LEU:O     | 2.19                     | 0.42              |
| 3:G:41:ALA:HB2    | 3:G:50:ILE:HG22   | 2.02                     | 0.42              |
| 3:G:69:LEU:HD12   | 3:G:79:VAL:CG2    | 2.35                     | 0.42              |
| 4:H:59:GLU:HG2    | 4:H:206:ASP:HB3   | 2.01                     | 0.42              |
| 4:H:228:ASP:N     | 4:H:228:ASP:OD1   | 2.53                     | 0.42              |
| 6:J:66:ASP:HB3    | 6:J:69:VAL:HG22   | 2.01                     | 0.42              |
| 6:J:95:ARG:HH12   | 6:J:101:PRO:HB3   | 1.82                     | 0.42              |
| 6:J:104:VAL:HG21  | 6:J:135:GLY:CA    | 2.49                     | 0.42              |
| 7:L:88:MET:HE3    | 7:L:134:ILE:HD11  | 2.01                     | 0.42              |
| 7:L:120:THR:O     | 7:L:120:THR:HG23  | 2.20                     | 0.42              |
| 7:L:205:LEU:HB3   | 7:L:210:VAL:HG21  | 2.02                     | 0.42              |
| 9:V:109:ASN:O     | 9:V:112:VAL:HG23  | 2.19                     | 0.42              |
| 9:V:348:PHE:CD2   | 9:V:361:PHE:CD2   | 3.07                     | 0.42              |
| 9:V:482:PHE:CD1   | 12:Y:377:LEU:HD22 | 2.55                     | 0.42              |
| 10:W:83:LEU:HD11  | 10:W:87:ILE:HD11  | 2.01                     | 0.42              |
| 11:X:334:ASN:HB3  | 11:X:354:ILE:HD11 | 2.01                     | 0.42              |
| 12:Y:387:ILE:HG23 | 13:Z:275:LEU:CD2  | 2.49                     | 0.42              |
| 17:d:90:ALA:O     | 17:d:94:MET:CG    | 2.68                     | 0.42              |
| 18:f:391:LEU:HG   | 18:f:414:LEU:CG   | 2.44                     | 0.42              |
| 18:f:419:LEU:HD21 | 18:f:822:VAL:HG13 | 2.02                     | 0.42              |
| 18:f:513:GLU:HA   | 18:f:554:TYR:CD2  | 2.48                     | 0.42              |
| 18:f:679:LEU:HD12 | 18:f:713:PHE:CE2  | 2.55                     | 0.42              |
| 18:f:797:LEU:HA   | 18:f:797:LEU:HD12 | 1.69                     | 0.42              |
| 18:f:828:ARG:HD2  | 18:f:874:LEU:HB2  | 2.00                     | 0.42              |
| 19:g:107:ILE:HB   | 19:g:111:GLU:CB   | 2.49                     | 0.42              |
| 20:u:165:LEU:HD12 | 20:u:166:LEU:N    | 2.34                     | 0.42              |
| 20:u:218:LEU:HG   | 20:u:220:LEU:HD22 | 2.00                     | 0.42              |
| 22:A:44:GLN:O     | 22:A:47:GLN:HB3   | 2.19                     | 0.42              |
| 22:A:113:ILE:HG23 | 22:A:123:VAL:HG22 | 2.01                     | 0.42              |
| 22:A:413:VAL:O    | 22:A:418:LYS:HG2  | 2.19                     | 0.42              |
| 23:B:133:VAL:HG11 | 23:B:157:HIS:HB3  | 2.01                     | 0.42              |
| 23:B:197:ILE:HD11 | 23:B:328:ILE:HD13 | 2.02                     | 0.42              |
| 23:B:278:ALA:O    | 23:B:279:PRO:C    | 2.63                     | 0.42              |
| 26:K:50:VAL:HG11  | 26:K:66:LYS:CB    | 2.44                     | 0.42              |
| 27:U:153:ILE:O    | 27:U:157:THR:HG22 | 2.20                     | 0.42              |
| 27:U:333:MET:HE2  | 27:U:333:MET:HB2  | 1.79                     | 0.42              |
| 27:U:366:HIS:O    | 27:U:370:VAL:HG23 | 2.20                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 27:U:390:LEU:O    | 27:U:390:LEU:HD23 | 2.19                     | 0.42              |
| 27:U:465:LEU:CD2  | 27:U:500:ASN:HD21 | 2.29                     | 0.42              |
| 27:U:483:LEU:HD12 | 27:U:483:LEU:HA   | 1.85                     | 0.42              |
| 1:C:73:VAL:O      | 1:C:73:VAL:CG1    | 2.67                     | 0.42              |
| 1:C:187:LEU:HD22  | 1:C:306:LEU:CD2   | 2.48                     | 0.42              |
| 1:C:292:ILE:O     | 1:C:293:MET:C     | 2.62                     | 0.42              |
| 1:C:340:ARG:HH12  | 12:Y:176:ARG:NH1  | 2.16                     | 0.42              |
| 2:D:309:MET:CE    | 2:D:327:LEU:HD21  | 2.42                     | 0.42              |
| 3:G:179:LEU:O     | 3:G:183:VAL:HG12  | 2.20                     | 0.42              |
| 5:I:101:TYR:CD1   | 5:I:101:TYR:N     | 2.88                     | 0.42              |
| 6:J:23:GLN:NE2    | 6:J:150:SER:HB3   | 2.26                     | 0.42              |
| 8:M:67:PHE:N      | 8:M:67:PHE:CD1    | 2.87                     | 0.42              |
| 8:M:185:THR:HG23  | 8:M:185:THR:O     | 2.19                     | 0.42              |
| 9:V:169:LEU:HD12  | 9:V:172:VAL:HB    | 2.01                     | 0.42              |
| 9:V:410:ILE:HD13  | 9:V:410:ILE:HA    | 1.81                     | 0.42              |
| 9:V:451:ILE:O     | 17:d:279:TYR:HA   | 2.19                     | 0.42              |
| 10:W:149:LEU:HD12 | 10:W:149:LEU:O    | 2.19                     | 0.42              |
| 10:W:347:GLY:HA2  | 10:W:350:ARG:HH11 | 1.84                     | 0.42              |
| 10:W:369:TYR:CD2  | 14:a:312:MET:SD   | 3.11                     | 0.42              |
| 11:X:86:ALA:O     | 11:X:89:VAL:HG12  | 2.20                     | 0.42              |
| 11:X:110:CYS:O    | 11:X:114:ILE:HG12 | 2.19                     | 0.42              |
| 11:X:133:LEU:HD11 | 11:X:137:TYR:CE1  | 2.54                     | 0.42              |
| 11:X:254:MET:HE3  | 11:X:254:MET:HB3  | 1.76                     | 0.42              |
| 12:Y:220:VAL:CG2  | 12:Y:249:VAL:HG11 | 2.48                     | 0.42              |
| 13:Z:39:LEU:HD23  | 13:Z:53:SER:HB2   | 2.01                     | 0.42              |
| 14:a:40:GLN:O     | 14:a:44:PHE:HB2   | 2.20                     | 0.42              |
| 14:a:61:GLU:O     | 14:a:65:SER:CB    | 2.68                     | 0.42              |
| 14:a:129:GLN:HG3  | 14:a:130:VAL:HG12 | 2.02                     | 0.42              |
| 14:a:313:LYS:O    | 14:a:314:ALA:C    | 2.62                     | 0.42              |
| 15:b:7:MET:HB2    | 15:b:97:LEU:HD13  | 2.01                     | 0.42              |
| 15:b:128:ALA:HB1  | 15:b:159:THR:HG23 | 2.01                     | 0.42              |
| 17:d:200:LEU:HD13 | 17:d:208:PHE:CD2  | 2.55                     | 0.42              |
| 17:d:275:ILE:CD1  | 17:d:290:ILE:HG22 | 2.50                     | 0.42              |
| 18:f:107:LYS:O    | 18:f:107:LYS:HD3  | 2.19                     | 0.42              |
| 18:f:138:GLU:HG3  | 18:f:141:LYS:CE   | 2.49                     | 0.42              |
| 18:f:203:GLU:O    | 18:f:207:LEU:N    | 2.47                     | 0.42              |
| 18:f:344:VAL:CG1  | 18:f:345:PRO:HD2  | 2.49                     | 0.42              |
| 18:f:737:ASN:OD1  | 18:f:737:ASN:N    | 2.53                     | 0.42              |
| 19:g:161:SER:O    | 19:g:165:ALA:HB3  | 2.20                     | 0.42              |
| 20:u:125:ASP:HA   | 20:u:266:ILE:HD13 | 2.01                     | 0.42              |
| 22:A:147:TYR:N    | 22:A:147:TYR:CD1  | 2.87                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:A:214:LEU:HD12 | 22:A:214:LEU:N    | 2.33                     | 0.42              |
| 22:A:394:MET:SD   | 23:B:211:TYR:HE2  | 2.43                     | 0.42              |
| 23:B:365:PHE:CE2  | 23:B:395:ILE:HD12 | 2.54                     | 0.42              |
| 24:E:90:SER:O     | 24:E:93:LYS:HG3   | 2.20                     | 0.42              |
| 25:F:154:ASN:HB3  | 25:F:157:SER:OG   | 2.20                     | 0.42              |
| 25:F:201:ALA:HB2  | 25:F:350:ARG:NH1  | 2.35                     | 0.42              |
| 26:K:65:GLU:O     | 26:K:78:MET:SD    | 2.78                     | 0.42              |
| 27:U:45:ILE:HD13  | 27:U:45:ILE:N     | 2.33                     | 0.42              |
| 27:U:422:LEU:CD2  | 27:U:426:TYR:HE2  | 2.32                     | 0.42              |
| 27:U:556:MET:O    | 27:U:589:ALA:HA   | 2.19                     | 0.42              |
| 27:U:899:ARG:HG2  | 27:U:917:THR:OG1  | 2.20                     | 0.42              |
| 27:U:903:PHE:CD1  | 27:U:915:LYS:HE3  | 2.55                     | 0.42              |
| 1:C:127:LEU:HD12  | 1:C:127:LEU:HA    | 1.87                     | 0.42              |
| 1:C:163:GLU:HB3   | 23:B:404:LEU:CD1  | 2.50                     | 0.42              |
| 2:D:45:LYS:CA     | 2:D:45:LYS:HE2    | 2.50                     | 0.42              |
| 2:D:58:GLU:HA     | 2:D:61:ILE:HG22   | 2.01                     | 0.42              |
| 2:D:239:TYR:HA    | 21:v:15:UNK:O     | 2.20                     | 0.42              |
| 2:D:261:ILE:HA    | 2:D:306:LYS:O     | 2.20                     | 0.42              |
| 2:D:274:ARG:HA    | 2:D:286:GLN:OE1   | 2.20                     | 0.42              |
| 3:G:7:ALA:O       | 3:G:10:ASP:HB2    | 2.20                     | 0.42              |
| 3:G:73:THR:HB     | 3:G:76:ILE:HD12   | 2.01                     | 0.42              |
| 3:G:143:ILE:HD11  | 3:G:220:VAL:HG22  | 2.02                     | 0.42              |
| 3:G:174:GLU:H     | 3:G:174:GLU:CD    | 2.23                     | 0.42              |
| 3:G:232:GLU:CD    | 3:G:232:GLU:N     | 2.72                     | 0.42              |
| 6:J:116:GLN:HE22  | 26:K:87:THR:HG1   | 1.57                     | 0.42              |
| 6:J:145:TYR:CD1   | 6:J:155:ALA:HB2   | 2.54                     | 0.42              |
| 8:M:23:VAL:CG1    | 8:M:154:SER:HB3   | 2.49                     | 0.42              |
| 8:M:25:TYR:C      | 8:M:28:LYS:HG2    | 2.44                     | 0.42              |
| 8:M:30:VAL:HG13   | 8:M:78:ALA:O      | 2.19                     | 0.42              |
| 8:M:66:LEU:HD12   | 8:M:75:MET:O      | 2.20                     | 0.42              |
| 8:M:67:PHE:CZ     | 8:M:85:ARG:HD2    | 2.55                     | 0.42              |
| 9:V:65:ARG:O      | 9:V:69:THR:N      | 2.35                     | 0.42              |
| 9:V:225:ASP:OD1   | 9:V:225:ASP:N     | 2.53                     | 0.42              |
| 9:V:241:ARG:NH1   | 9:V:241:ARG:HB2   | 2.35                     | 0.42              |
| 9:V:389:ASP:OD1   | 9:V:389:ASP:N     | 2.53                     | 0.42              |
| 9:V:464:ILE:HG22  | 9:V:465:ASP:H     | 1.85                     | 0.42              |
| 10:W:55:ARG:HH12  | 10:W:93:ARG:CD    | 2.32                     | 0.42              |
| 11:X:76:PHE:CZ    | 11:X:80:ILE:HG21  | 2.55                     | 0.42              |
| 11:X:87:ARG:O     | 11:X:91:SER:OG    | 2.22                     | 0.42              |
| 11:X:153:LEU:HD23 | 11:X:153:LEU:HA   | 1.86                     | 0.42              |
| 11:X:385:LEU:CD2  | 11:X:387:ILE:HD11 | 2.48                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 12:Y:48:ASN:CB    | 12:Y:50:MET:HE2   | 2.44                     | 0.42              |
| 12:Y:205:VAL:HG21 | 12:Y:246:ILE:HG12 | 2.02                     | 0.42              |
| 13:Z:174:HIS:O    | 13:Z:177:ARG:HB2  | 2.20                     | 0.42              |
| 14:a:112:ILE:HA   | 14:a:115:LYS:CG   | 2.47                     | 0.42              |
| 14:a:135:ILE:HD11 | 14:a:158:LEU:CD2  | 2.49                     | 0.42              |
| 14:a:313:LYS:HE2  | 14:a:317:VAL:HG23 | 2.00                     | 0.42              |
| 15:b:26:LEU:HD21  | 15:b:80:PRO:CD    | 2.49                     | 0.42              |
| 16:c:163:ILE:HD11 | 16:c:172:HIS:HA   | 2.01                     | 0.42              |
| 16:c:199:HIS:CD2  | 16:c:199:HIS:N    | 2.88                     | 0.42              |
| 18:f:282:PHE:CE1  | 18:f:307:LEU:HD13 | 2.55                     | 0.42              |
| 18:f:441:LYS:CD   | 18:f:469:TYR:HE2  | 2.31                     | 0.42              |
| 18:f:463:LEU:HD23 | 18:f:463:LEU:O    | 2.19                     | 0.42              |
| 18:f:650:GLN:O    | 18:f:653:ALA:N    | 2.53                     | 0.42              |
| 18:f:821:LEU:HD23 | 18:f:821:LEU:N    | 2.34                     | 0.42              |
| 18:f:833:PHE:HA   | 18:f:839:PRO:HA   | 2.02                     | 0.42              |
| 19:g:108:THR:HG22 | 19:g:109:GLY:H    | 1.84                     | 0.42              |
| 20:u:126:LEU:HD13 | 20:u:175:VAL:HG11 | 2.01                     | 0.42              |
| 22:A:168:GLU:OE1  | 22:A:168:GLU:HA   | 2.20                     | 0.42              |
| 22:A:176:ASP:O    | 22:A:176:ASP:OD1  | 2.38                     | 0.42              |
| 22:A:333:ARG:HH11 | 25:F:394:ALA:HB1  | 1.84                     | 0.42              |
| 22:A:372:LEU:HD13 | 22:A:372:LEU:C    | 2.45                     | 0.42              |
| 22:A:376:LEU:O    | 22:A:418:LYS:HE2  | 2.19                     | 0.42              |
| 23:B:221:GLY:O    | 23:B:348:ASP:N    | 2.52                     | 0.42              |
| 25:F:201:ALA:O    | 25:F:205:PRO:HG2  | 2.19                     | 0.42              |
| 25:F:254:PRO:HA   | 25:F:290:ALA:CB   | 2.49                     | 0.42              |
| 25:F:370:SER:HA   | 25:F:373:MET:HE3  | 2.00                     | 0.42              |
| 26:K:81:LEU:HD12  | 26:K:81:LEU:H     | 1.84                     | 0.42              |
| 26:K:90:ASP:OD1   | 26:K:90:ASP:O     | 2.37                     | 0.42              |
| 26:K:109:VAL:HG22 | 26:K:154:PHE:HD2  | 1.82                     | 0.42              |
| 26:K:146:VAL:HG11 | 26:K:222:PRO:HG3  | 2.01                     | 0.42              |
| 27:U:419:ALA:HB3  | 27:U:450:HIS:CE1  | 2.55                     | 0.42              |
| 27:U:637:VAL:HG11 | 27:U:652:ALA:HA   | 2.02                     | 0.42              |
| 1:C:23:TYR:CD1    | 1:C:24:TYR:CD1    | 3.08                     | 0.42              |
| 1:C:23:TYR:CE1    | 27:U:105:ILE:HD12 | 2.55                     | 0.42              |
| 2:D:41:TYR:CG     | 27:U:152:GLY:HA3  | 2.55                     | 0.42              |
| 2:D:387:VAL:HG13  | 24:E:158:LEU:HD21 | 2.00                     | 0.42              |
| 2:D:391:ARG:NH2   | 2:D:395:LEU:HB2   | 2.34                     | 0.42              |
| 4:H:176:LYS:HZ2   | 4:H:176:LYS:HG2   | 1.64                     | 0.42              |
| 7:L:155:ASP:HB2   | 8:M:62:SER:HB2    | 2.00                     | 0.42              |
| 7:L:230:SER:HA    | 7:L:233:LEU:HB2   | 2.01                     | 0.42              |
| 9:V:93:PHE:HD1    | 9:V:96:ARG:HH21   | 1.68                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 9:V:119:GLY:HA3   | 9:V:147:PHE:O     | 2.20                     | 0.42              |
| 9:V:192:MET:HG2   | 9:V:192:MET:H     | 1.64                     | 0.42              |
| 9:V:244:ALA:CB    | 9:V:279:GLN:HE21  | 2.29                     | 0.42              |
| 10:W:60:MET:N     | 10:W:60:MET:SD    | 2.93                     | 0.42              |
| 10:W:287:VAL:HA   | 10:W:290:ILE:CG2  | 2.45                     | 0.42              |
| 11:X:66:LEU:HD12  | 11:X:69:LEU:HD23  | 2.00                     | 0.42              |
| 11:X:178:HIS:HD2  | 11:X:183:LEU:CD1  | 2.32                     | 0.42              |
| 12:Y:205:VAL:HG21 | 12:Y:246:ILE:CG1  | 2.49                     | 0.42              |
| 12:Y:228:MET:CE   | 12:Y:259:TYR:CZ   | 3.01                     | 0.42              |
| 13:Z:149:THR:CG2  | 13:Z:150:PRO:HD2  | 2.42                     | 0.42              |
| 13:Z:176:LEU:C    | 13:Z:178:ASP:N    | 2.77                     | 0.42              |
| 14:a:77:VAL:HA    | 14:a:80:ILE:CD1   | 2.50                     | 0.42              |
| 14:a:217:LEU:O    | 14:a:223:GLU:HG2  | 2.20                     | 0.42              |
| 15:b:76:HIS:O     | 15:b:77:THR:C     | 2.63                     | 0.42              |
| 16:c:31:VAL:HG21  | 16:c:141:VAL:HG11 | 2.02                     | 0.42              |
| 16:c:259:VAL:O    | 16:c:262:GLU:HB2  | 2.20                     | 0.42              |
| 16:c:285:GLU:O    | 16:c:288:VAL:N    | 2.53                     | 0.42              |
| 17:d:136:LEU:HB2  | 17:d:141:LEU:HD21 | 2.01                     | 0.42              |
| 17:d:293:PHE:CD1  | 17:d:298:LYS:HE3  | 2.46                     | 0.42              |
| 18:f:170:TRP:CD2  | 18:f:211:ILE:HG23 | 2.54                     | 0.42              |
| 18:f:231:LEU:HD21 | 18:f:853:VAL:HG22 | 2.02                     | 0.42              |
| 18:f:298:LEU:HD23 | 18:f:298:LEU:HA   | 1.73                     | 0.42              |
| 18:f:513:GLU:HB2  | 18:f:554:TYR:HE2  | 1.78                     | 0.42              |
| 18:f:723:TYR:O    | 18:f:761:MET:CE   | 2.68                     | 0.42              |
| 23:B:52:VAL:HG23  | 23:B:64:LYS:HB2   | 2.00                     | 0.42              |
| 24:E:40:TYR:HE1   | 25:F:76:ASN:HB3   | 1.85                     | 0.42              |
| 24:E:374:VAL:C    | 24:E:378:LYS:HB2  | 2.44                     | 0.42              |
| 25:F:74:LYS:NZ    | 25:F:78:GLU:HG3   | 2.34                     | 0.42              |
| 25:F:151:VAL:HB   | 25:F:160:ILE:CG2  | 2.50                     | 0.42              |
| 27:U:177:LEU:HD12 | 27:U:204:ILE:CD1  | 2.34                     | 0.42              |
| 27:U:247:GLN:HG3  | 27:U:904:LYS:CB   | 2.50                     | 0.42              |
| 27:U:658:ILE:HG12 | 27:U:763:VAL:HG11 | 2.01                     | 0.42              |
| 27:U:802:TYR:OH   | 27:U:882:ALA:HB3  | 2.19                     | 0.42              |
| 27:U:844:LYS:O    | 27:U:847:GLU:HB2  | 2.20                     | 0.42              |
| 27:U:873:PRO:HB2  | 27:U:876:GLN:CD   | 2.45                     | 0.42              |
| 1:C:78:ARG:NH1    | 23:B:165:ASP:O    | 2.52                     | 0.42              |
| 1:C:338:LEU:HD13  | 1:C:342:ILE:HG21  | 2.02                     | 0.42              |
| 1:C:370:ALA:CB    | 1:C:375:ARG:HH21  | 2.32                     | 0.42              |
| 3:G:73:THR:CG2    | 3:G:74:GLU:H      | 2.33                     | 0.42              |
| 3:G:243:ALA:O     | 10:W:92:LYS:CE    | 2.67                     | 0.42              |
| 4:H:26:LEU:HD23   | 4:H:26:LEU:HA     | 1.93                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:I:82:ASP:HA     | 5:I:85:VAL:CG1    | 2.50                     | 0.42              |
| 6:J:158:ALA:HB3   | 26:K:58:LEU:CD2   | 2.26                     | 0.42              |
| 6:J:184:ASP:O     | 6:J:188:ILE:HD12  | 2.19                     | 0.42              |
| 7:L:35:THR:N      | 7:L:161:ILE:O     | 2.36                     | 0.42              |
| 7:L:67:ASP:N      | 7:L:70:ILE:O      | 2.51                     | 0.42              |
| 9:V:81:GLN:O      | 9:V:84:LYS:HB3    | 2.19                     | 0.42              |
| 10:W:263:TRP:CE2  | 10:W:264:GLN:HG3  | 2.54                     | 0.42              |
| 12:Y:11:LEU:HG    | 12:Y:212:GLU:OE1  | 2.20                     | 0.42              |
| 12:Y:55:GLU:H     | 12:Y:55:GLU:HG2   | 1.64                     | 0.42              |
| 13:Z:225:GLN:C    | 13:Z:227:ILE:H    | 2.27                     | 0.42              |
| 14:a:159:SER:CB   | 14:a:168:ASN:HD21 | 2.29                     | 0.42              |
| 14:a:320:VAL:HG12 | 14:a:322:GLY:H    | 1.83                     | 0.42              |
| 16:c:25:VAL:HG13  | 16:c:29:GLU:OE1   | 2.20                     | 0.42              |
| 17:d:163:SER:HA   | 17:d:166:ARG:CG   | 2.49                     | 0.42              |
| 17:d:282:ILE:O    | 17:d:315:TYR:HA   | 2.20                     | 0.42              |
| 18:f:250:ARG:HG2  | 18:f:250:ARG:H    | 1.57                     | 0.42              |
| 18:f:407:MET:HB3  | 18:f:407:MET:HE3  | 1.82                     | 0.42              |
| 18:f:483:PHE:HB2  | 18:f:517:VAL:CG1  | 2.48                     | 0.42              |
| 18:f:505:MET:HE1  | 18:f:519:ALA:HA   | 2.02                     | 0.42              |
| 18:f:596:ASP:OD1  | 18:f:608:LYS:HE3  | 2.20                     | 0.42              |
| 19:g:107:ILE:HG13 | 19:g:115:LYS:HZ3  | 1.81                     | 0.42              |
| 22:A:103:ASN:O    | 22:A:104:ALA:C    | 2.63                     | 0.42              |
| 22:A:381:THR:O    | 22:A:385:ILE:HG12 | 2.20                     | 0.42              |
| 23:B:165:ASP:OD1  | 23:B:165:ASP:O    | 2.37                     | 0.42              |
| 23:B:249:ARG:HG2  | 23:B:249:ARG:HH11 | 1.85                     | 0.42              |
| 24:E:171:LEU:CD1  | 24:E:279:THR:HG22 | 2.37                     | 0.42              |
| 26:K:83:LYS:HE3   | 26:K:83:LYS:HB2   | 1.89                     | 0.42              |
| 27:U:11:LEU:HB2   | 27:U:23:ALA:HB2   | 2.02                     | 0.42              |
| 27:U:422:LEU:HG   | 27:U:426:TYR:OH   | 2.20                     | 0.42              |
| 27:U:790:GLY:H    | 27:U:880:ASN:HB3  | 1.85                     | 0.42              |
| 1:C:213:ARG:HG2   | 1:C:213:ARG:HH11  | 1.84                     | 0.41              |
| 1:C:400:SER:CB    | 4:H:26:LEU:HD22   | 2.44                     | 0.41              |
| 2:D:151:ILE:HG21  | 2:D:250:VAL:HG22  | 2.02                     | 0.41              |
| 3:G:178:PHE:CD2   | 3:G:201:CYS:HA    | 2.55                     | 0.41              |
| 4:H:101:TYR:CD1   | 4:H:101:TYR:N     | 2.87                     | 0.41              |
| 5:I:76:VAL:HG13   | 5:I:132:VAL:HG23  | 2.01                     | 0.41              |
| 6:J:189:LYS:O     | 6:J:193:LYS:HG3   | 2.20                     | 0.41              |
| 7:L:69:HIS:NE2    | 7:L:103:LEU:O     | 2.30                     | 0.41              |
| 7:L:95:SER:CB     | 7:L:103:LEU:HB2   | 2.50                     | 0.41              |
| 8:M:70:ASP:CG     | 8:M:71:ARG:H      | 2.28                     | 0.41              |
| 10:W:110:THR:O    | 10:W:114:GLU:HG2  | 2.20                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 11:X:51:LEU:HD12  | 11:X:51:LEU:O     | 2.19                     | 0.41              |
| 11:X:141:LYS:HE3  | 11:X:143:TYR:OH   | 2.20                     | 0.41              |
| 11:X:414:LEU:CD2  | 13:Z:273:HIS:HA   | 2.50                     | 0.41              |
| 13:Z:230:LEU:O    | 13:Z:230:LEU:HD23 | 2.19                     | 0.41              |
| 14:a:68:GLU:OE1   | 14:a:71:VAL:HB    | 2.20                     | 0.41              |
| 14:a:114:CYS:O    | 14:a:117:ALA:HB3  | 2.21                     | 0.41              |
| 14:a:115:LYS:O    | 14:a:118:ILE:CG2  | 2.67                     | 0.41              |
| 14:a:365:MET:HA   | 14:a:368:GLU:CG   | 2.49                     | 0.41              |
| 16:c:183:HIS:CD2  | 27:U:770:TRP:HZ2  | 2.38                     | 0.41              |
| 17:d:293:PHE:HZ   | 17:d:302:TYR:CE2  | 2.37                     | 0.41              |
| 18:f:209:MET:HE2  | 23:B:59:ARG:HD3   | 2.01                     | 0.41              |
| 18:f:478:ARG:HH12 | 18:f:510:SER:HG   | 1.67                     | 0.41              |
| 18:f:711:SER:CA   | 18:f:729:MET:HE3  | 2.49                     | 0.41              |
| 18:f:807:ARG:H    | 18:f:807:ARG:HG3  | 1.65                     | 0.41              |
| 19:g:165:ALA:HA   | 19:g:168:ASN:CB   | 2.50                     | 0.41              |
| 23:B:127:VAL:O    | 23:B:127:VAL:HG12 | 2.20                     | 0.41              |
| 24:E:289:LEU:HD23 | 24:E:289:LEU:HA   | 1.88                     | 0.41              |
| 25:F:154:ASN:OD1  | 25:F:155:LYS:N    | 2.53                     | 0.41              |
| 25:F:222:GLY:HA2  | 25:F:328:VAL:O    | 2.19                     | 0.41              |
| 26:K:113:THR:HG23 | 26:K:143:PHE:CD2  | 2.55                     | 0.41              |
| 27:U:24:LEU:CD1   | 27:U:48:LEU:HD23  | 2.50                     | 0.41              |
| 27:U:163:PHE:CD1  | 27:U:163:PHE:C    | 2.96                     | 0.41              |
| 27:U:405:THR:HG21 | 27:U:438:GLN:HA   | 2.01                     | 0.41              |
| 27:U:462:LEU:HD12 | 27:U:462:LEU:HA   | 1.76                     | 0.41              |
| 27:U:486:MET:HE2  | 27:U:781:LEU:HD21 | 2.02                     | 0.41              |
| 27:U:675:MET:O    | 27:U:678:ASP:N    | 2.49                     | 0.41              |
| 27:U:756:HIS:HB3  | 27:U:759:SER:HB3  | 2.02                     | 0.41              |
| 1:C:354:ALA:CB    | 1:C:391:MET:HE1   | 2.51                     | 0.41              |
| 2:D:303:VAL:O     | 2:D:303:VAL:HG13  | 2.20                     | 0.41              |
| 2:D:327:LEU:O     | 2:D:330:LYS:NZ    | 2.53                     | 0.41              |
| 2:D:384:MET:CE    | 24:E:167:PRO:HG3  | 2.45                     | 0.41              |
| 3:G:9:PHE:O       | 3:G:11:ARG:N      | 2.54                     | 0.41              |
| 4:H:40:ALA:O      | 4:H:42:ASN:N      | 2.53                     | 0.41              |
| 5:I:241:GLU:OE2   | 5:I:241:GLU:HA    | 2.20                     | 0.41              |
| 6:J:83:VAL:HG23   | 6:J:114:LEU:HD23  | 2.02                     | 0.41              |
| 7:L:15:PRO:O      | 8:M:28:LYS:NZ     | 2.48                     | 0.41              |
| 9:V:121:PHE:HE1   | 9:V:167:LEU:CB    | 2.32                     | 0.41              |
| 9:V:236:ARG:CD    | 9:V:240:LEU:HD21  | 2.50                     | 0.41              |
| 10:W:22:ALA:O     | 10:W:25:ASP:HB3   | 2.21                     | 0.41              |
| 10:W:326:MET:HE3  | 10:W:327:GLU:N    | 2.34                     | 0.41              |
| 10:W:346:GLU:HG3  | 10:W:350:ARG:HH22 | 1.84                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 11:X:114:ILE:HD11 | 11:X:130:GLU:CA   | 2.50                     | 0.41              |
| 11:X:240:ASP:OD2  | 11:X:278:ARG:NH2  | 2.53                     | 0.41              |
| 12:Y:279:GLU:HB2  | 12:Y:296:VAL:CG2  | 2.48                     | 0.41              |
| 13:Z:262:LEU:HD12 | 13:Z:262:LEU:O    | 2.21                     | 0.41              |
| 14:a:38:THR:CB    | 14:a:71:VAL:HG13  | 2.49                     | 0.41              |
| 14:a:81:LEU:O     | 14:a:84:VAL:HG12  | 2.21                     | 0.41              |
| 14:a:94:LEU:HA    | 14:a:97:LEU:CD2   | 2.50                     | 0.41              |
| 15:b:23:PRO:O     | 15:b:24:THR:OG1   | 2.31                     | 0.41              |
| 15:b:109:ILE:HB   | 15:b:138:VAL:CG2  | 2.49                     | 0.41              |
| 15:b:172:THR:O    | 15:b:172:THR:CG2  | 2.67                     | 0.41              |
| 16:c:40:LYS:HZ3   | 16:c:40:LYS:HB2   | 1.85                     | 0.41              |
| 16:c:161:ARG:O    | 16:c:201:TYR:CE1  | 2.74                     | 0.41              |
| 17:d:218:LYS:HE2  | 17:d:222:THR:HB   | 2.01                     | 0.41              |
| 18:f:378:ASN:HB2  | 18:f:398:TRP:HH2  | 1.85                     | 0.41              |
| 18:f:391:LEU:HD23 | 18:f:417:ILE:HD12 | 2.01                     | 0.41              |
| 18:f:792:ALA:HB1  | 18:f:824:ALA:CB   | 2.50                     | 0.41              |
| 19:g:109:GLY:O    | 19:g:112:LEU:HB3  | 2.20                     | 0.41              |
| 22:A:126:SER:O    | 22:A:129:VAL:HG12 | 2.21                     | 0.41              |
| 22:A:212:VAL:HA   | 22:A:339:ARG:O    | 2.20                     | 0.41              |
| 23:B:424:GLU:O    | 23:B:428:TYR:CE1  | 2.73                     | 0.41              |
| 24:E:247:THR:HG23 | 24:E:250:ASP:OD2  | 2.19                     | 0.41              |
| 24:E:313:LEU:O    | 24:E:317:ALA:CB   | 2.68                     | 0.41              |
| 25:F:66:LEU:HA    | 25:F:66:LEU:HD13  | 1.83                     | 0.41              |
| 25:F:188:ILE:HG12 | 25:F:235:LEU:CG   | 2.50                     | 0.41              |
| 25:F:330:ALA:HB3  | 25:F:348:LEU:CD1  | 2.50                     | 0.41              |
| 26:K:51:GLU:HA    | 26:K:215:ILE:HG22 | 2.02                     | 0.41              |
| 27:U:187:LEU:C    | 27:U:188:MET:HE2  | 2.43                     | 0.41              |
| 27:U:213:PHE:O    | 27:U:216:VAL:HG12 | 2.20                     | 0.41              |
| 27:U:353:LEU:HA   | 27:U:353:LEU:HD23 | 1.81                     | 0.41              |
| 27:U:443:LEU:HD13 | 27:U:464:GLN:HG3  | 2.02                     | 0.41              |
| 27:U:443:LEU:HD13 | 27:U:464:GLN:CG   | 2.50                     | 0.41              |
| 27:U:641:SER:O    | 27:U:675:MET:HE2  | 2.19                     | 0.41              |
| 27:U:792:ASN:HD21 | 27:U:796:LYS:CE   | 2.32                     | 0.41              |
| 27:U:827:LYS:HB2  | 27:U:827:LYS:HE2  | 1.81                     | 0.41              |
| 1:C:27:LYS:O      | 1:C:30:GLU:HG3    | 2.21                     | 0.41              |
| 1:C:168:PRO:HG3   | 1:C:175:PHE:CZ    | 2.55                     | 0.41              |
| 2:D:45:LYS:HE2    | 2:D:45:LYS:HA     | 2.02                     | 0.41              |
| 2:D:410:ASP:N     | 2:D:410:ASP:OD1   | 2.53                     | 0.41              |
| 4:H:75:VAL:HG23   | 4:H:135:LEU:CB    | 2.35                     | 0.41              |
| 4:H:121:TYR:O     | 4:H:127:VAL:HG23  | 2.20                     | 0.41              |
| 5:I:17:ARG:HG2    | 6:J:28:LYS:HZ3    | 1.84                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:I:119:GLN:O     | 5:I:122:THR:N     | 2.52                     | 0.41              |
| 5:I:124:PHE:HE1   | 6:J:118:TYR:CE1   | 2.35                     | 0.41              |
| 7:L:6:TYR:HE1     | 8:M:9:LEU:HD12    | 1.84                     | 0.41              |
| 7:L:108:LEU:HD12  | 7:L:108:LEU:C     | 2.46                     | 0.41              |
| 7:L:147:THR:O     | 7:L:147:THR:OG1   | 2.28                     | 0.41              |
| 8:M:137:LEU:O     | 8:M:148:LEU:HA    | 2.19                     | 0.41              |
| 8:M:149:TYR:CD1   | 8:M:159:GLY:CA    | 3.03                     | 0.41              |
| 9:V:80:LYS:O      | 9:V:84:LYS:N      | 2.53                     | 0.41              |
| 9:V:82:LEU:HD22   | 9:V:162:GLU:HG3   | 2.03                     | 0.41              |
| 9:V:191:LEU:HD12  | 9:V:195:ILE:HG23  | 2.02                     | 0.41              |
| 9:V:205:LEU:HD22  | 9:V:205:LEU:N     | 2.35                     | 0.41              |
| 9:V:440:LYS:HD2   | 9:V:444:ASP:OD1   | 2.20                     | 0.41              |
| 10:W:72:LYS:HD2   | 10:W:76:GLU:CD    | 2.45                     | 0.41              |
| 10:W:125:ILE:HA   | 10:W:145:LEU:HD12 | 2.02                     | 0.41              |
| 10:W:451:MET:CE   | 13:Z:100:LYS:HA   | 2.50                     | 0.41              |
| 11:X:125:LEU:C    | 11:X:128:ALA:H    | 2.28                     | 0.41              |
| 11:X:200:ILE:HG13 | 11:X:201:TYR:N    | 2.31                     | 0.41              |
| 11:X:351:SER:HB2  | 11:X:356:LEU:O    | 2.19                     | 0.41              |
| 12:Y:309:GLU:OE2  | 12:Y:309:GLU:CA   | 2.63                     | 0.41              |
| 13:Z:10:VAL:HG21  | 13:Z:49:ASP:OD1   | 2.20                     | 0.41              |
| 13:Z:17:LEU:HD21  | 16:c:35:SER:O     | 2.20                     | 0.41              |
| 13:Z:69:PHE:CE2   | 15:b:96:ALA:HA    | 2.55                     | 0.41              |
| 14:a:135:ILE:HG13 | 14:a:158:LEU:CD2  | 2.51                     | 0.41              |
| 14:a:193:GLN:HB3  | 14:a:225:LEU:HD13 | 2.01                     | 0.41              |
| 14:a:281:THR:HG23 | 14:a:335:TRP:CE3  | 2.55                     | 0.41              |
| 14:a:312:MET:HA   | 14:a:312:MET:CE   | 2.44                     | 0.41              |
| 18:f:515:ALA:O    | 18:f:518:THR:HB   | 2.19                     | 0.41              |
| 19:g:168:ASN:O    | 19:g:171:LEU:N    | 2.52                     | 0.41              |
| 22:A:83:ASP:CG    | 23:B:137:SER:H    | 2.28                     | 0.41              |
| 22:A:189:GLU:OE1  | 22:A:189:GLU:HA   | 2.19                     | 0.41              |
| 22:A:272:ILE:HD13 | 22:A:272:ILE:N    | 2.34                     | 0.41              |
| 22:A:292:ASP:HB2  | 23:B:300:GLY:CA   | 2.50                     | 0.41              |
| 24:E:40:TYR:HE1   | 25:F:76:ASN:CB    | 2.33                     | 0.41              |
| 24:E:55:GLN:OE1   | 25:F:135:PRO:HD3  | 2.21                     | 0.41              |
| 24:E:122:MET:CE   | 25:F:344:ARG:NH1  | 2.80                     | 0.41              |
| 25:F:226:TYR:CD1  | 25:F:226:TYR:C    | 2.99                     | 0.41              |
| 25:F:294:LYS:HB3  | 25:F:295:ARG:NH2  | 2.36                     | 0.41              |
| 26:K:227:HIS:NE2  | 26:K:229:PHE:O    | 2.53                     | 0.41              |
| 27:U:202:VAL:O    | 27:U:205:TYR:HB2  | 2.20                     | 0.41              |
| 27:U:466:LYS:HE2  | 27:U:466:LYS:HB2  | 1.91                     | 0.41              |
| 1:C:256:SER:O     | 1:C:257:SER:C     | 2.64                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:277:LEU:HD23  | 1:C:310:ARG:HD2   | 2.03                     | 0.41              |
| 2:D:126:PRO:O     | 2:D:127:ASN:OD1   | 2.38                     | 0.41              |
| 2:D:239:TYR:O     | 2:D:242:GLU:HG2   | 2.20                     | 0.41              |
| 3:G:138:MET:HE3   | 3:G:138:MET:HB3   | 1.66                     | 0.41              |
| 4:H:71:HIS:C      | 4:H:72:ILE:HG13   | 2.45                     | 0.41              |
| 4:H:80:GLY:O      | 4:H:81:PRO:C      | 2.63                     | 0.41              |
| 4:H:118:MET:HE2   | 4:H:150:ASP:O     | 2.20                     | 0.41              |
| 5:I:239:LYS:O     | 5:I:242:GLU:HG2   | 2.20                     | 0.41              |
| 7:L:24:TYR:HD2    | 26:K:15:PHE:O     | 2.04                     | 0.41              |
| 9:V:74:ASP:O      | 9:V:78:HIS:N      | 2.40                     | 0.41              |
| 9:V:175:MET:HG3   | 9:V:184:ALA:HB2   | 2.03                     | 0.41              |
| 9:V:201:ARG:HH12  | 9:V:241:ARG:HD3   | 1.84                     | 0.41              |
| 9:V:212:TYR:CD2   | 9:V:213:TYR:HD1   | 2.38                     | 0.41              |
| 9:V:435:GLU:OE1   | 9:V:453:HIS:NE2   | 2.52                     | 0.41              |
| 10:W:436:MET:HE3  | 10:W:436:MET:HB2  | 1.96                     | 0.41              |
| 11:X:155:ARG:HG2  | 11:X:155:ARG:HH11 | 1.85                     | 0.41              |
| 11:X:407:MET:C    | 11:X:410:VAL:HG12 | 2.45                     | 0.41              |
| 14:a:119:GLY:O    | 14:a:123:LEU:HB2  | 2.20                     | 0.41              |
| 14:a:244:ASN:ND2  | 14:a:246:GLU:HB3  | 2.35                     | 0.41              |
| 14:a:277:LEU:HD21 | 14:a:333:MET:HE3  | 2.02                     | 0.41              |
| 14:a:335:TRP:NE1  | 14:a:337:GLN:HB3  | 2.34                     | 0.41              |
| 14:a:352:ARG:HG2  | 14:a:352:ARG:HH11 | 1.86                     | 0.41              |
| 15:b:104:ASN:OD1  | 15:b:104:ASN:C    | 2.63                     | 0.41              |
| 15:b:138:VAL:O    | 15:b:168:SER:HB3  | 2.21                     | 0.41              |
| 15:b:184:ILE:HA   | 15:b:188:ILE:HB   | 2.00                     | 0.41              |
| 17:d:146:ASP:HA   | 17:d:149:GLU:HB2  | 2.03                     | 0.41              |
| 17:d:269:ASP:O    | 17:d:272:ALA:HB3  | 2.21                     | 0.41              |
| 18:f:90:THR:HG23  | 23:B:411:ARG:HA   | 2.02                     | 0.41              |
| 18:f:242:GLU:CD   | 18:f:245:ASN:HD21 | 2.28                     | 0.41              |
| 18:f:430:ASP:HB2  | 19:g:169:PHE:N    | 2.36                     | 0.41              |
| 18:f:478:ARG:NH2  | 18:f:509:LYS:HZ2  | 2.19                     | 0.41              |
| 22:A:258:ARG:HG3  | 22:A:301:GLU:OE2  | 2.20                     | 0.41              |
| 23:B:71:TYR:O     | 23:B:75:GLU:N     | 2.46                     | 0.41              |
| 23:B:233:THR:O    | 23:B:237:LYS:HG3  | 2.20                     | 0.41              |
| 23:B:371:ARG:HG3  | 23:B:371:ARG:HH11 | 1.86                     | 0.41              |
| 23:B:409:GLU:HB3  | 23:B:411:ARG:HH12 | 1.85                     | 0.41              |
| 24:E:271:HIS:C    | 24:E:272:ARG:HH21 | 2.28                     | 0.41              |
| 25:F:220:PRO:CG   | 25:F:350:ARG:HD3  | 2.49                     | 0.41              |
| 25:F:251:LEU:O    | 25:F:252:ALA:C    | 2.63                     | 0.41              |
| 25:F:253:GLY:N    | 25:F:254:PRO:CD   | 2.83                     | 0.41              |
| 25:F:376:SER:O    | 25:F:379:VAL:HG23 | 2.20                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 26:K:225:ASN:O    | 26:K:228:MET:SD   | 2.79                     | 0.41              |
| 27:U:37:GLU:H     | 27:U:37:GLU:CD    | 2.26                     | 0.41              |
| 27:U:368:ALA:CA   | 27:U:371:ILE:HG22 | 2.51                     | 0.41              |
| 27:U:469:SER:HG   | 27:U:471:ASP:CG   | 2.12                     | 0.41              |
| 27:U:831:ALA:O    | 27:U:836:THR:CB   | 2.68                     | 0.41              |
| 27:U:880:ASN:N    | 27:U:881:PRO:HD2  | 2.36                     | 0.41              |
| 1:C:82:LYS:HD2    | 1:C:82:LYS:HA     | 1.75                     | 0.41              |
| 1:C:251:ILE:HG21  | 1:C:301:LEU:HD11  | 2.01                     | 0.41              |
| 2:D:225:ALA:HB1   | 2:D:259:PRO:O     | 2.20                     | 0.41              |
| 2:D:355:SER:OG    | 2:D:357:GLU:CD    | 2.64                     | 0.41              |
| 4:H:12:THR:O      | 4:H:12:THR:OG1    | 2.38                     | 0.41              |
| 4:H:14:SER:OG     | 4:H:18:LYS:N      | 2.50                     | 0.41              |
| 4:H:111:VAL:CG1   | 4:H:155:TYR:HB2   | 2.50                     | 0.41              |
| 4:H:144:PRO:O     | 4:H:145:TYR:HD1   | 2.03                     | 0.41              |
| 4:H:179:ASN:OD1   | 4:H:179:ASN:C     | 2.63                     | 0.41              |
| 4:H:184:LEU:O     | 4:H:188:ILE:HD12  | 2.20                     | 0.41              |
| 5:I:105:ILE:O     | 5:I:107:CYS:N     | 2.47                     | 0.41              |
| 5:I:158:GLY:N     | 6:J:58:THR:HG21   | 2.35                     | 0.41              |
| 7:L:72:ILE:HD12   | 7:L:72:ILE:O      | 2.20                     | 0.41              |
| 7:L:133:LEU:HA    | 7:L:145:PHE:O     | 2.20                     | 0.41              |
| 7:L:160:SER:CB    | 7:L:168:ALA:HB3   | 2.50                     | 0.41              |
| 8:M:120:HIS:HB2   | 8:M:155:GLY:HA3   | 2.02                     | 0.41              |
| 8:M:181:MET:H     | 8:M:181:MET:HG3   | 1.59                     | 0.41              |
| 10:W:263:TRP:CZ3  | 10:W:295:LYS:HB3  | 2.56                     | 0.41              |
| 10:W:371:THR:O    | 10:W:414:ASN:HA   | 2.20                     | 0.41              |
| 11:X:57:LEU:HB3   | 11:X:66:LEU:HD13  | 2.03                     | 0.41              |
| 12:Y:61:LEU:O     | 12:Y:63:TRP:HD1   | 2.04                     | 0.41              |
| 12:Y:316:LEU:HD11 | 12:Y:331:ASP:HB2  | 2.02                     | 0.41              |
| 13:Z:156:GLU:HG2  | 13:Z:157:HIS:H    | 1.86                     | 0.41              |
| 13:Z:201:LEU:O    | 13:Z:201:LEU:HD12 | 2.20                     | 0.41              |
| 13:Z:246:VAL:CG2  | 17:d:330:ILE:HD11 | 2.46                     | 0.41              |
| 14:a:5:PRO:HA     | 14:a:8:LEU:HD21   | 2.01                     | 0.41              |
| 14:a:18:GLN:HA    | 14:a:21:VAL:CG2   | 2.51                     | 0.41              |
| 14:a:78:GLU:OE1   | 14:a:82:HIS:HE1   | 2.03                     | 0.41              |
| 14:a:84:VAL:HG21  | 14:a:93:ALA:CB    | 2.50                     | 0.41              |
| 14:a:293:PHE:CD2  | 14:a:294:GLU:HG3  | 2.55                     | 0.41              |
| 16:c:61:PHE:HD1   | 16:c:67:VAL:HG22  | 1.86                     | 0.41              |
| 17:d:199:LEU:N    | 17:d:199:LEU:HD23 | 2.36                     | 0.41              |
| 17:d:283:LEU:HA   | 17:d:315:TYR:CD1  | 2.55                     | 0.41              |
| 18:f:608:LYS:O    | 18:f:612:LEU:N    | 2.43                     | 0.41              |
| 18:f:801:VAL:HG23 | 18:f:802:SER:N    | 2.36                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 18:f:828:ARG:HD3  | 18:f:829:MET:N    | 2.35                     | 0.41              |
| 18:f:872:VAL:HG12 | 18:f:873:LEU:N    | 2.35                     | 0.41              |
| 19:g:170:GLN:O    | 19:g:171:LEU:C    | 2.63                     | 0.41              |
| 22:A:172:VAL:HG23 | 22:A:176:ASP:OD2  | 2.20                     | 0.41              |
| 22:A:334:PRO:HG2  | 25:F:394:ALA:C    | 2.44                     | 0.41              |
| 22:A:367:ASP:O    | 22:A:368:ILE:C    | 2.64                     | 0.41              |
| 22:A:373:LEU:HD11 | 22:A:409:PHE:CB   | 2.49                     | 0.41              |
| 23:B:66:GLU:HG2   | 27:U:834:SER:CB   | 2.36                     | 0.41              |
| 24:E:251:ARG:HG3  | 24:E:255:ARG:CZ   | 2.50                     | 0.41              |
| 24:E:308:ALA:O    | 24:E:312:ILE:N    | 2.42                     | 0.41              |
| 25:F:272:PHE:CE2  | 25:F:320:PHE:HE2  | 2.38                     | 0.41              |
| 25:F:288:LEU:HB3  | 25:F:332:THR:HG1  | 1.83                     | 0.41              |
| 27:U:54:PHE:HB3   | 27:U:57:ARG:HG3   | 2.01                     | 0.41              |
| 27:U:181:LEU:HA   | 27:U:201:LEU:CD1  | 2.51                     | 0.41              |
| 27:U:194:ARG:HG2  | 27:U:194:ARG:HH11 | 1.85                     | 0.41              |
| 27:U:332:GLU:OE2  | 27:U:453:HIS:HE1  | 2.03                     | 0.41              |
| 27:U:509:GLY:HA3  | 27:U:544:ILE:CG1  | 2.27                     | 0.41              |
| 27:U:636:VAL:HG13 | 27:U:637:VAL:N    | 2.35                     | 0.41              |
| 27:U:653:ALA:HA   | 27:U:672:LEU:HD21 | 2.03                     | 0.41              |
| 2:D:296:MET:CE    | 2:D:309:MET:HE2   | 2.38                     | 0.41              |
| 3:G:84:THR:HB     | 8:M:156:VAL:HG12  | 2.01                     | 0.41              |
| 3:G:208:ILE:HG22  | 3:G:209:ASP:N     | 2.36                     | 0.41              |
| 4:H:34:PRO:CG     | 4:H:49:GLU:HG2    | 2.49                     | 0.41              |
| 5:I:98:LEU:O      | 5:I:102:GLN:HA    | 2.21                     | 0.41              |
| 5:I:159:TRP:CE2   | 6:J:54:GLN:HB3    | 2.56                     | 0.41              |
| 6:J:4:ASP:HB2     | 6:J:21:TYR:CE2    | 2.55                     | 0.41              |
| 6:J:152:THR:HG22  | 26:K:83:LYS:HG3   | 2.03                     | 0.41              |
| 8:M:36:ALA:HB3    | 8:M:78:ALA:HB2    | 2.02                     | 0.41              |
| 8:M:206:ASP:OD1   | 8:M:206:ASP:N     | 2.54                     | 0.41              |
| 9:V:69:THR:O      | 9:V:73:GLU:HG3    | 2.21                     | 0.41              |
| 9:V:184:ALA:CA    | 9:V:187:ILE:HB    | 2.40                     | 0.41              |
| 9:V:358:MET:N     | 9:V:359:PRO:CD    | 2.84                     | 0.41              |
| 10:W:102:ALA:C    | 10:W:106:GLN:HE22 | 2.29                     | 0.41              |
| 10:W:242:SER:HA   | 10:W:245:LYS:HE3  | 2.03                     | 0.41              |
| 11:X:272:SER:O    | 11:X:277:LEU:CD2  | 2.68                     | 0.41              |
| 11:X:371:ASP:O    | 11:X:372:LYS:HB2  | 2.21                     | 0.41              |
| 12:Y:22:LEU:HD23  | 12:Y:22:LEU:HA    | 1.75                     | 0.41              |
| 12:Y:247:LEU:O    | 12:Y:250:LEU:HB2  | 2.20                     | 0.41              |
| 13:Z:54:PHE:CG    | 13:Z:78:MET:HG2   | 2.55                     | 0.41              |
| 14:a:295:GLU:HA   | 14:a:298:LYS:CE   | 2.51                     | 0.41              |
| 14:a:349:MET:HB2  | 14:a:349:MET:HE3  | 1.66                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 15:b:61:LEU:H     | 15:b:61:LEU:HD12  | 1.85                     | 0.41              |
| 15:b:98:LYS:HB2   | 15:b:98:LYS:HE3   | 1.79                     | 0.41              |
| 17:d:93:GLY:O     | 17:d:97:GLN:HG3   | 2.20                     | 0.41              |
| 17:d:232:LEU:HD12 | 17:d:232:LEU:HA   | 1.82                     | 0.41              |
| 17:d:244:VAL:HG11 | 17:d:267:ILE:HD13 | 1.99                     | 0.41              |
| 17:d:251:ILE:HD12 | 17:d:257:THR:OG1  | 2.21                     | 0.41              |
| 17:d:254:GLU:H    | 17:d:254:GLU:CD   | 2.29                     | 0.41              |
| 18:f:172:GLU:HG2  | 18:f:172:GLU:O    | 2.20                     | 0.41              |
| 18:f:450:ILE:HG12 | 18:f:822:VAL:HG11 | 2.01                     | 0.41              |
| 18:f:685:THR:HA   | 18:f:688:ARG:HD2  | 2.02                     | 0.41              |
| 18:f:722:SER:OG   | 18:f:758:ASN:OD1  | 2.25                     | 0.41              |
| 18:f:759:LEU:O    | 18:f:763:ARG:HB2  | 2.21                     | 0.41              |
| 18:f:844:VAL:O    | 18:f:844:VAL:HG23 | 2.20                     | 0.41              |
| 19:g:89:LEU:CD2   | 19:g:155:VAL:HG21 | 2.50                     | 0.41              |
| 19:g:116:ILE:HD13 | 19:g:136:LEU:HD11 | 2.02                     | 0.41              |
| 20:u:177:LEU:HD22 | 20:u:265:PHE:HD2  | 1.86                     | 0.41              |
| 22:A:113:ILE:O    | 22:A:113:ILE:HG13 | 2.17                     | 0.41              |
| 22:A:167:GLU:O    | 22:A:167:GLU:HG2  | 2.21                     | 0.41              |
| 22:A:230:ALA:CA   | 22:A:233:THR:HG23 | 2.47                     | 0.41              |
| 22:A:279:ALA:O    | 23:B:307:ARG:HD3  | 2.21                     | 0.41              |
| 22:A:395:PHE:CE2  | 22:A:411:GLU:HB3  | 2.55                     | 0.41              |
| 23:B:259:TYR:HB2  | 23:B:262:ASP:CB   | 2.44                     | 0.41              |
| 23:B:376:ASP:OD1  | 23:B:376:ASP:N    | 2.54                     | 0.41              |
| 24:E:135:ILE:HD11 | 24:E:186:ALA:CB   | 2.50                     | 0.41              |
| 24:E:193:CYS:HB2  | 24:E:227:PRO:HG2  | 2.01                     | 0.41              |
| 24:E:304:PRO:HG2  | 24:E:340:GLY:CA   | 2.50                     | 0.41              |
| 25:F:202:ILE:HG13 | 25:F:329:ILE:HD11 | 2.02                     | 0.41              |
| 25:F:203:VAL:HG22 | 25:F:244:THR:CB   | 2.50                     | 0.41              |
| 25:F:280:PRO:CB   | 25:F:325:GLN:HB3  | 2.50                     | 0.41              |
| 25:F:307:GLN:O    | 25:F:311:LEU:HD23 | 2.20                     | 0.41              |
| 26:K:90:ASP:O     | 26:K:94:VAL:HG23  | 2.21                     | 0.41              |
| 27:U:27:LEU:HD23  | 27:U:27:LEU:HA    | 1.88                     | 0.41              |
| 27:U:185:MET:HE2  | 27:U:222:PHE:HE2  | 1.86                     | 0.41              |
| 27:U:246:TYR:CE2  | 27:U:794:ASP:HB3  | 2.55                     | 0.41              |
| 27:U:247:GLN:CG   | 27:U:904:LYS:HD2  | 2.49                     | 0.41              |
| 27:U:504:ASP:HB2  | 27:U:535:TYR:OH   | 2.21                     | 0.41              |
| 27:U:895:PRO:HG2  | 27:U:902:PRO:HD3  | 2.03                     | 0.41              |
| 1:C:328:ILE:HD11  | 29:C:501:ATP:N6   | 2.36                     | 0.41              |
| 2:D:143:LEU:HG    | 24:E:64:LEU:HD11  | 2.03                     | 0.41              |
| 2:D:185:LEU:HD13  | 2:D:225:ALA:HB2   | 2.02                     | 0.41              |
| 2:D:238:LYS:CG    | 2:D:239:TYR:H     | 2.34                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:H:24:TYR:O      | 4:H:27:ALA:HB3    | 2.21                     | 0.41              |
| 4:H:36:VAL:HG13   | 4:H:195:LEU:HD23  | 2.02                     | 0.41              |
| 4:H:134:LEU:O     | 4:H:148:GLN:HA    | 2.20                     | 0.41              |
| 4:H:226:VAL:HG12  | 4:H:230:LEU:HD12  | 2.02                     | 0.41              |
| 5:I:240:HIS:O     | 5:I:244:GLU:HG2   | 2.20                     | 0.41              |
| 6:J:86:ARG:O      | 6:J:86:ARG:HD3    | 2.21                     | 0.41              |
| 7:L:185:ASN:O     | 7:L:188:VAL:HG12  | 2.20                     | 0.41              |
| 9:V:79:VAL:HG12   | 9:V:83:GLU:OE2    | 2.19                     | 0.41              |
| 10:W:49:SER:HA    | 10:W:52:LYS:HZ3   | 1.85                     | 0.41              |
| 10:W:87:ILE:O     | 10:W:91:SER:HB3   | 2.21                     | 0.41              |
| 10:W:212:LYS:HA   | 10:W:212:LYS:CE   | 2.50                     | 0.41              |
| 10:W:369:TYR:N    | 10:W:369:TYR:CD1  | 2.89                     | 0.41              |
| 10:W:378:MET:SD   | 10:W:413:ILE:CD1  | 3.09                     | 0.41              |
| 11:X:53:LEU:HD23  | 11:X:53:LEU:HA    | 1.92                     | 0.41              |
| 11:X:115:GLU:HG3  | 11:X:116:TRP:N    | 2.36                     | 0.41              |
| 12:Y:301:ILE:HD13 | 12:Y:342:ARG:HB3  | 2.01                     | 0.41              |
| 13:Z:48:LEU:HD23  | 13:Z:120:VAL:CG1  | 2.50                     | 0.41              |
| 13:Z:144:VAL:HG21 | 14:a:178:ARG:HD3  | 2.01                     | 0.41              |
| 14:a:82:HIS:O     | 14:a:86:GLN:CB    | 2.69                     | 0.41              |
| 14:a:84:VAL:HG23  | 14:a:93:ALA:HB2   | 2.02                     | 0.41              |
| 14:a:130:VAL:HG23 | 14:a:133:GLU:HB3  | 2.03                     | 0.41              |
| 14:a:132:LYS:HZ3  | 14:a:162:TYR:CB   | 2.34                     | 0.41              |
| 14:a:186:LYS:HE2  | 14:a:190:VAL:HG22 | 2.03                     | 0.41              |
| 14:a:250:THR:HA   | 14:a:253:THR:HG22 | 2.01                     | 0.41              |
| 15:b:14:GLU:N     | 15:b:82:GLY:O     | 2.45                     | 0.41              |
| 15:b:51:LEU:CD1   | 15:b:61:LEU:HB2   | 2.50                     | 0.41              |
| 18:f:218:GLU:O    | 18:f:258:LYS:CD   | 2.68                     | 0.41              |
| 18:f:329:ASN:O    | 18:f:332:ALA:HB3  | 2.21                     | 0.41              |
| 18:f:435:SER:HB3  | 18:f:440:ILE:HG12 | 2.03                     | 0.41              |
| 18:f:459:CYS:CB   | 19:g:154:MET:HB2  | 2.51                     | 0.41              |
| 18:f:493:ASN:HA   | 18:f:498:LEU:HD11 | 2.02                     | 0.41              |
| 19:g:88:PHE:O     | 19:g:155:VAL:HB   | 2.21                     | 0.41              |
| 19:g:103:THR:HG23 | 19:g:104:ARG:O    | 2.20                     | 0.41              |
| 19:g:109:GLY:CA   | 19:g:145:GLN:HE22 | 2.34                     | 0.41              |
| 20:u:199:ASN:OD1  | 20:u:199:ASN:N    | 2.52                     | 0.41              |
| 22:A:121:PHE:CE2  | 22:A:147:TYR:CE2  | 3.07                     | 0.41              |
| 23:B:151:LEU:HB2  | 23:B:161:GLY:O    | 2.20                     | 0.41              |
| 23:B:347:ILE:HD13 | 23:B:347:ILE:HA   | 1.85                     | 0.41              |
| 24:E:233:ASP:O    | 24:E:235:ILE:HG13 | 2.19                     | 0.41              |
| 25:F:181:PRO:HB2  | 25:F:183:GLU:OE1  | 2.21                     | 0.41              |
| 26:K:66:LYS:NZ    | 26:K:78:MET:O     | 2.53                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 27:U:71:LEU:HD23  | 27:U:71:LEU:C     | 2.45                     | 0.41              |
| 27:U:136:LYS:HG3  | 27:U:137:MET:N    | 2.35                     | 0.41              |
| 27:U:199:ARG:O    | 27:U:202:VAL:HG13 | 2.21                     | 0.41              |
| 27:U:399:TRP:O    | 27:U:402:PHE:HB3  | 2.21                     | 0.41              |
| 27:U:405:THR:O    | 27:U:445:ALA:HB2  | 2.20                     | 0.41              |
| 27:U:669:ILE:HD11 | 27:U:695:MET:CG   | 2.46                     | 0.41              |
| 27:U:879:ASP:OD1  | 27:U:925:VAL:HG21 | 2.21                     | 0.41              |
| 28:e:61:GLU:O     | 28:e:65:TYR:HD2   | 2.03                     | 0.41              |
| 1:C:358:GLU:HA    | 2:D:324:PRO:HB2   | 2.02                     | 0.41              |
| 2:D:144:PRO:HD2   | 24:E:64:LEU:HD22  | 2.01                     | 0.41              |
| 3:G:98:ALA:O      | 3:G:101:TRP:N     | 2.53                     | 0.41              |
| 7:L:7:ASP:OD1     | 7:L:20:HIS:HB3    | 2.20                     | 0.41              |
| 8:M:77:VAL:CB     | 8:M:84:ALA:HB1    | 2.51                     | 0.41              |
| 8:M:116:ALA:C     | 8:M:117:MET:HE2   | 2.45                     | 0.41              |
| 8:M:173:LYS:C     | 8:M:177:GLU:HG3   | 2.45                     | 0.41              |
| 8:M:197:ILE:HG21  | 8:M:211:LEU:CD1   | 2.51                     | 0.41              |
| 9:V:79:VAL:HG12   | 9:V:83:GLU:CD     | 2.46                     | 0.41              |
| 9:V:159:LEU:HA    | 9:V:159:LEU:HD23  | 1.77                     | 0.41              |
| 9:V:345:ARG:CG    | 28:e:41:ASP:O     | 2.68                     | 0.41              |
| 10:W:230:MET:HE3  | 10:W:230:MET:O    | 2.21                     | 0.41              |
| 10:W:263:TRP:CH2  | 10:W:264:GLN:HG2  | 2.56                     | 0.41              |
| 10:W:366:MET:HE1  | 10:W:381:LEU:HB2  | 2.01                     | 0.41              |
| 10:W:448:LYS:HE3  | 10:W:448:LYS:HB3  | 1.87                     | 0.41              |
| 13:Z:20:VAL:HG23  | 16:c:216:MET:HE3  | 2.03                     | 0.41              |
| 13:Z:39:LEU:HD11  | 13:Z:95:TYR:HB3   | 2.01                     | 0.41              |
| 13:Z:113:LYS:HE3  | 13:Z:113:LYS:HB3  | 1.81                     | 0.41              |
| 13:Z:130:ASP:O    | 13:Z:131:LEU:C    | 2.63                     | 0.41              |
| 14:a:111:VAL:CG2  | 14:a:115:LYS:HE3  | 2.50                     | 0.41              |
| 14:a:112:ILE:CG1  | 14:a:138:VAL:HG11 | 2.51                     | 0.41              |
| 14:a:304:VAL:HA   | 14:a:307:VAL:HG12 | 2.02                     | 0.41              |
| 14:a:321:LYS:HG3  | 14:a:336:VAL:CG2  | 2.49                     | 0.41              |
| 15:b:38:HIS:HE1   | 15:b:72:LEU:CD1   | 2.31                     | 0.41              |
| 15:b:130:ARG:HH21 | 15:b:131:LEU:HD23 | 1.84                     | 0.41              |
| 16:c:31:VAL:O     | 16:c:205:ILE:HD12 | 2.21                     | 0.41              |
| 17:d:149:GLU:CD   | 17:d:187:TYR:HB2  | 2.46                     | 0.41              |
| 18:f:69:SER:C     | 18:f:73:PRO:HG2   | 2.46                     | 0.41              |
| 18:f:90:THR:HG23  | 23:B:412:MET:H    | 1.86                     | 0.41              |
| 18:f:189:LYS:NZ   | 18:f:216:MET:HE3  | 2.35                     | 0.41              |
| 18:f:193:PRO:HG3  | 18:f:220:ASP:OD2  | 2.20                     | 0.41              |
| 18:f:233:LEU:CD1  | 18:f:252:ALA:HB2  | 2.51                     | 0.41              |
| 18:f:553:THR:HG22 | 18:f:809:ILE:HD11 | 2.03                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 18:f:833:PHE:HA   | 18:f:838:ARG:O    | 2.20                     | 0.41              |
| 20:u:275:MET:CA   | 20:u:275:MET:HE2  | 2.50                     | 0.41              |
| 22:A:206:ILE:CG2  | 25:F:404:GLY:HA3  | 2.50                     | 0.41              |
| 22:A:293:ASN:O    | 22:A:297:ARG:HG3  | 2.21                     | 0.41              |
| 22:A:333:ARG:HG2  | 22:A:334:PRO:HD2  | 2.03                     | 0.41              |
| 23:B:200:SER:HB2  | 23:B:219:PRO:O    | 2.21                     | 0.41              |
| 24:E:273:VAL:HG22 | 24:E:274:LYS:N    | 2.35                     | 0.41              |
| 24:E:317:ALA:O    | 24:E:318:GLY:C    | 2.64                     | 0.41              |
| 26:K:149:LYS:O    | 26:K:149:LYS:HG3  | 2.21                     | 0.41              |
| 27:U:147:TYR:C    | 27:U:149:GLN:H    | 2.29                     | 0.41              |
| 27:U:554:LEU:CD2  | 27:U:761:VAL:HG22 | 2.48                     | 0.41              |
| 27:U:791:LEU:HD11 | 27:U:794:ASP:O    | 2.21                     | 0.41              |
| 1:C:45:LEU:HA     | 1:C:45:LEU:HD23   | 1.84                     | 0.41              |
| 1:C:49:ARG:NH2    | 27:U:639:LEU:O    | 2.45                     | 0.41              |
| 1:C:71:SER:HG     | 2:D:112:TYR:HD2   | 1.69                     | 0.41              |
| 1:C:151:ILE:HG12  | 1:C:198:LEU:CD2   | 2.50                     | 0.41              |
| 1:C:275:GLU:HG2   | 23:B:253:SER:HB3  | 2.02                     | 0.41              |
| 2:D:84:SER:HB3    | 16:c:152:LYS:NZ   | 2.36                     | 0.41              |
| 2:D:238:LYS:O     | 2:D:239:TYR:HB2   | 2.20                     | 0.41              |
| 2:D:410:ASP:CG    | 2:D:411:GLU:H     | 2.29                     | 0.41              |
| 4:H:65:VAL:HG22   | 4:H:75:VAL:HG11   | 1.97                     | 0.41              |
| 4:H:93:LEU:HD23   | 4:H:93:LEU:HA     | 1.81                     | 0.41              |
| 5:I:49:ARG:H      | 5:I:49:ARG:HG2    | 1.63                     | 0.41              |
| 5:I:56:LEU:HD23   | 5:I:56:LEU:C      | 2.45                     | 0.41              |
| 5:I:108:GLU:CA    | 5:I:148:TYR:HE2   | 2.34                     | 0.41              |
| 5:I:134:LEU:HG    | 5:I:136:TYR:CZ    | 2.55                     | 0.41              |
| 5:I:218:ARG:HA    | 5:I:218:ARG:HD2   | 1.93                     | 0.41              |
| 6:J:132:LEU:HD23  | 6:J:132:LEU:HA    | 1.79                     | 0.41              |
| 7:L:10:VAL:O      | 7:L:10:VAL:HG22   | 2.20                     | 0.41              |
| 7:L:18:ARG:HD2    | 7:L:23:GLU:OE2    | 2.21                     | 0.41              |
| 7:L:39:LYS:O      | 7:L:39:LYS:HG3    | 2.19                     | 0.41              |
| 7:L:55:GLU:HB2    | 26:K:182:GLN:HG3  | 2.02                     | 0.41              |
| 7:L:90:GLN:OE1    | 7:L:90:GLN:HA     | 2.21                     | 0.41              |
| 7:L:158:ALA:H     | 8:M:57:LEU:HD22   | 1.85                     | 0.41              |
| 8:M:66:LEU:CD1    | 8:M:76:ALA:HA     | 2.50                     | 0.41              |
| 9:V:69:THR:HG23   | 9:V:70:VAL:N      | 2.35                     | 0.41              |
| 9:V:73:GLU:HG3    | 9:V:147:PHE:HE2   | 1.85                     | 0.41              |
| 9:V:122:THR:HG22  | 9:V:128:ARG:HD2   | 2.01                     | 0.41              |
| 9:V:166:TYR:O     | 9:V:170:LEU:HD13  | 2.20                     | 0.41              |
| 9:V:168:GLN:O     | 9:V:172:VAL:N     | 2.40                     | 0.41              |
| 9:V:276:PHE:HD2   | 9:V:288:TYR:CD2   | 2.39                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 10:W:40:LEU:HB3   | 10:W:41:GLN:H     | 1.54                     | 0.41              |
| 10:W:86:ASN:C     | 10:W:90:LEU:HG    | 2.43                     | 0.41              |
| 10:W:275:ILE:HG23 | 10:W:309:PHE:CZ   | 2.54                     | 0.41              |
| 11:X:377:ILE:HG21 | 12:Y:312:ARG:CB   | 2.50                     | 0.41              |
| 12:Y:95:LEU:CG    | 12:Y:99:GLU:HG3   | 2.51                     | 0.41              |
| 13:Z:6:VAL:HG22   | 13:Z:139:ILE:HD11 | 2.02                     | 0.41              |
| 13:Z:38:VAL:HG11  | 13:Z:91:ILE:HG23  | 2.03                     | 0.41              |
| 13:Z:237:LEU:HB3  | 13:Z:238:PRO:HD2  | 2.02                     | 0.41              |
| 14:a:89:ASP:OD1   | 14:a:92:VAL:HG12  | 2.19                     | 0.41              |
| 14:a:142:LEU:O    | 14:a:142:LEU:HG   | 2.19                     | 0.41              |
| 14:a:143:ASN:C    | 14:a:144:ASN:OD1  | 2.64                     | 0.41              |
| 14:a:186:LYS:HG3  | 14:a:188:LEU:O    | 2.20                     | 0.41              |
| 14:a:219:HIS:ND1  | 14:a:220:PRO:HD2  | 2.36                     | 0.41              |
| 14:a:302:ILE:HD11 | 14:a:306:GLU:OE2  | 2.21                     | 0.41              |
| 15:b:15:TYR:C     | 15:b:17:ARG:H     | 2.29                     | 0.41              |
| 15:b:77:THR:O     | 15:b:77:THR:HG23  | 2.21                     | 0.41              |
| 15:b:97:LEU:CG    | 15:b:107:MET:CE   | 2.99                     | 0.41              |
| 15:b:118:GLU:O    | 15:b:118:GLU:HG2  | 2.20                     | 0.41              |
| 15:b:161:ASN:OD1  | 15:b:161:ASN:N    | 2.53                     | 0.41              |
| 16:c:32:TYR:HA    | 16:c:206:ASN:O    | 2.19                     | 0.41              |
| 16:c:137:SER:CB   | 20:u:273:THR:HG22 | 2.51                     | 0.41              |
| 17:d:138:LYS:N    | 17:d:138:LYS:HD2  | 2.36                     | 0.41              |
| 17:d:141:LEU:O    | 17:d:145:ARG:HB3  | 2.21                     | 0.41              |
| 17:d:188:MET:HG3  | 17:d:189:HIS:N    | 2.36                     | 0.41              |
| 17:d:233:GLU:OE2  | 17:d:233:GLU:C    | 2.64                     | 0.41              |
| 17:d:243:LYS:HB2  | 17:d:243:LYS:HE3  | 1.84                     | 0.41              |
| 17:d:248:LYS:HE3  | 17:d:248:LYS:HB3  | 1.89                     | 0.41              |
| 17:d:291:LEU:HD11 | 17:d:308:TRP:CZ3  | 2.56                     | 0.41              |
| 18:f:110:TYR:CE1  | 18:f:119:LYS:HG3  | 2.55                     | 0.41              |
| 18:f:231:LEU:HD22 | 18:f:852:VAL:HG13 | 2.03                     | 0.41              |
| 18:f:266:LEU:HD12 | 18:f:266:LEU:HA   | 1.94                     | 0.41              |
| 18:f:325:GLN:NE2  | 18:f:329:ASN:OD1  | 2.48                     | 0.41              |
| 18:f:367:SER:HB3  | 18:f:370:MET:HG3  | 2.02                     | 0.41              |
| 18:f:385:PHE:CZ   | 18:f:773:LYS:HD2  | 2.56                     | 0.41              |
| 18:f:446:LEU:O    | 18:f:450:ILE:N    | 2.45                     | 0.41              |
| 18:f:447:ALA:C    | 18:f:450:ILE:HG22 | 2.46                     | 0.41              |
| 18:f:557:TRP:HZ2  | 18:f:809:ILE:HG23 | 1.85                     | 0.41              |
| 18:f:754:LYS:HD2  | 18:f:754:LYS:HA   | 1.73                     | 0.41              |
| 18:f:807:ARG:O    | 18:f:812:GLY:N    | 2.54                     | 0.41              |
| 19:g:88:PHE:O     | 19:g:155:VAL:CB   | 2.69                     | 0.41              |
| 19:g:122:LEU:HD22 | 19:g:127:ILE:CD1  | 2.51                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 20:u:156:PHE:CD2  | 20:u:259:ARG:HG2  | 2.56                     | 0.41              |
| 20:u:246:ILE:HD12 | 20:u:246:ILE:N    | 2.35                     | 0.41              |
| 22:A:134:ILE:CD1  | 22:A:152:PRO:HG3  | 2.51                     | 0.41              |
| 22:A:433:ASN:ND2  | 26:K:66:LYS:HG2   | 2.36                     | 0.41              |
| 23:B:121:ALA:HB3  | 23:B:135:ILE:CD1  | 2.43                     | 0.41              |
| 23:B:197:ILE:O    | 23:B:197:ILE:CG1  | 2.64                     | 0.41              |
| 23:B:430:LYS:O    | 23:B:431:GLN:C    | 2.64                     | 0.41              |
| 24:E:60:VAL:O     | 24:E:61:LEU:HD23  | 2.20                     | 0.41              |
| 24:E:61:LEU:O     | 24:E:62:LYS:HB2   | 2.21                     | 0.41              |
| 24:E:90:SER:O     | 24:E:91:LYS:C     | 2.63                     | 0.41              |
| 24:E:105:LEU:HD23 | 24:E:105:LEU:HA   | 1.98                     | 0.41              |
| 24:E:178:THR:HG21 | 24:E:301:ILE:O    | 2.20                     | 0.41              |
| 24:E:261:LEU:HD11 | 24:E:288:ALA:HB3  | 2.03                     | 0.41              |
| 24:E:356:ARG:HH22 | 25:F:200:GLU:HG2  | 1.86                     | 0.41              |
| 25:F:189:GLY:O    | 29:F:501:ATP:N6   | 2.48                     | 0.41              |
| 25:F:195:ILE:HA   | 25:F:236:LEU:HD11 | 2.02                     | 0.41              |
| 25:F:233:LYS:HG2  | 25:F:233:LYS:H    | 1.61                     | 0.41              |
| 25:F:268:VAL:CG1  | 25:F:313:LEU:HA   | 2.50                     | 0.41              |
| 25:F:388:THR:HG22 | 25:F:424:ILE:CD1  | 2.51                     | 0.41              |
| 26:K:32:LYS:HD3   | 26:K:32:LYS:HA    | 1.79                     | 0.41              |
| 26:K:91:LYS:HG2   | 26:K:119:LEU:HD23 | 2.02                     | 0.41              |
| 26:K:230:THR:CG2  | 26:K:233:GLU:OE1  | 2.68                     | 0.41              |
| 27:U:167:ILE:N    | 27:U:167:ILE:HD13 | 2.35                     | 0.41              |
| 27:U:342:LEU:HD13 | 27:U:342:LEU:HA   | 1.87                     | 0.41              |
| 27:U:391:GLU:OE2  | 27:U:391:GLU:CA   | 2.69                     | 0.41              |
| 27:U:557:TYR:HD1  | 27:U:588:MET:HE3  | 1.85                     | 0.41              |
| 27:U:577:ILE:HD12 | 27:U:580:ARG:NH1  | 2.36                     | 0.41              |
| 27:U:717:ILE:HG23 | 27:U:718:ASN:N    | 2.36                     | 0.41              |
| 1:C:131:VAL:O     | 1:C:132:ASP:C     | 2.64                     | 0.41              |
| 1:C:148:TYR:H     | 1:C:206:HIS:HE1   | 1.69                     | 0.41              |
| 2:D:159:LYS:N     | 2:D:159:LYS:HD2   | 2.36                     | 0.41              |
| 2:D:338:ARG:NE    | 11:X:234:GLU:OE2  | 2.53                     | 0.41              |
| 2:D:398:ASP:OD1   | 2:D:398:ASP:N     | 2.52                     | 0.41              |
| 4:H:50:LYS:HD2    | 4:H:62:VAL:O      | 2.20                     | 0.41              |
| 4:H:101:TYR:HD1   | 4:H:101:TYR:N     | 2.18                     | 0.41              |
| 4:H:179:ASN:C     | 4:H:181:ASP:H     | 2.29                     | 0.41              |
| 4:H:222:THR:OG1   | 4:H:223:PRO:HD2   | 2.21                     | 0.41              |
| 5:I:86:LEU:HD12   | 5:I:86:LEU:HA     | 1.82                     | 0.41              |
| 6:J:38:ARG:NH2    | 6:J:182:GLU:O     | 2.42                     | 0.41              |
| 7:L:14:SER:HB3    | 7:L:18:ARG:O      | 2.21                     | 0.41              |
| 7:L:39:LYS:NZ     | 7:L:143:HIS:HA    | 2.36                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:L:45:VAL:CG2    | 7:L:188:VAL:HG23  | 2.42                     | 0.41              |
| 7:L:84:LEU:HD12   | 7:L:130:VAL:HG11  | 2.03                     | 0.41              |
| 8:M:69:VAL:HG23   | 8:M:75:MET:HE2    | 2.01                     | 0.41              |
| 8:M:136:MET:HA    | 8:M:149:TYR:O     | 2.20                     | 0.41              |
| 9:V:68:ASP:O      | 9:V:72:LEU:HD22   | 2.21                     | 0.41              |
| 9:V:282:ASN:ND2   | 12:Y:385:ARG:CB   | 2.81                     | 0.41              |
| 9:V:334:VAL:CG1   | 9:V:395:ILE:HD13  | 2.50                     | 0.41              |
| 9:V:403:ILE:HD12  | 9:V:403:ILE:HA    | 1.80                     | 0.41              |
| 11:X:93:LEU:HD22  | 11:X:129:LEU:HD13 | 2.00                     | 0.41              |
| 12:Y:26:LEU:HD23  | 12:Y:26:LEU:HA    | 1.83                     | 0.41              |
| 12:Y:29:PRO:HA    | 12:Y:32:ARG:NH2   | 2.37                     | 0.41              |
| 12:Y:73:MET:O     | 12:Y:77:ASN:N     | 2.37                     | 0.41              |
| 12:Y:276:ALA:O    | 12:Y:280:GLN:HG2  | 2.21                     | 0.41              |
| 12:Y:314:LEU:HD11 | 12:Y:319:MET:SD   | 2.61                     | 0.41              |
| 13:Z:10:VAL:CG2   | 13:Z:49:ASP:OD1   | 2.68                     | 0.41              |
| 13:Z:33:LYS:O     | 13:Z:34:ARG:C     | 2.63                     | 0.41              |
| 14:a:60:TYR:CZ    | 14:a:64:ILE:HD12  | 2.56                     | 0.41              |
| 14:a:291:LEU:HD12 | 14:a:331:VAL:O    | 2.21                     | 0.41              |
| 15:b:123:ASP:O    | 15:b:126:LYS:HG2  | 2.21                     | 0.41              |
| 17:d:241:TYR:OH   | 17:d:270:GLU:OE2  | 2.38                     | 0.41              |
| 18:f:226:TYR:HA   | 18:f:229:VAL:CG1  | 2.50                     | 0.41              |
| 18:f:372:LEU:HG   | 18:f:372:LEU:H    | 1.68                     | 0.41              |
| 18:f:423:ASP:OD2  | 19:g:91:PRO:HD3   | 2.20                     | 0.41              |
| 19:g:108:THR:CG2  | 19:g:109:GLY:N    | 2.84                     | 0.41              |
| 19:g:122:LEU:HD22 | 19:g:127:ILE:HD13 | 2.03                     | 0.41              |
| 22:A:117:GLN:H    | 22:A:117:GLN:CD   | 2.29                     | 0.41              |
| 22:A:161:VAL:HG23 | 22:A:256:MET:SD   | 2.61                     | 0.41              |
| 23:B:123:VAL:HG13 | 23:B:133:VAL:HG22 | 2.02                     | 0.41              |
| 23:B:125:THR:HB   | 23:B:129:SER:OG   | 2.21                     | 0.41              |
| 24:E:141:GLN:OE1  | 24:E:141:GLN:N    | 2.43                     | 0.41              |
| 25:F:238:ARG:O    | 25:F:241:ALA:HB3  | 2.21                     | 0.41              |
| 27:U:14:GLU:CB    | 27:U:19:LEU:HD23  | 2.48                     | 0.41              |
| 27:U:815:ALA:HB1  | 27:U:816:PRO:CD   | 2.51                     | 0.41              |
| 2:D:205:TYR:CG    | 2:D:314:ALA:CB    | 3.05                     | 0.40              |
| 2:D:229:ARG:HG2   | 2:D:229:ARG:NH1   | 2.35                     | 0.40              |
| 3:G:17:SER:OG     | 3:G:21:ARG:O      | 2.28                     | 0.40              |
| 3:G:232:GLU:HA    | 3:G:235:ILE:CD1   | 2.47                     | 0.40              |
| 5:I:89:GLU:HA     | 5:I:89:GLU:OE1    | 2.21                     | 0.40              |
| 6:J:10:PHE:CE2    | 26:K:27:ALA:HB2   | 2.57                     | 0.40              |
| 6:J:69:VAL:HG12   | 6:J:104:VAL:HG23  | 2.04                     | 0.40              |
| 6:J:137:ASP:C     | 6:J:139:ASP:N     | 2.78                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 8:M:124:LEU:HD23  | 8:M:124:LEU:HA    | 1.86                     | 0.40              |
| 9:V:200:ARG:HE    | 9:V:200:ARG:HB3   | 1.57                     | 0.40              |
| 9:V:316:ALA:O     | 9:V:318:GLN:N     | 2.54                     | 0.40              |
| 9:V:340:GLY:HA2   | 9:V:405:THR:HG1   | 1.86                     | 0.40              |
| 9:V:367:VAL:CG2   | 9:V:398:LEU:HD21  | 2.51                     | 0.40              |
| 9:V:471:GLU:HB3   | 9:V:472:PRO:HD3   | 2.03                     | 0.40              |
| 10:W:185:PHE:O    | 10:W:188:GLU:N    | 2.54                     | 0.40              |
| 11:X:66:LEU:HD12  | 11:X:66:LEU:HA    | 1.78                     | 0.40              |
| 12:Y:19:ILE:HG22  | 12:Y:150:PHE:CZ   | 2.55                     | 0.40              |
| 12:Y:62:ASP:OD1   | 12:Y:62:ASP:C     | 2.65                     | 0.40              |
| 12:Y:121:LEU:CD2  | 12:Y:147:ILE:HG21 | 2.51                     | 0.40              |
| 12:Y:334:LEU:HD23 | 12:Y:334:LEU:HA   | 1.87                     | 0.40              |
| 12:Y:387:ILE:HG12 | 13:Z:276:ILE:CG1  | 2.39                     | 0.40              |
| 13:Z:283:ARG:O    | 13:Z:286:GLU:HB3  | 2.21                     | 0.40              |
| 14:a:37:LEU:HD21  | 14:a:64:ILE:HD11  | 2.03                     | 0.40              |
| 14:a:99:LYS:HA    | 14:a:102:GLU:HG2  | 2.03                     | 0.40              |
| 14:a:190:VAL:HG12 | 14:a:194:GLN:OE1  | 2.21                     | 0.40              |
| 14:a:210:VAL:O    | 14:a:210:VAL:CG2  | 2.70                     | 0.40              |
| 14:a:221:VAL:C    | 14:a:225:LEU:HD12 | 2.45                     | 0.40              |
| 15:b:5:SER:CB     | 15:b:64:LEU:HD11  | 2.51                     | 0.40              |
| 15:b:33:VAL:HG12  | 15:b:75:LEU:HD11  | 2.01                     | 0.40              |
| 15:b:49:VAL:HG23  | 15:b:71:ILE:HG12  | 2.03                     | 0.40              |
| 16:c:72:VAL:HG21  | 16:c:112:TYR:CE1  | 2.56                     | 0.40              |
| 18:f:160:ARG:HH11 | 18:f:160:ARG:HB3  | 1.86                     | 0.40              |
| 18:f:173:LEU:HD21 | 18:f:181:ARG:HG3  | 2.03                     | 0.40              |
| 18:f:231:LEU:CD2  | 18:f:852:VAL:HG13 | 2.51                     | 0.40              |
| 18:f:316:ASP:C    | 18:f:319:GLU:HG3  | 2.46                     | 0.40              |
| 18:f:407:MET:CB   | 18:f:440:ILE:HG22 | 2.51                     | 0.40              |
| 18:f:479:LEU:CD1  | 18:f:514:VAL:HG22 | 2.51                     | 0.40              |
| 18:f:723:TYR:OH   | 18:f:757:ASN:HB2  | 2.21                     | 0.40              |
| 18:f:894:LEU:HD12 | 18:f:894:LEU:N    | 2.35                     | 0.40              |
| 19:g:108:THR:HB   | 19:g:111:GLU:OE1  | 2.20                     | 0.40              |
| 22:A:262:GLU:HA   | 22:A:262:GLU:OE1  | 2.21                     | 0.40              |
| 22:A:409:PHE:O    | 22:A:413:VAL:N    | 2.45                     | 0.40              |
| 23:B:112:LEU:HD12 | 23:B:112:LEU:HA   | 1.92                     | 0.40              |
| 24:E:300:HIS:ND1  | 24:E:301:ILE:N    | 2.69                     | 0.40              |
| 24:E:318:GLY:O    | 24:E:319:PRO:C    | 2.63                     | 0.40              |
| 25:F:129:ARG:HH11 | 25:F:129:ARG:CG   | 2.34                     | 0.40              |
| 25:F:188:ILE:HD11 | 25:F:235:LEU:O    | 2.22                     | 0.40              |
| 26:K:50:VAL:HG11  | 26:K:66:LYS:CE    | 2.49                     | 0.40              |
| 27:U:351:MET:HE1  | 27:U:354:LYS:NZ   | 2.36                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 27:U:560:MET:HE1  | 27:U:593:SER:HB2  | 2.03                     | 0.40              |
| 27:U:650:TYR:CD1  | 27:U:650:TYR:C    | 2.99                     | 0.40              |
| 27:U:773:PHE:N    | 27:U:774:PRO:CD   | 2.83                     | 0.40              |
| 28:e:18:GLU:H     | 28:e:18:GLU:CD    | 2.22                     | 0.40              |
| 28:e:48:VAL:O     | 28:e:48:VAL:HG13  | 2.21                     | 0.40              |
| 1:C:254:ILE:HA    | 1:C:269:VAL:HG22  | 2.02                     | 0.40              |
| 2:D:380:GLN:OE1   | 24:E:165:ILE:HB   | 2.22                     | 0.40              |
| 2:D:388:ARG:CZ    | 2:D:388:ARG:HB2   | 2.50                     | 0.40              |
| 3:G:132:ARG:HB2   | 8:M:12:SER:HA     | 2.02                     | 0.40              |
| 5:I:65:ILE:HD13   | 5:I:75:SER:CB     | 2.51                     | 0.40              |
| 6:J:16:LEU:O      | 6:J:20:GLU:HG3    | 2.21                     | 0.40              |
| 7:L:144:ILE:HD13  | 7:L:144:ILE:HA    | 1.86                     | 0.40              |
| 8:M:33:SER:CB     | 8:M:79:GLY:CA     | 2.99                     | 0.40              |
| 8:M:164:ALA:CB    | 8:M:172:ALA:CB    | 2.99                     | 0.40              |
| 8:M:170:GLN:O     | 8:M:174:THR:HG23  | 2.20                     | 0.40              |
| 9:V:129:ASP:O     | 9:V:133:PRO:HG3   | 2.21                     | 0.40              |
| 9:V:213:TYR:CD1   | 9:V:213:TYR:N     | 2.89                     | 0.40              |
| 9:V:303:SER:HA    | 9:V:339:LEU:CD2   | 2.51                     | 0.40              |
| 9:V:348:PHE:CD1   | 9:V:348:PHE:N     | 2.89                     | 0.40              |
| 10:W:60:MET:HA    | 10:W:63:THR:OG1   | 2.21                     | 0.40              |
| 10:W:177:MET:HG3  | 10:W:181:GLU:OE1  | 2.21                     | 0.40              |
| 10:W:267:LEU:C    | 10:W:270:VAL:HG12 | 2.45                     | 0.40              |
| 10:W:407:ASP:OD2  | 11:X:344:ARG:HD3  | 2.22                     | 0.40              |
| 11:X:380:GLN:CB   | 12:Y:314:LEU:HA   | 2.49                     | 0.40              |
| 11:X:420:LYS:HE3  | 16:c:264:LYS:NZ   | 2.36                     | 0.40              |
| 13:Z:93:GLY:HA3   | 13:Z:120:VAL:O    | 2.21                     | 0.40              |
| 13:Z:120:VAL:O    | 13:Z:120:VAL:HG13 | 2.21                     | 0.40              |
| 13:Z:205:LEU:HD23 | 13:Z:205:LEU:HA   | 1.79                     | 0.40              |
| 13:Z:252:LYS:HE2  | 13:Z:252:LYS:HA   | 2.03                     | 0.40              |
| 14:a:162:TYR:HB3  | 14:a:168:ASN:HD22 | 1.86                     | 0.40              |
| 14:a:251:LEU:HA   | 14:a:254:ALA:HB3  | 2.03                     | 0.40              |
| 14:a:293:PHE:CD1  | 14:a:329:LYS:HB3  | 2.56                     | 0.40              |
| 15:b:100:ARG:NH1  | 15:b:107:MET:SD   | 2.95                     | 0.40              |
| 15:b:150:THR:CG2  | 15:b:152:LYS:HG2  | 2.51                     | 0.40              |
| 16:c:177:THR:HB   | 27:U:773:PHE:H    | 1.86                     | 0.40              |
| 18:f:217:LEU:CD2  | 18:f:229:VAL:CG2  | 2.96                     | 0.40              |
| 18:f:432:TYR:O    | 18:f:434:TYR:N    | 2.53                     | 0.40              |
| 18:f:560:LEU:HD12 | 18:f:801:VAL:CG2  | 2.51                     | 0.40              |
| 18:f:613:LEU:CD1  | 23:B:74:MET:HE3   | 2.51                     | 0.40              |
| 19:g:163:GLU:O    | 19:g:167:LYS:HG3  | 2.21                     | 0.40              |
| 20:u:165:LEU:HD12 | 20:u:165:LEU:C    | 2.46                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:A:176:ASP:OD1  | 22:A:357:ILE:CG2  | 2.70                     | 0.40              |
| 23:B:293:LYS:HE3  | 23:B:293:LYS:HB2  | 1.67                     | 0.40              |
| 23:B:366:GLN:HA   | 23:B:369:THR:HG23 | 2.03                     | 0.40              |
| 24:E:98:VAL:CG2   | 24:E:107:ILE:HG12 | 2.49                     | 0.40              |
| 24:E:100:LEU:HA   | 24:E:107:ILE:HA   | 2.03                     | 0.40              |
| 24:E:364:GLN:O    | 24:E:365:GLU:C    | 2.64                     | 0.40              |
| 25:F:93:VAL:HG23  | 25:F:151:VAL:HG22 | 2.02                     | 0.40              |
| 25:F:185:TYR:HD1  | 25:F:239:ALA:HB1  | 1.82                     | 0.40              |
| 25:F:224:LEU:HD12 | 25:F:225:MET:N    | 2.36                     | 0.40              |
| 27:U:151:ILE:HD13 | 27:U:163:PHE:CD1  | 2.57                     | 0.40              |
| 27:U:518:LEU:HD23 | 27:U:554:LEU:HD13 | 2.02                     | 0.40              |
| 27:U:602:LEU:HD11 | 27:U:621:SER:CB   | 2.50                     | 0.40              |
| 27:U:615:ARG:O    | 27:U:618:ALA:HB3  | 2.21                     | 0.40              |
| 1:C:69:GLN:HB2    | 1:C:118:ASN:CB    | 2.51                     | 0.40              |
| 1:C:145:ASP:OD1   | 1:C:145:ASP:N     | 2.52                     | 0.40              |
| 1:C:165:ILE:HD11  | 1:C:292:ILE:CD1   | 2.52                     | 0.40              |
| 1:C:267:SER:O     | 1:C:271:ARG:NH1   | 2.53                     | 0.40              |
| 3:G:102:LYS:HG3   | 3:G:107:TYR:C     | 2.46                     | 0.40              |
| 4:H:48:THR:HG22   | 4:H:65:VAL:HG23   | 2.03                     | 0.40              |
| 6:J:104:VAL:HG12  | 6:J:145:TYR:CD2   | 2.57                     | 0.40              |
| 6:J:211:MET:HE3   | 6:J:217:LEU:HD12  | 2.03                     | 0.40              |
| 7:L:19:ILE:CD1    | 8:M:129:ARG:NE    | 2.84                     | 0.40              |
| 7:L:38:LEU:HD23   | 7:L:38:LEU:H      | 1.86                     | 0.40              |
| 9:V:213:TYR:HD1   | 9:V:213:TYR:N     | 2.20                     | 0.40              |
| 9:V:228:ARG:HB2   | 9:V:257:ASN:HD21  | 1.86                     | 0.40              |
| 9:V:363:LEU:O     | 9:V:366:ALA:N     | 2.55                     | 0.40              |
| 9:V:442:ILE:HD12  | 9:V:451:ILE:HG13  | 2.03                     | 0.40              |
| 10:W:23:THR:CA    | 10:W:26:GLN:HG2   | 2.45                     | 0.40              |
| 10:W:77:ALA:O     | 10:W:78:LYS:HB2   | 2.20                     | 0.40              |
| 10:W:172:GLU:OE2  | 10:W:186:ILE:HD11 | 2.20                     | 0.40              |
| 10:W:245:LYS:HG3  | 10:W:286:LEU:HD11 | 2.03                     | 0.40              |
| 10:W:377:ARG:HA   | 10:W:377:ARG:HD2  | 1.60                     | 0.40              |
| 11:X:386:ILE:N    | 11:X:386:ILE:HD13 | 2.35                     | 0.40              |
| 11:X:414:LEU:HA   | 11:X:414:LEU:HD23 | 1.80                     | 0.40              |
| 12:Y:59:LYS:HG2   | 12:Y:60:SER:N     | 2.36                     | 0.40              |
| 14:a:80:ILE:C     | 14:a:83:VAL:HB    | 2.46                     | 0.40              |
| 14:a:102:GLU:HA   | 14:a:105:LYS:HG3  | 2.02                     | 0.40              |
| 14:a:226:ARG:HB3  | 14:a:226:ARG:CZ   | 2.52                     | 0.40              |
| 15:b:60:VAL:O     | 15:b:62:THR:N     | 2.55                     | 0.40              |
| 15:b:130:ARG:HD2  | 15:b:134:GLU:CD   | 2.46                     | 0.40              |
| 15:b:142:ASN:OD1  | 15:b:142:ASN:C    | 2.63                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 16:c:84:VAL:HG11  | 20:u:280:ARG:HB2  | 2.02                     | 0.40              |
| 16:c:190:GLN:OE1  | 16:c:190:GLN:N    | 2.54                     | 0.40              |
| 17:d:136:LEU:HD22 | 17:d:140:GLN:HE22 | 1.85                     | 0.40              |
| 17:d:145:ARG:HH22 | 17:d:185:SER:N    | 2.19                     | 0.40              |
| 17:d:241:TYR:HB3  | 17:d:271:ILE:HD11 | 2.04                     | 0.40              |
| 18:f:237:VAL:CG1  | 18:f:249:LEU:HD23 | 2.51                     | 0.40              |
| 18:f:266:LEU:CD2  | 18:f:294:MET:HA   | 2.51                     | 0.40              |
| 18:f:371:ASN:O    | 18:f:374:SER:HB2  | 2.22                     | 0.40              |
| 18:f:599:ALA:HB3  | 18:f:600:TYR:CD1  | 2.57                     | 0.40              |
| 18:f:620:PHE:CE2  | 18:f:647:GLY:HA2  | 2.56                     | 0.40              |
| 18:f:723:TYR:O    | 18:f:761:MET:HE1  | 2.21                     | 0.40              |
| 18:f:771:LEU:CD1  | 18:f:778:LEU:HD21 | 2.46                     | 0.40              |
| 19:g:90:PRO:HG2   | 19:g:157:GLU:CA   | 2.52                     | 0.40              |
| 19:g:100:LEU:HD22 | 19:g:100:LEU:N    | 2.29                     | 0.40              |
| 19:g:105:LEU:O    | 19:g:143:GLU:HG3  | 2.20                     | 0.40              |
| 19:g:107:ILE:HD11 | 19:g:115:LYS:HB3  | 2.03                     | 0.40              |
| 19:g:165:ALA:HA   | 19:g:169:PHE:N    | 2.36                     | 0.40              |
| 22:A:35:THR:CG2   | 22:A:36:TYR:N     | 2.84                     | 0.40              |
| 22:A:278:ASP:HB2  | 23:B:310:LEU:HD23 | 1.99                     | 0.40              |
| 23:B:176:VAL:HB   | 23:B:247:PHE:O    | 2.21                     | 0.40              |
| 24:E:40:TYR:CZ    | 25:F:72:LYS:HB3   | 2.57                     | 0.40              |
| 24:E:54:GLY:O     | 24:E:102:MET:HE2  | 2.21                     | 0.40              |
| 25:F:371:ARG:HG3  | 25:F:371:ARG:H    | 1.69                     | 0.40              |
| 26:K:162:PHE:O    | 26:K:162:PHE:CG   | 2.74                     | 0.40              |
| 27:U:103:LYS:O    | 27:U:106:ASP:N    | 2.55                     | 0.40              |
| 27:U:469:SER:CB   | 27:U:471:ASP:OD2  | 2.69                     | 0.40              |
| 27:U:489:ALA:HA   | 27:U:519:VAL:O    | 2.22                     | 0.40              |
| 27:U:606:ALA:HB2  | 27:U:618:ALA:HB1  | 2.02                     | 0.40              |
| 1:C:49:ARG:NH1    | 2:D:60:TYR:OH     | 2.54                     | 0.40              |
| 1:C:191:PRO:HG2   | 1:C:319:PRO:HD3   | 2.04                     | 0.40              |
| 1:C:311:ILE:O     | 1:C:311:ILE:HG22  | 2.20                     | 0.40              |
| 2:D:201:GLY:HA2   | 2:D:307:VAL:O     | 2.22                     | 0.40              |
| 2:D:217:LYS:HA    | 24:E:267:PHE:CE2  | 2.55                     | 0.40              |
| 2:D:370:ILE:HD12  | 2:D:375:ILE:CG1   | 2.52                     | 0.40              |
| 3:G:211:LYS:HE2   | 3:G:213:SER:H     | 1.87                     | 0.40              |
| 4:H:63:HIS:HB3    | 4:H:220:ARG:NE    | 2.36                     | 0.40              |
| 4:H:210:VAL:O     | 4:H:221:LEU:HG    | 2.20                     | 0.40              |
| 5:I:17:ARG:CZ     | 5:I:19:TYR:HE1    | 2.34                     | 0.40              |
| 5:I:229:LYS:O     | 5:I:232:GLU:HG2   | 2.22                     | 0.40              |
| 6:J:35:VAL:HG22   | 6:J:191:VAL:CG2   | 2.51                     | 0.40              |
| 6:J:43:LEU:HD23   | 6:J:43:LEU:N      | 2.36                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:J:45:VAL:CG1    | 6:J:61:LYS:HD2    | 2.50                     | 0.40              |
| 6:J:185:ASP:HA    | 6:J:188:ILE:HD12  | 2.03                     | 0.40              |
| 7:L:72:ILE:CD1    | 7:L:74:ILE:HG23   | 2.51                     | 0.40              |
| 7:L:83:LEU:CD1    | 26:K:125:GLU:HB3  | 2.50                     | 0.40              |
| 8:M:27:MET:HA     | 8:M:153:PRO:HG2   | 2.04                     | 0.40              |
| 8:M:175:GLU:HB3   | 8:M:196:ILE:CD1   | 2.51                     | 0.40              |
| 8:M:232:ARG:CZ    | 8:M:232:ARG:HB2   | 2.51                     | 0.40              |
| 9:V:93:PHE:HA     | 9:V:96:ARG:NH2    | 2.33                     | 0.40              |
| 9:V:231:LEU:HB2   | 9:V:254:LEU:HD13  | 2.03                     | 0.40              |
| 9:V:403:ILE:CG1   | 9:V:428:LEU:HD21  | 2.51                     | 0.40              |
| 10:W:40:LEU:HD12  | 10:W:40:LEU:HA    | 1.78                     | 0.40              |
| 10:W:272:LEU:O    | 10:W:275:ILE:HB   | 2.21                     | 0.40              |
| 10:W:307:LYS:HG3  | 10:W:308:LEU:N    | 2.36                     | 0.40              |
| 10:W:374:THR:HB   | 10:W:376:LYS:NZ   | 2.37                     | 0.40              |
| 11:X:167:VAL:CG1  | 11:X:210:LEU:HD11 | 2.52                     | 0.40              |
| 11:X:168:GLU:O    | 11:X:172:LEU:HD23 | 2.22                     | 0.40              |
| 11:X:339:ILE:CG2  | 11:X:339:ILE:O    | 2.70                     | 0.40              |
| 13:Z:94:TRP:O     | 13:Z:121:LEU:HA   | 2.21                     | 0.40              |
| 13:Z:185:GLY:O    | 13:Z:189:GLN:HB2  | 2.21                     | 0.40              |
| 13:Z:212:LEU:HD11 | 14:a:346:ILE:CD1  | 2.51                     | 0.40              |
| 13:Z:228:TYR:HD1  | 13:Z:229:GLN:N    | 2.20                     | 0.40              |
| 14:a:112:ILE:HA   | 14:a:115:LYS:CB   | 2.52                     | 0.40              |
| 14:a:116:THR:C    | 14:a:120:ALA:H    | 2.12                     | 0.40              |
| 14:a:122:LYS:HE2  | 14:a:130:VAL:CG1  | 2.51                     | 0.40              |
| 15:b:24:THR:CG2   | 15:b:25:ARG:N     | 2.85                     | 0.40              |
| 15:b:51:LEU:O     | 15:b:51:LEU:HD12  | 2.22                     | 0.40              |
| 15:b:73:SER:HB2   | 25:F:61:ARG:HH21  | 1.87                     | 0.40              |
| 15:b:107:MET:HG3  | 15:b:136:VAL:HG22 | 2.04                     | 0.40              |
| 17:d:120:LYS:O    | 17:d:123:LEU:HB2  | 2.22                     | 0.40              |
| 17:d:223:ASN:OD1  | 17:d:226:ILE:HG13 | 2.22                     | 0.40              |
| 17:d:251:ILE:O    | 17:d:251:ILE:CG1  | 2.70                     | 0.40              |
| 18:f:114:ALA:C    | 18:f:116:GLY:H    | 2.29                     | 0.40              |
| 18:f:270:LEU:CD1  | 18:f:787:LEU:HD11 | 2.47                     | 0.40              |
| 18:f:471:LEU:H    | 18:f:471:LEU:HD23 | 1.86                     | 0.40              |
| 19:g:148:ALA:N    | 19:g:151:VAL:HG21 | 2.35                     | 0.40              |
| 22:A:240:VAL:HB   | 22:A:274:PHE:HA   | 2.04                     | 0.40              |
| 23:B:272:ARG:O    | 23:B:276:GLU:HB2  | 2.22                     | 0.40              |
| 23:B:292:THR:O    | 23:B:309:MET:CE   | 2.69                     | 0.40              |
| 24:E:153:LEU:HD13 | 24:E:191:LEU:HD23 | 2.02                     | 0.40              |
| 24:E:280:ASN:OD1  | 24:E:280:ASN:C    | 2.64                     | 0.40              |
| 24:E:363:VAL:CG1  | 24:E:365:GLU:HB2  | 2.51                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 25:F:134:LEU:HD12 | 25:F:160:ILE:HG12 | 2.02                     | 0.40              |
| 26:K:67:ILE:HA    | 26:K:76:CYS:O     | 2.22                     | 0.40              |
| 27:U:222:PHE:CD1  | 27:U:222:PHE:N    | 2.89                     | 0.40              |
| 27:U:461:LEU:HD13 | 27:U:481:LEU:N    | 2.36                     | 0.40              |
| 27:U:620:GLU:C    | 27:U:620:GLU:CD   | 2.89                     | 0.40              |
| 2:D:81:ARG:CZ     | 2:D:81:ARG:HB2    | 2.50                     | 0.40              |
| 2:D:257:ASN:OD1   | 2:D:257:ASN:N     | 2.53                     | 0.40              |
| 2:D:354:LEU:HD23  | 2:D:354:LEU:HA    | 1.86                     | 0.40              |
| 3:G:46:ASP:O      | 3:G:222:VAL:HG23  | 2.22                     | 0.40              |
| 3:G:93:ARG:NH2    | 3:G:121:ILE:HG13  | 2.37                     | 0.40              |
| 3:G:199:ILE:HD11  | 3:G:215:ILE:HD13  | 2.04                     | 0.40              |
| 4:H:127:VAL:HG23  | 4:H:127:VAL:O     | 2.21                     | 0.40              |
| 4:H:157:ALA:HB3   | 5:I:57:ASP:O      | 2.21                     | 0.40              |
| 5:I:101:TYR:N     | 5:I:101:TYR:HD1   | 2.19                     | 0.40              |
| 5:I:132:VAL:HG13  | 5:I:132:VAL:O     | 2.22                     | 0.40              |
| 7:L:87:PHE:CD2    | 7:L:112:ILE:HD12  | 2.57                     | 0.40              |
| 7:L:98:VAL:HG12   | 7:L:99:PHE:HD1    | 1.86                     | 0.40              |
| 7:L:105:VAL:HG13  | 7:L:134:ILE:CG2   | 2.51                     | 0.40              |
| 8:M:234:GLU:O     | 8:M:238:TYR:N     | 2.40                     | 0.40              |
| 9:V:237:THR:C     | 9:V:241:ARG:HH12  | 2.29                     | 0.40              |
| 9:V:295:ILE:HD13  | 9:V:295:ILE:HA    | 1.89                     | 0.40              |
| 10:W:216:GLU:H    | 10:W:219:THR:CG2  | 2.33                     | 0.40              |
| 10:W:373:ILE:HA   | 14:a:326:GLU:CB   | 2.44                     | 0.40              |
| 11:X:88:LEU:O     | 11:X:92:LEU:N     | 2.35                     | 0.40              |
| 11:X:248:ILE:HD12 | 11:X:248:ILE:HA   | 1.85                     | 0.40              |
| 12:Y:95:LEU:HB3   | 12:Y:99:GLU:CG    | 2.52                     | 0.40              |
| 13:Z:63:LYS:C     | 13:Z:65:ASP:H     | 2.30                     | 0.40              |
| 13:Z:126:VAL:HG13 | 13:Z:127:LYS:N    | 2.37                     | 0.40              |
| 13:Z:170:VAL:CG1  | 13:Z:171:GLY:N    | 2.85                     | 0.40              |
| 13:Z:222:ILE:CG2  | 13:Z:227:ILE:HD13 | 2.52                     | 0.40              |
| 14:a:65:SER:HA    | 14:a:68:GLU:OE1   | 2.21                     | 0.40              |
| 14:a:111:VAL:HG22 | 14:a:115:LYS:CE   | 2.51                     | 0.40              |
| 14:a:157:ASP:O    | 14:a:161:LYS:HG2  | 2.21                     | 0.40              |
| 14:a:216:LEU:CD1  | 14:a:237:LEU:HB3  | 2.48                     | 0.40              |
| 14:a:285:PRO:HG2  | 14:a:288:HIS:HB2  | 2.03                     | 0.40              |
| 14:a:296:ILE:CG2  | 14:a:307:VAL:HG23 | 2.46                     | 0.40              |
| 15:b:3:LEU:HD23   | 15:b:44:ASN:ND2   | 2.37                     | 0.40              |
| 15:b:16:MET:HE3   | 15:b:26:LEU:HD12  | 2.03                     | 0.40              |
| 15:b:51:LEU:HD11  | 15:b:61:LEU:HB2   | 2.02                     | 0.40              |
| 16:c:92:GLN:OE1   | 16:c:96:LEU:HD12  | 2.21                     | 0.40              |
| 17:d:207:GLU:O    | 17:d:211:GLU:HB2  | 2.22                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 17:d:323:GLN:C    | 17:d:324:LYS:HG3  | 2.47                     | 0.40              |
| 18:f:78:LEU:O     | 18:f:82:ILE:HB    | 2.20                     | 0.40              |
| 18:f:131:MET:HE1  | 22:A:36:TYR:CD1   | 2.56                     | 0.40              |
| 18:f:369:ARG:O    | 18:f:372:LEU:N    | 2.55                     | 0.40              |
| 18:f:425:GLY:O    | 18:f:429:ILE:N    | 2.54                     | 0.40              |
| 18:f:465:LEU:CD1  | 19:g:173:GLU:HG2  | 2.51                     | 0.40              |
| 18:f:473:ASN:OD1  | 18:f:509:LYS:HE3  | 2.22                     | 0.40              |
| 18:f:539:LEU:HG   | 18:f:540:GLN:OE1  | 2.21                     | 0.40              |
| 18:f:661:ALA:HB2  | 23:B:71:TYR:OH    | 2.22                     | 0.40              |
| 18:f:670:MET:HE2  | 18:f:670:MET:HB2  | 1.94                     | 0.40              |
| 18:f:698:SER:OG   | 18:f:703:ARG:NH2  | 2.54                     | 0.40              |
| 18:f:830:LEU:HD13 | 18:f:874:LEU:HD11 | 2.04                     | 0.40              |
| 19:g:145:GLN:HG3  | 19:g:147:VAL:CG2  | 2.47                     | 0.40              |
| 23:B:103:ARG:HE   | 23:B:160:ILE:HG23 | 1.86                     | 0.40              |
| 23:B:114:GLU:HG3  | 23:B:116:ILE:CD1  | 2.52                     | 0.40              |
| 24:E:143:ARG:HB3  | 24:E:143:ARG:NH1  | 2.37                     | 0.40              |
| 24:E:182:LEU:HD12 | 24:E:182:LEU:C    | 2.47                     | 0.40              |
| 24:E:237:ALA:HB3  | 24:E:238:ILE:HD12 | 2.04                     | 0.40              |
| 25:F:341:ALA:O    | 25:F:347:ARG:CD   | 2.65                     | 0.40              |
| 26:K:190:THR:HG23 | 26:K:192:LYS:H    | 1.86                     | 0.40              |
| 27:U:14:GLU:HB2   | 27:U:19:LEU:CD2   | 2.48                     | 0.40              |
| 27:U:265:ILE:HG21 | 27:U:326:ILE:HG23 | 1.94                     | 0.40              |
| 27:U:583:MET:HE3  | 27:U:602:LEU:CD2  | 2.50                     | 0.40              |
| 27:U:772:TRP:CD1  | 27:U:774:PRO:HD2  | 2.56                     | 0.40              |
| 27:U:792:ASN:ND2  | 27:U:796:LYS:HG2  | 2.36                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

| Mol | Chain | Analysed      | Favoured  | Allowed | Outliers | Percentiles |
|-----|-------|---------------|-----------|---------|----------|-------------|
| 1   | C     | 384/406 (95%) | 349 (91%) | 32 (8%) | 3 (1%)   | 16 49       |

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| Mol | Chain | Analysed         | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|------------------|------------|----------|----------|-------------|-----|
| 2   | D     | 378/418 (90%)    | 330 (87%)  | 44 (12%) | 4 (1%)   | 11          | 42  |
| 3   | G     | 237/246 (96%)    | 217 (92%)  | 17 (7%)  | 3 (1%)   | 9           | 39  |
| 4   | H     | 230/234 (98%)    | 212 (92%)  | 18 (8%)  | 0        | 100         | 100 |
| 5   | I     | 246/261 (94%)    | 232 (94%)  | 13 (5%)  | 1 (0%)   | 30          | 62  |
| 6   | J     | 237/248 (96%)    | 213 (90%)  | 24 (10%) | 0        | 100         | 100 |
| 7   | L     | 236/263 (90%)    | 227 (96%)  | 9 (4%)   | 0        | 100         | 100 |
| 8   | M     | 238/255 (93%)    | 219 (92%)  | 19 (8%)  | 0        | 100         | 100 |
| 9   | V     | 441/534 (83%)    | 415 (94%)  | 24 (5%)  | 2 (0%)   | 24          | 58  |
| 10  | W     | 436/456 (96%)    | 415 (95%)  | 20 (5%)  | 1 (0%)   | 43          | 74  |
| 11  | X     | 376/422 (89%)    | 354 (94%)  | 22 (6%)  | 0        | 100         | 100 |
| 12  | Y     | 378/389 (97%)    | 362 (96%)  | 16 (4%)  | 0        | 100         | 100 |
| 13  | Z     | 284/324 (88%)    | 252 (89%)  | 29 (10%) | 3 (1%)   | 11          | 42  |
| 14  | a     | 371/376 (99%)    | 331 (89%)  | 40 (11%) | 0        | 100         | 100 |
| 15  | b     | 189/377 (50%)    | 158 (84%)  | 31 (16%) | 0        | 100         | 100 |
| 16  | c     | 287/424 (68%)    | 239 (83%)  | 45 (16%) | 3 (1%)   | 12          | 44  |
| 17  | d     | 267/350 (76%)    | 246 (92%)  | 20 (8%)  | 1 (0%)   | 30          | 62  |
| 18  | f     | 824/908 (91%)    | 757 (92%)  | 66 (8%)  | 1 (0%)   | 48          | 79  |
| 19  | g     | 93/601 (16%)     | 68 (73%)   | 25 (27%) | 0        | 100         | 100 |
| 20  | u     | 170/289 (59%)    | 162 (95%)  | 6 (4%)   | 2 (1%)   | 10          | 41  |
| 22  | A     | 403/433 (93%)    | 373 (93%)  | 28 (7%)  | 2 (0%)   | 24          | 58  |
| 23  | B     | 392/440 (89%)    | 351 (90%)  | 40 (10%) | 1 (0%)   | 36          | 67  |
| 24  | E     | 339/389 (87%)    | 297 (88%)  | 33 (10%) | 9 (3%)   | 4           | 27  |
| 25  | F     | 353/439 (80%)    | 307 (87%)  | 45 (13%) | 1 (0%)   | 36          | 67  |
| 26  | K     | 224/241 (93%)    | 209 (93%)  | 15 (7%)  | 0        | 100         | 100 |
| 27  | U     | 834/953 (88%)    | 731 (88%)  | 98 (12%) | 5 (1%)   | 21          | 53  |
| 28  | e     | 37/70 (53%)      | 34 (92%)   | 3 (8%)   | 0        | 100         | 100 |
| All | All   | 8884/10746 (83%) | 8060 (91%) | 782 (9%) | 42 (0%)  | 26          | 58  |

All (42) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 82  | LYS  |
| 2   | D     | 413 | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | G     | 10  | ASP  |
| 3   | G     | 11  | ARG  |
| 3   | G     | 184 | LYS  |
| 10  | W     | 41  | GLN  |
| 13  | Z     | 146 | ASP  |
| 13  | Z     | 226 | ILE  |
| 16  | c     | 116 | PRO  |
| 16  | c     | 145 | VAL  |
| 16  | c     | 285 | GLU  |
| 18  | f     | 433 | LEU  |
| 22  | A     | 367 | ASP  |
| 23  | B     | 278 | ALA  |
| 24  | E     | 122 | MET  |
| 24  | E     | 267 | PHE  |
| 24  | E     | 268 | ASP  |
| 24  | E     | 328 | TYR  |
| 24  | E     | 357 | ALA  |
| 27  | U     | 42  | VAL  |
| 1   | C     | 81  | ASP  |
| 2   | D     | 219 | VAL  |
| 9   | V     | 318 | GLN  |
| 17  | d     | 332 | SER  |
| 24  | E     | 295 | LEU  |
| 27  | U     | 172 | ASP  |
| 27  | U     | 242 | LEU  |
| 27  | U     | 812 | ALA  |
| 1   | C     | 355 | SER  |
| 2   | D     | 324 | PRO  |
| 2   | D     | 411 | GLU  |
| 5   | I     | 107 | CYS  |
| 9   | V     | 494 | MET  |
| 22  | A     | 116 | LYS  |
| 24  | E     | 125 | GLU  |
| 24  | E     | 304 | PRO  |
| 20  | u     | 119 | ILE  |
| 20  | u     | 279 | LYS  |
| 13  | Z     | 177 | ARG  |
| 24  | E     | 297 | ARG  |
| 25  | F     | 203 | VAL  |
| 27  | U     | 815 | ALA  |

### 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   | C     | 338/352 (96%)  | 322 (95%) | 16 (5%)  | 23          | 50 |
| 2   | D     | 333/366 (91%)  | 309 (93%) | 24 (7%)  | 13          | 38 |
| 3   | G     | 192/210 (91%)  | 184 (96%) | 8 (4%)   | 26          | 52 |
| 4   | H     | 190/191 (100%) | 182 (96%) | 8 (4%)   | 26          | 52 |
| 5   | I     | 191/221 (86%)  | 179 (94%) | 12 (6%)  | 16          | 43 |
| 6   | J     | 158/211 (75%)  | 151 (96%) | 7 (4%)   | 25          | 51 |
| 7   | L     | 198/224 (88%)  | 193 (98%) | 5 (2%)   | 42          | 63 |
| 8   | M     | 192/212 (91%)  | 179 (93%) | 13 (7%)  | 14          | 41 |
| 9   | V     | 391/460 (85%)  | 376 (96%) | 15 (4%)  | 29          | 56 |
| 10  | W     | 403/416 (97%)  | 386 (96%) | 17 (4%)  | 26          | 52 |
| 11  | X     | 325/362 (90%)  | 313 (96%) | 12 (4%)  | 30          | 56 |
| 12  | Y     | 335/344 (97%)  | 324 (97%) | 11 (3%)  | 33          | 58 |
| 13  | Z     | 257/295 (87%)  | 246 (96%) | 11 (4%)  | 26          | 52 |
| 14  | a     | 333/336 (99%)  | 314 (94%) | 19 (6%)  | 18          | 45 |
| 15  | b     | 167/312 (54%)  | 154 (92%) | 13 (8%)  | 11          | 37 |
| 16  | c     | 252/359 (70%)  | 238 (94%) | 14 (6%)  | 19          | 46 |
| 17  | d     | 237/294 (81%)  | 232 (98%) | 5 (2%)   | 47          | 66 |
| 18  | f     | 702/763 (92%)  | 685 (98%) | 17 (2%)  | 43          | 64 |
| 19  | g     | 85/527 (16%)   | 82 (96%)  | 3 (4%)   | 32          | 57 |
| 20  | u     | 156/253 (62%)  | 146 (94%) | 10 (6%)  | 16          | 43 |
| 22  | A     | 350/372 (94%)  | 329 (94%) | 21 (6%)  | 17          | 44 |
| 23  | B     | 348/385 (90%)  | 328 (94%) | 20 (6%)  | 18          | 45 |
| 24  | E     | 298/341 (87%)  | 226 (76%) | 72 (24%) | 1           | 4  |
| 25  | F     | 304/379 (80%)  | 269 (88%) | 35 (12%) | 5           | 24 |
| 26  | K     | 189/204 (93%)  | 182 (96%) | 7 (4%)   | 30          | 56 |
| 27  | U     | 718/816 (88%)  | 684 (95%) | 34 (5%)  | 23          | 50 |

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| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|----------|-------------|----|
| 28  | e     | 37/63 (59%)     | 35 (95%)   | 2 (5%)   | 20          | 47 |
| All | All   | 7679/9268 (83%) | 7248 (94%) | 431 (6%) | 21          | 46 |

All (431) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 23  | TYR  |
| 1   | C     | 24  | TYR  |
| 1   | C     | 38  | LYS  |
| 1   | C     | 41  | ASN  |
| 1   | C     | 105 | ILE  |
| 1   | C     | 119 | ASP  |
| 1   | C     | 206 | HIS  |
| 1   | C     | 254 | ILE  |
| 1   | C     | 269 | VAL  |
| 1   | C     | 293 | MET  |
| 1   | C     | 295 | THR  |
| 1   | C     | 333 | SER  |
| 1   | C     | 339 | THR  |
| 1   | C     | 346 | LYS  |
| 1   | C     | 350 | LEU  |
| 1   | C     | 362 | VAL  |
| 2   | D     | 54  | LEU  |
| 2   | D     | 60  | TYR  |
| 2   | D     | 76  | GLN  |
| 2   | D     | 93  | LEU  |
| 2   | D     | 105 | SER  |
| 2   | D     | 110 | ASN  |
| 2   | D     | 155 | THR  |
| 2   | D     | 164 | TYR  |
| 2   | D     | 166 | ASP  |
| 2   | D     | 167 | ILE  |
| 2   | D     | 170 | MET  |
| 2   | D     | 171 | ASP  |
| 2   | D     | 224 | THR  |
| 2   | D     | 231 | VAL  |
| 2   | D     | 238 | LYS  |
| 2   | D     | 253 | LEU  |
| 2   | D     | 272 | THR  |
| 2   | D     | 313 | ARG  |
| 2   | D     | 324 | PRO  |
| 2   | D     | 347 | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | D     | 370 | ILE  |
| 2   | D     | 371 | SER  |
| 2   | D     | 374 | ASP  |
| 2   | D     | 414 | HIS  |
| 3   | G     | 14  | THR  |
| 3   | G     | 87  | SER  |
| 3   | G     | 115 | CYS  |
| 3   | G     | 131 | MET  |
| 3   | G     | 166 | THR  |
| 3   | G     | 171 | LYS  |
| 3   | G     | 215 | ILE  |
| 3   | G     | 244 | GLU  |
| 4   | H     | 3   | GLU  |
| 4   | H     | 4   | ARG  |
| 4   | H     | 16  | SER  |
| 4   | H     | 39  | LYS  |
| 4   | H     | 48  | THR  |
| 4   | H     | 87  | VAL  |
| 4   | H     | 89  | ARG  |
| 4   | H     | 219 | ARG  |
| 5   | I     | 9   | THR  |
| 5   | I     | 10  | THR  |
| 5   | I     | 19  | TYR  |
| 5   | I     | 38  | LEU  |
| 5   | I     | 80  | THR  |
| 5   | I     | 93  | ILE  |
| 5   | I     | 99  | LEU  |
| 5   | I     | 153 | SER  |
| 5   | I     | 163 | CYS  |
| 5   | I     | 164 | ILE  |
| 5   | I     | 174 | MET  |
| 5   | I     | 206 | LEU  |
| 6   | J     | 8   | THR  |
| 6   | J     | 26  | VAL  |
| 6   | J     | 55  | ASP  |
| 6   | J     | 84  | ILE  |
| 6   | J     | 94  | HIS  |
| 6   | J     | 108 | THR  |
| 6   | J     | 144 | LEU  |
| 7   | L     | 11  | THR  |
| 7   | L     | 53  | GLN  |
| 7   | L     | 114 | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 7   | L     | 170 | THR  |
| 7   | L     | 212 | ILE  |
| 8   | M     | 49  | VAL  |
| 8   | M     | 50  | GLU  |
| 8   | M     | 66  | LEU  |
| 8   | M     | 75  | MET  |
| 8   | M     | 87  | LEU  |
| 8   | M     | 115 | VAL  |
| 8   | M     | 123 | THR  |
| 8   | M     | 154 | SER  |
| 8   | M     | 158 | TYR  |
| 8   | M     | 169 | ARG  |
| 8   | M     | 181 | MET  |
| 8   | M     | 199 | ILE  |
| 8   | M     | 227 | VAL  |
| 9   | V     | 61  | GLU  |
| 9   | V     | 65  | ARG  |
| 9   | V     | 72  | LEU  |
| 9   | V     | 89  | LYS  |
| 9   | V     | 94  | VAL  |
| 9   | V     | 223 | LYS  |
| 9   | V     | 285 | TRP  |
| 9   | V     | 310 | THR  |
| 9   | V     | 353 | LEU  |
| 9   | V     | 403 | ILE  |
| 9   | V     | 410 | ILE  |
| 9   | V     | 425 | LYS  |
| 9   | V     | 464 | ILE  |
| 9   | V     | 478 | GLN  |
| 9   | V     | 490 | SER  |
| 10  | W     | 73  | MET  |
| 10  | W     | 139 | GLU  |
| 10  | W     | 145 | LEU  |
| 10  | W     | 166 | LEU  |
| 10  | W     | 205 | ILE  |
| 10  | W     | 209 | ILE  |
| 10  | W     | 224 | LEU  |
| 10  | W     | 230 | MET  |
| 10  | W     | 243 | ILE  |
| 10  | W     | 259 | GLU  |
| 10  | W     | 265 | GLN  |
| 10  | W     | 288 | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 10  | W     | 338 | THR  |
| 10  | W     | 352 | LYS  |
| 10  | W     | 377 | ARG  |
| 10  | W     | 388 | GLU  |
| 10  | W     | 402 | ILE  |
| 11  | X     | 51  | LEU  |
| 11  | X     | 89  | VAL  |
| 11  | X     | 129 | LEU  |
| 11  | X     | 136 | LEU  |
| 11  | X     | 169 | VAL  |
| 11  | X     | 195 | THR  |
| 11  | X     | 237 | GLU  |
| 11  | X     | 261 | LEU  |
| 11  | X     | 265 | GLU  |
| 11  | X     | 284 | THR  |
| 11  | X     | 310 | ARG  |
| 11  | X     | 373 | LYS  |
| 12  | Y     | 30  | GLU  |
| 12  | Y     | 104 | MET  |
| 12  | Y     | 109 | GLU  |
| 12  | Y     | 121 | LEU  |
| 12  | Y     | 141 | VAL  |
| 12  | Y     | 143 | TYR  |
| 12  | Y     | 181 | LYS  |
| 12  | Y     | 191 | ILE  |
| 12  | Y     | 221 | THR  |
| 12  | Y     | 325 | VAL  |
| 12  | Y     | 378 | ASN  |
| 13  | Z     | 8   | LYS  |
| 13  | Z     | 15  | VAL  |
| 13  | Z     | 53  | SER  |
| 13  | Z     | 106 | ILE  |
| 13  | Z     | 121 | LEU  |
| 13  | Z     | 130 | ASP  |
| 13  | Z     | 187 | LEU  |
| 13  | Z     | 195 | VAL  |
| 13  | Z     | 228 | TYR  |
| 13  | Z     | 233 | VAL  |
| 13  | Z     | 276 | ILE  |
| 14  | a     | 32  | LYS  |
| 14  | a     | 69  | HIS  |
| 14  | a     | 112 | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 14  | a     | 127 | ASP  |
| 14  | a     | 143 | ASN  |
| 14  | a     | 158 | LEU  |
| 14  | a     | 211 | PHE  |
| 14  | a     | 212 | ASN  |
| 14  | a     | 216 | LEU  |
| 14  | a     | 252 | LYS  |
| 14  | a     | 274 | LEU  |
| 14  | a     | 292 | THR  |
| 14  | a     | 320 | VAL  |
| 14  | a     | 327 | VAL  |
| 14  | a     | 328 | ASP  |
| 14  | a     | 346 | ILE  |
| 14  | a     | 358 | THR  |
| 14  | a     | 362 | SER  |
| 14  | a     | 374 | ILE  |
| 15  | b     | 33  | VAL  |
| 15  | b     | 34  | ASN  |
| 15  | b     | 48  | ASN  |
| 15  | b     | 64  | LEU  |
| 15  | b     | 75  | LEU  |
| 15  | b     | 78  | VAL  |
| 15  | b     | 90  | ILE  |
| 15  | b     | 97  | LEU  |
| 15  | b     | 113 | VAL  |
| 15  | b     | 134 | GLU  |
| 15  | b     | 135 | LYS  |
| 15  | b     | 166 | THR  |
| 15  | b     | 181 | ASP  |
| 16  | c     | 51  | MET  |
| 16  | c     | 60  | GLU  |
| 16  | c     | 66  | THR  |
| 16  | c     | 69  | VAL  |
| 16  | c     | 88  | ASP  |
| 16  | c     | 115 | HIS  |
| 16  | c     | 129 | THR  |
| 16  | c     | 143 | VAL  |
| 16  | c     | 180 | ASN  |
| 16  | c     | 192 | LEU  |
| 16  | c     | 199 | HIS  |
| 16  | c     | 231 | LEU  |
| 16  | c     | 261 | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 16  | c     | 284 | LEU  |
| 17  | d     | 140 | GLN  |
| 17  | d     | 188 | MET  |
| 17  | d     | 219 | ASP  |
| 17  | d     | 280 | GLU  |
| 17  | d     | 282 | ILE  |
| 18  | f     | 60  | VAL  |
| 18  | f     | 82  | ILE  |
| 18  | f     | 111 | GLU  |
| 18  | f     | 162 | LEU  |
| 18  | f     | 205 | CYS  |
| 18  | f     | 219 | LYS  |
| 18  | f     | 249 | LEU  |
| 18  | f     | 296 | PHE  |
| 18  | f     | 372 | LEU  |
| 18  | f     | 381 | VAL  |
| 18  | f     | 404 | ASP  |
| 18  | f     | 433 | LEU  |
| 18  | f     | 434 | TYR  |
| 18  | f     | 440 | ILE  |
| 18  | f     | 573 | ILE  |
| 18  | f     | 721 | VAL  |
| 18  | f     | 800 | LEU  |
| 19  | g     | 101 | LEU  |
| 19  | g     | 131 | ILE  |
| 19  | g     | 166 | ARG  |
| 20  | u     | 157 | LEU  |
| 20  | u     | 165 | LEU  |
| 20  | u     | 169 | VAL  |
| 20  | u     | 213 | GLU  |
| 20  | u     | 243 | SER  |
| 20  | u     | 245 | THR  |
| 20  | u     | 250 | SER  |
| 20  | u     | 263 | PHE  |
| 20  | u     | 268 | THR  |
| 20  | u     | 289 | HIS  |
| 22  | A     | 34  | LYS  |
| 22  | A     | 38  | GLN  |
| 22  | A     | 46  | LYS  |
| 22  | A     | 59  | ILE  |
| 22  | A     | 65  | ILE  |
| 22  | A     | 77  | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 22  | A     | 95  | VAL  |
| 22  | A     | 123 | VAL  |
| 22  | A     | 145 | ASN  |
| 22  | A     | 171 | ASP  |
| 22  | A     | 184 | ILE  |
| 22  | A     | 207 | GLU  |
| 22  | A     | 233 | THR  |
| 22  | A     | 240 | VAL  |
| 22  | A     | 322 | ASN  |
| 22  | A     | 326 | THR  |
| 22  | A     | 332 | MET  |
| 22  | A     | 342 | GLU  |
| 22  | A     | 390 | THR  |
| 22  | A     | 403 | ILE  |
| 22  | A     | 431 | THR  |
| 23  | B     | 52  | VAL  |
| 23  | B     | 56  | THR  |
| 23  | B     | 57  | GLN  |
| 23  | B     | 72  | LEU  |
| 23  | B     | 86  | LYS  |
| 23  | B     | 177 | GLU  |
| 23  | B     | 203 | LEU  |
| 23  | B     | 250 | VAL  |
| 23  | B     | 255 | LEU  |
| 23  | B     | 256 | ILE  |
| 23  | B     | 290 | ILE  |
| 23  | B     | 309 | MET  |
| 23  | B     | 325 | VAL  |
| 23  | B     | 332 | ASN  |
| 23  | B     | 383 | LEU  |
| 23  | B     | 401 | GLU  |
| 23  | B     | 429 | LYS  |
| 23  | B     | 430 | LYS  |
| 23  | B     | 431 | GLN  |
| 23  | B     | 438 | LEU  |
| 24  | E     | 35  | GLU  |
| 24  | E     | 37  | THR  |
| 24  | E     | 38  | LYS  |
| 24  | E     | 42  | LYS  |
| 24  | E     | 47  | LEU  |
| 24  | E     | 53  | VAL  |
| 24  | E     | 56  | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 24  | E     | 65  | THR  |
| 24  | E     | 75  | ASN  |
| 24  | E     | 81  | VAL  |
| 24  | E     | 85  | ARG  |
| 24  | E     | 88  | ASP  |
| 24  | E     | 100 | LEU  |
| 24  | E     | 103 | THR  |
| 24  | E     | 113 | ARG  |
| 24  | E     | 114 | GLU  |
| 24  | E     | 115 | VAL  |
| 24  | E     | 116 | ASP  |
| 24  | E     | 120 | TYR  |
| 24  | E     | 125 | GLU  |
| 24  | E     | 130 | VAL  |
| 24  | E     | 135 | ILE  |
| 24  | E     | 138 | LEU  |
| 24  | E     | 139 | SER  |
| 24  | E     | 190 | GLN  |
| 24  | E     | 193 | CYS  |
| 24  | E     | 194 | ASN  |
| 24  | E     | 196 | LEU  |
| 24  | E     | 198 | VAL  |
| 24  | E     | 201 | SER  |
| 24  | E     | 203 | ILE  |
| 24  | E     | 204 | VAL  |
| 24  | E     | 205 | ASP  |
| 24  | E     | 206 | LYS  |
| 24  | E     | 208 | ILE  |
| 24  | E     | 216 | ARG  |
| 24  | E     | 218 | MET  |
| 24  | E     | 223 | ARG  |
| 24  | E     | 224 | ASP  |
| 24  | E     | 229 | ILE  |
| 24  | E     | 245 | GLU  |
| 24  | E     | 268 | ASP  |
| 24  | E     | 272 | ARG  |
| 24  | E     | 277 | MET  |
| 24  | E     | 279 | THR  |
| 24  | E     | 285 | LEU  |
| 24  | E     | 286 | ASP  |
| 24  | E     | 297 | ARG  |
| 24  | E     | 298 | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 24  | E     | 301 | ILE  |
| 24  | E     | 302 | ASP  |
| 24  | E     | 303 | LEU  |
| 24  | E     | 304 | PRO  |
| 24  | E     | 307 | GLN  |
| 24  | E     | 309 | ARG  |
| 24  | E     | 322 | LYS  |
| 24  | E     | 323 | HIS  |
| 24  | E     | 326 | ILE  |
| 24  | E     | 335 | SER  |
| 24  | E     | 339 | ASN  |
| 24  | E     | 343 | LEU  |
| 24  | E     | 344 | ARG  |
| 24  | E     | 352 | MET  |
| 24  | E     | 356 | ARG  |
| 24  | E     | 359 | HIS  |
| 24  | E     | 360 | ASP  |
| 24  | E     | 363 | VAL  |
| 24  | E     | 364 | GLN  |
| 24  | E     | 373 | LYS  |
| 24  | E     | 377 | SER  |
| 24  | E     | 378 | LYS  |
| 24  | E     | 379 | LYS  |
| 25  | F     | 59  | VAL  |
| 25  | F     | 61  | ARG  |
| 25  | F     | 62  | VAL  |
| 25  | F     | 66  | LEU  |
| 25  | F     | 71  | ASP  |
| 25  | F     | 74  | LYS  |
| 25  | F     | 75  | GLU  |
| 25  | F     | 76  | ASN  |
| 25  | F     | 77  | SER  |
| 25  | F     | 79  | LYS  |
| 25  | F     | 81  | LYS  |
| 25  | F     | 143 | GLU  |
| 25  | F     | 162 | GLU  |
| 25  | F     | 193 | LYS  |
| 25  | F     | 195 | ILE  |
| 25  | F     | 209 | LYS  |
| 25  | F     | 211 | LYS  |
| 25  | F     | 213 | GLU  |
| 25  | F     | 215 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 25  | F     | 217 | ILE  |
| 25  | F     | 218 | GLN  |
| 25  | F     | 221 | LYS  |
| 25  | F     | 233 | LYS  |
| 25  | F     | 250 | LYS  |
| 25  | F     | 276 | LYS  |
| 25  | F     | 295 | ARG  |
| 25  | F     | 309 | THR  |
| 25  | F     | 335 | VAL  |
| 25  | F     | 337 | ILE  |
| 25  | F     | 397 | LYS  |
| 25  | F     | 399 | VAL  |
| 25  | F     | 402 | GLU  |
| 25  | F     | 424 | ILE  |
| 25  | F     | 428 | GLN  |
| 25  | F     | 435 | LEU  |
| 26  | K     | 14  | THR  |
| 26  | K     | 36  | THR  |
| 26  | K     | 38  | ILE  |
| 26  | K     | 67  | ILE  |
| 26  | K     | 152 | GLN  |
| 26  | K     | 184 | VAL  |
| 26  | K     | 201 | ILE  |
| 27  | U     | 46  | GLU  |
| 27  | U     | 69  | TYR  |
| 27  | U     | 99  | THR  |
| 27  | U     | 112 | CYS  |
| 27  | U     | 124 | LYS  |
| 27  | U     | 127 | ASP  |
| 27  | U     | 147 | TYR  |
| 27  | U     | 151 | ILE  |
| 27  | U     | 177 | LEU  |
| 27  | U     | 204 | ILE  |
| 27  | U     | 208 | LEU  |
| 27  | U     | 219 | CYS  |
| 27  | U     | 233 | LEU  |
| 27  | U     | 236 | LEU  |
| 27  | U     | 244 | MET  |
| 27  | U     | 254 | GLU  |
| 27  | U     | 263 | SER  |
| 27  | U     | 364 | VAL  |
| 27  | U     | 365 | CYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 27  | U     | 373 | ASN  |
| 27  | U     | 462 | LEU  |
| 27  | U     | 467 | ASN  |
| 27  | U     | 531 | ASP  |
| 27  | U     | 585 | THR  |
| 27  | U     | 586 | VAL  |
| 27  | U     | 602 | LEU  |
| 27  | U     | 633 | CYS  |
| 27  | U     | 675 | MET  |
| 27  | U     | 691 | SER  |
| 27  | U     | 717 | ILE  |
| 27  | U     | 786 | THR  |
| 27  | U     | 835 | ILE  |
| 27  | U     | 870 | GLU  |
| 27  | U     | 889 | LEU  |
| 28  | e     | 41  | ASP  |
| 28  | e     | 63  | HIS  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (108) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 69  | GLN  |
| 1   | C     | 278 | ASN  |
| 2   | D     | 57  | GLN  |
| 2   | D     | 83  | GLN  |
| 2   | D     | 222 | HIS  |
| 2   | D     | 376 | ASN  |
| 2   | D     | 380 | GLN  |
| 2   | D     | 412 | GLN  |
| 3   | G     | 75  | ASN  |
| 3   | G     | 127 | GLN  |
| 4   | H     | 52  | GLN  |
| 4   | H     | 112 | GLN  |
| 5   | I     | 142 | HIS  |
| 5   | I     | 146 | GLN  |
| 5   | I     | 198 | ASN  |
| 5   | I     | 240 | HIS  |
| 6   | J     | 92  | GLN  |
| 6   | J     | 116 | GLN  |
| 6   | J     | 146 | GLN  |
| 6   | J     | 159 | ASN  |
| 7   | L     | 8   | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 7   | L     | 53  | GLN  |
| 7   | L     | 59  | HIS  |
| 8   | M     | 147 | GLN  |
| 9   | V     | 177 | ASN  |
| 9   | V     | 232 | HIS  |
| 9   | V     | 247 | GLN  |
| 9   | V     | 257 | ASN  |
| 9   | V     | 282 | ASN  |
| 10  | W     | 189 | GLN  |
| 10  | W     | 440 | ASN  |
| 11  | X     | 44  | GLN  |
| 11  | X     | 48  | GLN  |
| 11  | X     | 127 | GLN  |
| 11  | X     | 380 | GLN  |
| 11  | X     | 406 | ASN  |
| 12  | Y     | 14  | ASN  |
| 12  | Y     | 280 | GLN  |
| 14  | a     | 12  | GLN  |
| 14  | a     | 168 | ASN  |
| 14  | a     | 305 | ASN  |
| 15  | b     | 99  | HIS  |
| 15  | b     | 101 | GLN  |
| 15  | b     | 142 | ASN  |
| 15  | b     | 161 | ASN  |
| 16  | c     | 44  | HIS  |
| 16  | c     | 101 | GLN  |
| 16  | c     | 197 | ASN  |
| 16  | c     | 241 | ASN  |
| 16  | c     | 256 | ASN  |
| 16  | c     | 295 | ASN  |
| 17  | d     | 127 | ASN  |
| 17  | d     | 190 | GLN  |
| 17  | d     | 195 | ASN  |
| 17  | d     | 202 | GLN  |
| 17  | d     | 234 | GLN  |
| 17  | d     | 338 | GLN  |
| 18  | f     | 198 | HIS  |
| 18  | f     | 325 | GLN  |
| 18  | f     | 329 | ASN  |
| 18  | f     | 355 | ASN  |
| 18  | f     | 387 | GLN  |
| 18  | f     | 614 | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 18  | f     | 701 | ASN  |
| 18  | f     | 752 | HIS  |
| 18  | f     | 766 | GLN  |
| 18  | f     | 782 | HIS  |
| 18  | f     | 790 | GLN  |
| 18  | f     | 868 | HIS  |
| 18  | f     | 876 | HIS  |
| 19  | g     | 135 | GLN  |
| 20  | u     | 183 | GLN  |
| 22  | A     | 296 | GLN  |
| 22  | A     | 314 | ASN  |
| 22  | A     | 433 | ASN  |
| 23  | B     | 242 | GLN  |
| 23  | B     | 277 | HIS  |
| 24  | E     | 39  | GLN  |
| 24  | E     | 45  | ASN  |
| 24  | E     | 190 | GLN  |
| 24  | E     | 220 | ASN  |
| 24  | E     | 262 | ASN  |
| 24  | E     | 280 | ASN  |
| 25  | F     | 76  | ASN  |
| 25  | F     | 208 | HIS  |
| 25  | F     | 214 | ASN  |
| 25  | F     | 218 | GLN  |
| 25  | F     | 307 | GLN  |
| 25  | F     | 325 | GLN  |
| 25  | F     | 380 | ASN  |
| 26  | K     | 99  | HIS  |
| 26  | K     | 152 | GLN  |
| 26  | K     | 164 | GLN  |
| 27  | U     | 207 | ASN  |
| 27  | U     | 227 | GLN  |
| 27  | U     | 267 | ASN  |
| 27  | U     | 345 | ASN  |
| 27  | U     | 355 | ASN  |
| 27  | U     | 366 | HIS  |
| 27  | U     | 373 | ASN  |
| 27  | U     | 389 | ASN  |
| 27  | U     | 398 | ASN  |
| 27  | U     | 415 | HIS  |
| 27  | U     | 525 | ASN  |
| 27  | U     | 685 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 27  | U     | 697 | GLN  |
| 27  | U     | 708 | GLN  |
| 27  | U     | 749 | GLN  |

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 6 are monoatomic - leaving 6 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 | $\# Z  > 2$ |
| 31  | ADP  | E     | 501 | -    | 28,29,29     | 0.42 | 0           | 43,45,45    | 0.54 | 0           |
| 29  | ATP  | A     | 501 | 30   | 32,33,33     | 0.55 | 0           | 48,52,52    | 0.60 | 0           |
| 29  | ATP  | B     | 501 | 30   | 32,33,33     | 0.59 | 1 (3%)      | 48,52,52    | 0.39 | 0           |
| 31  | ADP  | D     | 501 | 30   | 28,29,29     | 0.46 | 0           | 43,45,45    | 0.52 | 0           |
| 29  | ATP  | F     | 501 | 30   | 32,33,33     | 0.57 | 0           | 48,52,52    | 0.63 | 0           |
| 29  | ATP  | C     | 501 | 30   | 32,33,33     | 0.60 | 0           | 48,52,52    | 0.63 | 0           |

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

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|-----|------|---------|------------|---------|
| 31  | ADP  | E     | 501 | -    | -       | 5/16/32/32 | 0/3/3/3 |
| 29  | ATP  | A     | 501 | 30   | -       | 2/22/38/38 | 0/3/3/3 |
| 29  | ATP  | B     | 501 | 30   | -       | 6/22/38/38 | 0/3/3/3 |
| 31  | ADP  | D     | 501 | 30   | -       | 6/16/32/32 | 0/3/3/3 |
| 29  | ATP  | F     | 501 | 30   | -       | 6/22/38/38 | 0/3/3/3 |
| 29  | ATP  | C     | 501 | 30   | -       | 8/22/38/38 | 0/3/3/3 |

All (1) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 29  | B     | 501 | ATP  | PB-O3B | -2.06 | 1.57        | 1.59     |

There are no bond angle outliers.

There are no chirality outliers.

All (33) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 29  | C     | 501 | ATP  | C5'-O5'-PA-O2A  |
| 29  | C     | 501 | ATP  | C5'-O5'-PA-O3A  |
| 29  | B     | 501 | ATP  | C5'-O5'-PA-O1A  |
| 29  | B     | 501 | ATP  | C5'-O5'-PA-O2A  |
| 29  | B     | 501 | ATP  | C5'-O5'-PA-O3A  |
| 29  | B     | 501 | ATP  | O4'-C4'-C5'-O5' |
| 29  | F     | 501 | ATP  | C5'-O5'-PA-O1A  |
| 29  | F     | 501 | ATP  | C5'-O5'-PA-O2A  |
| 29  | F     | 501 | ATP  | C5'-O5'-PA-O3A  |
| 31  | D     | 501 | ADP  | C5'-O5'-PA-O2A  |
| 31  | D     | 501 | ADP  | C5'-O5'-PA-O3A  |
| 31  | E     | 501 | ADP  | PA-O3A-PB-O3B   |
| 31  | E     | 501 | ADP  | C5'-O5'-PA-O2A  |
| 31  | E     | 501 | ADP  | C5'-O5'-PA-O3A  |
| 29  | A     | 501 | ATP  | O4'-C4'-C5'-O5' |
| 31  | D     | 501 | ADP  | O4'-C4'-C5'-O5' |
| 29  | C     | 501 | ATP  | O4'-C4'-C5'-O5' |
| 29  | C     | 501 | ATP  | C3'-C4'-C5'-O5' |
| 29  | F     | 501 | ATP  | C3'-C4'-C5'-O5' |
| 31  | D     | 501 | ADP  | C3'-C4'-C5'-O5' |
| 29  | B     | 501 | ATP  | C3'-C4'-C5'-O5' |
| 29  | F     | 501 | ATP  | O4'-C4'-C5'-O5' |

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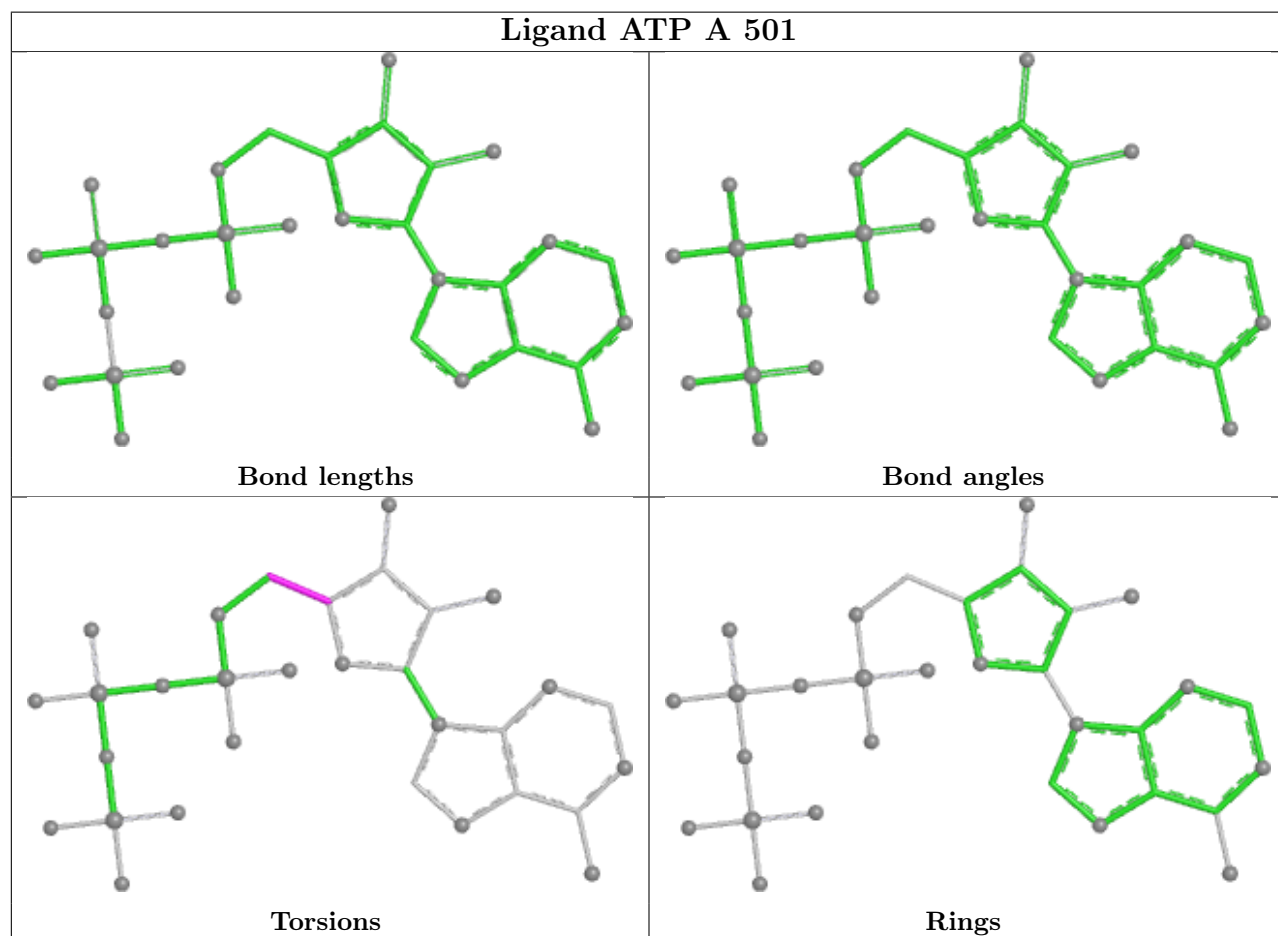
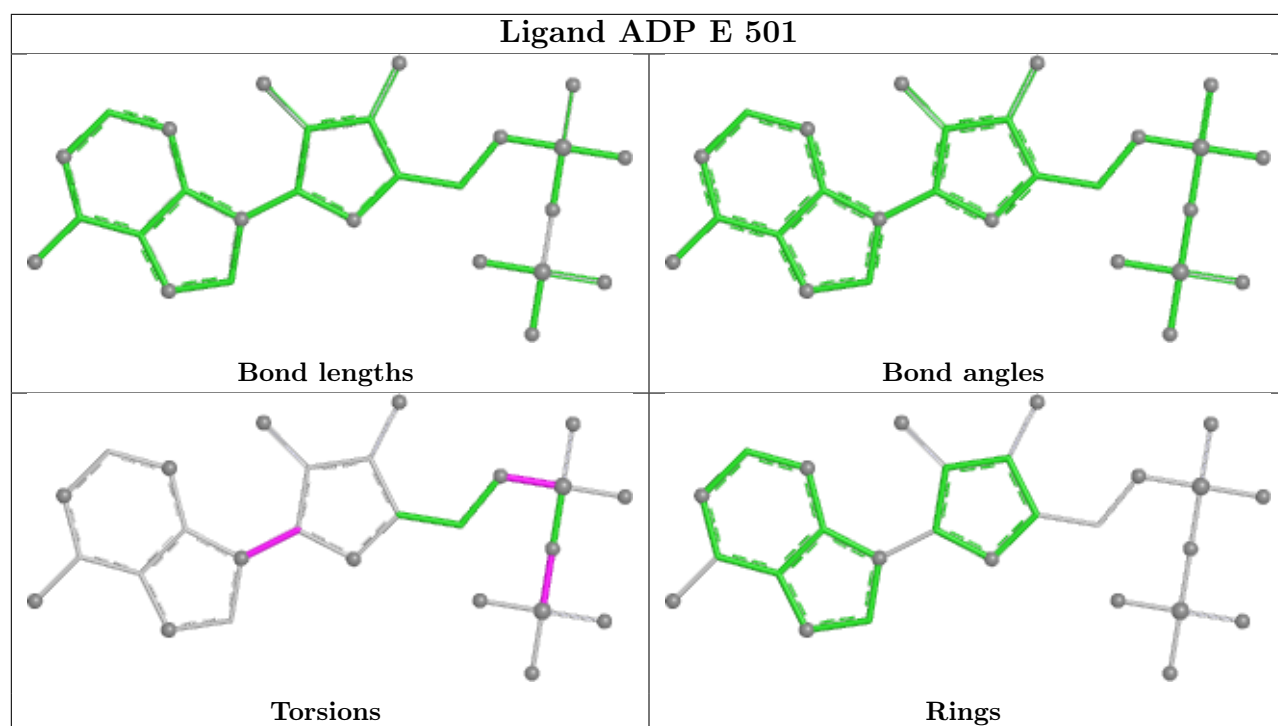
| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 29  | A     | 501 | ATP  | C3'-C4'-C5'-O5' |
| 29  | B     | 501 | ATP  | PB-O3B-PG-O3G   |
| 29  | C     | 501 | ATP  | PB-O3A-PA-O2A   |
| 29  | C     | 501 | ATP  | C5'-O5'-PA-O1A  |
| 29  | C     | 501 | ATP  | C4'-C5'-O5'-PA  |
| 29  | F     | 501 | ATP  | PB-O3B-PG-O1G   |
| 29  | C     | 501 | ATP  | PB-O3A-PA-O1A   |
| 31  | D     | 501 | ADP  | C2'-C1'-N9-C8   |
| 31  | E     | 501 | ADP  | C2'-C1'-N9-C8   |
| 31  | D     | 501 | ADP  | C2'-C1'-N9-C4   |
| 31  | E     | 501 | ADP  | C2'-C1'-N9-C4   |

There are no ring outliers.

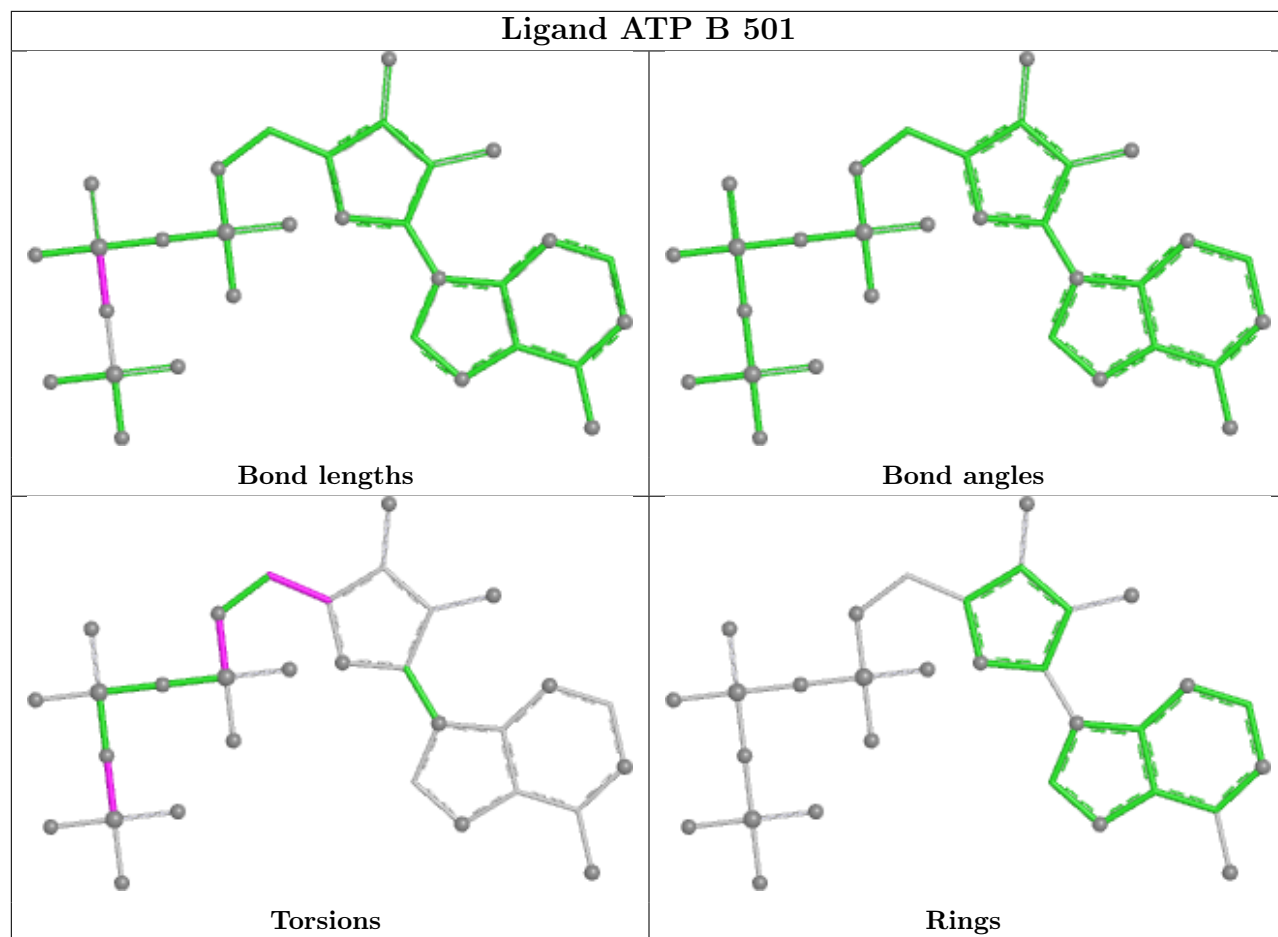
5 monomers are involved in 19 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 29  | A     | 501 | ATP  | 2       | 0            |
| 29  | B     | 501 | ATP  | 5       | 0            |
| 31  | D     | 501 | ADP  | 1       | 0            |
| 29  | F     | 501 | ATP  | 9       | 0            |
| 29  | C     | 501 | ATP  | 2       | 0            |

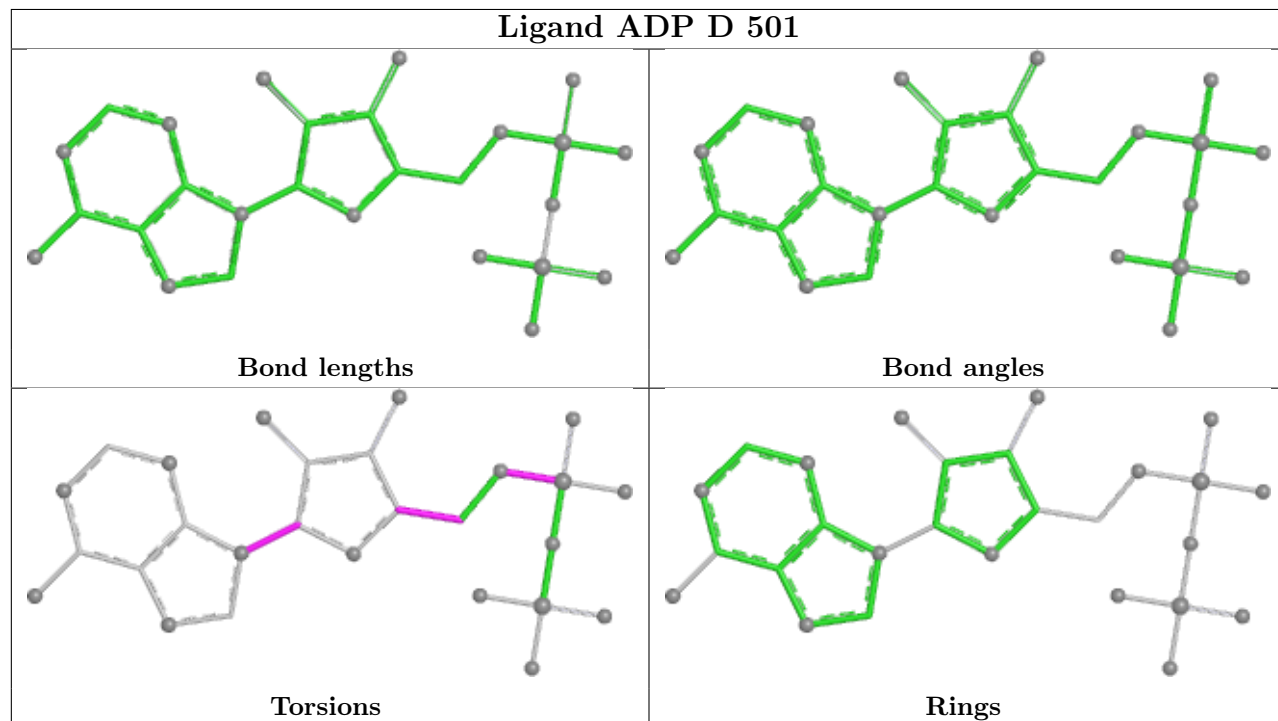
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



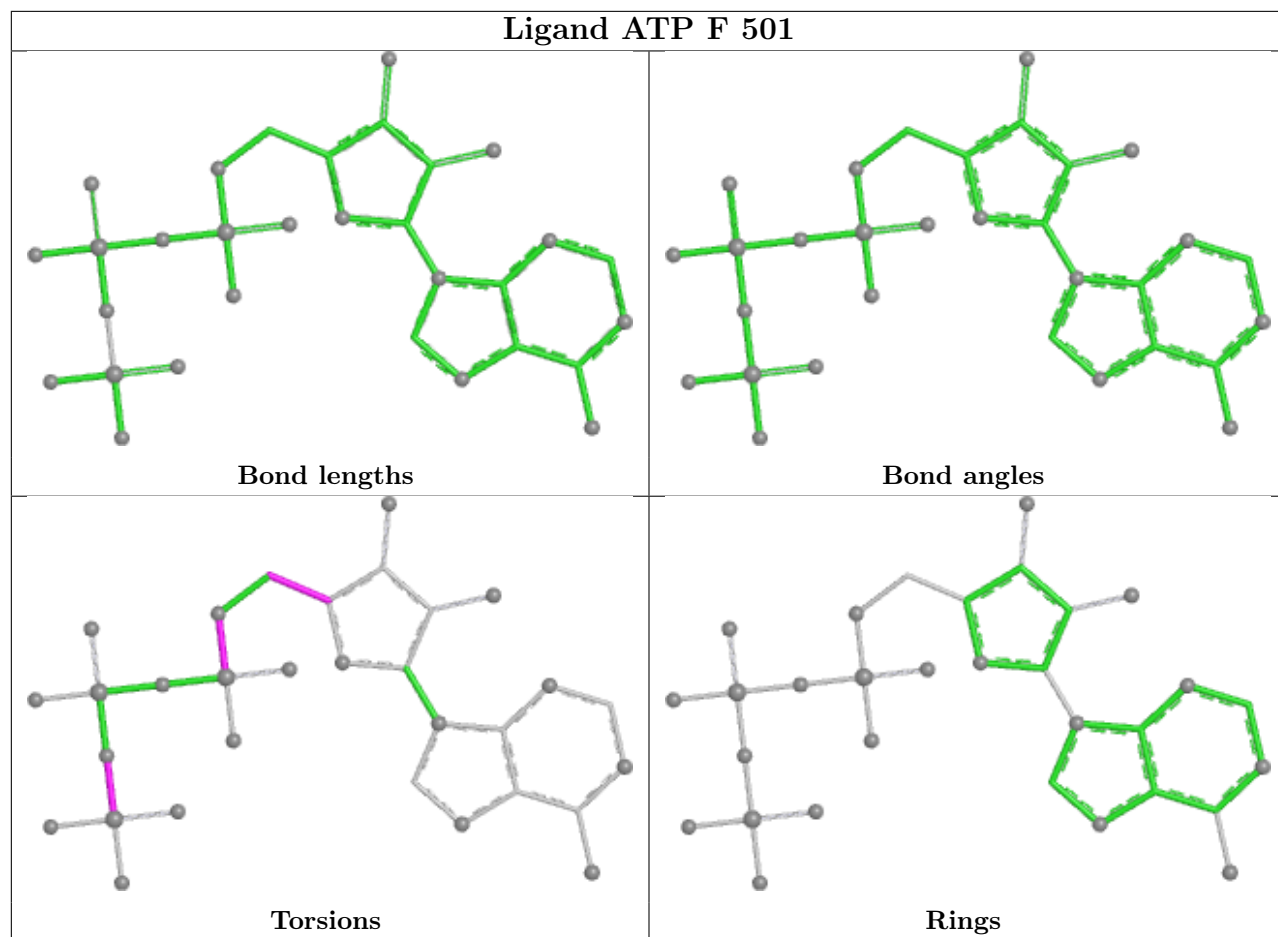
## Ligand ATP B 501

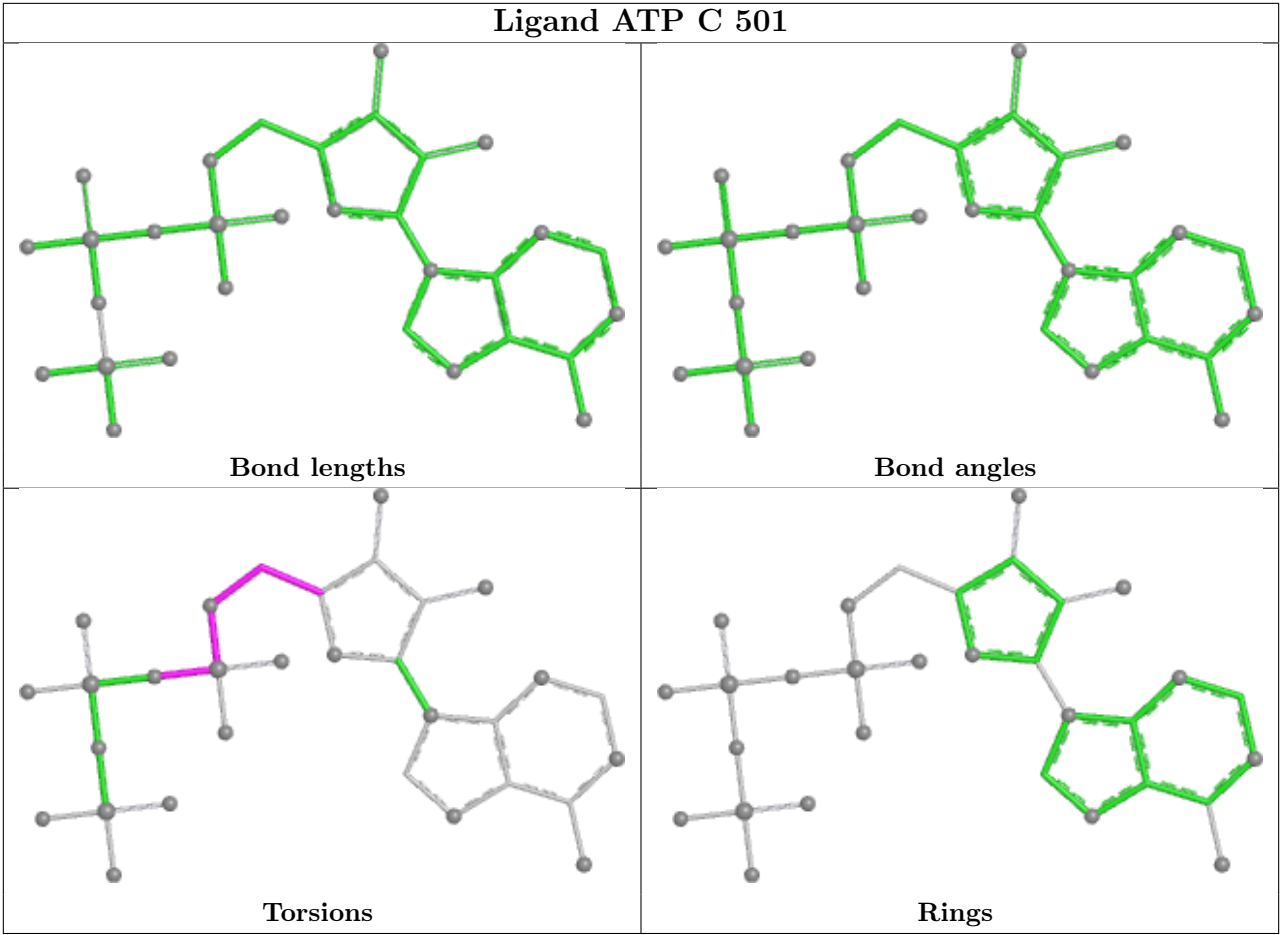


## Ligand ADP D 501



## Ligand ATP F 501





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

| Mol | Chain | Number of breaks |
|-----|-------|------------------|
| 18  | f     | 1                |

All chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1     | f     | 646:MET   | C      | 647:GLY   | N      | 3.77         |

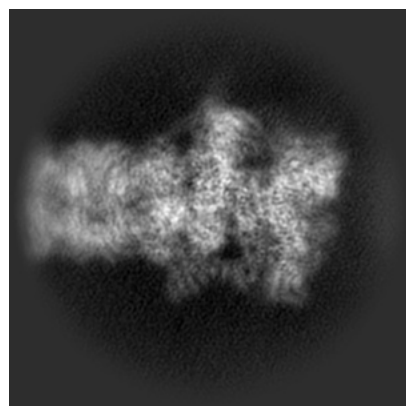
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-47722. These allow visual inspection of the internal detail of the map and identification of artifacts.

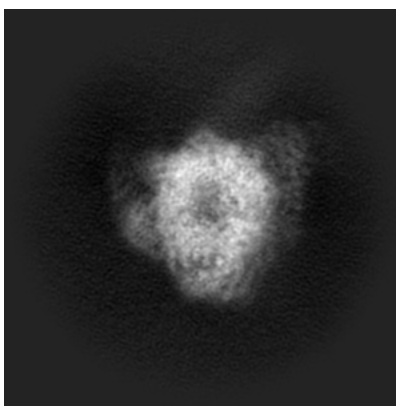
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

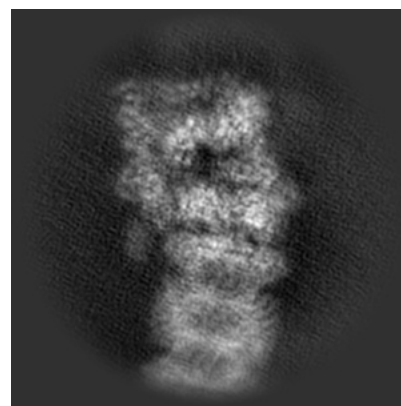
#### 6.1.1 Primary map



X

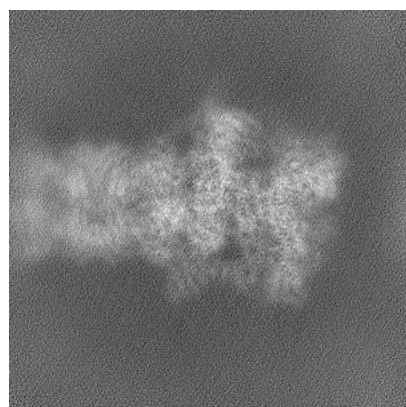


Y

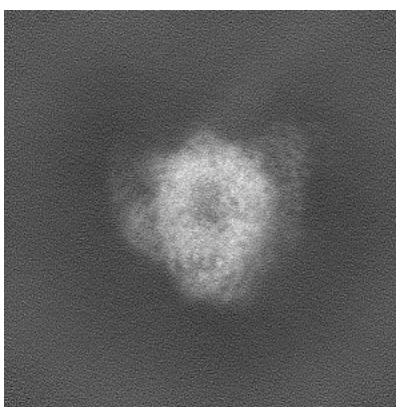


Z

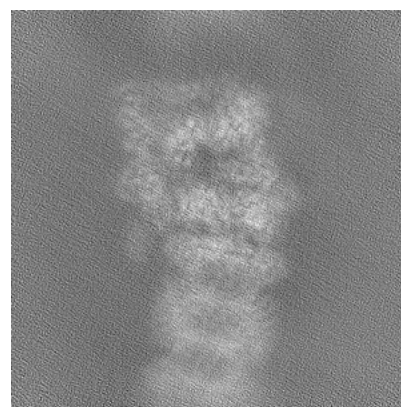
#### 6.1.2 Raw map



X



Y

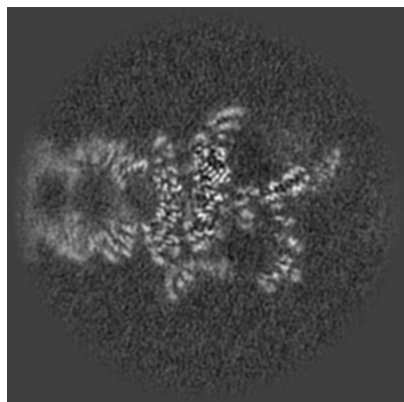


Z

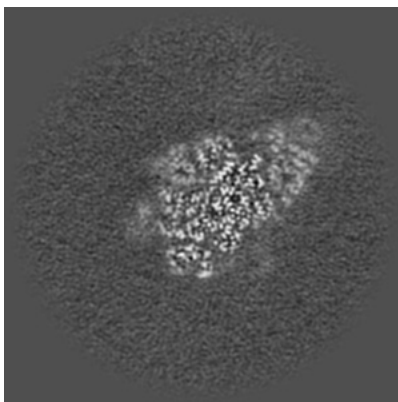
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

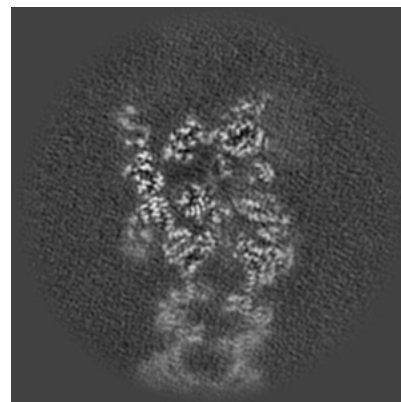
### 6.2.1 Primary map



X Index: 170

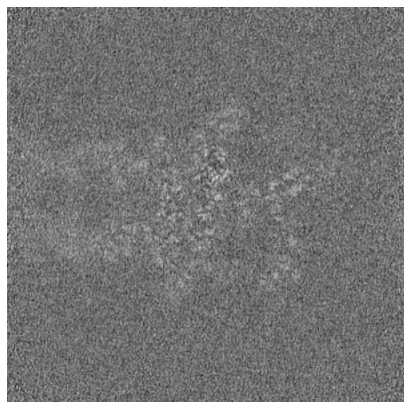


Y Index: 170

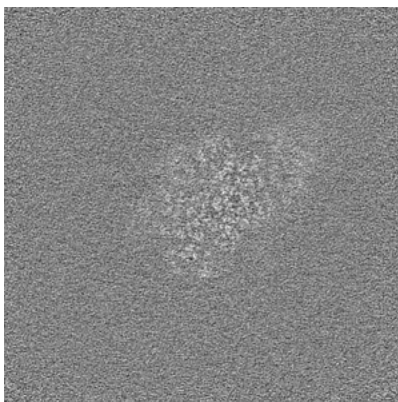


Z Index: 170

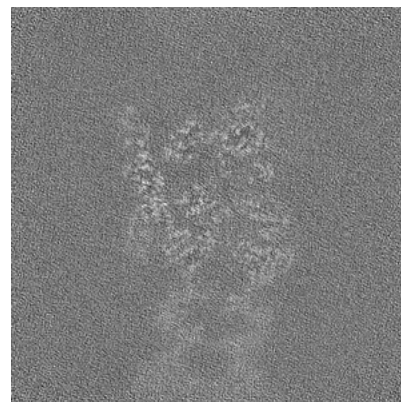
### 6.2.2 Raw map



X Index: 170



Y Index: 170

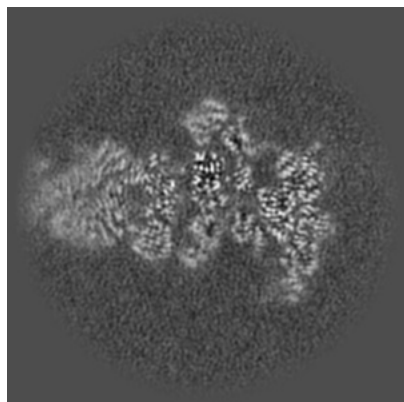


Z Index: 170

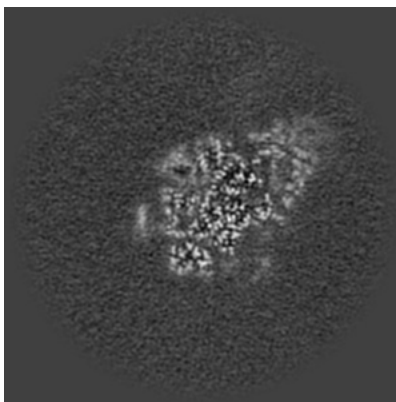
The images above show central slices of the map in three orthogonal directions.

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

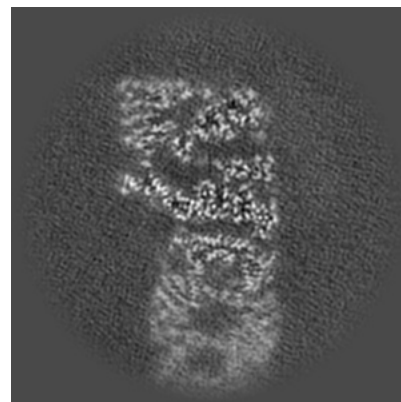
### 6.3.1 Primary map



X Index: 200

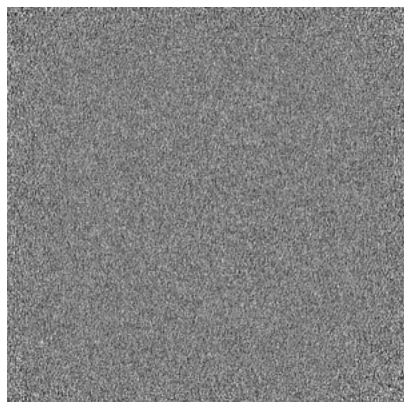


Y Index: 172

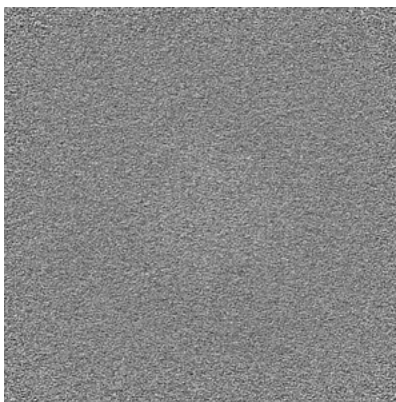


Z Index: 192

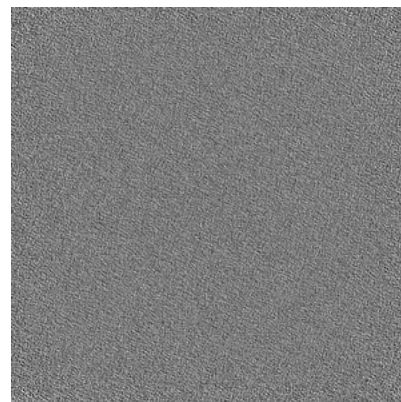
### 6.3.2 Raw map



X Index: 0



Y Index: 0

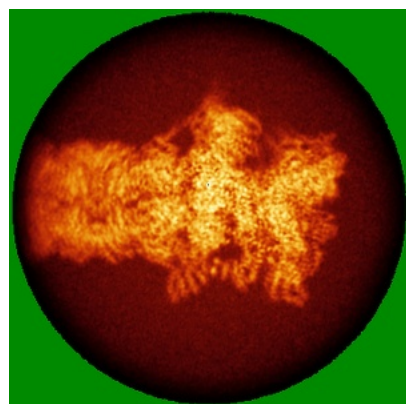


Z Index: 0

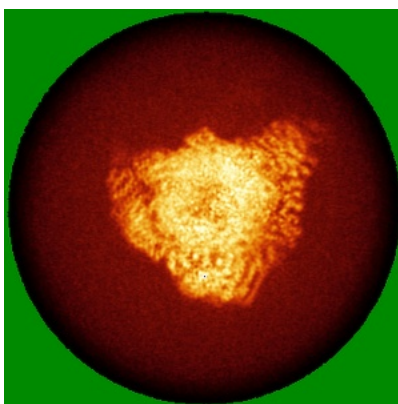
The images above show the largest variance slices of the map in three orthogonal directions.

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

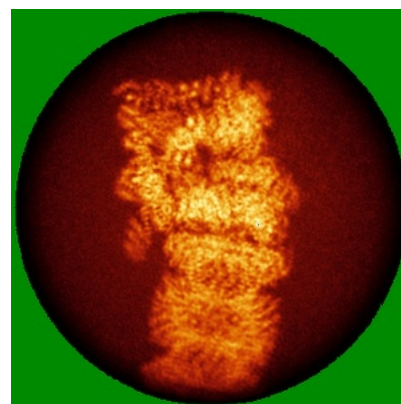
### 6.4.1 Primary map



X

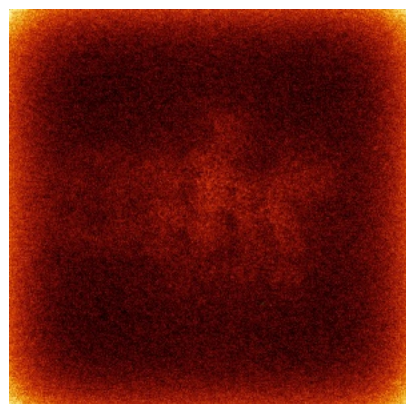


Y

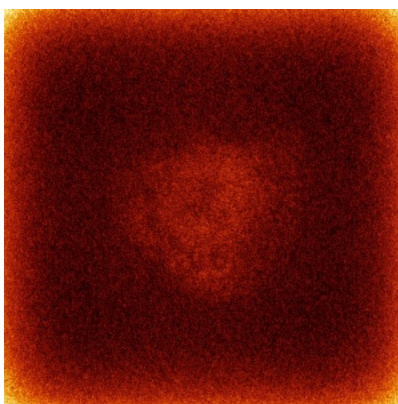


Z

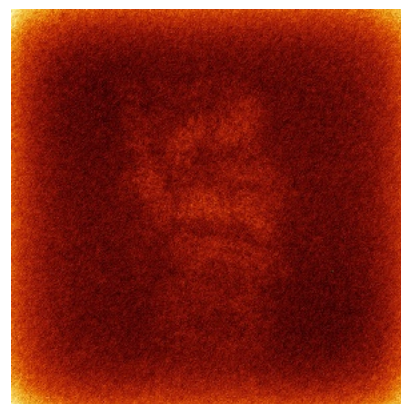
### 6.4.2 Raw map



X



Y

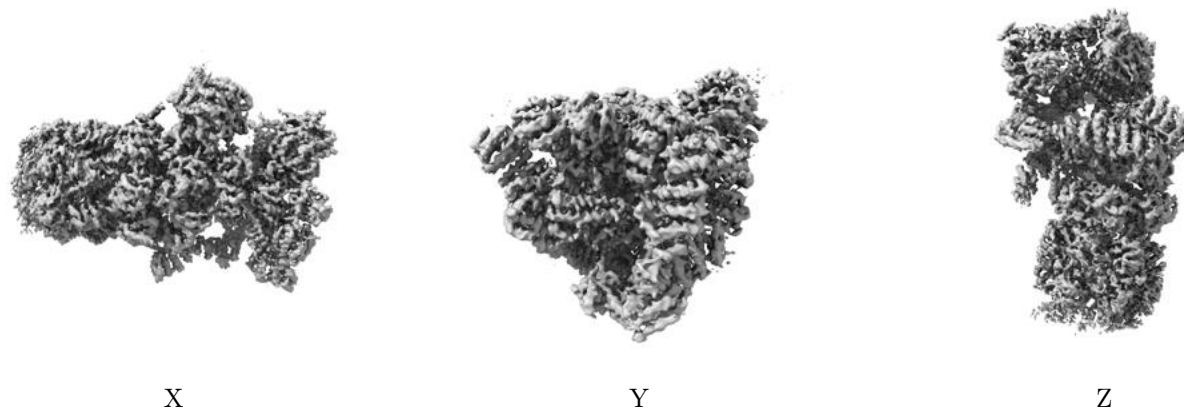


Z

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

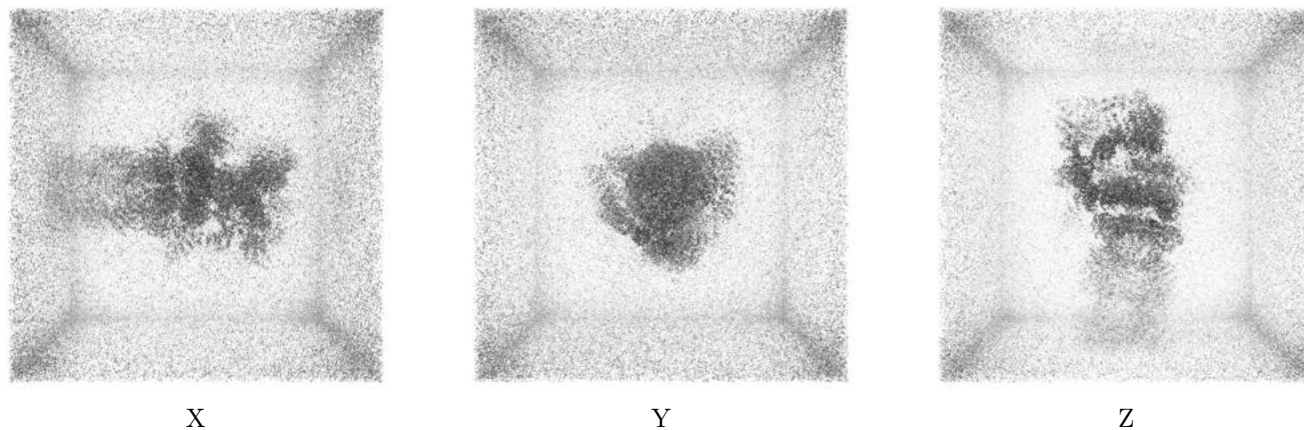
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.15. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



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

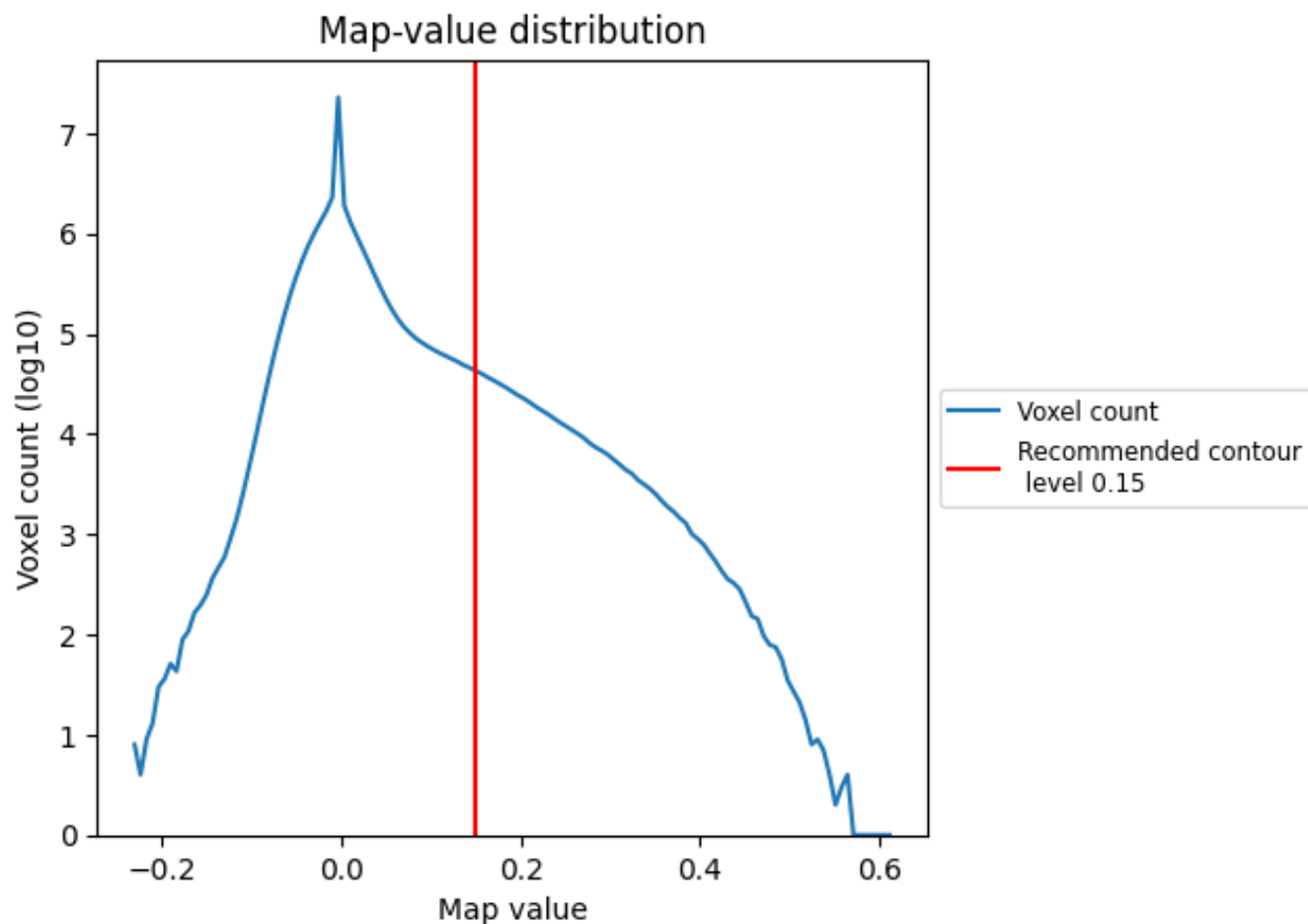
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

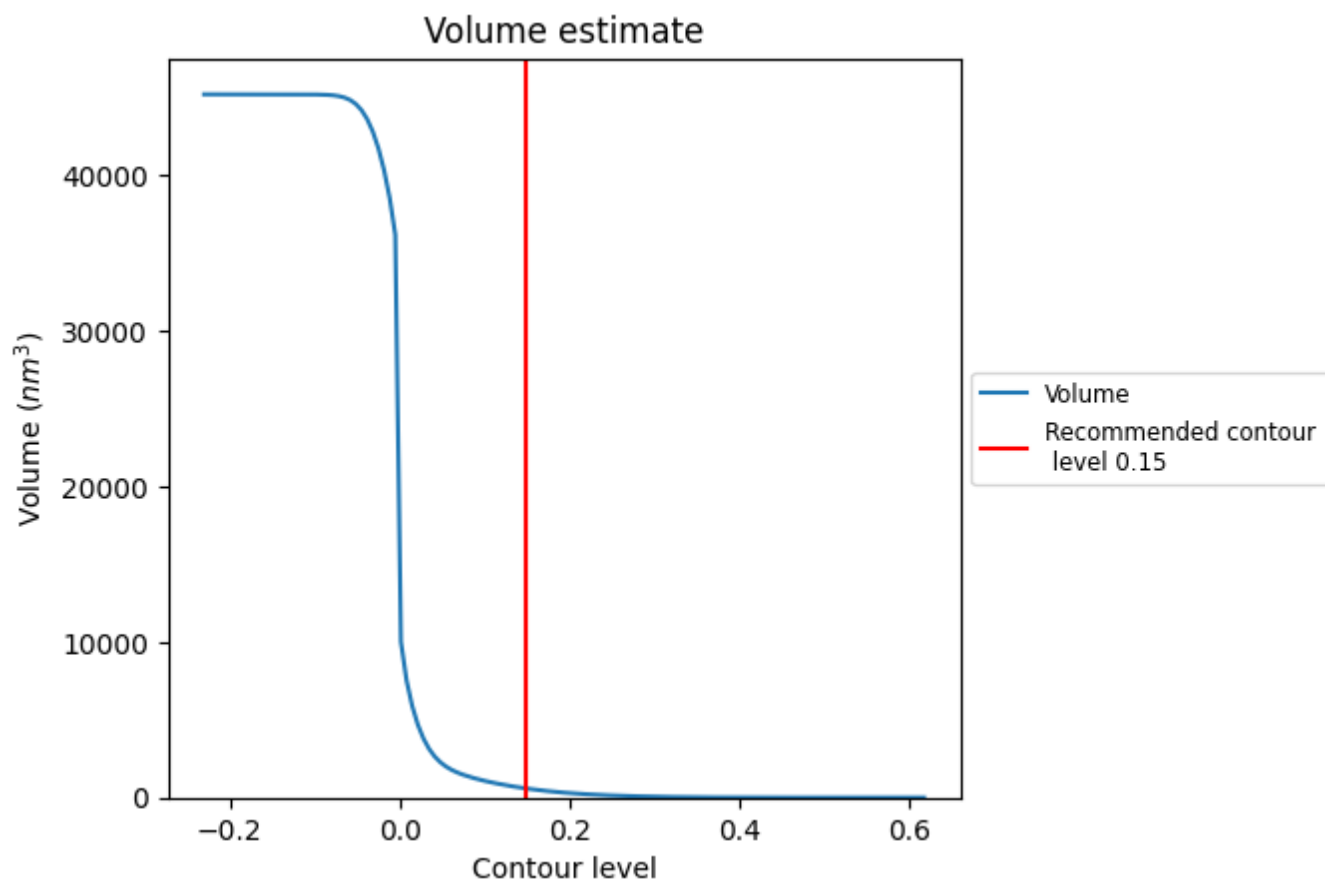
This section contains the results of statistical analysis of the map.

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



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

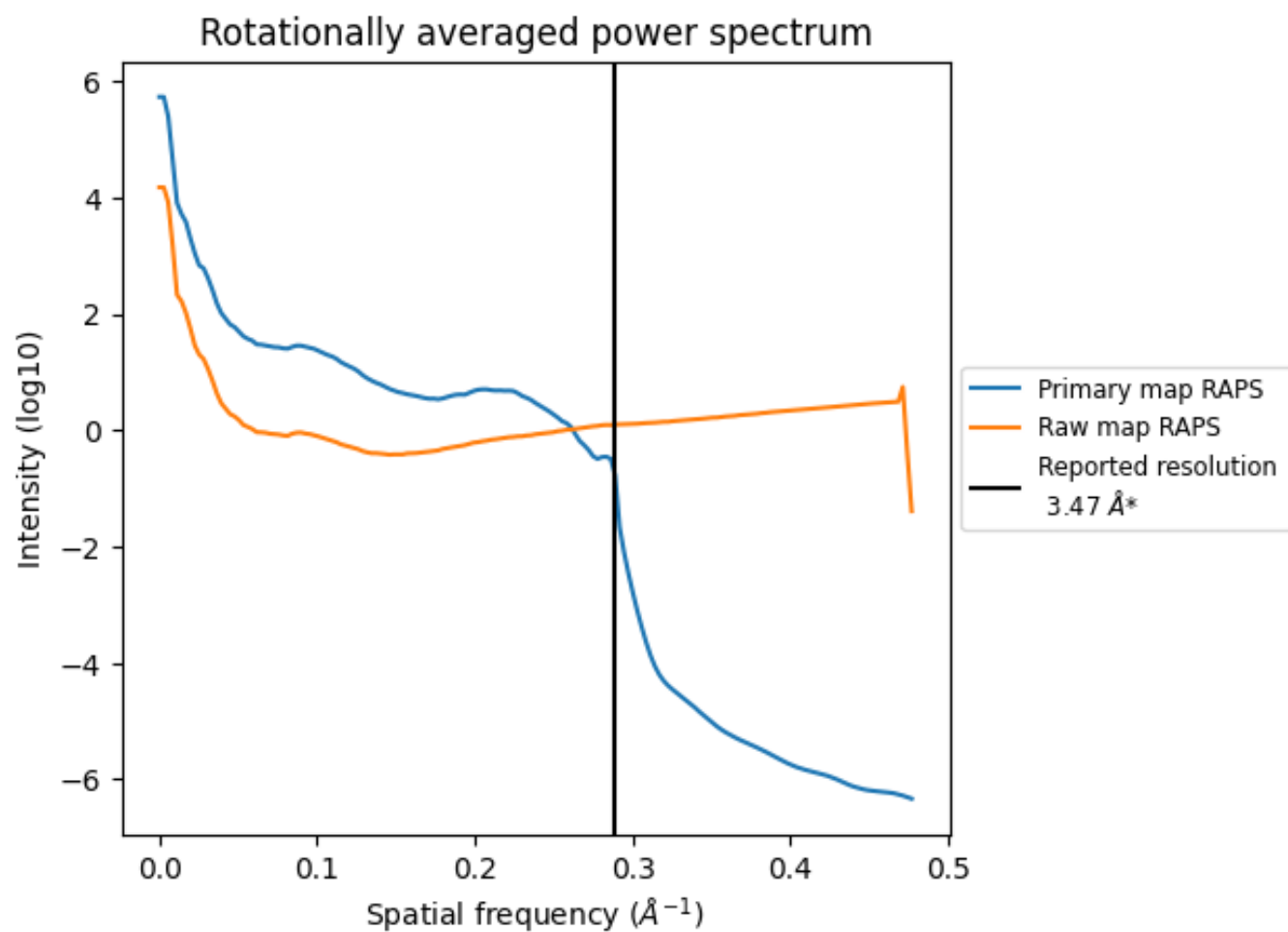
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 582 nm<sup>3</sup>; this corresponds to an approximate mass of 526 kDa.

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

### 7.3 Rotationally averaged power spectrum ⓘ

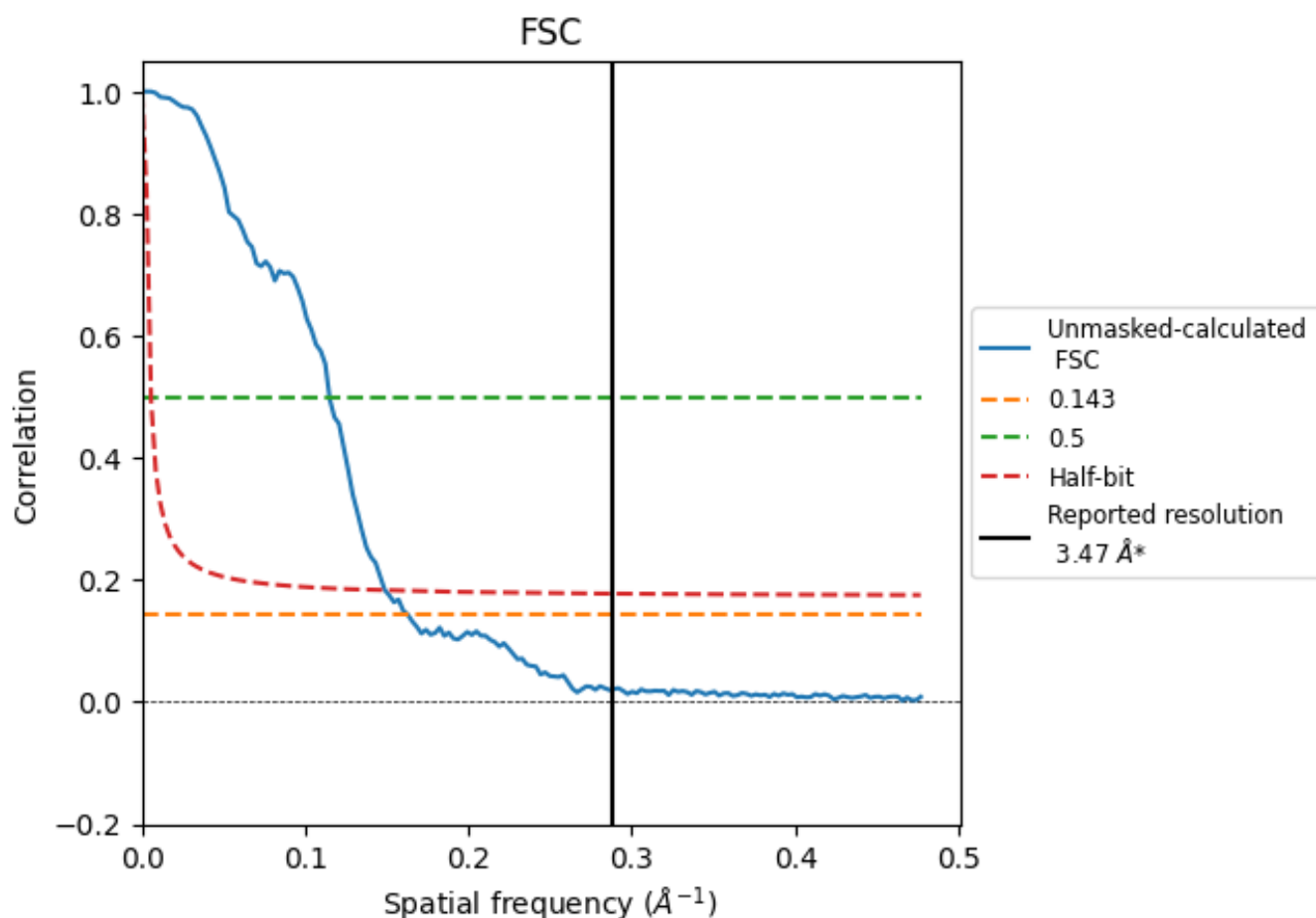


\*Reported resolution corresponds to spatial frequency of 0.288 Å<sup>-1</sup>

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

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.288  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

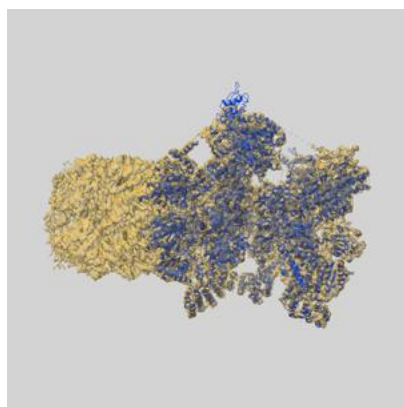
| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |      |          |
|---------------------------|------------------------------------|------|----------|
|                           | 0.143                              | 0.5  | Half-bit |
| Reported by author        | 3.47                               | -    | -        |
| Author-provided FSC curve | -                                  | -    | -        |
| Unmasked-calculated*      | 6.14                               | 8.71 | 6.71     |

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.14 differs from the reported value 3.47 by more than 10 %

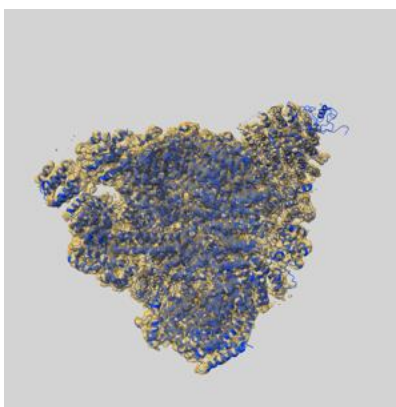
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-47722 and PDB model 9E8J. Per-residue inclusion information can be found in section 3 on page 14.

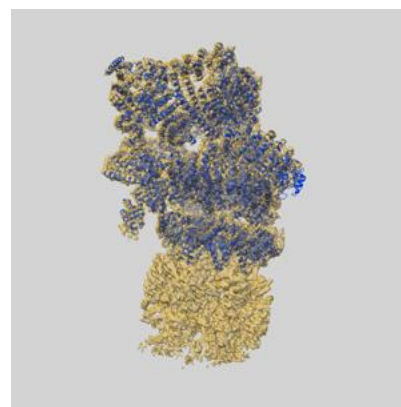
### 9.1 Map-model overlay [i](#)



X



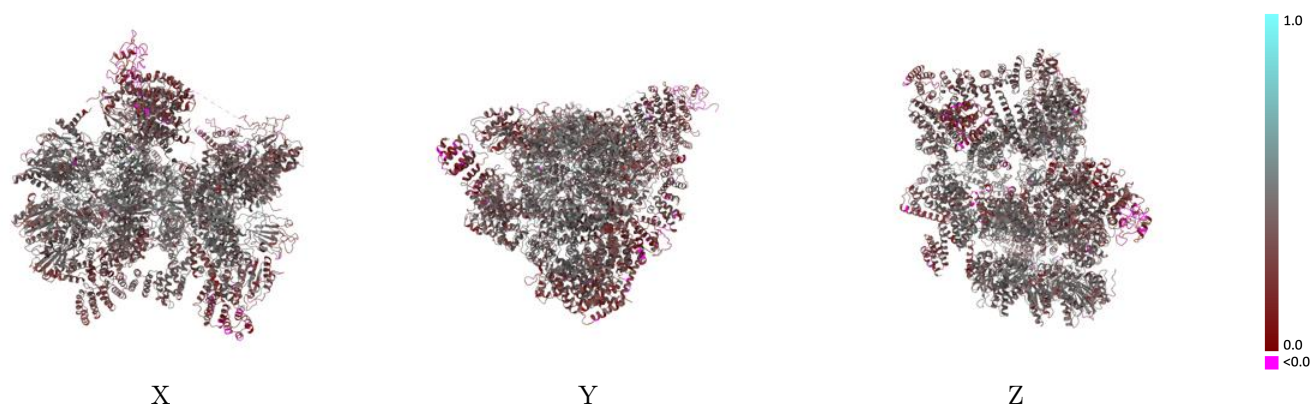
Y



Z

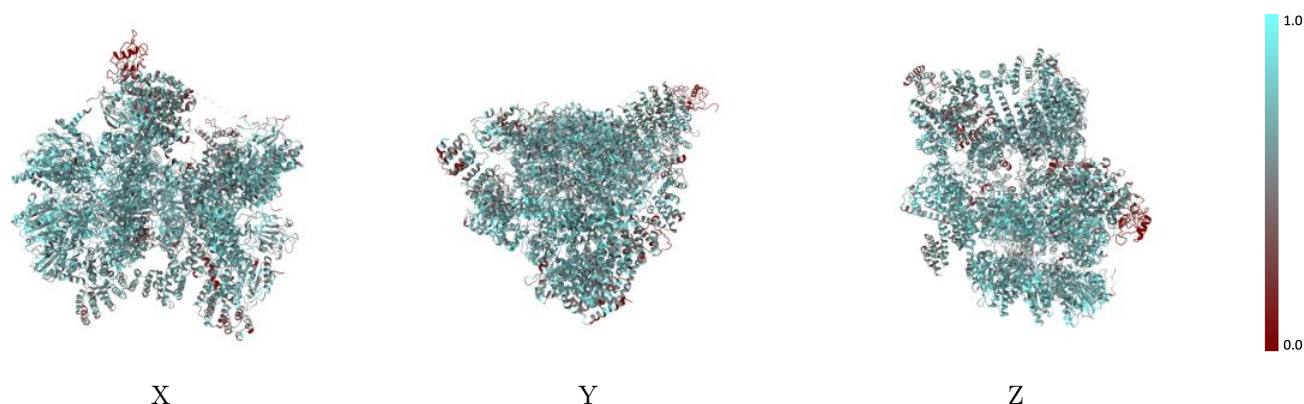
The images above show the 3D surface view of the map at the recommended contour level 0.15 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



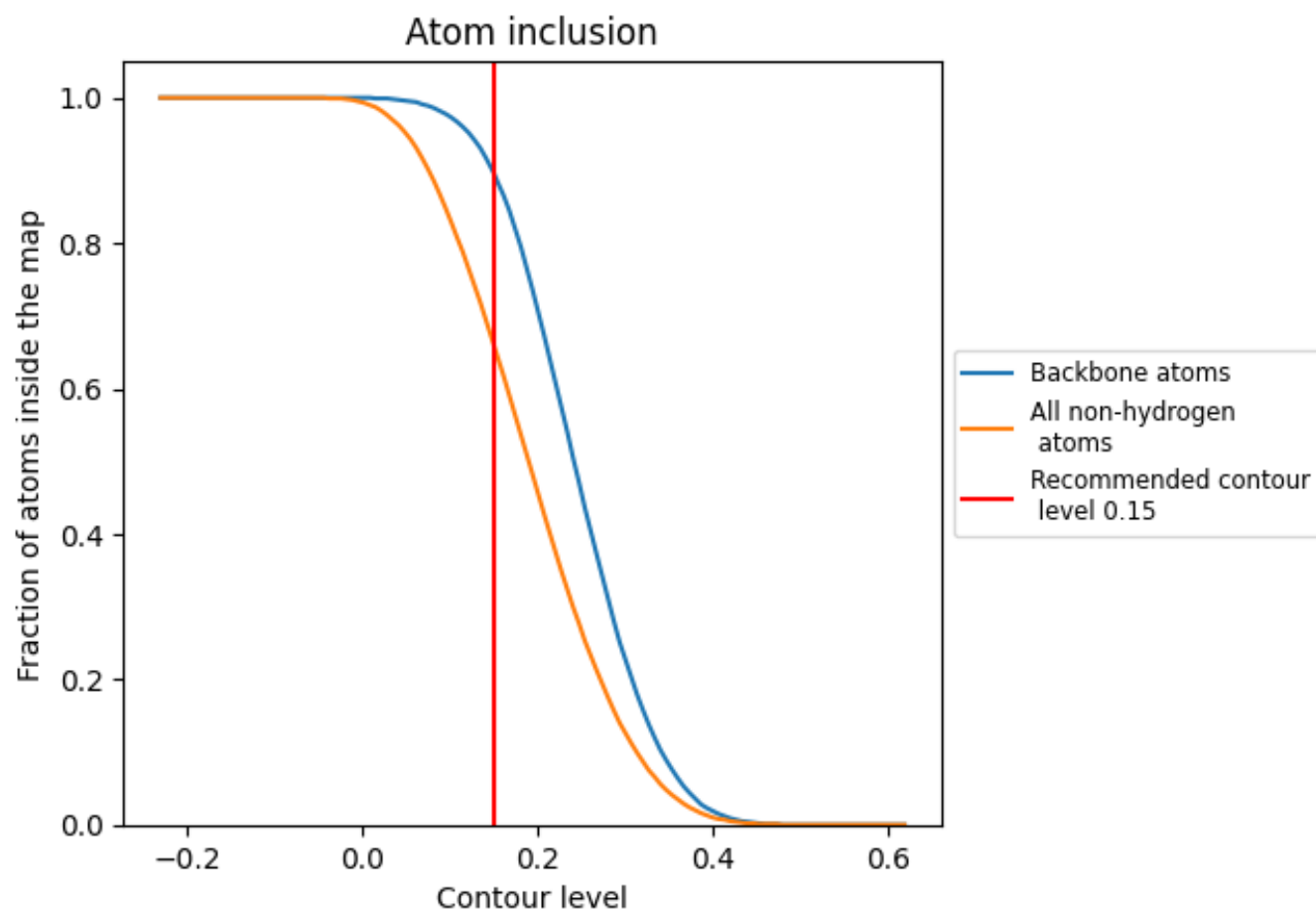
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.15).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 66% 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 (0.15) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| All   |  0.6600   |  0.3750   |
| A     |  0.6760   |  0.4140   |
| B     |  0.6950   |  0.4400   |
| C     |  0.7280   |  0.4500   |
| D     |  0.7200   |  0.4410   |
| E     |  0.6320   |  0.3570   |
| F     |  0.6100   |  0.3610   |
| G     |  0.7180   |  0.4170   |
| H     |  0.7320   |  0.4250   |
| I     |  0.7260   |  0.4060   |
| J     |  0.7320   |  0.4070   |
| K     |  0.7160   |  0.4060   |
| L     |  0.7280   |  0.4090   |
| M     |  0.6940   |  0.3900   |
| U     |  0.6620  |  0.3720  |
| V     |  0.6050 |  0.3250 |
| W     |  0.6270 |  0.3530 |
| X     |  0.6910 |  0.3810 |
| Y     |  0.7620 |  0.4110 |
| Z     |  0.7200 |  0.4240 |
| a     |  0.6000 |  0.2920 |
| b     |  0.6070 |  0.3340 |
| c     |  0.6740 |  0.4080 |
| d     |  0.5530 |  0.2890 |
| e     |  0.6670 |  0.3560 |
| f     |  0.6100 |  0.3150 |
| g     |  0.0200 |  0.0650 |
| u     |  0.5690 |  0.3850 |
| v     |  0.9270 |  0.5470 |

