



## Full wwPDB EM Validation Report ⓘ

Mar 10, 2026 – 04:49 AM UTC

PDB ID : 5ZZ8 / pdb\_00005zz8  
EMDB ID : EMD-6976  
Title : Structure of the Herpes simplex virus type 2 C-capsid with capsid-vertex-specific component  
Authors : Wang, J.L.; Yuan, S.; Zhu, D.J.; Tang, H.; Wang, N.; Chen, W.Y.; Gao, Q.; Li, Y.H.; Wang, J.Z.; Liu, H.R.; Zhang, X.Z.; Rao, Z.H.; Wang, X.X.  
Deposited on : 2018-05-31  
Resolution : 3.75 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  
MolProbity : 4-5-2 with Phenix2.0  
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

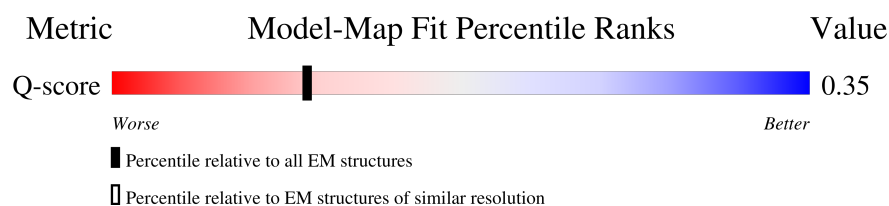
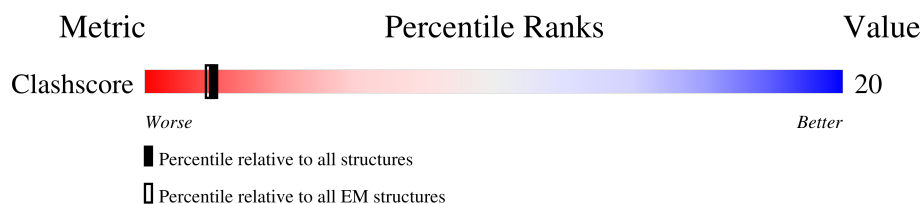
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

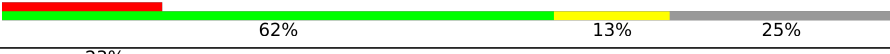
The reported resolution of this entry is 3.75 Å.

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                       | -                                                        |
| Q-score    | -                           | 25397                       | 10301 ( 3.25 - 4.25 )                                    |

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   | 1     | 466    |  |
| 1   | Q     | 466    |  |
| 1   | T     | 466    |  |
| 1   | W     | 466    |  |
| 1   | w     | 466    |  |
| 2   | 2     | 318    |  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 2   | 3     | 318    |                  |
| 2   | R     | 318    |                  |
| 2   | S     | 318    |                  |
| 2   | U     | 318    |                  |
| 2   | V     | 318    |                  |
| 2   | X     | 318    |                  |
| 2   | Y     | 318    |                  |
| 2   | x     | 318    |                  |
| 2   | y     | 318    |                  |
| 3   | A     | 1374   |                  |
| 3   | B     | 1374   |                  |
| 3   | C     | 1374   |                  |
| 3   | D     | 1374   |                  |
| 3   | E     | 1374   |                  |
| 3   | F     | 1374   |                  |
| 3   | G     | 1374   |                  |
| 3   | H     | 1374   |                  |
| 3   | I     | 1374   |                  |
| 3   | J     | 1374   |                  |
| 3   | K     | 1374   |                  |
| 3   | L     | 1374   |                  |
| 3   | M     | 1374   |                  |
| 3   | N     | 1374   |                  |
| 3   | O     | 1374   |                  |
| 3   | P     | 1374   |                  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 4   | b     | 112    | 79%<br>          |
| 4   | c     | 112    | 79%<br>          |
| 4   | d     | 112    | 78%<br>          |
| 4   | e     | 112    | 79%<br>          |
| 4   | f     | 112    | 79%<br>          |
| 4   | g     | 112    | 79%<br>          |
| 4   | h     | 112    | 71%<br>          |
| 4   | i     | 112    | 71%<br>          |
| 4   | j     | 112    | 70%<br>          |
| 4   | k     | 112    | 70%<br>          |
| 4   | l     | 112    | 72%<br>          |
| 4   | m     | 112    | 71%<br>          |
| 4   | n     | 112    | 79%<br>          |
| 4   | o     | 112    | 77%<br>          |
| 4   | p     | 112    | 74%<br>          |
| 5   | q     | 702    | 15%<br>          |
| 6   | r     | 585    |                  |
| 6   | s     | 585    |                  |
| 7   | t     | 3122   |                  |
| 7   | u     | 3122   |                  |

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 218714 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 VP19C.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 1   | Q     | 350      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2589  | 1620 | 493 | 461 | 15 |         |       |
| 1   | T     | 350      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2595  | 1623 | 496 | 461 | 15 |         |       |
| 1   | W     | 350      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2577  | 1613 | 490 | 459 | 15 |         |       |
| 1   | 1     | 350      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2589  | 1620 | 493 | 461 | 15 |         |       |
| 1   | w     | 350      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2595  | 1623 | 496 | 461 | 15 |         |       |

- Molecule 2 is a protein called VP23.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 2   | R     | 286      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2102  | 1343 | 374 | 379 | 6  |         |       |
| 2   | S     | 308      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2337  | 1484 | 413 | 429 | 11 |         |       |
| 2   | U     | 286      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2102  | 1343 | 374 | 379 | 6  |         |       |
| 2   | V     | 308      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2337  | 1484 | 413 | 429 | 11 |         |       |
| 2   | X     | 286      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2102  | 1343 | 374 | 379 | 6  |         |       |
| 2   | Y     | 308      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2337  | 1484 | 413 | 429 | 11 |         |       |
| 2   | 3     | 286      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2102  | 1343 | 374 | 379 | 6  |         |       |
| 2   | 2     | 308      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2334  | 1481 | 413 | 429 | 11 |         |       |
| 2   | x     | 286      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2102  | 1343 | 374 | 379 | 6  |         |       |
| 2   | y     | 308      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2328  | 1478 | 410 | 429 | 11 |         |       |

- Molecule 3 is a protein called Major capsid protein.

| Mol | Chain | Residues | Atoms |      |      |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
| 3   | I     | 1362     | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 10418 | 6584 | 1873 | 1905 | 56 |         |       |
| 3   | J     | 1364     | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 10408 | 6582 | 1863 | 1907 | 56 |         |       |
| 3   | K     | 1364     | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 10414 | 6585 | 1866 | 1907 | 56 |         |       |
| 3   | L     | 1362     | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 10422 | 6586 | 1873 | 1907 | 56 |         |       |
| 3   | M     | 1366     | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 10449 | 6603 | 1877 | 1913 | 56 |         |       |
| 3   | A     | 1259     | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 9646  | 6107 | 1725 | 1762 | 52 |         |       |
| 3   | H     | 1362     | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 10416 | 6583 | 1873 | 1905 | 55 |         |       |
| 3   | N     | 1362     | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 10397 | 6574 | 1868 | 1899 | 56 |         |       |
| 3   | O     | 1366     | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 10417 | 6585 | 1877 | 1899 | 56 |         |       |
| 3   | P     | 1364     | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 10407 | 6582 | 1866 | 1903 | 56 |         |       |
| 3   | B     | 1357     | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 10349 | 6542 | 1854 | 1897 | 56 |         |       |
| 3   | C     | 1356     | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 10355 | 6545 | 1857 | 1897 | 56 |         |       |
| 3   | D     | 1364     | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 10413 | 6583 | 1872 | 1902 | 56 |         |       |
| 3   | E     | 1362     | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 10405 | 6578 | 1870 | 1901 | 56 |         |       |
| 3   | F     | 1362     | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 10392 | 6571 | 1862 | 1903 | 56 |         |       |
| 3   | G     | 1346     | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 10261 | 6487 | 1845 | 1874 | 55 |         |       |

- Molecule 4 is a protein called VP26.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 4   | h     | 101      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 773   | 489 | 143 | 138 | 3 |         |       |
| 4   | i     | 101      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 773   | 489 | 143 | 138 | 3 |         |       |
| 4   | j     | 101      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 773   | 489 | 143 | 138 | 3 |         |       |

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| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 4   | k     | 101      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 773   | 489 | 143 | 138 | 3 |         |       |
| 4   | l     | 101      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 773   | 489 | 143 | 138 | 3 |         |       |
| 4   | m     | 101      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 773   | 489 | 143 | 138 | 3 |         |       |
| 4   | n     | 101      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 773   | 489 | 143 | 138 | 3 |         |       |
| 4   | o     | 101      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 773   | 489 | 143 | 138 | 3 |         |       |
| 4   | p     | 101      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 773   | 489 | 143 | 138 | 3 |         |       |
| 4   | b     | 101      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 773   | 489 | 143 | 138 | 3 |         |       |
| 4   | c     | 101      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 773   | 489 | 143 | 138 | 3 |         |       |
| 4   | d     | 101      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 773   | 489 | 143 | 138 | 3 |         |       |
| 4   | e     | 101      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 773   | 489 | 143 | 138 | 3 |         |       |
| 4   | f     | 101      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 773   | 489 | 143 | 138 | 3 |         |       |
| 4   | g     | 101      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 773   | 489 | 143 | 138 | 3 |         |       |

- Molecule 5 is a protein called UL17.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 5   | q     | 554      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4241  | 2700 | 774 | 749 | 18 |         |       |

- Molecule 6 is a protein called UL25.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 6   | r     | 94       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 764   | 490 | 136 | 136 | 2 |         |       |
| 6   | s     | 80       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 651   | 413 | 123 | 114 | 1 |         |       |

- Molecule 7 is a protein called UL36.

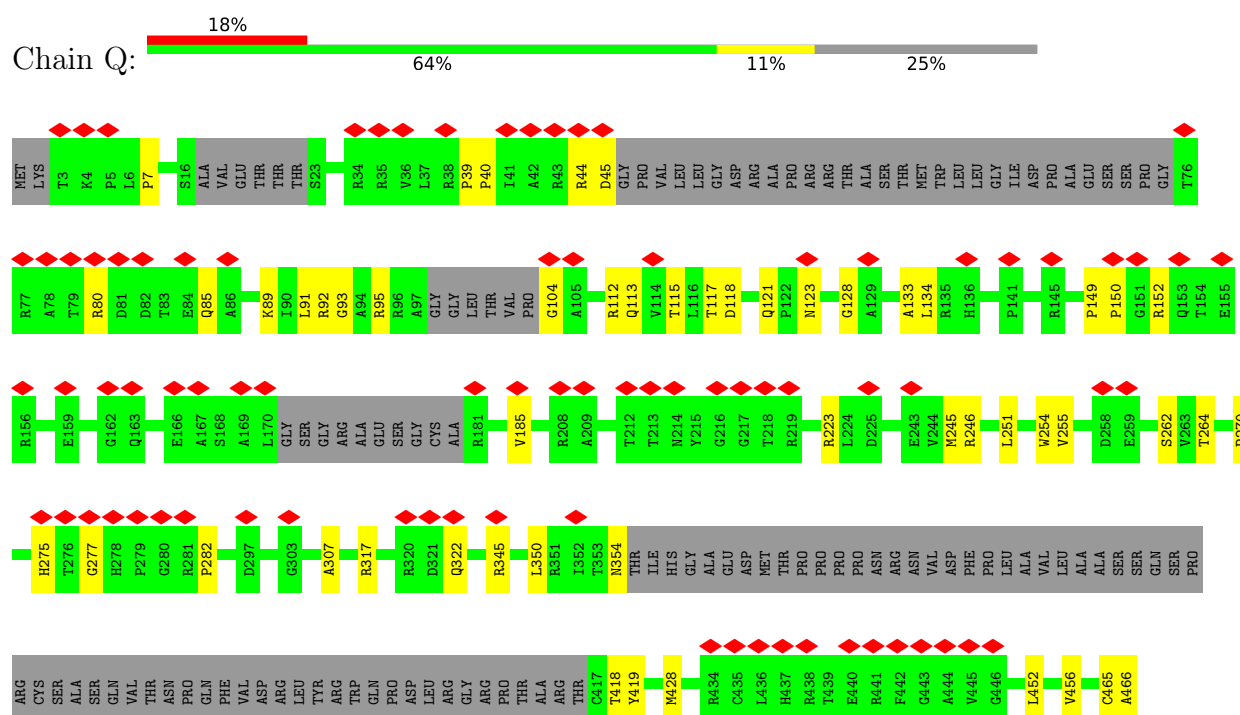
| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 7   | t     | 47       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 383   | 234 | 87 | 60 | 2 |         |       |
| 7   | u     | 47       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 383   | 234 | 87 | 60 | 2 |         |       |



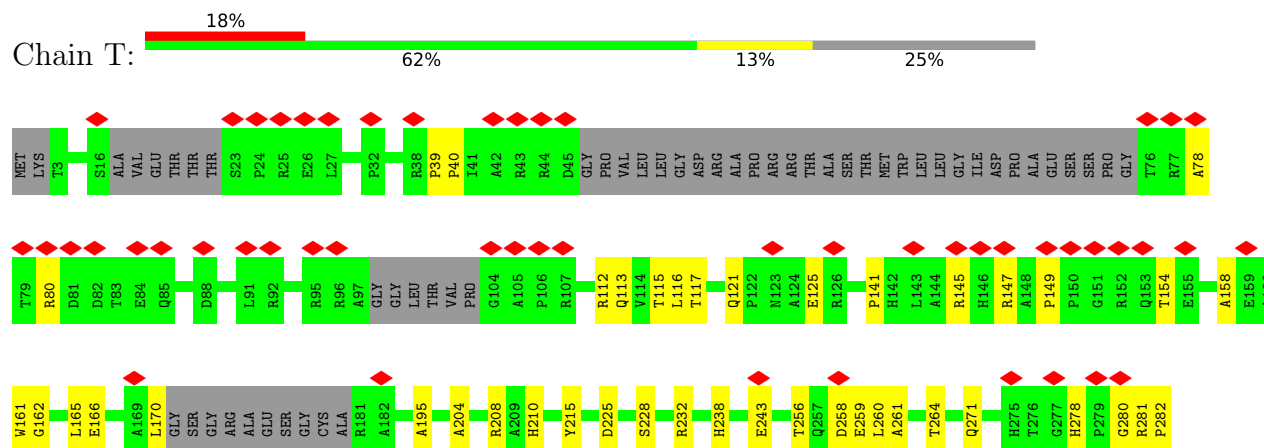
### 3 Residue-property plots

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.

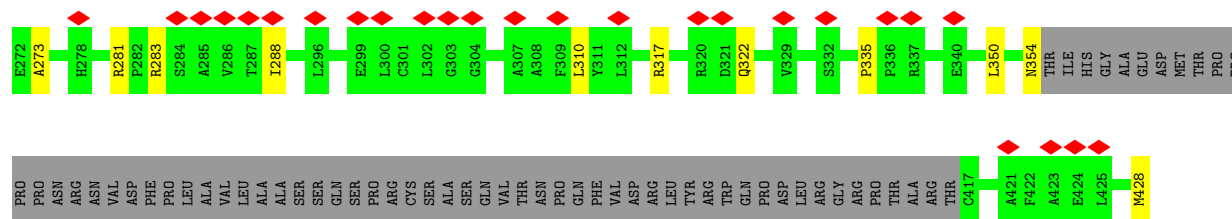
#### • Molecule 1: VP19C



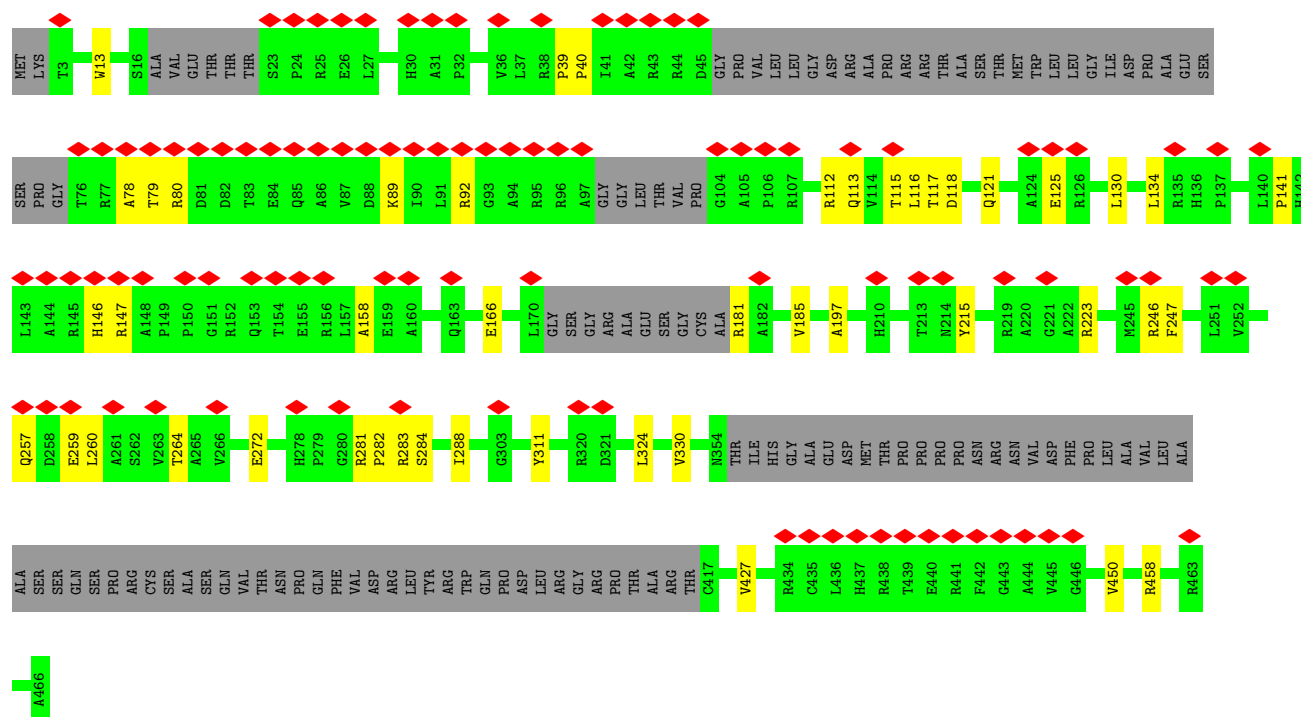
#### • Molecule 1: VP19C



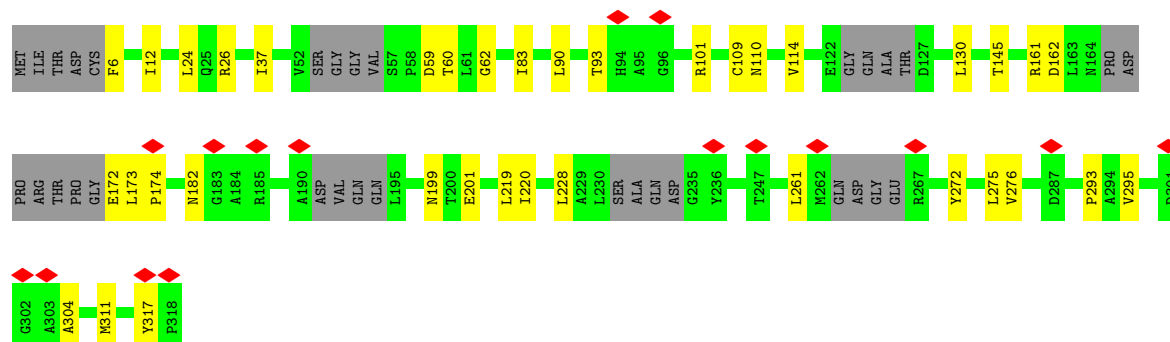
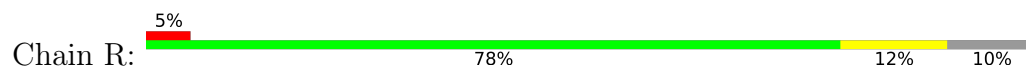




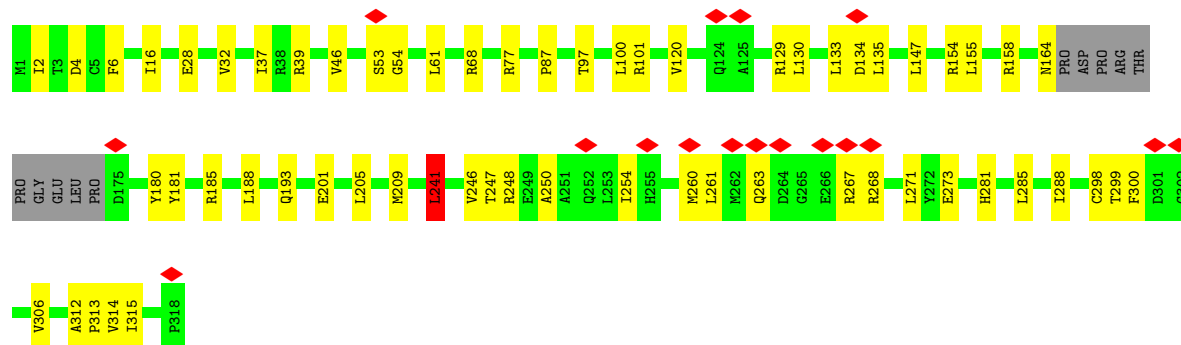
• Molecule 1: VP19C



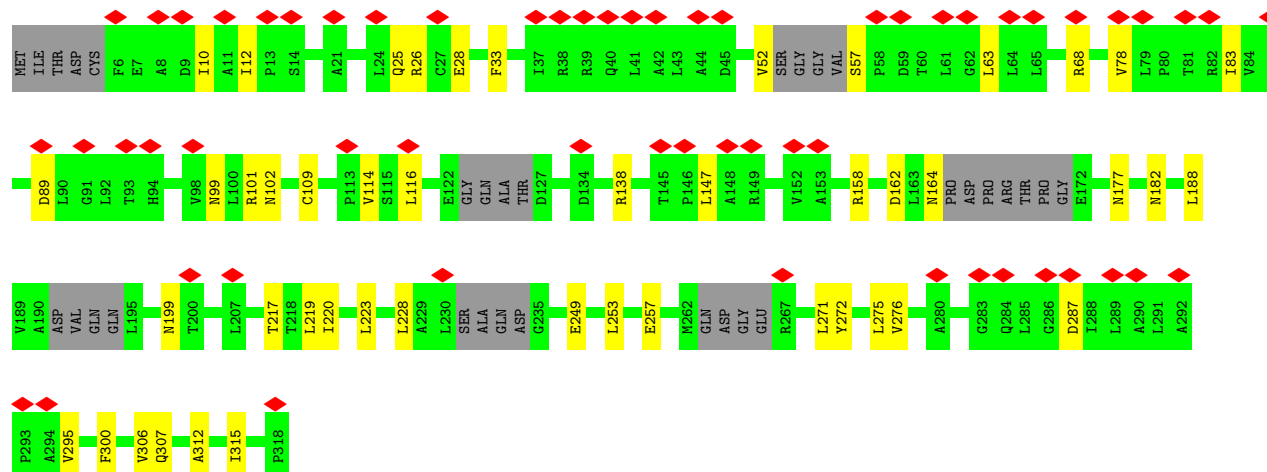
• Molecule 2: VP23



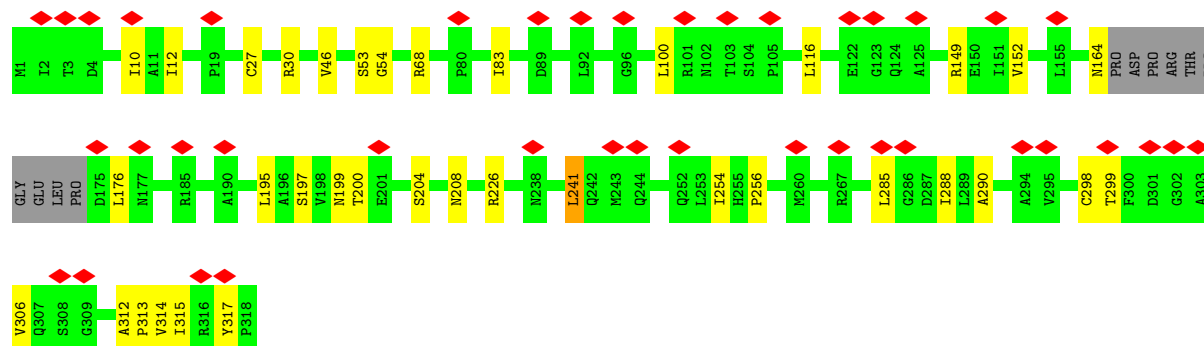
## • Molecule 2: VP23

Chain S: 

## • Molecule 2: VP23

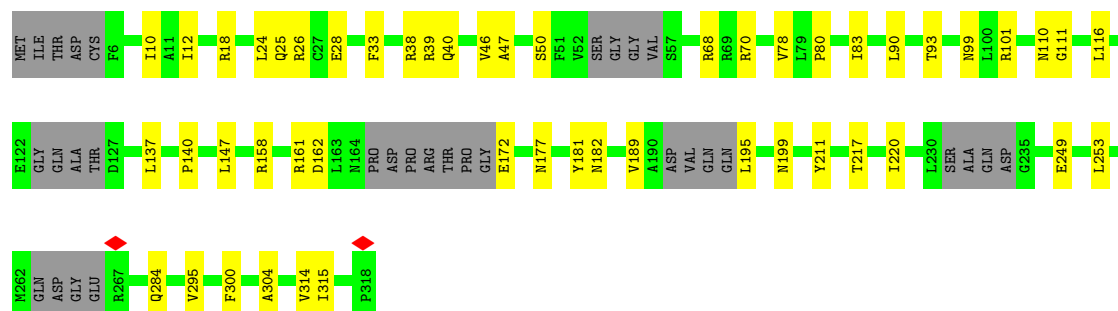
Chain U: 

## • Molecule 2: VP23

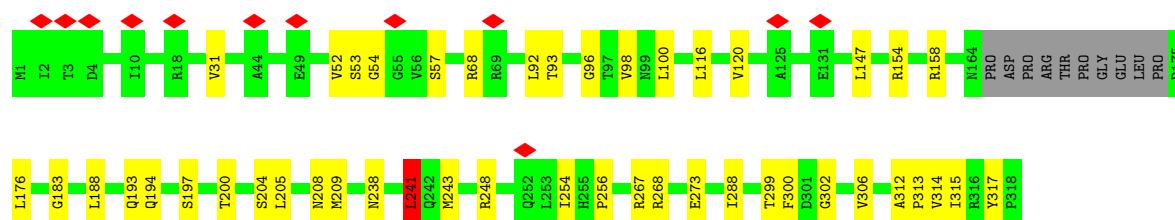
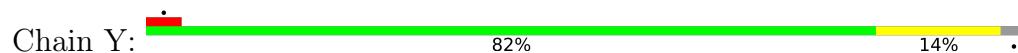
Chain V: 

## • Molecule 2: VP23

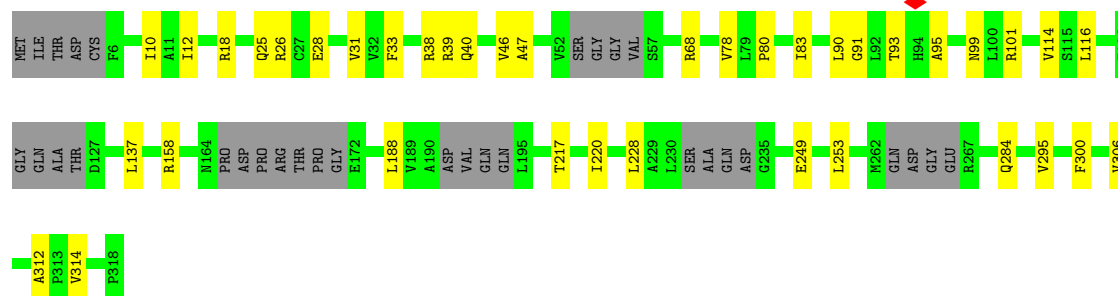
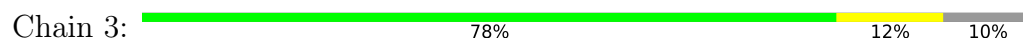
Chain X: 



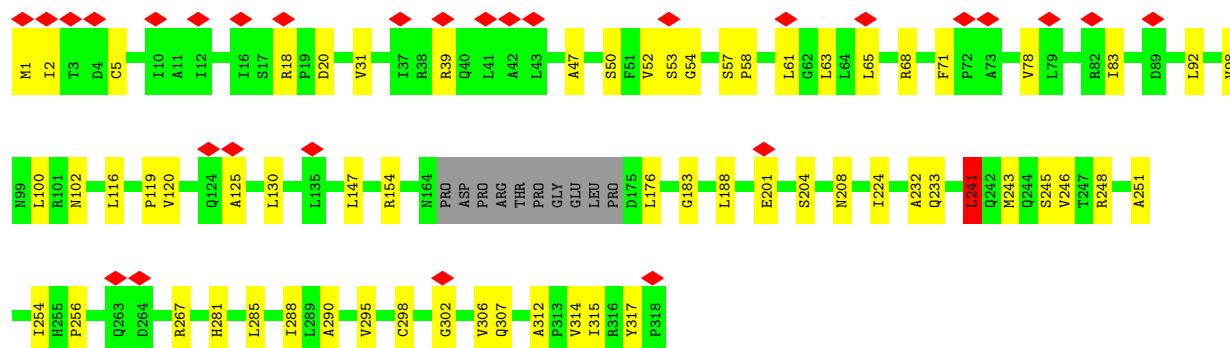
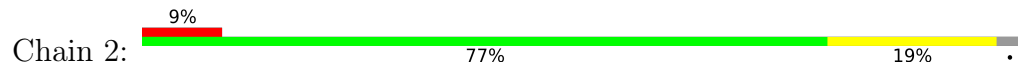
- Molecule 2: VP23



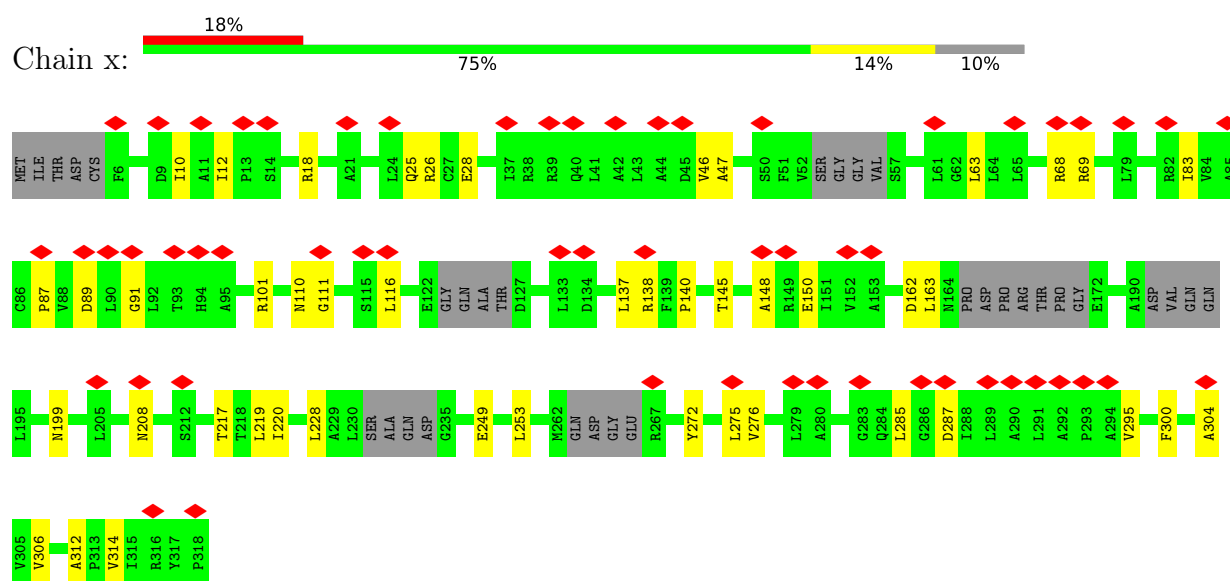
- Molecule 2: VP23



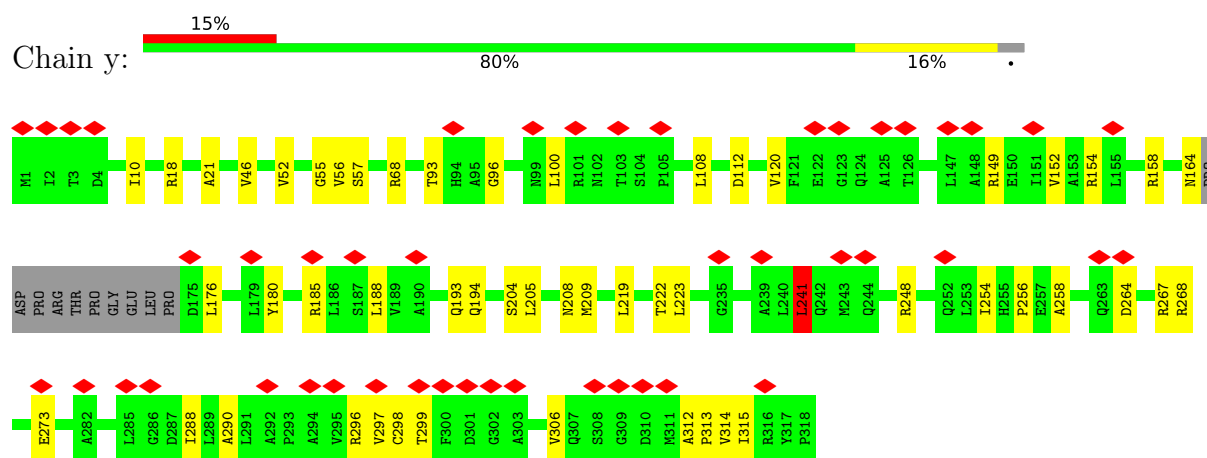
- Molecule 2: VP23



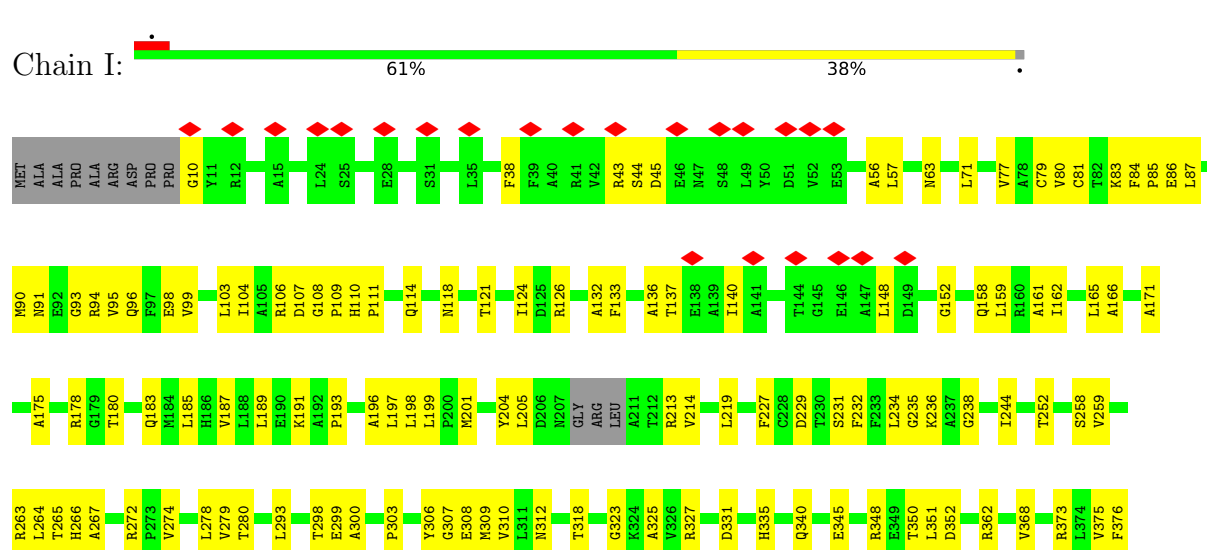
- Molecule 2: VP23

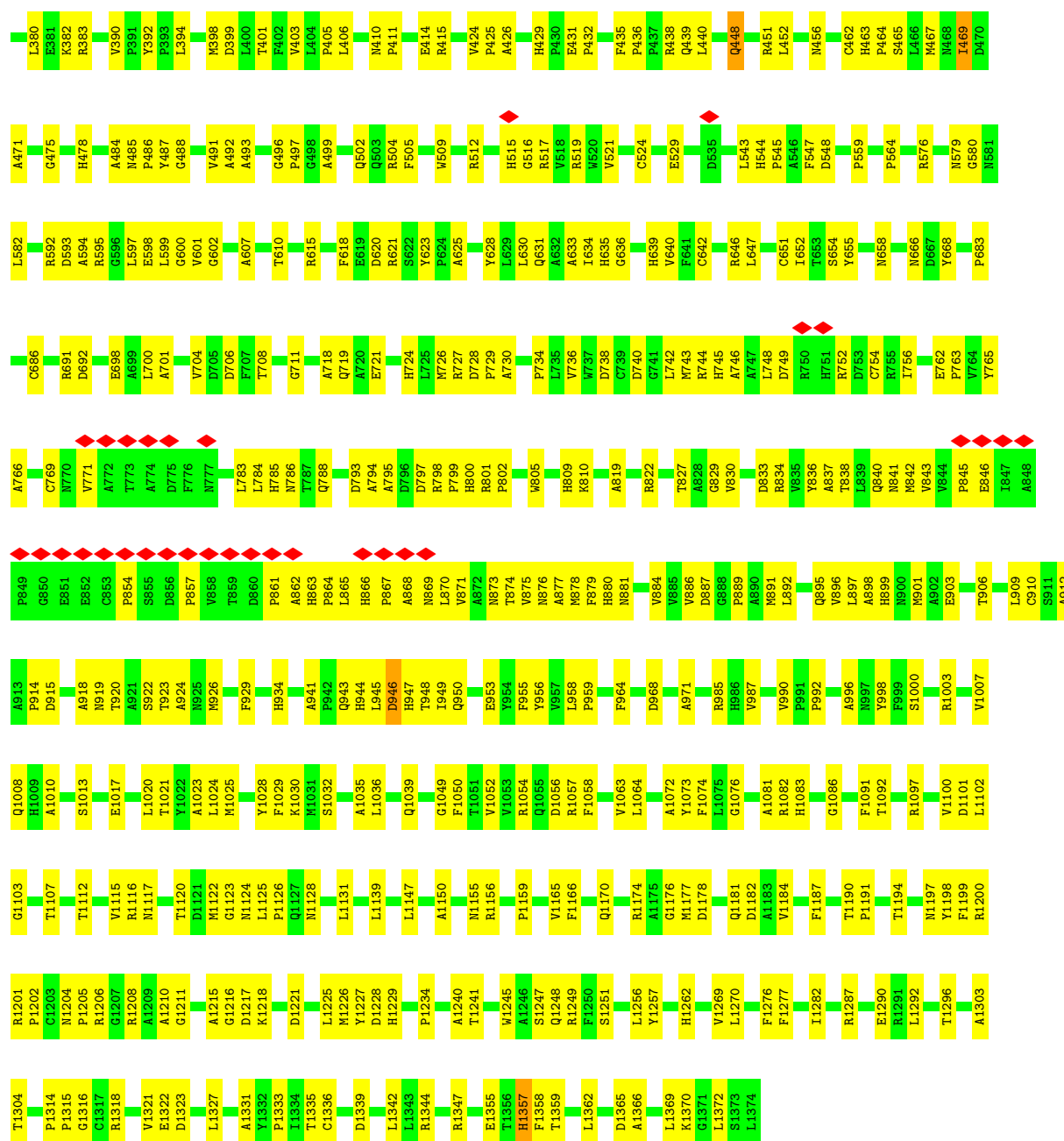


• Molecule 2: VP23



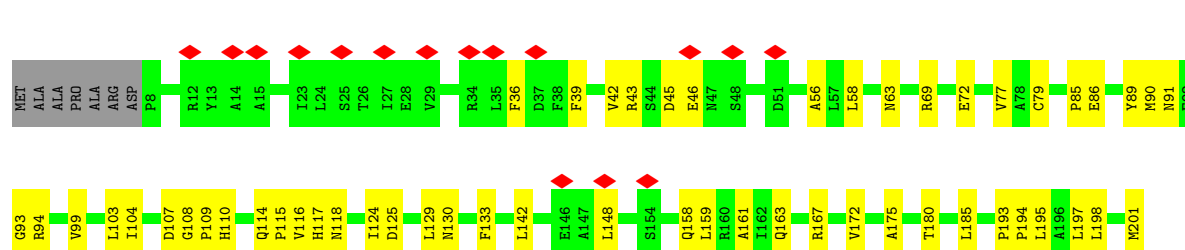
• Molecule 3: Major capsid protein

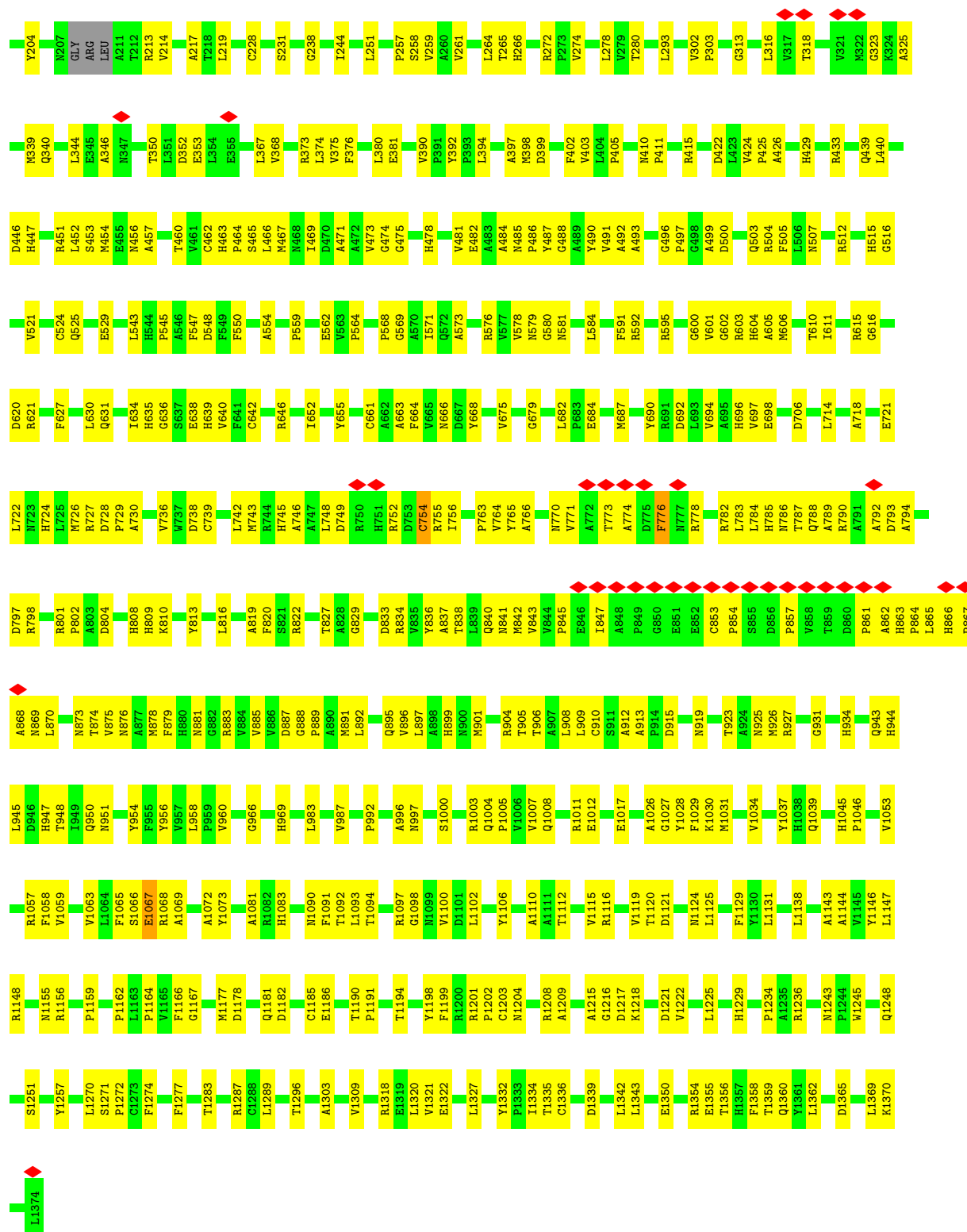




### • Molecule 3: Major capsid protein

Chain J:

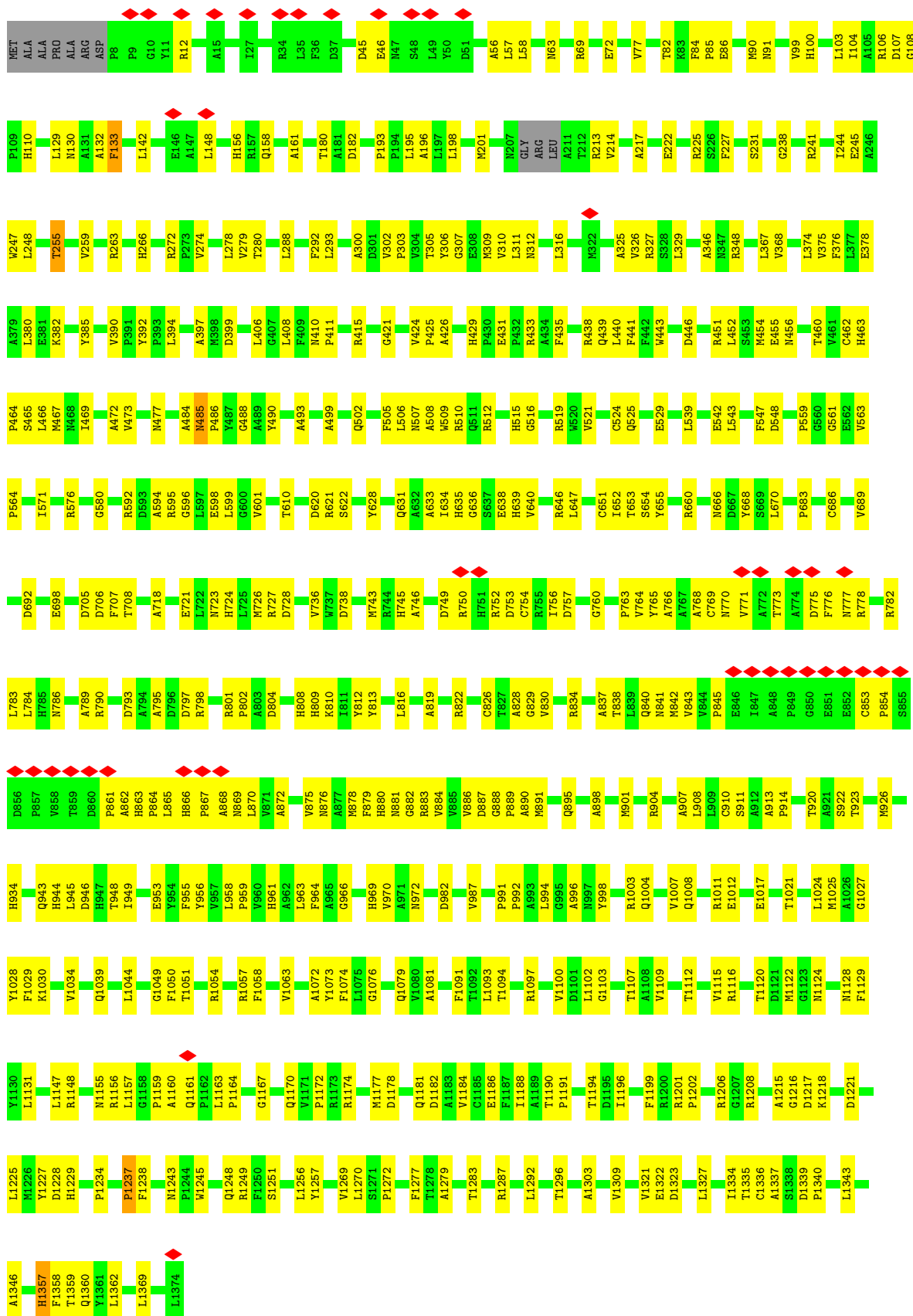




• Molecule 3: Major capsid protein

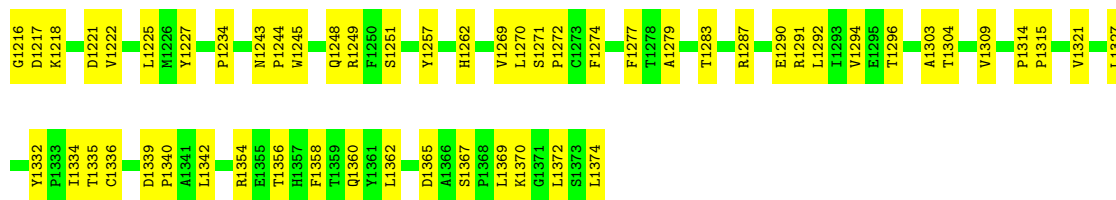
Chain K: 65% 33%



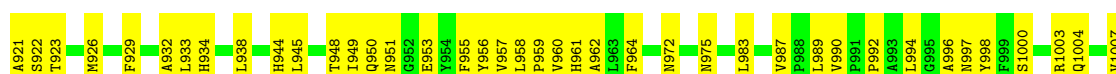
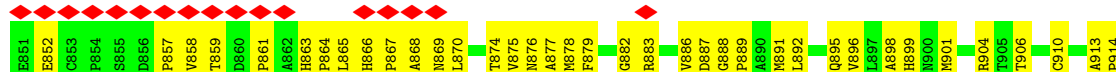
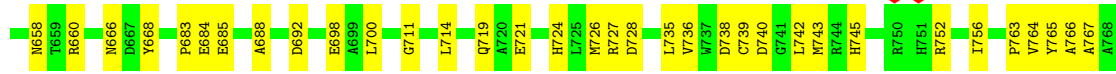
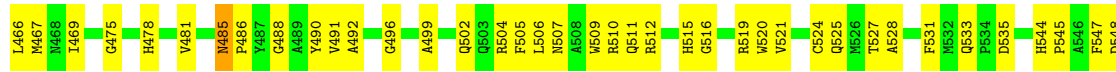
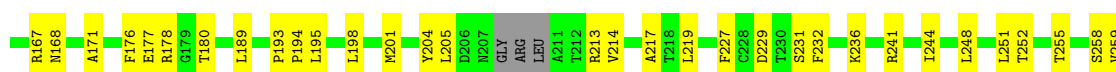


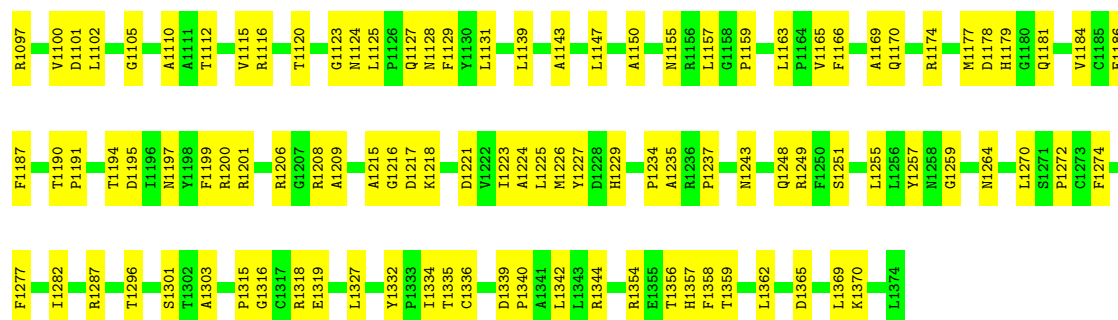
• Molecule 3: Major capsid protein



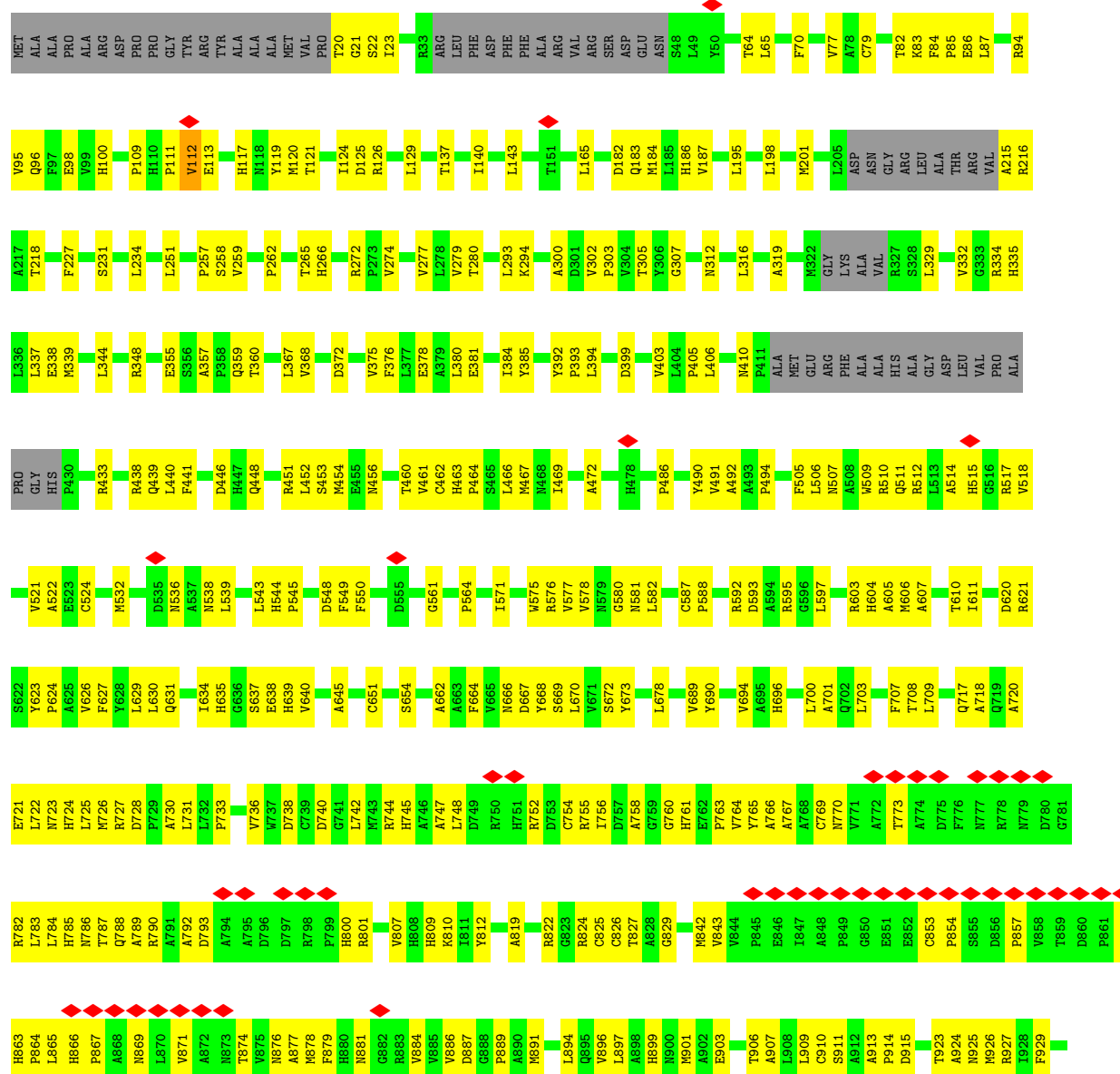


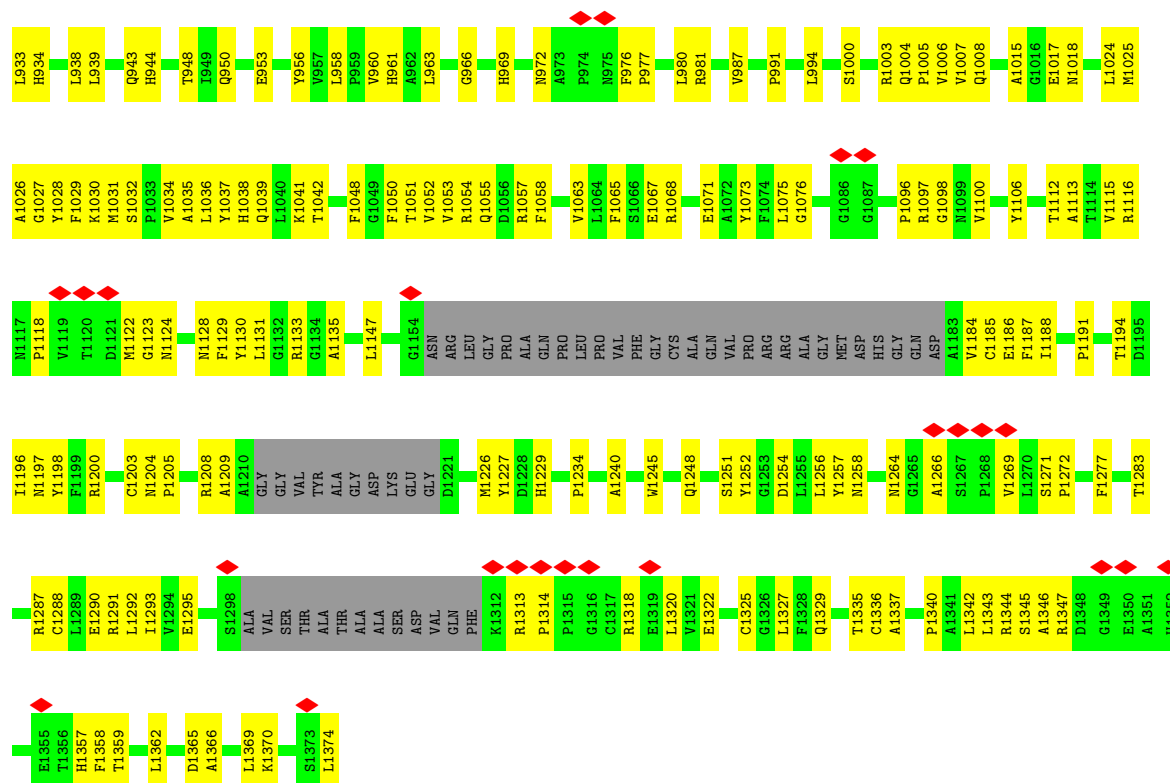
• Molecule 3: Major capsid protein



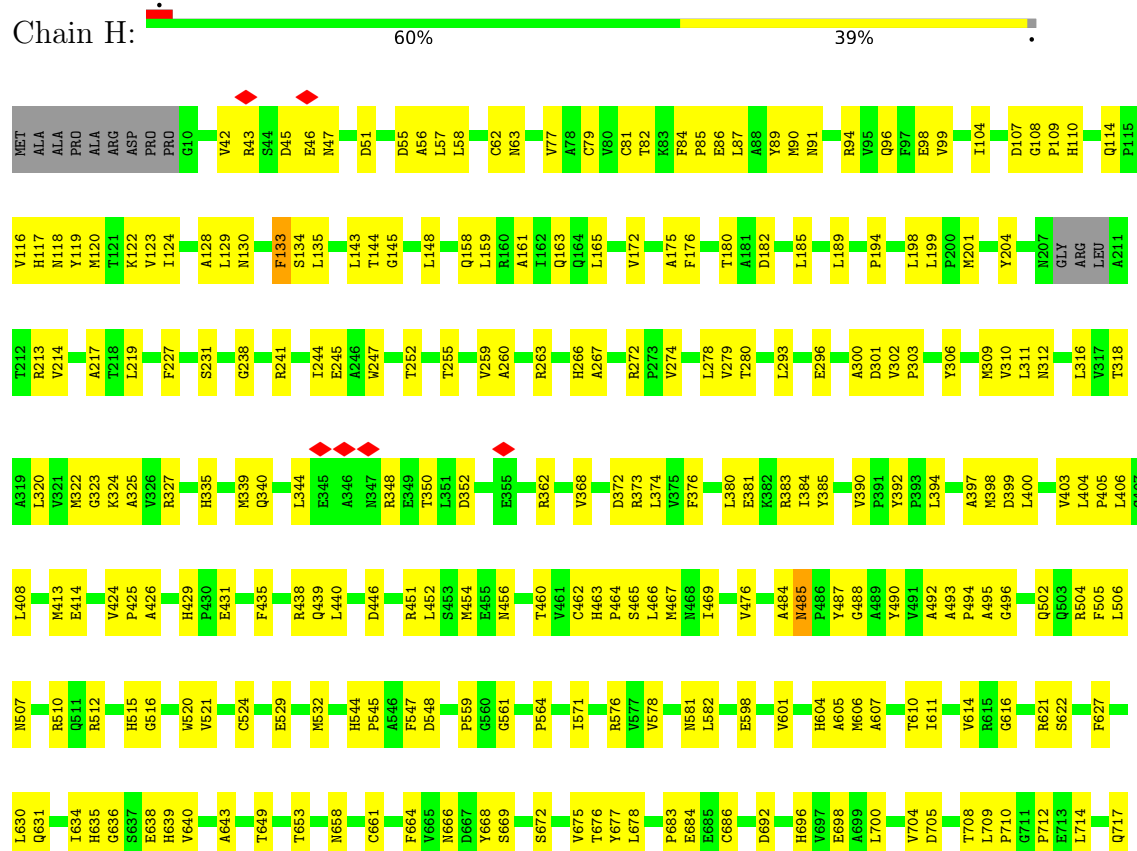


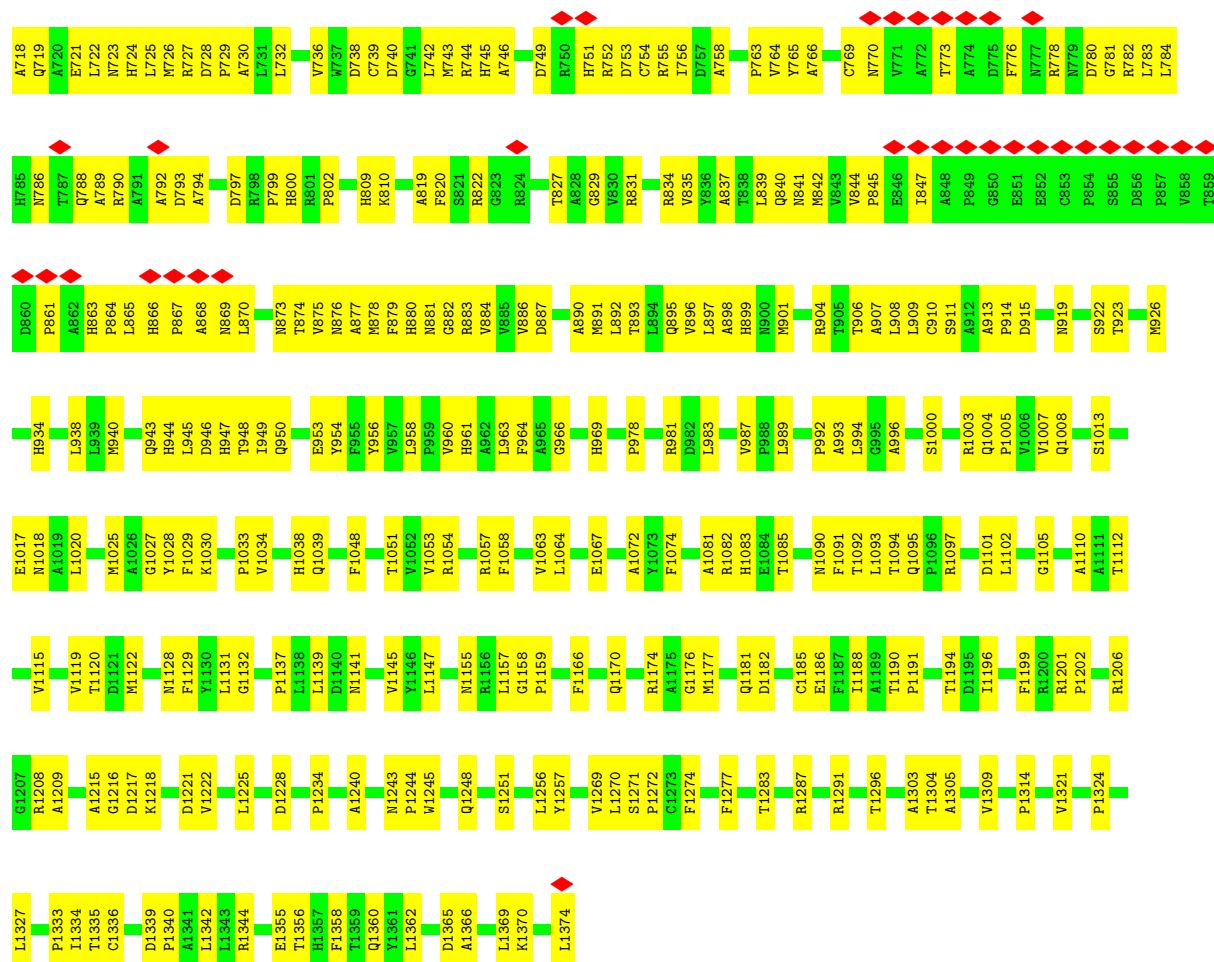
### • Molecule 3: Major capsid protein



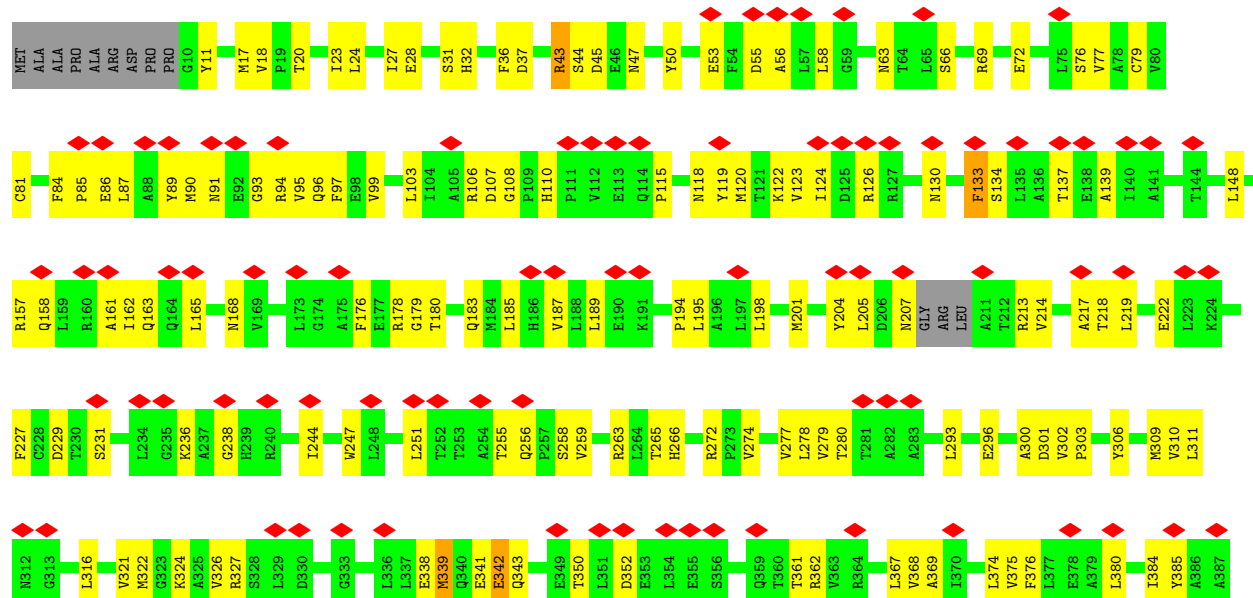


### • Molecule 3: Major capsid protein

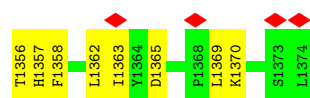




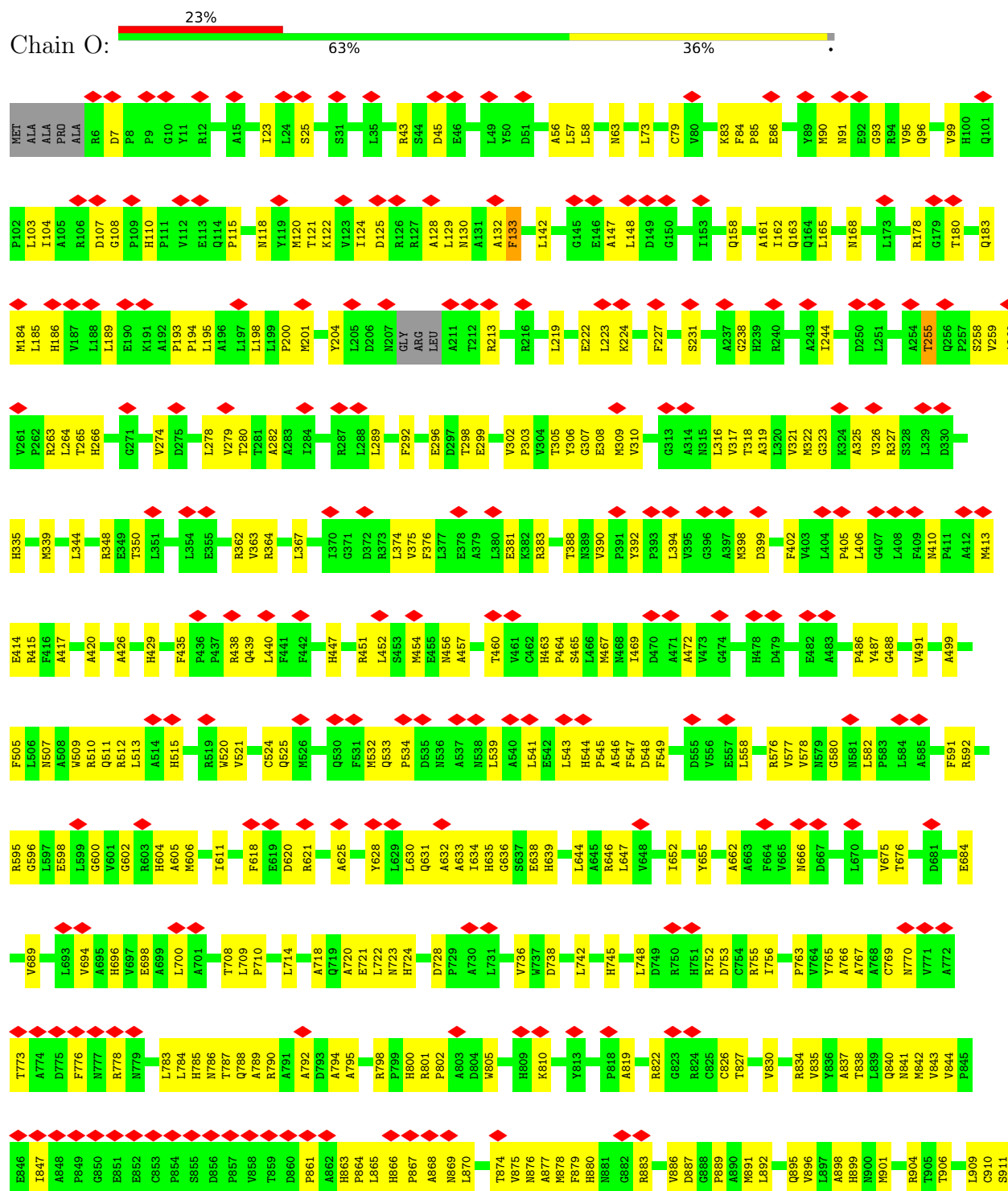
### • Molecule 3: Major capsid protein



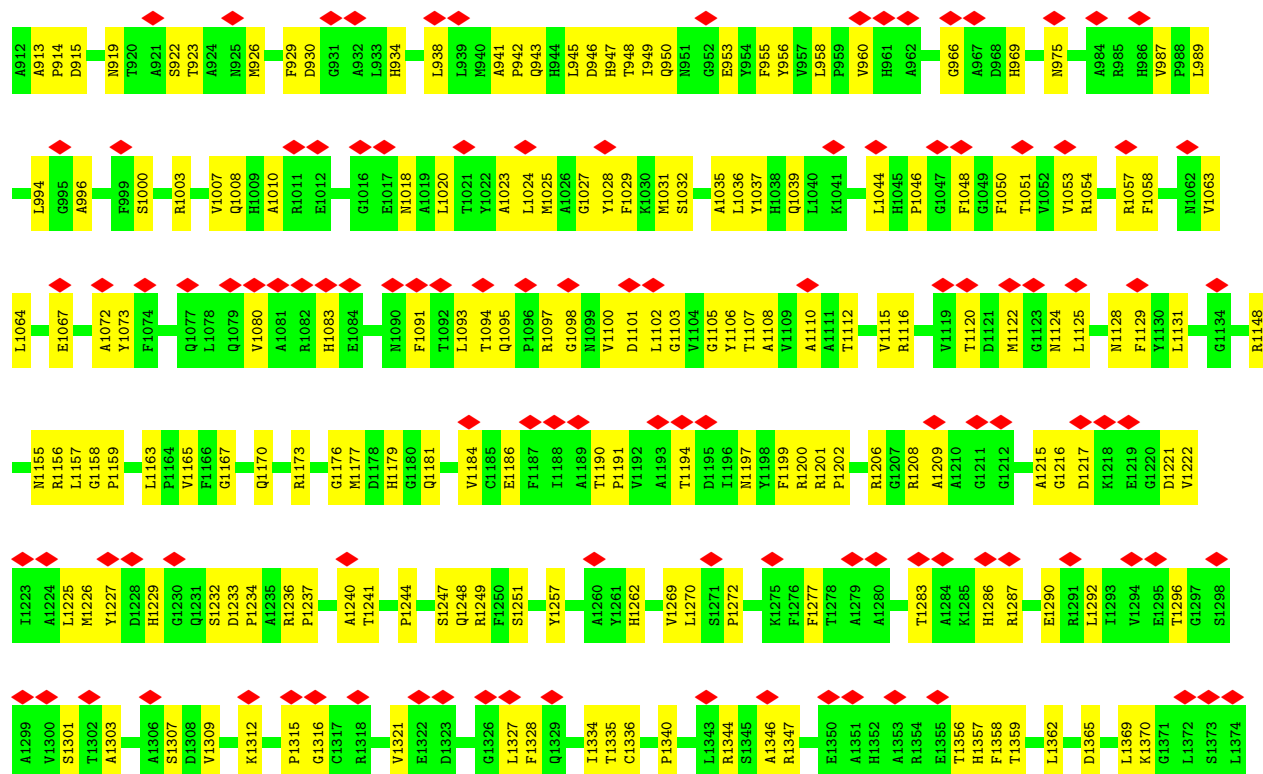




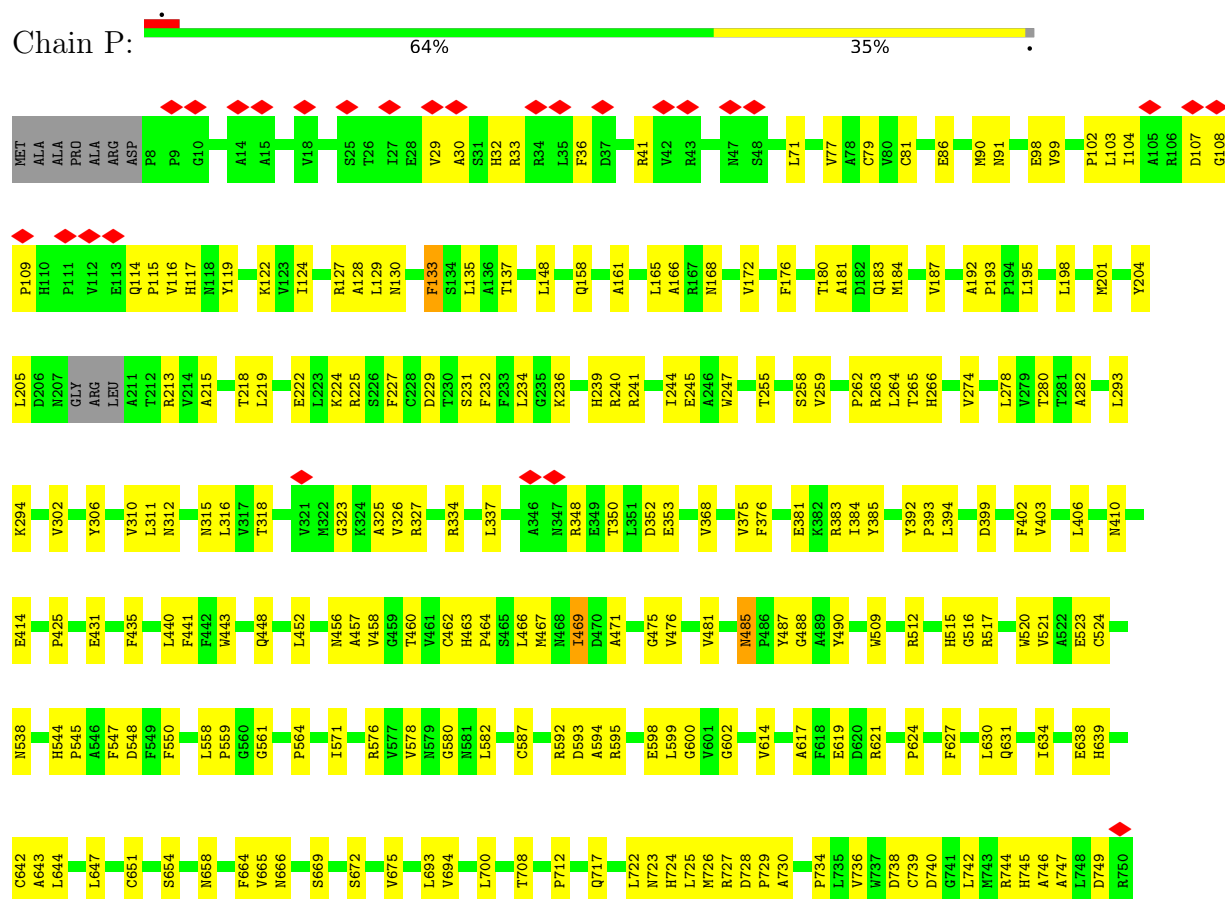
### • Molecule 3: Major capsid protein

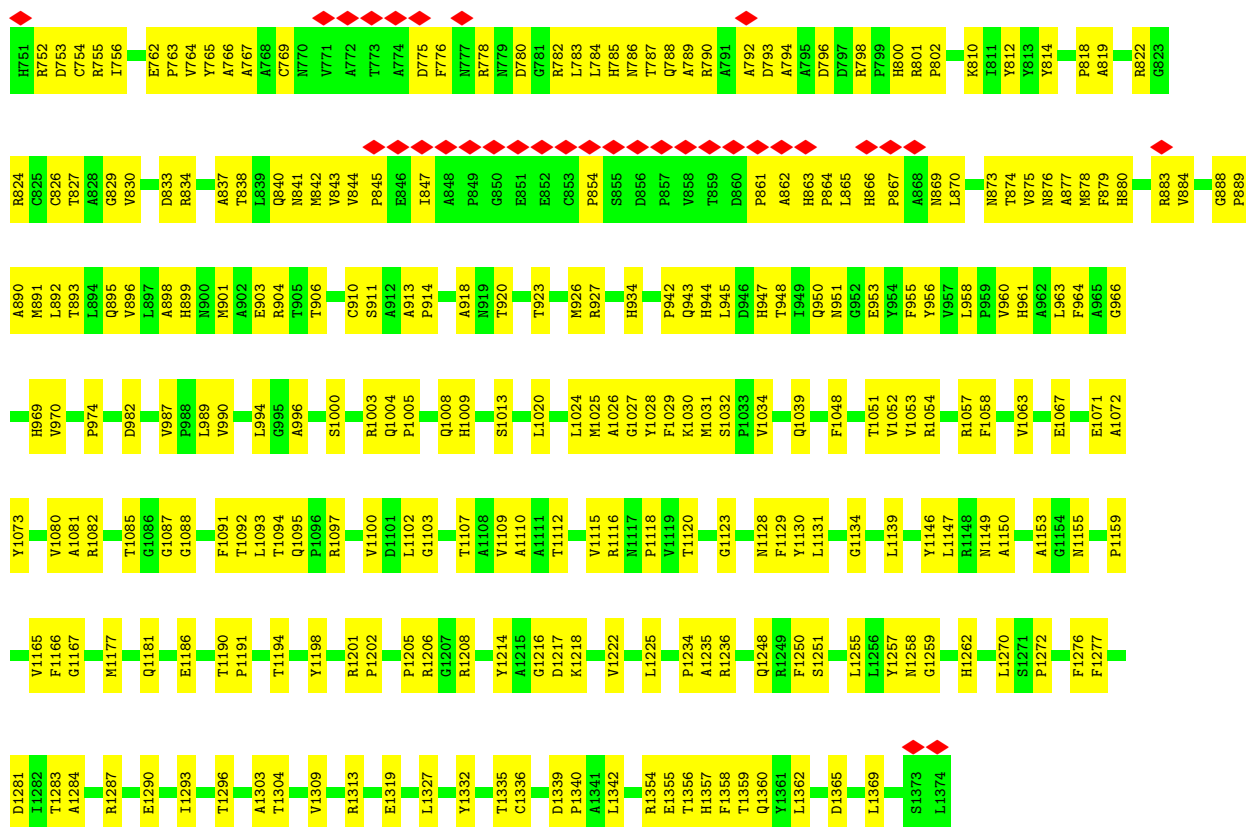






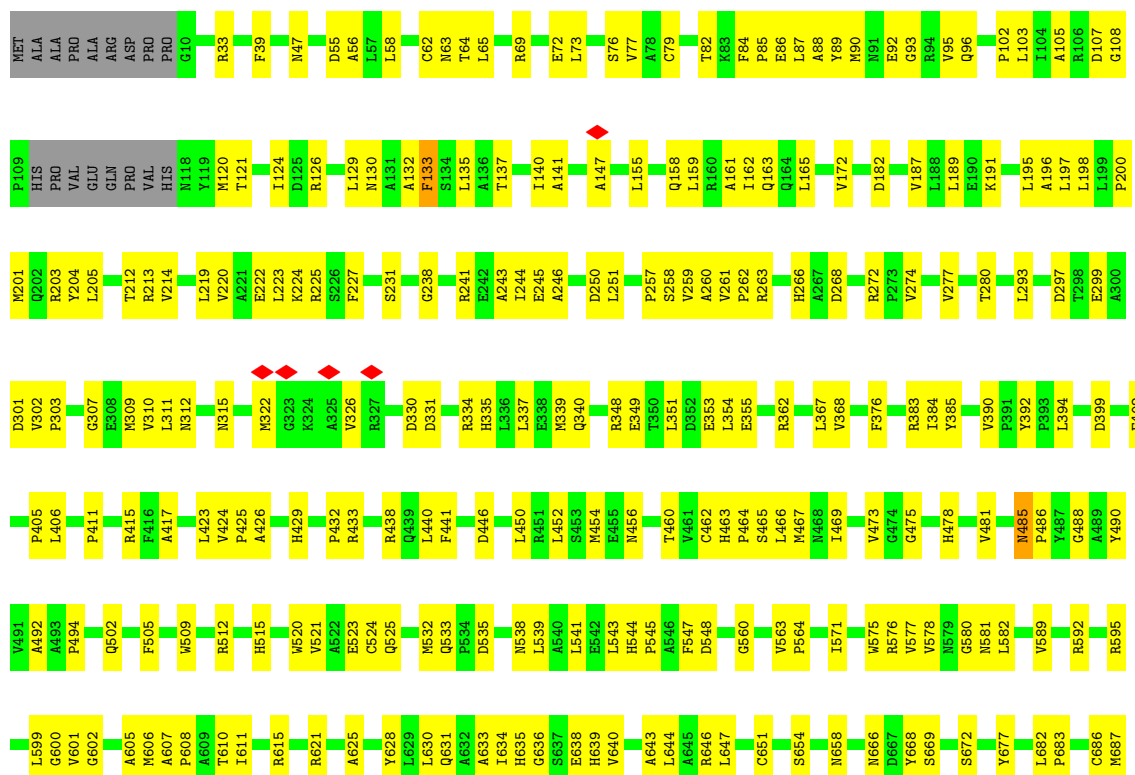
- Molecule 3: Major capsid protein

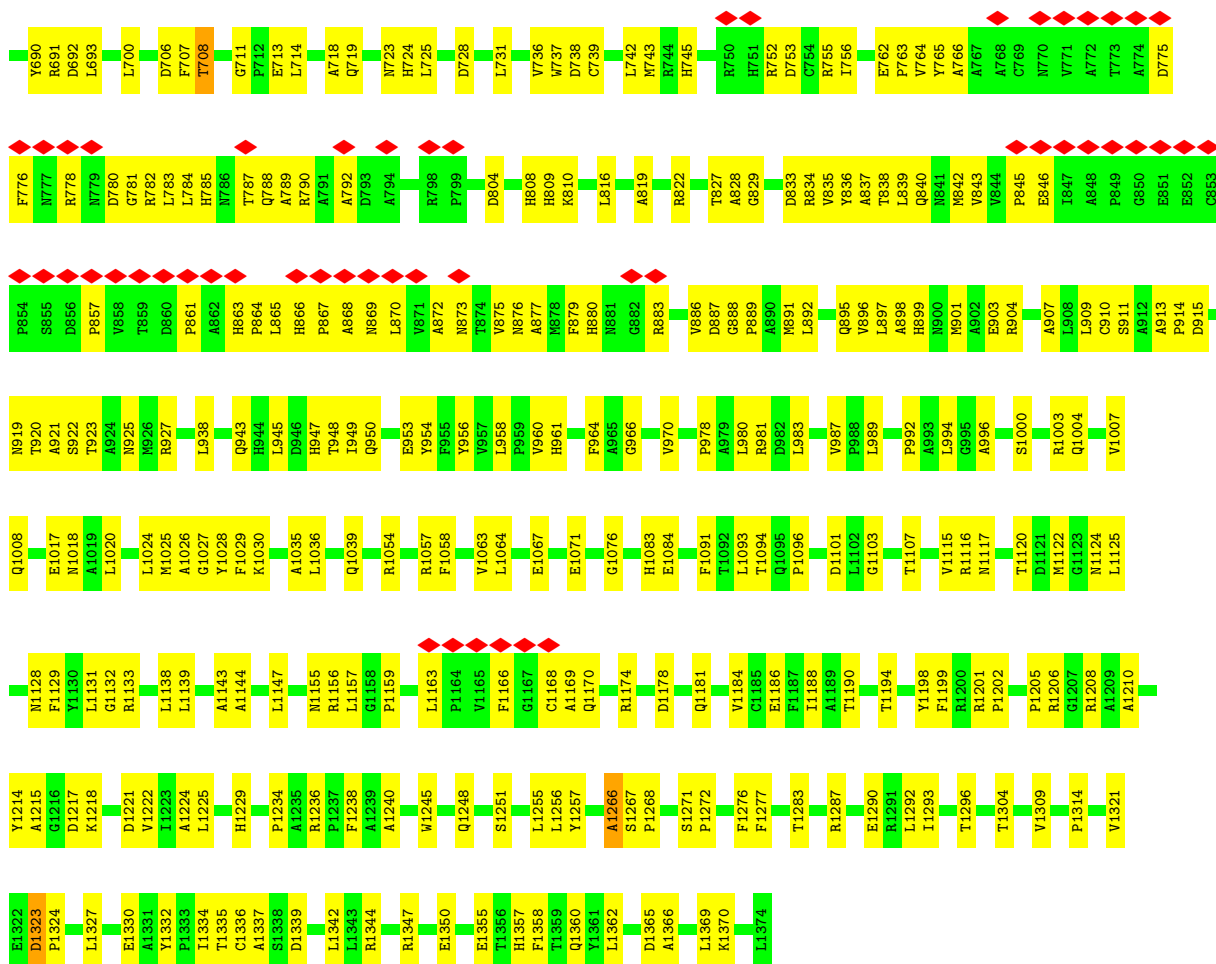




### • Molecule 3: Major capsid protein

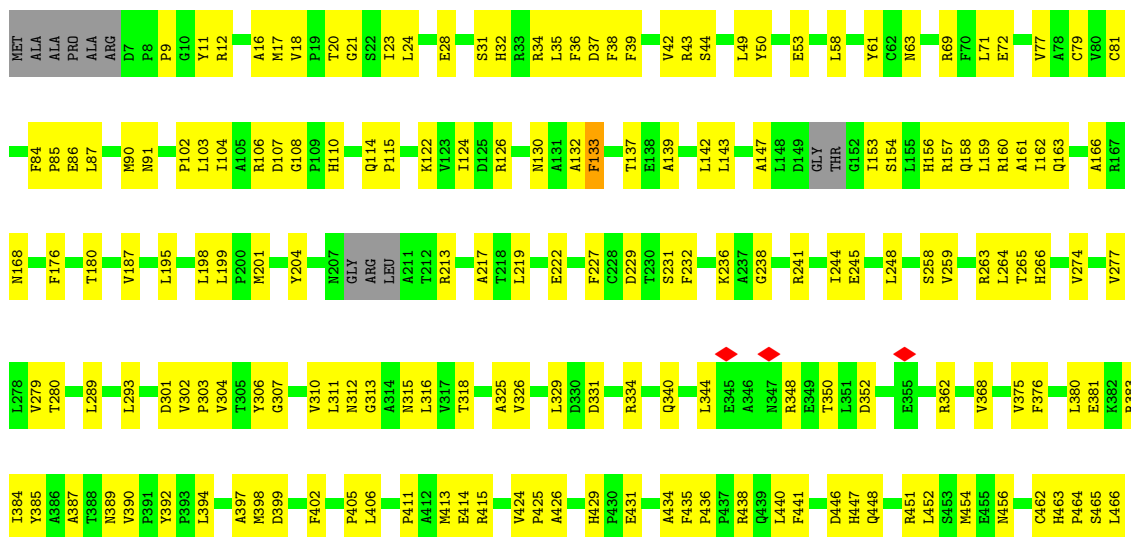
Chain B:

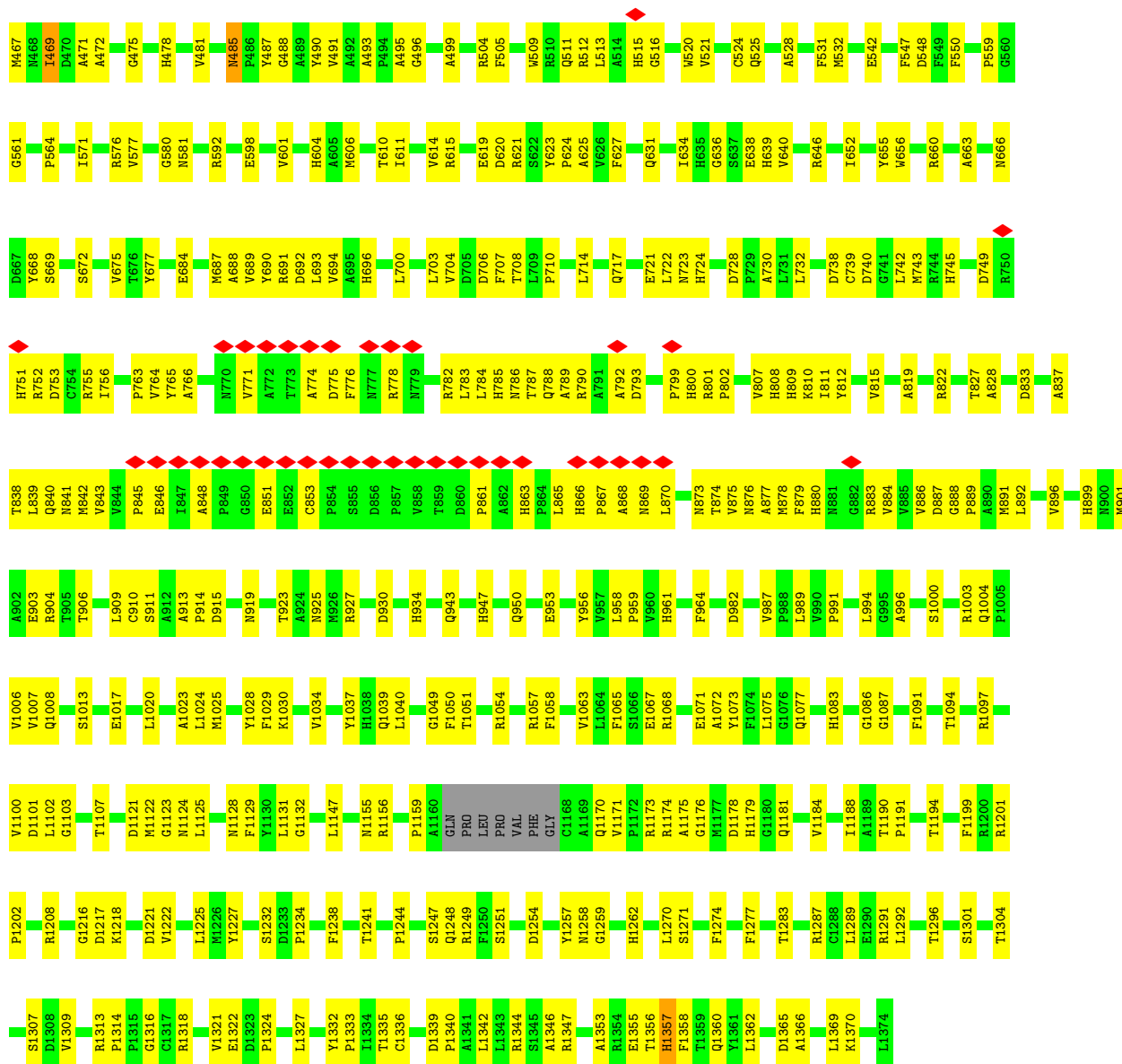




### • Molecule 3: Major capsid protein

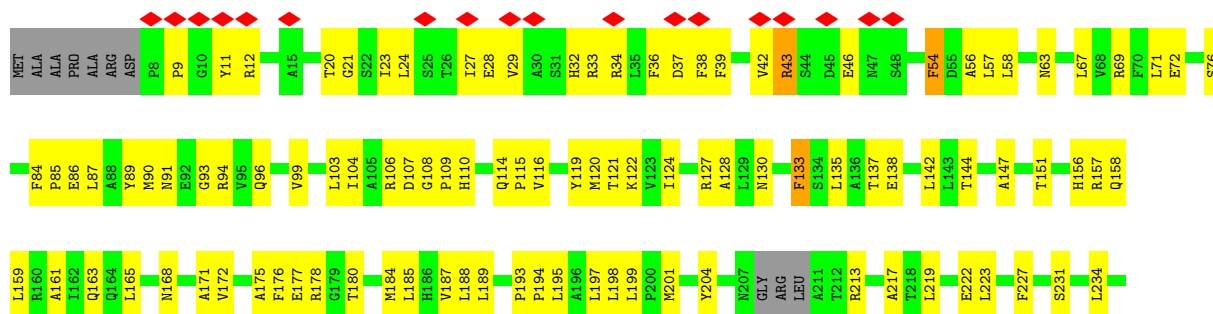
Chain C: 60% 39%

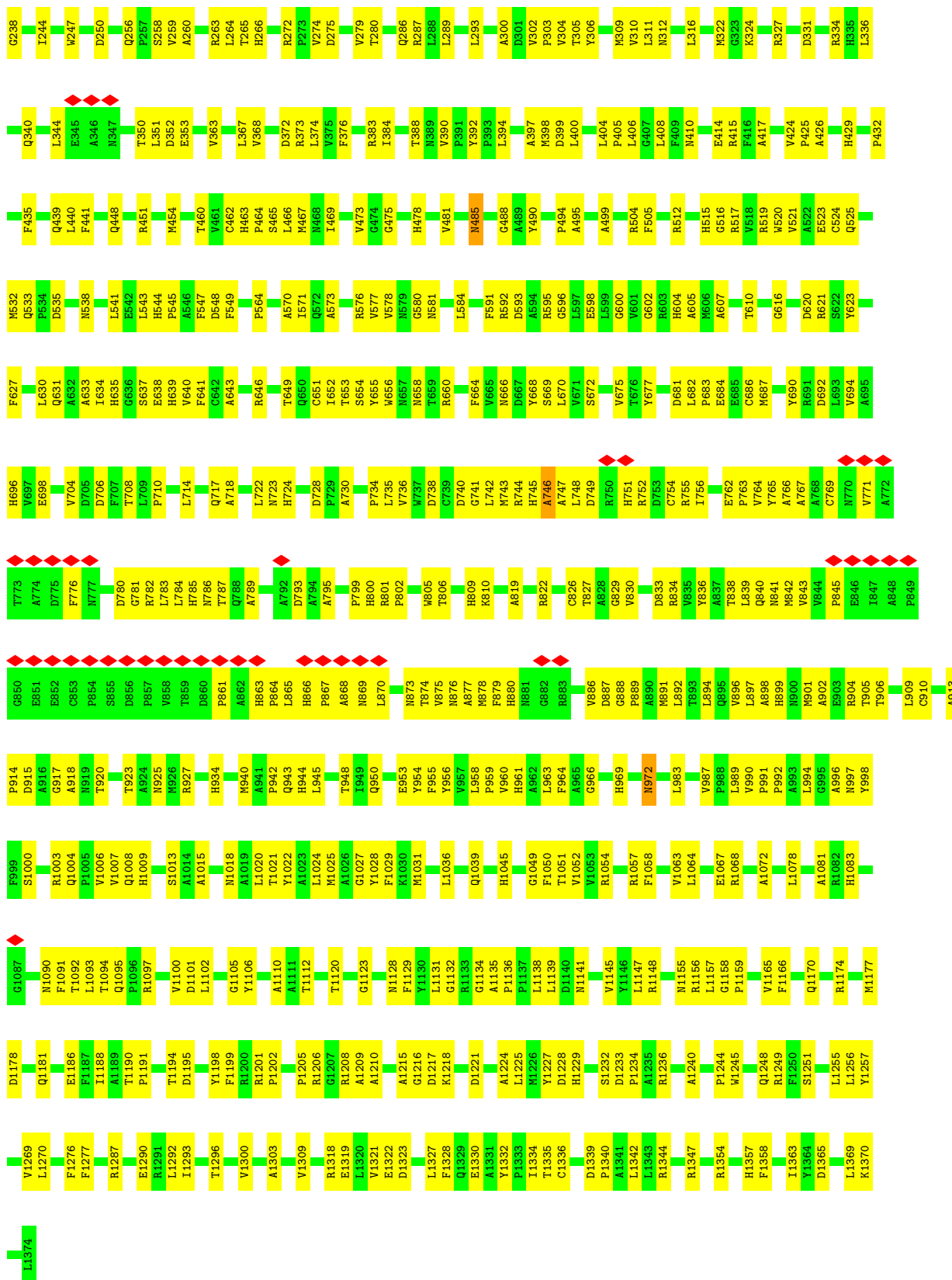




• Molecule 3: Major capsid protein

Chain D: 56% 43%



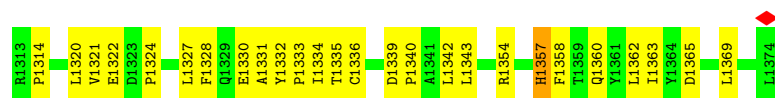


- Molecule 3: Major capsid protein

Chain E:

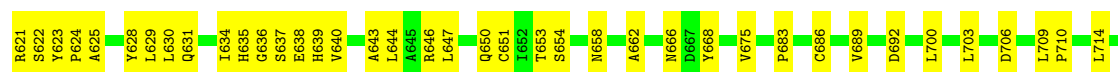


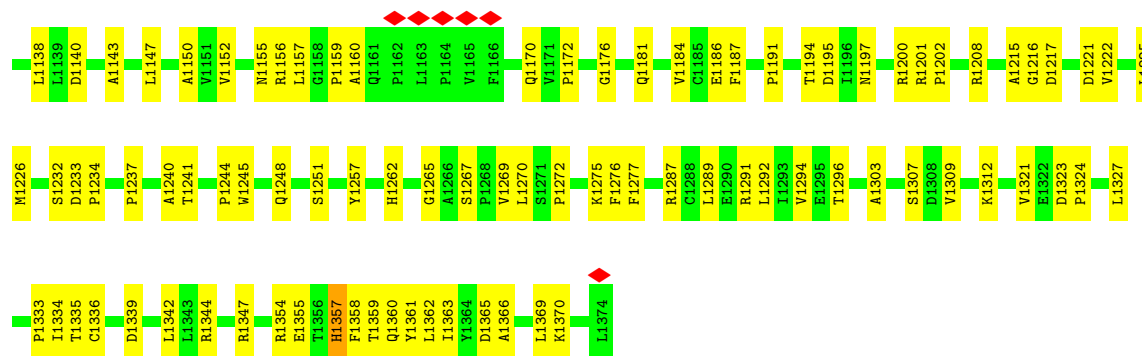
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|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|--|
| MET  | ALA  | ALA  | PRO  | ALA  | ARG  | ASP  | PRO  | G10  | Y11  | R12  | R33  | R34  | L35  | F38  | V42  | R43  | S44  | D51  | V52  | D55  | L57  | L58  | G59  | N63  | T64  | L65  | S66  | R69  | F70  | L71  | E72  | L73  | C79  | V80  | C81  | T82  | R83  | F84  | P85  | E86  | L87  | A88  | Y89  | N90  | N91  | Q96  | V99  |  |
|      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |  |
| P200 | M201 | Y204 | N207 | GLY  | ARG  | LEU  | L311 | A211 | T212 | R213 | V214 | A217 | L218 | L219 | E222 | L223 | F227 | S231 | F232 | F233 | L234 | G238 | L244 | T255 | S258 | V259 | R263 | L264 | T265 | H266 | A267 | D268 | T269 | R270 | P273 | V274 | L278 | D279 | T280 | L289 | P194 | F292 | L293 | D301 | V302 |      |      |  |
| P303 | V304 | T305 | Y306 | G307 | E308 | M309 | V310 | L311 | N312 | N315 | L316 | A319 | L320 | V321 | M322 | G323 | K324 | A325 | V326 | R327 | Q340 | E341 | E342 | R348 | R362 | L367 | V368 | V375 | F376 | R383 | L384 | Y385 | V390 | P391 | Y392 | P393 | L394 | M398 | D399 | L400 | F402 | V403 | L404 | P405 | L408 | F409 | N410 |  |
|      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |  |
|      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |  |
|      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |  |
|      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |  |
|      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |  |
|      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |  |
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|      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |  |
|      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |  |
|      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |  |
|      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |  |
|      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |  |
|      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |  |
|      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |  |
|      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |  |
|      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |  |
|      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |  |
|      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |  |
|      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |  |
|      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |  |
|      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |  |
|      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |  |
|      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |  |
|      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |  |
|      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |  |
|      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |  |



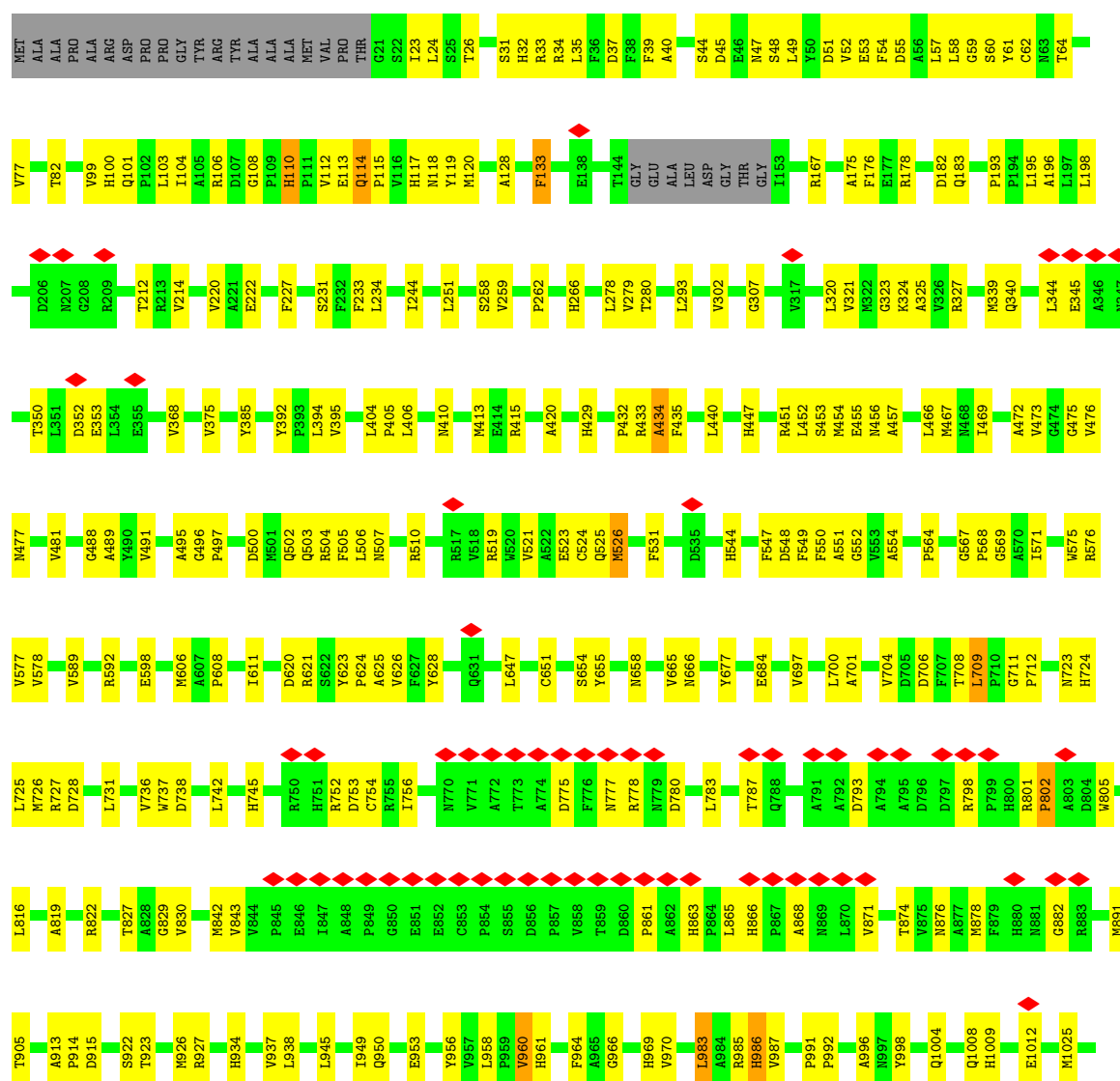
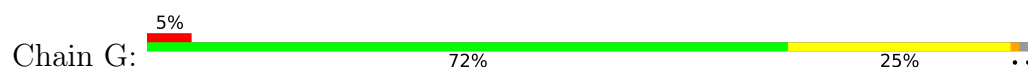
### • Molecule 3: Major capsid protein

Chain F: 60% 38%

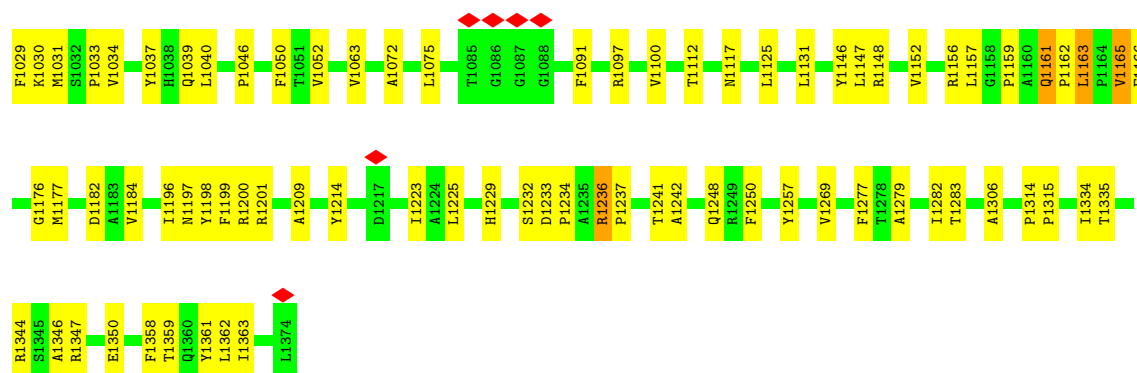




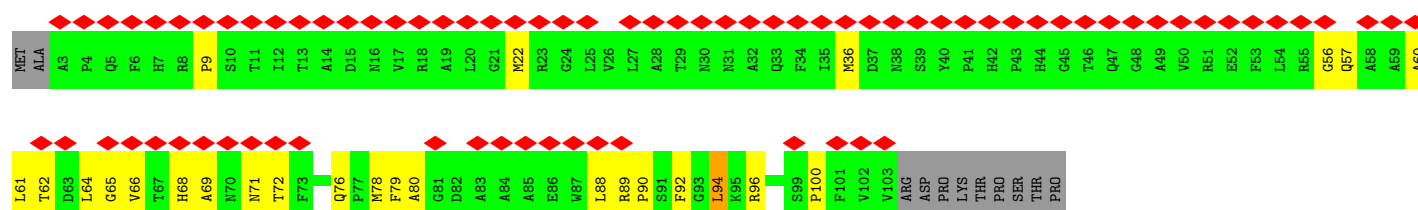
• Molecule 3: Major capsid protein



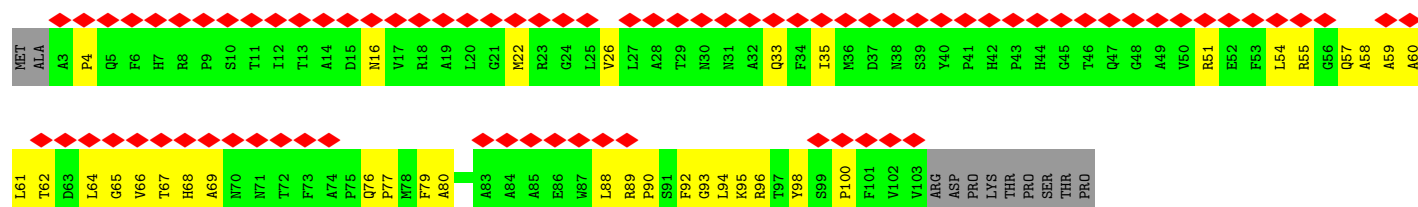




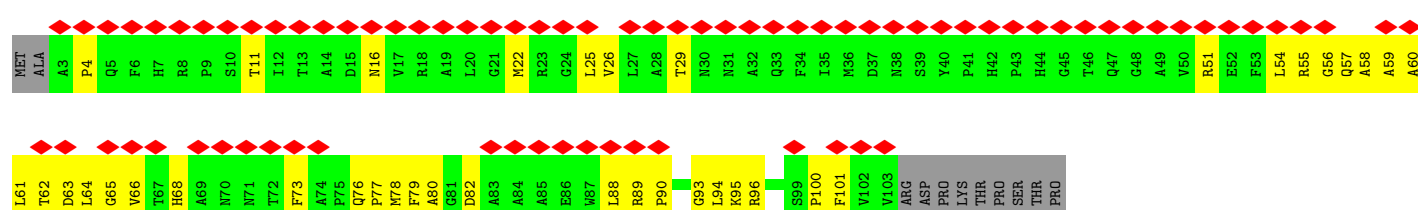
• Molecule 4: VP26



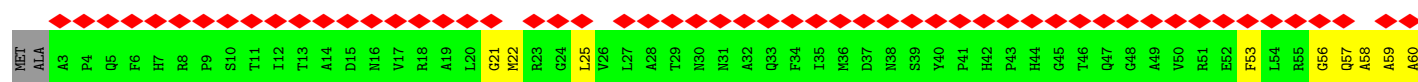
• Molecule 4: VP26



• Molecule 4: VP26

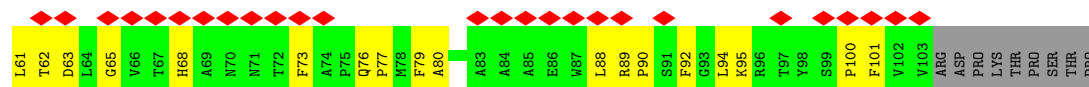


• Molecule 4: VP26

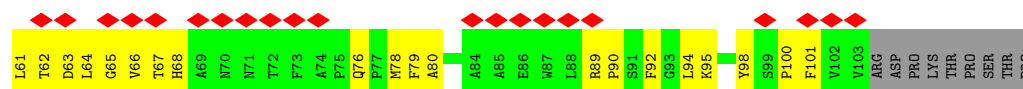
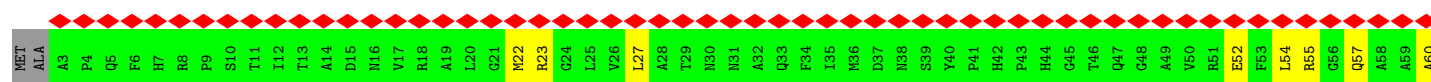
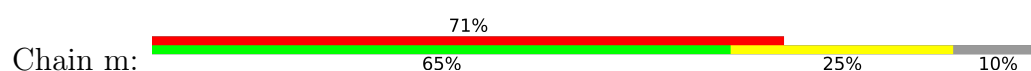




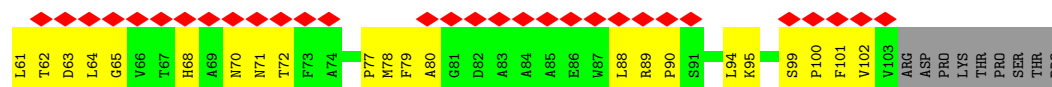
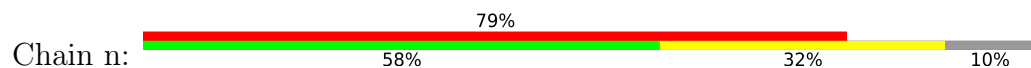
## ● Molecule 4: VP26



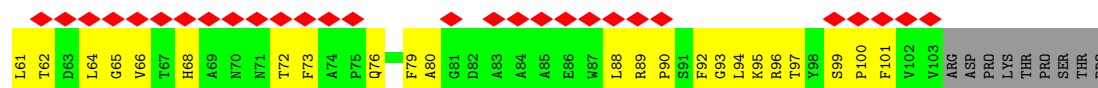
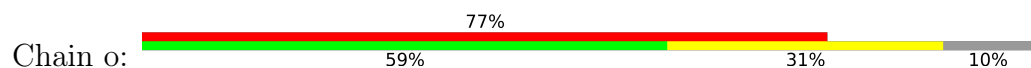
## ● Molecule 4: VP26



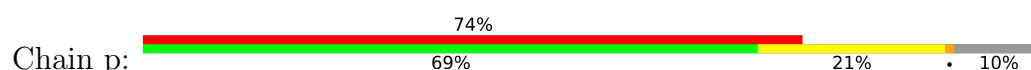
## ● Molecule 4: VP26

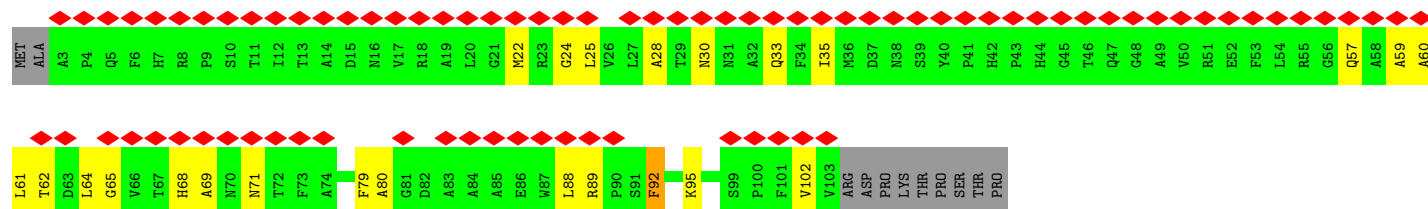


## ● Molecule 4: VP26

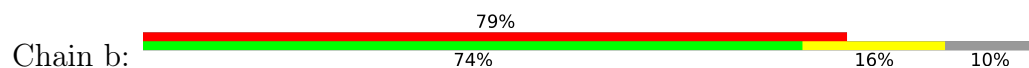


## ● Molecule 4: VP26

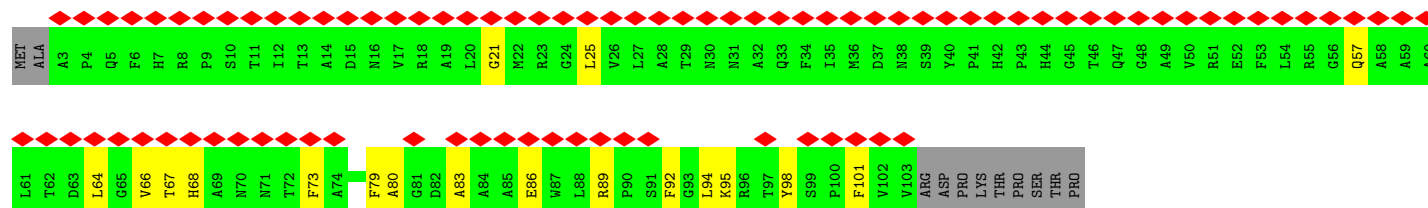
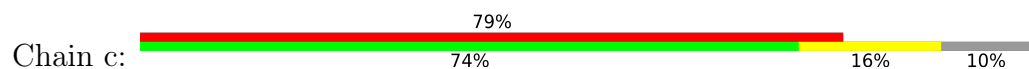




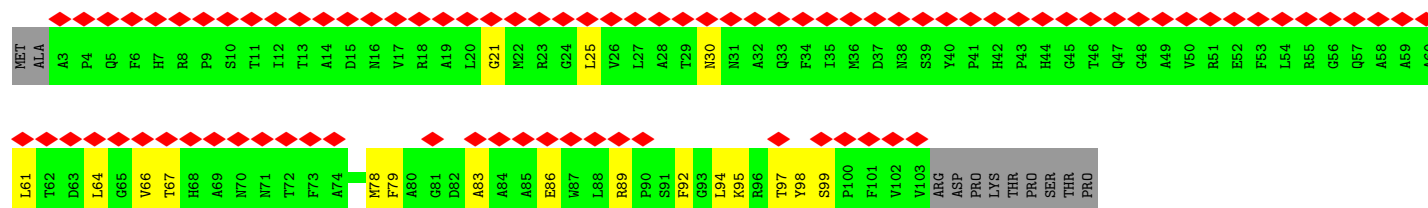
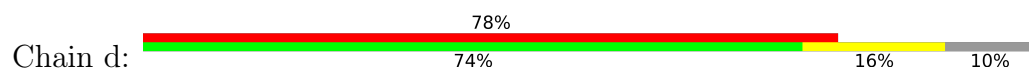
• Molecule 4: VP26



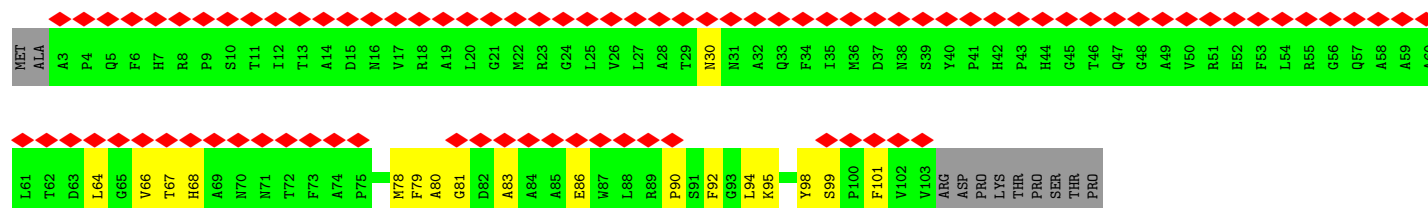
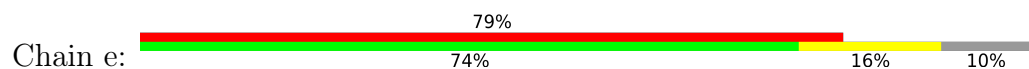
• Molecule 4: VP26



• Molecule 4: VP26

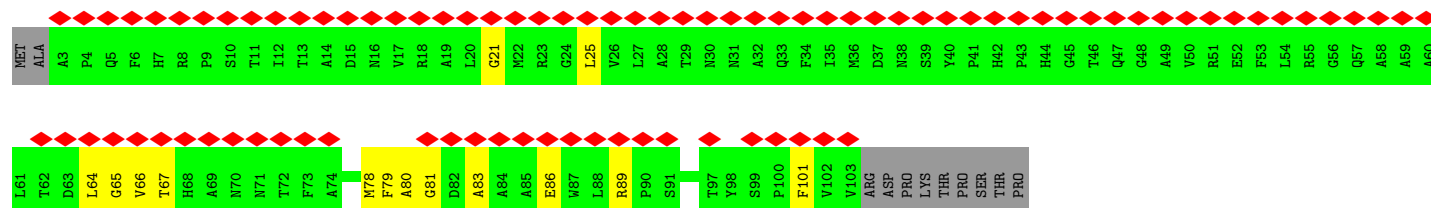


• Molecule 4: VP26



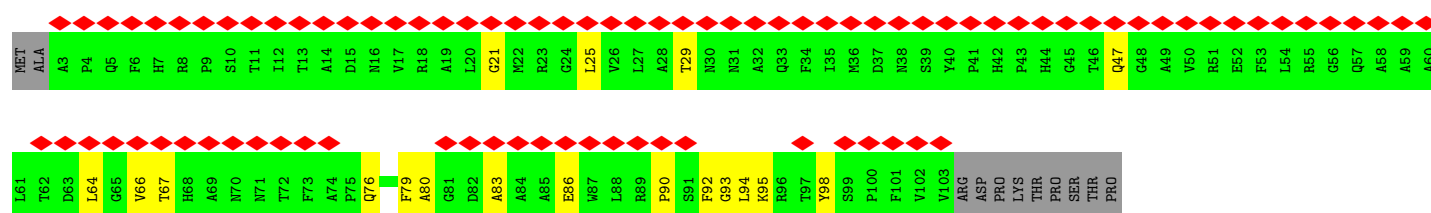
- Molecule 4: VP26

Chain f: 



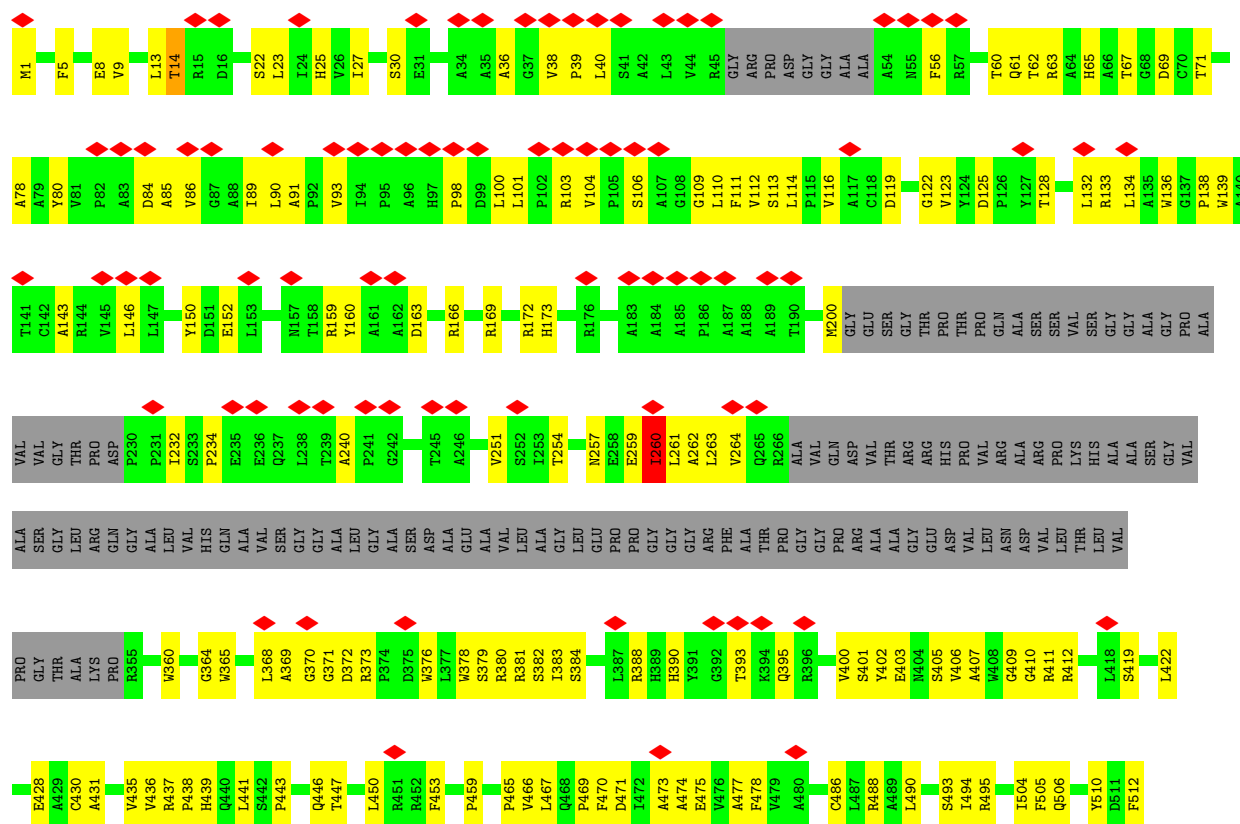
- Molecule 4: VP26

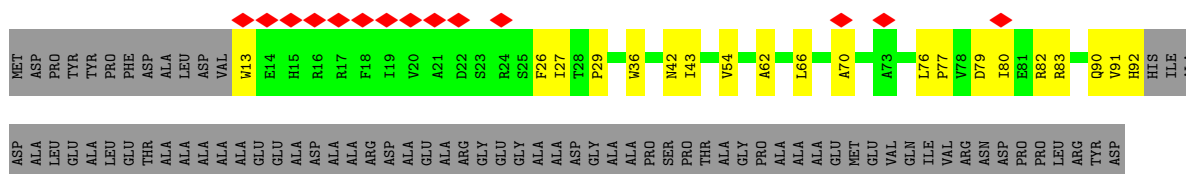
Chain g: 



- Molecule 5: UL17

Chain q: 







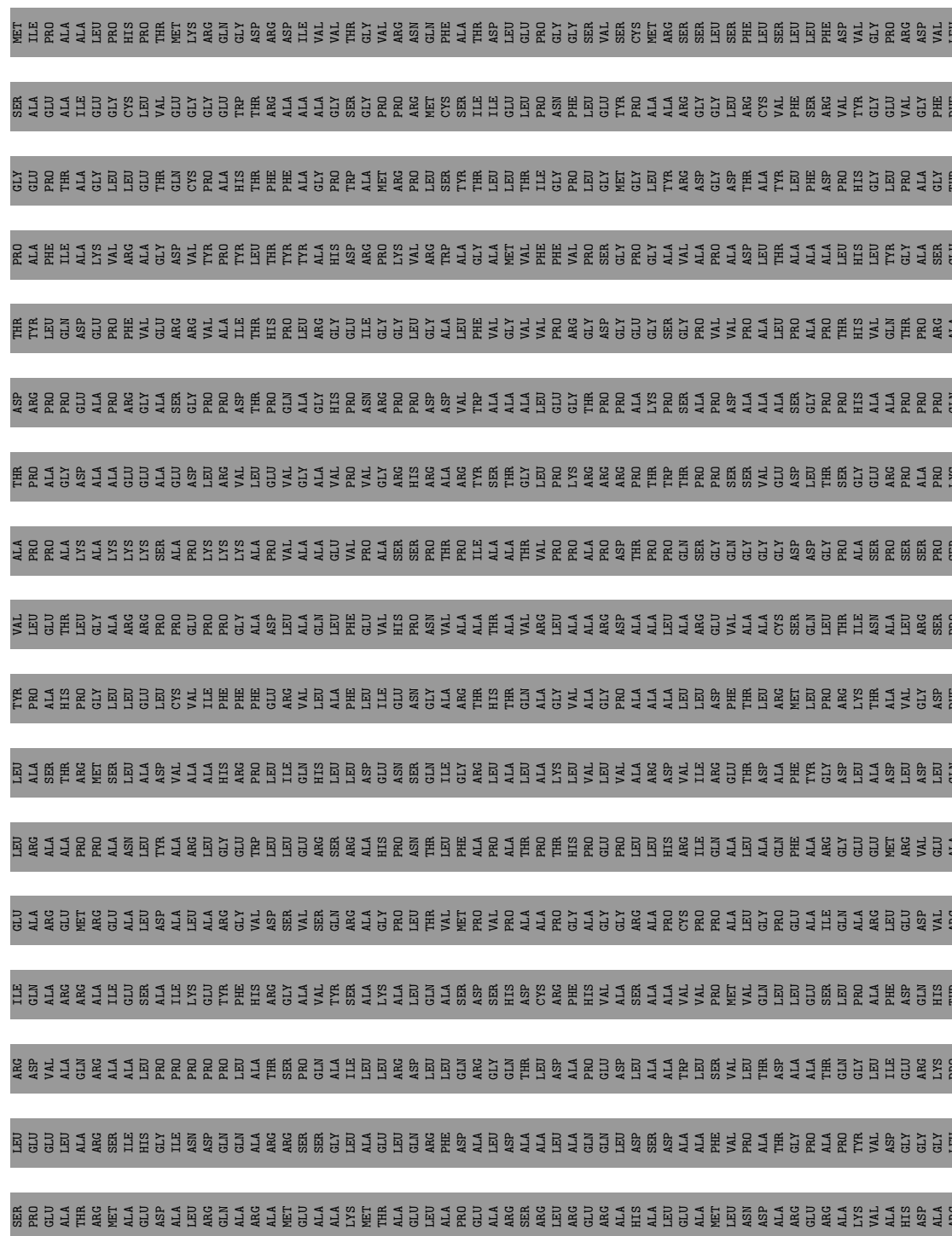






- Molecule 7: UL36

Chain u:  98%







## 4 Experimental information

| Property                             | Value                      | Source    |
|--------------------------------------|----------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE            | Depositor |
| Imposed symmetry                     | POINT, C1                  | Depositor |
| Number of particles used             | 56901                      | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF          | Depositor |
| CTF correction method                | NONE                       | Depositor |
| Microscope                           | FEI TITAN KRIOS            | Depositor |
| Voltage (kV)                         | 300                        | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 30                         | Depositor |
| Minimum defocus (nm)                 | Not provided               |           |
| Maximum defocus (nm)                 | Not provided               |           |
| Magnification                        | Not provided               |           |
| Image detector                       | GATAN K2 QUANTUM (4k x 4k) | Depositor |
| Maximum map value                    | 16.874                     | Depositor |
| Minimum map value                    | -9.664                     | Depositor |
| Average map value                    | 0.008                      | Depositor |
| Map value standard deviation         | 0.739                      | Depositor |
| Recommended contour level            | 1                          | Depositor |
| Map size ( $\text{\AA}$ )            | 1656.0, 1656.0, 1656.0     | wwPDB     |
| Map dimensions                       | 1200, 1200, 1200           | wwPDB     |
| Map angles ( $^\circ$ )              | 90.0, 90.0, 90.0           | wwPDB     |
| Pixel spacing ( $\text{\AA}$ )       | 1.38, 1.38, 1.38           | Depositor |

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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   | 1     | 0.36         | 0/2641         | 0.63        | 3/3594 (0.1%)   |
| 1   | Q     | 0.28         | 0/2641         | 0.59        | 4/3594 (0.1%)   |
| 1   | T     | 0.28         | 0/2647         | 0.60        | 3/3601 (0.1%)   |
| 1   | W     | 0.29         | 0/2629         | 0.65        | 1/3579 (0.0%)   |
| 1   | w     | 0.25         | 0/2647         | 0.59        | 3/3601 (0.1%)   |
| 2   | 2     | 0.51         | 0/2374         | 0.71        | 2/3247 (0.1%)   |
| 2   | 3     | 0.47         | 0/2134         | 0.69        | 1/2921 (0.0%)   |
| 2   | R     | 0.30         | 0/2134         | 0.61        | 1/2921 (0.0%)   |
| 2   | S     | 0.30         | 0/2377         | 0.60        | 2/3251 (0.1%)   |
| 2   | U     | 0.34         | 0/2134         | 0.66        | 1/2921 (0.0%)   |
| 2   | V     | 0.32         | 0/2377         | 0.60        | 2/3251 (0.1%)   |
| 2   | X     | 0.39         | 0/2134         | 0.68        | 0/2921          |
| 2   | Y     | 0.39         | 0/2377         | 0.64        | 2/3251 (0.1%)   |
| 2   | x     | 0.31         | 0/2134         | 0.62        | 1/2921 (0.0%)   |
| 2   | y     | 0.31         | 0/2368         | 0.59        | 2/3240 (0.1%)   |
| 3   | A     | 0.42         | 0/9879         | 0.61        | 0/13481         |
| 3   | B     | 0.69         | 5/10603 (0.0%) | 0.74        | 0/14473         |
| 3   | C     | 0.69         | 3/10610 (0.0%) | 0.77        | 5/14483 (0.0%)  |
| 3   | D     | 0.69         | 3/10672 (0.0%) | 0.79        | 4/14569 (0.0%)  |
| 3   | E     | 0.71         | 2/10663 (0.0%) | 0.81        | 7/14556 (0.0%)  |
| 3   | F     | 0.70         | 1/10649 (0.0%) | 0.79        | 3/14539 (0.0%)  |
| 3   | G     | 0.40         | 1/10514 (0.0%) | 0.71        | 32/14356 (0.2%) |
| 3   | H     | 0.52         | 0/10674        | 0.70        | 2/14570 (0.0%)  |
| 3   | I     | 0.55         | 1/10676 (0.0%) | 0.72        | 6/14572 (0.0%)  |
| 3   | J     | 0.56         | 1/10668 (0.0%) | 0.72        | 1/14567 (0.0%)  |
| 3   | K     | 0.55         | 1/10674 (0.0%) | 0.72        | 4/14574 (0.0%)  |
| 3   | L     | 0.55         | 2/10680 (0.0%) | 0.69        | 0/14577         |
| 3   | M     | 0.50         | 1/10709 (0.0%) | 0.68        | 6/14619 (0.0%)  |
| 3   | N     | 0.52         | 2/10654 (0.0%) | 0.69        | 1/14544 (0.0%)  |
| 3   | O     | 0.51         | 2/10676 (0.0%) | 0.69        | 0/14577         |
| 3   | P     | 0.57         | 2/10667 (0.0%) | 0.71        | 0/14565         |
| 4   | b     | 0.25         | 0/795          | 0.46        | 0/1084          |
| 4   | c     | 0.25         | 0/795          | 0.46        | 0/1084          |
| 4   | d     | 0.25         | 0/795          | 0.46        | 0/1084          |

| Mol | Chain | Bond lengths |                  | Bond angles |                   |
|-----|-------|--------------|------------------|-------------|-------------------|
|     |       | RMSZ         | # Z  >5          | RMSZ        | # Z  >5           |
| 4   | e     | 0.25         | 0/795            | 0.46        | 0/1084            |
| 4   | f     | 0.25         | 0/795            | 0.46        | 0/1084            |
| 4   | g     | 0.25         | 0/795            | 0.46        | 0/1084            |
| 4   | h     | 0.21         | 0/795            | 0.55        | 0/1084            |
| 4   | i     | 0.22         | 0/795            | 0.55        | 0/1084            |
| 4   | j     | 0.23         | 0/795            | 0.58        | 0/1084            |
| 4   | k     | 0.21         | 0/795            | 0.55        | 0/1084            |
| 4   | l     | 0.24         | 0/795            | 0.58        | 0/1084            |
| 4   | m     | 0.23         | 0/795            | 0.56        | 0/1084            |
| 4   | n     | 0.20         | 0/795            | 0.53        | 0/1084            |
| 4   | o     | 0.20         | 0/795            | 0.54        | 0/1084            |
| 4   | p     | 0.22         | 0/795            | 0.56        | 0/1084            |
| 5   | q     | 0.26         | 0/4350           | 0.58        | 3/5934 (0.1%)     |
| 6   | r     | 0.20         | 0/786            | 0.51        | 0/1074            |
| 6   | s     | 0.23         | 0/667            | 0.55        | 0/908             |
| 7   | t     | 0.17         | 0/385            | 0.53        | 0/514             |
| 7   | u     | 0.19         | 0/385            | 0.54        | 0/514             |
| All | All   | 0.53         | 27/223914 (0.0%) | 0.70        | 102/305640 (0.0%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | 1     | 0                   | 2                   |
| 1   | Q     | 0                   | 3                   |
| 1   | T     | 0                   | 2                   |
| 1   | W     | 0                   | 2                   |
| 1   | w     | 0                   | 2                   |
| 2   | 2     | 0                   | 1                   |
| 2   | S     | 0                   | 1                   |
| 2   | U     | 0                   | 1                   |
| 2   | V     | 0                   | 1                   |
| 2   | X     | 0                   | 1                   |
| 2   | Y     | 0                   | 1                   |
| 2   | y     | 0                   | 1                   |
| 3   | A     | 0                   | 1                   |
| 3   | B     | 0                   | 3                   |
| 3   | C     | 0                   | 3                   |
| 3   | D     | 0                   | 2                   |
| 3   | E     | 0                   | 3                   |

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| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 3   | F     | 0                   | 4                   |
| 3   | G     | 0                   | 1                   |
| 3   | H     | 0                   | 1                   |
| 3   | I     | 0                   | 4                   |
| 3   | J     | 0                   | 3                   |
| 3   | K     | 0                   | 3                   |
| 3   | L     | 0                   | 2                   |
| 3   | M     | 0                   | 2                   |
| 3   | N     | 0                   | 5                   |
| 3   | O     | 0                   | 1                   |
| 3   | P     | 0                   | 2                   |
| 4   | h     | 0                   | 1                   |
| 4   | p     | 0                   | 1                   |
| 5   | q     | 0                   | 2                   |
| All | All   | 0                   | 62                  |

All (27) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|--------|-------------|----------|
| 3   | B     | 485  | ASN  | C-N   | -17.32 | 0.93        | 1.33     |
| 3   | C     | 485  | ASN  | C-N   | -13.26 | 0.97        | 1.34     |
| 3   | P     | 485  | ASN  | C-N   | -13.08 | 0.98        | 1.34     |
| 3   | L     | 485  | ASN  | C-N   | -12.99 | 0.98        | 1.34     |
| 3   | F     | 1116 | ARG  | C-N   | -11.58 | 1.11        | 1.33     |
| 3   | O     | 255  | THR  | C-N   | -10.15 | 1.21        | 1.33     |
| 3   | E     | 1312 | LYS  | C-N   | -8.38  | 1.16        | 1.33     |
| 3   | P     | 1134 | GLY  | C-N   | -8.33  | 1.21        | 1.33     |
| 3   | B     | 708  | THR  | C-N   | -8.25  | 1.21        | 1.33     |
| 3   | I     | 1331 | ALA  | C-N   | -7.89  | 1.21        | 1.33     |
| 3   | D     | 972  | ASN  | C-N   | -7.65  | 1.23        | 1.33     |
| 3   | K     | 255  | THR  | C-N   | -6.84  | 1.24        | 1.33     |
| 3   | M     | 975  | ASN  | C-N   | -6.73  | 1.23        | 1.33     |
| 3   | B     | 1266 | ALA  | C-N   | -6.70  | 1.23        | 1.33     |
| 3   | E     | 83   | LYS  | C-N   | -6.18  | 1.22        | 1.33     |
| 3   | N     | 76   | SER  | CA-C  | -6.00  | 1.44        | 1.52     |
| 3   | J     | 1203 | CYS  | C-N   | -5.96  | 1.26        | 1.33     |
| 3   | D     | 1134 | GLY  | C-N   | -5.90  | 1.24        | 1.33     |
| 3   | C     | 434  | ALA  | C-N   | -5.88  | 1.24        | 1.33     |
| 3   | O     | 975  | ASN  | C-N   | -5.73  | 1.23        | 1.33     |
| 3   | B     | 76   | SER  | CA-C  | -5.68  | 1.44        | 1.52     |
| 3   | L     | 76   | SER  | CA-C  | -5.44  | 1.45        | 1.52     |
| 3   | N     | 1255 | LEU  | CA-C  | -5.39  | 1.45        | 1.52     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 3   | G     | 1236 | ARG  | C-N   | 5.38  | 1.39        | 1.34     |
| 3   | D     | 76   | SER  | CA-C  | -5.32 | 1.45        | 1.52     |
| 3   | B     | 1323 | ASP  | C-N   | -5.12 | 1.27        | 1.34     |
| 3   | C     | 1238 | PHE  | CA-C  | -5.03 | 1.45        | 1.52     |

All (102) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms    | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 3   | D     | 43   | ARG  | N-CA-C   | -17.85 | 86.97       | 110.53   |
| 1   | W     | 199  | ASP  | N-CA-C   | 14.39  | 126.47      | 111.07   |
| 3   | N     | 339  | MET  | N-CA-C   | -9.66  | 100.75      | 111.28   |
| 3   | E     | 1116 | ARG  | N-CA-C   | -9.35  | 98.47       | 110.53   |
| 3   | I     | 83   | LYS  | CA-C-N   | -8.92  | 109.22      | 121.61   |
| 3   | I     | 83   | LYS  | C-N-CA   | -8.92  | 109.22      | 121.61   |
| 3   | K     | 1237 | PRO  | CA-N-CD  | -8.86  | 99.59       | 112.00   |
| 3   | G     | 802  | PRO  | CA-N-CD  | -8.62  | 99.93       | 112.00   |
| 3   | G     | 526  | MET  | N-CA-C   | 8.35   | 122.34      | 110.23   |
| 3   | E     | 761  | HIS  | CA-C-N   | 8.08   | 133.79      | 120.86   |
| 3   | E     | 761  | HIS  | C-N-CA   | 8.08   | 133.79      | 120.86   |
| 3   | G     | 1236 | ARG  | N-CA-C   | -7.78  | 94.24       | 109.10   |
| 3   | G     | 986  | HIS  | N-CA-C   | 7.36   | 119.30      | 111.28   |
| 3   | C     | 434  | ALA  | CA-C-N   | -7.17  | 110.45      | 121.92   |
| 3   | C     | 434  | ALA  | C-N-CA   | -7.17  | 110.45      | 121.92   |
| 3   | G     | 108  | GLY  | C-N-CD   | 7.13   | 136.30      | 120.60   |
| 3   | D     | 485  | ASN  | N-CA-C   | -6.45  | 95.56       | 109.81   |
| 3   | G     | 1030 | LYS  | N-CA-C   | 6.44   | 119.58      | 110.50   |
| 3   | E     | 232  | PHE  | CA-C-N   | -6.16  | 112.37      | 122.54   |
| 3   | E     | 232  | PHE  | C-N-CA   | -6.16  | 112.37      | 122.54   |
| 3   | D     | 746  | ALA  | N-CA-C   | -6.08  | 104.65      | 111.28   |
| 1   | T     | 39   | PRO  | C-N-CD   | -6.08  | 107.22      | 120.60   |
| 3   | G     | 983  | LEU  | N-CA-C   | 6.03   | 117.94      | 111.36   |
| 3   | G     | 1165 | VAL  | N-CA-C   | 5.96   | 116.70      | 110.62   |
| 2   | R     | 228  | LEU  | CA-CB-CG | 5.96   | 137.16      | 116.30   |
| 3   | G     | 1236 | ARG  | CA-C-N   | -5.95  | 114.10      | 120.47   |
| 3   | G     | 1236 | ARG  | C-N-CA   | -5.95  | 114.10      | 120.47   |
| 3   | G     | 564  | PRO  | O-C-N    | 5.91   | 123.92      | 121.15   |
| 3   | G     | 709  | LEU  | CA-C-N   | -5.84  | 113.75      | 119.76   |
| 3   | G     | 709  | LEU  | C-N-CA   | -5.84  | 113.75      | 119.76   |
| 3   | K     | 485  | ASN  | CA-C-N   | -5.84  | 114.03      | 121.91   |
| 3   | K     | 485  | ASN  | C-N-CA   | -5.84  | 114.03      | 121.91   |
| 3   | G     | 429  | HIS  | CA-C-N   | -5.83  | 114.60      | 120.31   |
| 3   | G     | 429  | HIS  | C-N-CA   | -5.83  | 114.60      | 120.31   |

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| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 1   | w     | 39   | PRO  | C-N-CD | -5.82 | 107.80      | 120.60   |
| 3   | G     | 960  | VAL  | N-CA-C | 5.78  | 116.56      | 110.72   |
| 1   | T     | 39   | PRO  | CA-C-N | 5.77  | 140.85      | 127.00   |
| 1   | T     | 39   | PRO  | C-N-CA | 5.77  | 140.85      | 127.00   |
| 3   | I     | 1331 | ALA  | CA-C-N | -5.73 | 105.77      | 122.21   |
| 3   | I     | 1331 | ALA  | C-N-CA | -5.73 | 105.77      | 122.21   |
| 5   | q     | 603  | ASN  | CA-C-N | 5.68  | 129.16      | 121.20   |
| 5   | q     | 603  | ASN  | C-N-CA | 5.68  | 129.16      | 121.20   |
| 1   | w     | 39   | PRO  | CA-C-N | 5.68  | 140.63      | 127.00   |
| 1   | w     | 39   | PRO  | C-N-CA | 5.68  | 140.63      | 127.00   |
| 3   | G     | 567  | GLY  | CA-C-N | -5.68 | 113.91      | 119.76   |
| 3   | G     | 567  | GLY  | C-N-CA | -5.68 | 113.91      | 119.76   |
| 2   | V     | 241  | LEU  | CA-C-N | 5.67  | 132.38      | 121.54   |
| 2   | V     | 241  | LEU  | C-N-CA | 5.67  | 132.38      | 121.54   |
| 5   | q     | 260  | ILE  | N-CA-C | 5.64  | 121.08      | 109.34   |
| 3   | E     | 485  | ASN  | N-CA-C | -5.63 | 99.25       | 109.44   |
| 3   | M     | 576  | ARG  | CA-C-N | -5.61 | 117.47      | 122.97   |
| 3   | M     | 576  | ARG  | C-N-CA | -5.61 | 117.47      | 122.97   |
| 3   | G     | 526  | MET  | CA-C-N | 5.60  | 128.82      | 120.87   |
| 3   | G     | 526  | MET  | C-N-CA | 5.60  | 128.82      | 120.87   |
| 3   | G     | 110  | HIS  | CA-C-N | -5.60 | 114.20      | 119.85   |
| 3   | G     | 110  | HIS  | C-N-CA | -5.60 | 114.20      | 119.85   |
| 3   | E     | 59   | GLY  | N-CA-C | 5.59  | 117.74      | 112.04   |
| 2   | y     | 241  | LEU  | CA-C-N | 5.56  | 132.16      | 121.54   |
| 2   | y     | 241  | LEU  | C-N-CA | 5.56  | 132.16      | 121.54   |
| 1   | l     | 39   | PRO  | C-N-CD | -5.55 | 108.38      | 120.60   |
| 3   | G     | 477  | ASN  | N-CA-C | 5.53  | 119.12      | 112.38   |
| 2   | S     | 241  | LEU  | CA-C-N | 5.50  | 132.06      | 121.54   |
| 2   | S     | 241  | LEU  | C-N-CA | 5.50  | 132.06      | 121.54   |
| 3   | G     | 1161 | GLN  | CA-C-N | -5.50 | 114.09      | 119.76   |
| 3   | G     | 1161 | GLN  | C-N-CA | -5.50 | 114.09      | 119.76   |
| 3   | G     | 434  | ALA  | N-CA-C | 5.50  | 117.27      | 111.28   |
| 3   | G     | 114  | GLN  | CA-C-N | -5.49 | 114.10      | 119.76   |
| 3   | G     | 114  | GLN  | C-N-CA | -5.49 | 114.10      | 119.76   |
| 3   | G     | 1163 | LEU  | CA-C-N | -5.46 | 114.33      | 119.85   |
| 3   | G     | 1163 | LEU  | C-N-CA | -5.46 | 114.33      | 119.85   |
| 3   | I     | 448  | GLN  | CA-C-N | -5.46 | 115.56      | 122.43   |
| 3   | I     | 448  | GLN  | C-N-CA | -5.46 | 115.56      | 122.43   |
| 3   | F     | 134  | SER  | N-CA-C | 5.43  | 117.89      | 110.24   |
| 3   | G     | 711  | GLY  | CA-C-N | -5.36 | 114.44      | 119.85   |
| 3   | G     | 711  | GLY  | C-N-CA | -5.36 | 114.44      | 119.85   |
| 1   | l     | 39   | PRO  | CA-C-N | 5.34  | 139.82      | 127.00   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 1   | 1     | 39   | PRO  | C-N-CA   | 5.34  | 139.82      | 127.00   |
| 3   | C     | 1121 | ASP  | CA-C-N   | -5.32 | 114.59      | 122.41   |
| 3   | C     | 1121 | ASP  | C-N-CA   | -5.32 | 114.59      | 122.41   |
| 3   | M     | 485  | ASN  | CA-C-N   | -5.30 | 113.49      | 120.96   |
| 3   | M     | 485  | ASN  | C-N-CA   | -5.30 | 113.49      | 120.96   |
| 3   | H     | 485  | ASN  | CA-C-N   | -5.28 | 113.52      | 120.96   |
| 3   | H     | 485  | ASN  | C-N-CA   | -5.28 | 113.52      | 120.96   |
| 2   | U     | 228  | LEU  | CA-CB-CG | 5.28  | 134.76      | 116.30   |
| 3   | M     | 975  | ASN  | CA-C-N   | -5.22 | 113.68      | 121.83   |
| 3   | M     | 975  | ASN  | C-N-CA   | -5.22 | 113.68      | 121.83   |
| 1   | Q     | 277  | GLY  | N-CA-C   | -5.22 | 108.00      | 113.58   |
| 3   | K     | 561  | GLY  | N-CA-C   | 5.19  | 119.02      | 112.79   |
| 2   | Y     | 241  | LEU  | CA-C-N   | 5.15  | 131.37      | 121.54   |
| 2   | Y     | 241  | LEU  | C-N-CA   | 5.15  | 131.37      | 121.54   |
| 3   | D     | 87   | LEU  | N-CA-C   | -5.14 | 103.70      | 111.56   |
| 2   | 3     | 228  | LEU  | CA-CB-CG | 5.11  | 134.17      | 116.30   |
| 1   | Q     | 39   | PRO  | CA-C-N   | 5.09  | 139.21      | 127.00   |
| 1   | Q     | 39   | PRO  | C-N-CA   | 5.09  | 139.21      | 127.00   |
| 2   | 2     | 241  | LEU  | CA-C-N   | 5.09  | 131.26      | 121.54   |
| 2   | 2     | 241  | LEU  | C-N-CA   | 5.09  | 131.26      | 121.54   |
| 1   | Q     | 39   | PRO  | C-N-CD   | -5.06 | 109.47      | 120.60   |
| 3   | J     | 776  | PHE  | CA-C-O   | -5.04 | 115.20      | 120.55   |
| 2   | x     | 228  | LEU  | CA-CB-CG | 5.04  | 133.93      | 116.30   |
| 3   | F     | 1312 | LYS  | CA-C-N   | -5.04 | 113.92      | 120.67   |
| 3   | F     | 1312 | LYS  | C-N-CA   | -5.04 | 113.92      | 120.67   |
| 3   | C     | 1357 | HIS  | N-CA-C   | -5.01 | 101.83      | 109.65   |

There are no chirality outliers.

All (62) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 1   | 1     | 40  | PRO  | Peptide |
| 1   | 1     | 80  | ARG  | Peptide |
| 2   | 2     | 241 | LEU  | Peptide |
| 3   | A     | 112 | VAL  | Peptide |
| 3   | B     | 133 | PHE  | Peptide |
| 3   | B     | 79  | CYS  | Peptide |
| 3   | B     | 966 | GLY  | Peptide |
| 3   | C     | 133 | PHE  | Peptide |
| 3   | C     | 447 | HIS  | Peptide |
| 3   | C     | 469 | ILE  | Peptide |
| 3   | D     | 133 | PHE  | Peptide |

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| Mol | Chain | Res  | Type | Group   |
|-----|-------|------|------|---------|
| 3   | D     | 54   | PHE  | Peptide |
| 3   | E     | 133  | PHE  | Peptide |
| 3   | E     | 1357 | HIS  | Peptide |
| 3   | E     | 908  | LEU  | Peptide |
| 3   | F     | 1138 | LEU  | Peptide |
| 3   | F     | 133  | PHE  | Peptide |
| 3   | F     | 1357 | HIS  | Peptide |
| 3   | F     | 749  | ASP  | Peptide |
| 3   | G     | 133  | PHE  | Peptide |
| 3   | H     | 133  | PHE  | Peptide |
| 3   | I     | 1357 | HIS  | Peptide |
| 3   | I     | 469  | ILE  | Peptide |
| 3   | I     | 794  | ALA  | Peptide |
| 3   | I     | 946  | ASP  | Peptide |
| 3   | J     | 1067 | GLU  | Peptide |
| 3   | J     | 754  | CYS  | Peptide |
| 3   | J     | 79   | CYS  | Peptide |
| 3   | K     | 133  | PHE  | Peptide |
| 3   | K     | 1357 | HIS  | Peptide |
| 3   | K     | 908  | LEU  | Peptide |
| 3   | L     | 103  | LEU  | Peptide |
| 3   | L     | 1067 | GLU  | Peptide |
| 3   | M     | 133  | PHE  | Peptide |
| 3   | M     | 79   | CYS  | Peptide |
| 3   | N     | 133  | PHE  | Peptide |
| 3   | N     | 341  | GLU  | Peptide |
| 3   | N     | 342  | GLU  | Peptide |
| 3   | N     | 43   | ARG  | Peptide |
| 3   | N     | 784  | LEU  | Peptide |
| 3   | O     | 133  | PHE  | Peptide |
| 3   | P     | 133  | PHE  | Peptide |
| 3   | P     | 469  | ILE  | Peptide |
| 1   | Q     | 40   | PRO  | Peptide |
| 1   | Q     | 7    | PRO  | Peptide |
| 1   | Q     | 80   | ARG  | Peptide |
| 2   | S     | 241  | LEU  | Peptide |
| 1   | T     | 40   | PRO  | Peptide |
| 1   | T     | 80   | ARG  | Peptide |
| 2   | U     | 315  | ILE  | Peptide |
| 2   | V     | 241  | LEU  | Peptide |
| 1   | W     | 40   | PRO  | Peptide |
| 1   | W     | 80   | ARG  | Peptide |

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| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 2   | X     | 315 | ILE  | Peptide |
| 2   | Y     | 241 | LEU  | Peptide |
| 4   | h     | 94  | LEU  | Peptide |
| 4   | p     | 92  | PHE  | Peptide |
| 5   | q     | 14  | THR  | Peptide |
| 5   | q     | 260 | ILE  | Peptide |
| 1   | w     | 40  | PRO  | Peptide |
| 1   | w     | 80  | ARG  | Peptide |
| 2   | y     | 241 | LEU  | Peptide |

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

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | 1     | 2589  | 0        | 2487     | 79      | 0            |
| 1   | Q     | 2589  | 0        | 2487     | 59      | 0            |
| 1   | T     | 2595  | 0        | 2497     | 120     | 0            |
| 1   | W     | 2577  | 0        | 2461     | 145     | 0            |
| 1   | w     | 2595  | 0        | 2496     | 79      | 0            |
| 2   | 2     | 2334  | 0        | 2405     | 55      | 0            |
| 2   | 3     | 2102  | 0        | 2108     | 65      | 0            |
| 2   | R     | 2102  | 0        | 2108     | 52      | 0            |
| 2   | S     | 2337  | 0        | 2414     | 82      | 0            |
| 2   | U     | 2102  | 0        | 2108     | 38      | 0            |
| 2   | V     | 2337  | 0        | 2417     | 22      | 0            |
| 2   | X     | 2102  | 0        | 2108     | 70      | 0            |
| 2   | Y     | 2337  | 0        | 2415     | 50      | 0            |
| 2   | x     | 2102  | 0        | 2108     | 35      | 0            |
| 2   | y     | 2328  | 0        | 2396     | 34      | 0            |
| 3   | A     | 9646  | 0        | 9463     | 422     | 0            |
| 3   | B     | 10349 | 0        | 10126    | 550     | 0            |
| 3   | C     | 10355 | 0        | 10128    | 567     | 0            |
| 3   | D     | 10413 | 0        | 10203    | 687     | 0            |
| 3   | E     | 10405 | 0        | 10194    | 549     | 0            |
| 3   | F     | 10392 | 0        | 10170    | 553     | 0            |
| 3   | G     | 10261 | 0        | 10036    | 607     | 0            |
| 3   | H     | 10416 | 0        | 10203    | 609     | 0            |
| 3   | I     | 10418 | 0        | 10211    | 557     | 0            |

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| Mol | Chain | Non-H  | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 3   | J     | 10408  | 0        | 10182    | 478     | 0            |
| 3   | K     | 10414  | 0        | 10193    | 400     | 0            |
| 3   | L     | 10422  | 0        | 10215    | 470     | 0            |
| 3   | M     | 10449  | 0        | 10232    | 601     | 0            |
| 3   | N     | 10397  | 0        | 10187    | 481     | 0            |
| 3   | O     | 10417  | 0        | 10204    | 473     | 0            |
| 3   | P     | 10407  | 0        | 10187    | 404     | 0            |
| 4   | b     | 773    | 0        | 748      | 43      | 0            |
| 4   | c     | 773    | 0        | 748      | 40      | 0            |
| 4   | d     | 773    | 0        | 748      | 38      | 0            |
| 4   | e     | 773    | 0        | 748      | 41      | 0            |
| 4   | f     | 773    | 0        | 748      | 14      | 0            |
| 4   | g     | 773    | 0        | 748      | 21      | 0            |
| 4   | h     | 773    | 0        | 748      | 45      | 0            |
| 4   | i     | 773    | 0        | 748      | 49      | 0            |
| 4   | j     | 773    | 0        | 748      | 46      | 0            |
| 4   | k     | 773    | 0        | 748      | 39      | 0            |
| 4   | l     | 773    | 0        | 748      | 41      | 0            |
| 4   | m     | 773    | 0        | 748      | 37      | 0            |
| 4   | n     | 773    | 0        | 748      | 38      | 0            |
| 4   | o     | 773    | 0        | 748      | 54      | 0            |
| 4   | p     | 773    | 0        | 748      | 22      | 0            |
| 5   | q     | 4241   | 0        | 4188     | 226     | 0            |
| 6   | r     | 764    | 0        | 740      | 92      | 0            |
| 6   | s     | 651    | 0        | 643      | 38      | 0            |
| 7   | t     | 383    | 0        | 418      | 13      | 0            |
| 7   | u     | 383    | 0        | 418      | 27      | 0            |
| All | All   | 218714 | 0        | 214776   | 8501    | 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 20.

All (8501) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:X:284:GLN:HG2  | 3:H:1166:PHE:CZ  | 1.16                     | 1.65              |
| 1:T:170:LEU:HD11 | 3:I:1262:HIS:CB  | 1.15                     | 1.61              |
| 3:H:339:MET:HE2  | 3:C:17:MET:CE    | 1.14                     | 1.60              |
| 2:S:300:PHE:CE2  | 3:A:111:PRO:CA   | 1.80                     | 1.59              |
| 2:S:300:PHE:HE2  | 3:A:111:PRO:CA   | 0.93                     | 1.58              |
| 1:T:161:TRP:CD1  | 3:I:1166:PHE:CE2 | 1.87                     | 1.57              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:W:352:ILE:CB   | 6:r:12:VAL:HG21  | 1.20                     | 1.56              |
| 3:N:322:MET:CE   | 3:E:324:LYS:HB2  | 1.08                     | 1.56              |
| 1:T:165:LEU:CD1  | 3:I:1166:PHE:CZ  | 1.91                     | 1.54              |
| 3:N:322:MET:HE1  | 3:E:324:LYS:CB   | 1.13                     | 1.54              |
| 3:H:322:MET:HE1  | 3:D:324:LYS:CB   | 1.09                     | 1.54              |
| 1:T:165:LEU:HD11 | 3:I:1166:PHE:CE2 | 1.39                     | 1.54              |
| 3:H:339:MET:CE   | 3:C:17:MET:HE2   | 1.30                     | 1.52              |
| 1:W:328:TYR:CE1  | 6:r:18:PHE:CZ    | 1.96                     | 1.51              |
| 2:S:300:PHE:CE2  | 3:A:111:PRO:CB   | 1.94                     | 1.49              |
| 1:I:141:PRO:CG   | 3:M:1166:PHE:CD2 | 1.96                     | 1.48              |
| 1:W:349:ARG:CB   | 6:r:14:GLU:HA    | 1.41                     | 1.48              |
| 2:3:300:PHE:CD2  | 3:M:1083:HIS:CD2 | 2.00                     | 1.48              |
| 2:Y:238:ASN:HD22 | 3:H:1137:PRO:CG  | 1.21                     | 1.48              |
| 3:A:329:LEU:CD1  | 3:G:61:TYR:HD2   | 1.24                     | 1.47              |
| 3:H:322:MET:CE   | 3:D:324:LYS:HB2  | 1.01                     | 1.46              |
| 1:T:170:LEU:HD11 | 3:I:1262:HIS:CG  | 1.49                     | 1.45              |
| 1:T:161:TRP:HD1  | 3:I:1166:PHE:CD2 | 1.32                     | 1.45              |
| 2:Y:238:ASN:ND2  | 3:H:1137:PRO:HG3 | 1.28                     | 1.45              |
| 1:w:272:GLU:HB3  | 1:w:283:ARG:NH2  | 1.25                     | 1.44              |
| 1:Q:44:ARG:HA    | 3:B:322:MET:CE   | 1.45                     | 1.43              |
| 1:Q:45:ASP:CA    | 3:B:322:MET:CB   | 1.94                     | 1.43              |
| 1:T:78:ALA:CB    | 3:I:308:GLU:OE1  | 1.66                     | 1.42              |
| 1:w:283:ARG:HE   | 3:N:47:ASN:ND2   | 0.98                     | 1.42              |
| 2:S:2:ILE:CD1    | 3:B:1084:GLU:O   | 1.68                     | 1.42              |
| 1:T:170:LEU:CD1  | 3:I:1262:HIS:HB2 | 1.49                     | 1.41              |
| 1:W:199:ASP:CB   | 6:r:17:ARG:HA    | 1.52                     | 1.40              |
| 1:W:352:ILE:CB   | 6:r:12:VAL:CG2   | 1.97                     | 1.40              |
| 1:W:344:GLU:OE1  | 6:r:13:TRP:CH2   | 1.75                     | 1.40              |
| 2:S:300:PHE:CE2  | 3:A:111:PRO:HB3  | 1.53                     | 1.39              |
| 5:q:172:ARG:HE   | 5:q:200:MET:CE   | 1.32                     | 1.39              |
| 1:Q:45:ASP:N     | 3:B:322:MET:HB3  | 1.10                     | 1.38              |
| 2:R:174:PRO:N    | 5:q:371:GLY:HA3  | 1.08                     | 1.38              |
| 2:3:300:PHE:HD2  | 3:M:1083:HIS:CD2 | 1.35                     | 1.38              |
| 1:T:161:TRP:NE1  | 3:I:1166:PHE:CE2 | 1.89                     | 1.37              |
| 1:Q:45:ASP:CA    | 3:B:322:MET:HB3  | 1.52                     | 1.37              |
| 1:T:280:GLY:O    | 3:H:51:ASP:CG    | 1.68                     | 1.37              |
| 1:W:344:GLU:O    | 6:r:13:TRP:CE3   | 1.65                     | 1.36              |
| 2:S:300:PHE:CD2  | 3:A:111:PRO:HB3  | 1.56                     | 1.36              |
| 2:U:300:PHE:CD2  | 3:I:1083:HIS:CD2 | 2.14                     | 1.36              |
| 3:G:554:ALA:CB   | 3:G:568:PRO:O    | 1.71                     | 1.36              |
| 3:N:89:TYR:HE1   | 3:D:157:ARG:NH2  | 1.22                     | 1.36              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:Q:45:ASP:C     | 3:B:322:MET:HB2   | 1.48                     | 1.35              |
| 3:N:256:GLN:OE1  | 3:D:27:ILE:CD1    | 1.71                     | 1.35              |
| 3:M:12:ARG:H     | 3:D:96:GLN:NE2    | 1.25                     | 1.35              |
| 3:B:263:ARG:N    | 3:G:59:GLY:O      | 1.56                     | 1.35              |
| 1:I:141:PRO:HG2  | 3:M:1166:PHE:CD2  | 1.53                     | 1.34              |
| 3:G:495:ALA:O    | 3:G:504:ARG:NH1   | 1.60                     | 1.34              |
| 2:2:39:ARG:HH22  | 3:N:1085:THR:CG2  | 1.37                     | 1.34              |
| 3:H:89:TYR:HE1   | 3:C:157:ARG:NH2   | 1.24                     | 1.34              |
| 3:G:99:VAL:O     | 3:G:118:ASN:N     | 1.59                     | 1.34              |
| 1:T:165:LEU:HG   | 3:I:1166:PHE:CZ   | 1.62                     | 1.34              |
| 1:w:283:ARG:NE   | 3:N:47:ASN:HD22   | 1.23                     | 1.34              |
| 2:2:39:ARG:NH2   | 3:N:1085:THR:CG2  | 1.87                     | 1.33              |
| 2:X:284:GLN:CG   | 3:H:1166:PHE:CZ   | 2.12                     | 1.33              |
| 3:H:339:MET:CE   | 3:C:17:MET:CE     | 1.91                     | 1.33              |
| 1:w:283:ARG:NH1  | 3:L:137:THR:OG1   | 1.62                     | 1.32              |
| 2:S:300:PHE:CD2  | 3:A:111:PRO:CB    | 2.09                     | 1.32              |
| 1:T:161:TRP:CD1  | 3:I:1166:PHE:CD2  | 2.11                     | 1.31              |
| 3:A:329:LEU:O    | 3:G:61:TYR:HE2    | 1.07                     | 1.31              |
| 3:G:524:CYS:HB3  | 3:G:1008:GLN:NE2  | 1.42                     | 1.31              |
| 1:W:328:TYR:CZ   | 6:r:18:PHE:CZ     | 2.08                     | 1.31              |
| 1:T:165:LEU:CG   | 3:I:1166:PHE:CZ   | 2.11                     | 1.31              |
| 2:R:174:PRO:N    | 5:q:371:GLY:CA    | 1.94                     | 1.30              |
| 3:B:225:ARG:NH2  | 3:G:447:HIS:NE2   | 1.79                     | 1.30              |
| 3:A:329:LEU:CD1  | 3:G:61:TYR:CD2    | 2.13                     | 1.30              |
| 3:F:448:GLN:NE2  | 3:G:1201:ARG:HH22 | 1.30                     | 1.29              |
| 2:X:18:ARG:NH1   | 2:3:18:ARG:HH12   | 1.27                     | 1.29              |
| 1:T:170:LEU:CD1  | 3:I:1262:HIS:CB   | 2.08                     | 1.29              |
| 2:R:173:LEU:C    | 5:q:371:GLY:CA    | 2.06                     | 1.29              |
| 1:Q:45:ASP:HA    | 3:B:322:MET:C     | 1.58                     | 1.29              |
| 1:T:158:ALA:HB1  | 3:I:1165:VAL:CG1  | 1.61                     | 1.29              |
| 1:W:198:TYR:O    | 1:W:201:ARG:CD    | 1.81                     | 1.29              |
| 3:J:469:ILE:HD11 | 3:J:547:PHE:CD1   | 1.66                     | 1.28              |
| 3:E:1117:ASN:ND2 | 3:F:222:GLU:OE2   | 1.66                     | 1.27              |
| 2:Y:238:ASN:ND2  | 3:H:1137:PRO:CG   | 1.85                     | 1.27              |
| 3:M:11:TYR:CE2   | 3:D:119:TYR:HB3   | 1.24                     | 1.27              |
| 1:Q:104:GLY:CA   | 3:B:1084:GLU:OE2  | 1.82                     | 1.27              |
| 1:W:166:GLU:HG2  | 3:C:1262:HIS:NE2  | 1.45                     | 1.26              |
| 2:Y:238:ASN:ND2  | 3:H:1137:PRO:CB   | 1.97                     | 1.26              |
| 2:2:2:ILE:CB     | 3:N:1084:GLU:O    | 1.81                     | 1.26              |
| 2:2:39:ARG:NH2   | 3:N:1085:THR:HG21 | 0.94                     | 1.26              |
| 3:A:329:LEU:O    | 3:G:61:TYR:CE2    | 1.86                     | 1.26              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:T:158:ALA:CB   | 3:I:1165:VAL:HG11 | 1.65                     | 1.26              |
| 1:T:165:LEU:CD1  | 3:I:1166:PHE:CE2  | 2.11                     | 1.25              |
| 1:w:283:ARG:NE   | 3:N:47:ASN:ND2    | 1.81                     | 1.25              |
| 1:W:348:GLY:O    | 6:r:12:VAL:HG13   | 1.34                     | 1.25              |
| 1:l:257:GLN:OE1  | 3:H:109:PRO:HD2   | 1.29                     | 1.25              |
| 2:R:173:LEU:C    | 5:q:371:GLY:HA2   | 1.58                     | 1.25              |
| 1:l:141:PRO:CG   | 3:M:1166:PHE:HD2  | 1.36                     | 1.25              |
| 1:w:79:THR:CA    | 3:O:308:GLU:OE2   | 1.83                     | 1.25              |
| 3:J:469:ILE:HD11 | 3:J:547:PHE:CE1   | 1.69                     | 1.25              |
| 5:q:172:ARG:CG   | 5:q:200:MET:HE2   | 1.66                     | 1.25              |
| 1:Q:104:GLY:HA3  | 3:B:1084:GLU:OE2  | 1.31                     | 1.25              |
| 2:S:2:ILE:HD13   | 3:B:1084:GLU:O    | 1.18                     | 1.25              |
| 3:N:326:VAL:HG21 | 3:E:321:VAL:CG1   | 1.65                     | 1.25              |
| 2:X:18:ARG:NH1   | 2:3:18:ARG:NH1    | 1.84                     | 1.24              |
| 2:X:40:GLN:NE2   | 3:H:128:ALA:HB3   | 1.50                     | 1.23              |
| 3:N:1260:ALA:O   | 3:N:1262:HIS:CD2  | 1.92                     | 1.22              |
| 1:T:161:TRP:CD1  | 3:I:1166:PHE:CZ   | 2.25                     | 1.22              |
| 3:F:432:PRO:O    | 3:G:413:MET:HE1   | 1.40                     | 1.21              |
| 3:G:469:ILE:HD11 | 3:G:547:PHE:CD2   | 1.76                     | 1.21              |
| 1:T:166:GLU:HG2  | 3:I:1262:HIS:NE2  | 1.55                     | 1.20              |
| 1:W:345:ARG:HG2  | 6:s:13:TRP:CZ3    | 1.74                     | 1.20              |
| 1:l:79:THR:HB    | 3:M:308:GLU:OE2   | 1.38                     | 1.20              |
| 1:W:29:GLY:HA3   | 3:H:144:THR:HA    | 1.22                     | 1.20              |
| 3:F:134:SER:OG   | 3:G:114:GLN:NE2   | 1.73                     | 1.20              |
| 3:A:329:LEU:HG   | 3:G:61:TYR:CE2    | 1.76                     | 1.20              |
| 1:W:328:TYR:CE1  | 6:r:18:PHE:CE1    | 2.28                     | 1.20              |
| 3:G:472:ALA:O    | 3:G:476:VAL:HG23  | 1.42                     | 1.20              |
| 1:T:158:ALA:HB1  | 3:I:1165:VAL:CG2  | 1.72                     | 1.19              |
| 3:B:261:VAL:HB   | 3:G:61:TYR:O      | 1.42                     | 1.19              |
| 1:W:349:ARG:CB   | 6:r:14:GLU:CA     | 2.19                     | 1.19              |
| 2:Y:238:ASN:HD22 | 3:H:1137:PRO:CB   | 1.55                     | 1.19              |
| 3:M:160:ARG:HD3  | 3:C:49:LEU:O      | 1.38                     | 1.19              |
| 3:G:949:ILE:HG23 | 3:G:953:GLU:OE1   | 1.41                     | 1.19              |
| 1:W:345:ARG:HG2  | 6:s:13:TRP:CE3    | 1.78                     | 1.19              |
| 3:M:28:GLU:OE2   | 3:C:389:ASN:OD1   | 1.61                     | 1.18              |
| 3:H:123:VAL:CG2  | 3:C:37:ASP:OD2    | 1.91                     | 1.18              |
| 1:l:141:PRO:HG3  | 3:M:1166:PHE:CD2  | 1.68                     | 1.18              |
| 3:M:11:TYR:HE2   | 3:D:119:TYR:CB    | 1.36                     | 1.18              |
| 3:M:134:SER:O    | 3:C:44:SER:OG     | 1.59                     | 1.18              |
| 3:N:256:GLN:OE1  | 3:D:27:ILE:HD11   | 1.01                     | 1.18              |
| 5:q:172:ARG:NE   | 5:q:200:MET:HE1   | 1.58                     | 1.18              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:S:300:PHE:CE2  | 3:A:111:PRO:HA    | 1.50                     | 1.18              |
| 3:G:829:GLY:C    | 3:G:956:TYR:CE1   | 2.21                     | 1.18              |
| 1:W:29:GLY:HA2   | 3:H:143:LEU:O     | 1.06                     | 1.18              |
| 3:G:505:PHE:CE1  | 3:G:991:PRO:HA    | 1.78                     | 1.18              |
| 5:q:172:ARG:CG   | 5:q:200:MET:CE    | 2.21                     | 1.17              |
| 1:Q:45:ASP:N     | 3:B:322:MET:CB    | 2.06                     | 1.17              |
| 2:R:174:PRO:CD   | 5:q:371:GLY:HA3   | 1.74                     | 1.17              |
| 3:G:103:LEU:HD11 | 3:G:115:PRO:HA    | 1.25                     | 1.17              |
| 1:W:25:ARG:O     | 3:H:144:THR:O     | 1.59                     | 1.16              |
| 3:H:89:TYR:CE1   | 3:C:157:ARG:NH2   | 2.13                     | 1.16              |
| 5:q:172:ARG:NE   | 5:q:200:MET:CE    | 2.06                     | 1.16              |
| 1:T:162:GLY:CA   | 3:I:1166:PHE:CD1  | 2.29                     | 1.16              |
| 3:M:29:VAL:CG1   | 3:D:120:MET:HE1   | 1.74                     | 1.16              |
| 3:A:329:LEU:HD11 | 3:G:61:TYR:CD2    | 1.71                     | 1.16              |
| 1:W:28:ALA:HB3   | 3:H:145:GLY:CA    | 1.75                     | 1.16              |
| 1:w:272:GLU:CB   | 1:w:283:ARG:NH2   | 1.89                     | 1.16              |
| 3:G:233:PHE:CE2  | 3:G:244:ILE:HG12  | 1.81                     | 1.16              |
| 1:T:162:GLY:HA2  | 3:I:1166:PHE:CD1  | 1.78                     | 1.15              |
| 3:G:524:CYS:HB3  | 3:G:1008:GLN:CD   | 1.69                     | 1.15              |
| 3:G:666:ASN:HB2  | 3:G:938:LEU:CD2   | 1.75                     | 1.15              |
| 3:J:469:ILE:CD1  | 3:J:547:PHE:CE1   | 2.29                     | 1.15              |
| 1:W:199:ASP:CB   | 6:r:17:ARG:CA     | 2.25                     | 1.15              |
| 3:N:89:TYR:CE1   | 3:D:157:ARG:NH2   | 2.15                     | 1.14              |
| 3:G:103:LEU:CD2  | 3:G:113:GLU:O     | 1.95                     | 1.14              |
| 2:S:300:PHE:HD2  | 3:A:111:PRO:CD    | 1.58                     | 1.14              |
| 1:T:170:LEU:CD1  | 3:I:1262:HIS:CG   | 2.28                     | 1.14              |
| 1:w:79:THR:HB    | 3:O:308:GLU:OE2   | 1.46                     | 1.14              |
| 3:G:99:VAL:O     | 3:G:118:ASN:HB2   | 1.44                     | 1.14              |
| 3:G:100:HIS:ND1  | 3:G:117:HIS:ND1   | 1.96                     | 1.14              |
| 3:A:1031:MET:HE1 | 3:A:1048:PHE:CE2  | 1.82                     | 1.14              |
| 1:w:79:THR:CB    | 3:O:308:GLU:OE2   | 1.95                     | 1.13              |
| 3:B:261:VAL:O    | 3:G:60:SER:HA     | 1.47                     | 1.13              |
| 3:M:20:THR:O     | 3:D:352:ASP:CB    | 1.96                     | 1.13              |
| 2:S:300:PHE:HD2  | 3:A:111:PRO:CG    | 1.62                     | 1.13              |
| 2:R:174:PRO:CA   | 5:q:371:GLY:HA3   | 1.79                     | 1.13              |
| 1:W:166:GLU:CG   | 3:C:1262:HIS:NE2  | 2.10                     | 1.13              |
| 3:B:261:VAL:CB   | 3:G:61:TYR:O      | 1.96                     | 1.13              |
| 1:T:158:ALA:CB   | 3:I:1165:VAL:HG21 | 1.79                     | 1.13              |
| 2:Y:248:ARG:HD3  | 3:H:1141:ASN:HD22 | 1.01                     | 1.13              |
| 3:F:390:VAL:HG21 | 3:G:104:ILE:CG1   | 1.78                     | 1.12              |
| 3:G:524:CYS:CB   | 3:G:1008:GLN:NE2  | 2.10                     | 1.13              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:3:284:GLN:HG2  | 3:D:1166:PHE:CZ   | 1.84                     | 1.12              |
| 1:W:28:ALA:HB3   | 3:H:145:GLY:HA3   | 1.13                     | 1.12              |
| 3:H:123:VAL:HG23 | 3:C:37:ASP:OD2    | 0.96                     | 1.12              |
| 3:G:801:ARG:HB3  | 3:G:802:PRO:HD3   | 1.26                     | 1.12              |
| 1:T:280:GLY:O    | 3:H:51:ASP:CB     | 1.97                     | 1.11              |
| 1:W:25:ARG:CB    | 3:H:145:GLY:O     | 1.90                     | 1.11              |
| 1:W:28:ALA:HB1   | 3:H:148:LEU:HD12  | 1.31                     | 1.11              |
| 1:W:349:ARG:CB   | 6:r:14:GLU:HG2    | 1.78                     | 1.11              |
| 3:H:339:MET:HE1  | 3:C:17:MET:HG2    | 1.31                     | 1.11              |
| 3:O:546:ALA:HA   | 3:O:1031:MET:HE1  | 1.14                     | 1.11              |
| 3:H:322:MET:HE3  | 3:D:324:LYS:HB2   | 1.16                     | 1.11              |
| 3:F:14:ALA:HB3   | 3:G:321:VAL:HG22  | 1.29                     | 1.11              |
| 3:G:524:CYS:CB   | 3:G:1008:GLN:CD   | 2.23                     | 1.11              |
| 3:M:61:TYR:HD1   | 3:C:21:GLY:O      | 1.33                     | 1.11              |
| 3:N:350:THR:HG21 | 3:D:21:GLY:CA     | 1.80                     | 1.10              |
| 3:G:233:PHE:HE2  | 3:G:244:ILE:HG12  | 1.05                     | 1.10              |
| 1:T:162:GLY:CA   | 3:I:1166:PHE:HD1  | 1.62                     | 1.10              |
| 2:3:40:GLN:HE22  | 3:D:128:ALA:HB3   | 1.09                     | 1.10              |
| 3:D:646:ARG:NH1  | 4:d:99:SER:HA     | 1.66                     | 1.10              |
| 3:B:677:TYR:HA   | 4:b:95:LYS:NZ     | 1.67                     | 1.10              |
| 1:W:29:GLY:CA    | 3:H:143:LEU:O     | 1.99                     | 1.10              |
| 3:J:469:ILE:CD1  | 3:J:547:PHE:CD1   | 2.33                     | 1.09              |
| 3:G:434:ALA:O    | 3:G:1359:THR:HG21 | 1.49                     | 1.09              |
| 2:3:284:GLN:HG2  | 3:D:1166:PHE:CE1  | 1.87                     | 1.09              |
| 3:H:324:LYS:HB2  | 3:D:322:MET:HE3   | 1.34                     | 1.09              |
| 3:B:872:ALA:HB2  | 4:g:76:GLN:HG2    | 1.23                     | 1.09              |
| 3:G:103:LEU:CD1  | 3:G:115:PRO:HA    | 1.82                     | 1.09              |
| 2:S:300:PHE:CD2  | 3:A:111:PRO:CD    | 2.35                     | 1.09              |
| 1:W:350:LEU:HD21 | 6:r:20:VAL:HG12   | 1.12                     | 1.09              |
| 3:M:29:VAL:HG11  | 3:D:120:MET:CE    | 1.81                     | 1.09              |
| 2:X:284:GLN:HG2  | 3:H:1166:PHE:CE1  | 1.87                     | 1.08              |
| 3:H:339:MET:HE1  | 3:C:17:MET:CG     | 1.82                     | 1.08              |
| 1:W:347:PHE:CE1  | 6:r:18:PHE:HD2    | 1.70                     | 1.08              |
| 3:N:350:THR:CG2  | 3:D:21:GLY:HA2    | 1.82                     | 1.08              |
| 1:W:194:CYS:O    | 1:W:198:TYR:CE2   | 2.05                     | 1.08              |
| 3:N:322:MET:HE1  | 3:E:324:LYS:HB3   | 1.16                     | 1.08              |
| 2:Y:248:ARG:HD3  | 3:H:1141:ASN:ND2  | 1.69                     | 1.08              |
| 3:G:99:VAL:O     | 3:G:118:ASN:CB    | 2.01                     | 1.08              |
| 3:G:526:MET:HE1  | 3:G:531:PHE:HD1   | 1.08                     | 1.07              |
| 3:G:666:ASN:CB   | 3:G:938:LEU:HD22  | 1.82                     | 1.07              |
| 1:W:350:LEU:HD21 | 6:r:20:VAL:CG1    | 1.84                     | 1.07              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:H:324:LYS:HB2  | 3:D:322:MET:CE   | 1.84                     | 1.07              |
| 3:N:96:GLN:NE2   | 3:D:12:ARG:H     | 1.52                     | 1.07              |
| 3:D:873:ASN:OD1  | 4:c:92:PHE:HB2   | 1.53                     | 1.07              |
| 1:Q:45:ASP:C     | 3:B:322:MET:CB   | 2.20                     | 1.07              |
| 2:x:18:ARG:N     | 3:O:7:ASP:OD2    | 1.88                     | 1.07              |
| 3:B:311:LEU:HD23 | 3:G:55:ASP:OD1   | 1.54                     | 1.07              |
| 1:T:165:LEU:HD11 | 3:I:1166:PHE:CZ  | 1.70                     | 1.06              |
| 1:l:158:ALA:HB1  | 3:M:1165:VAL:CG2 | 1.85                     | 1.06              |
| 1:w:79:THR:HA    | 3:O:308:GLU:OE2  | 1.50                     | 1.06              |
| 1:Q:104:GLY:N    | 3:B:1084:GLU:OE2 | 1.88                     | 1.06              |
| 3:B:310:VAL:O    | 3:G:55:ASP:HA    | 1.55                     | 1.06              |
| 1:Q:45:ASP:HA    | 3:B:322:MET:O    | 1.55                     | 1.06              |
| 3:A:1031:MET:HE1 | 3:A:1048:PHE:HE2 | 0.97                     | 1.06              |
| 1:Q:44:ARG:HA    | 3:B:322:MET:HE2  | 1.21                     | 1.06              |
| 1:Q:45:ASP:HA    | 3:B:322:MET:CB   | 1.66                     | 1.06              |
| 3:M:24:LEU:HD12  | 3:D:258:SER:O    | 1.56                     | 1.06              |
| 3:A:329:LEU:CG   | 3:G:61:TYR:CD2   | 2.38                     | 1.06              |
| 1:T:283:ARG:HD2  | 3:H:47:ASN:HB3   | 1.06                     | 1.06              |
| 1:W:198:TYR:O    | 1:W:201:ARG:HD3  | 1.41                     | 1.06              |
| 3:F:159:LEU:HD11 | 3:G:340:GLN:HA   | 1.06                     | 1.06              |
| 3:A:329:LEU:HG   | 3:G:61:TYR:CD2   | 1.91                     | 1.05              |
| 1:Q:44:ARG:CA    | 3:B:322:MET:CE   | 2.34                     | 1.05              |
| 1:Q:45:ASP:HA    | 3:B:322:MET:CA   | 1.86                     | 1.05              |
| 1:T:162:GLY:N    | 3:I:1166:PHE:CD1 | 2.13                     | 1.05              |
| 1:W:345:ARG:CG   | 6:s:13:TRP:CZ3   | 2.27                     | 1.05              |
| 3:F:873:ASN:HA   | 4:e:92:PHE:HB2   | 1.35                     | 1.05              |
| 1:l:281:ARG:NH1  | 3:L:51:ASP:OD2   | 1.90                     | 1.05              |
| 3:G:23:ILE:HD13  | 3:G:167:ARG:CD   | 1.86                     | 1.05              |
| 3:G:454:MET:HE1  | 3:G:1046:PRO:HD2 | 1.34                     | 1.04              |
| 3:N:322:MET:HE2  | 3:E:324:LYS:HB2  | 1.37                     | 1.04              |
| 5:q:172:ARG:HG2  | 5:q:200:MET:HE2  | 1.08                     | 1.04              |
| 1:l:141:PRO:HB2  | 3:M:1165:VAL:CG1 | 1.88                     | 1.04              |
| 1:T:165:LEU:HD12 | 3:I:1166:PHE:CZ  | 1.89                     | 1.04              |
| 2:2:39:ARG:NH1   | 3:N:1083:HIS:HD2 | 1.53                     | 1.04              |
| 1:Q:45:ASP:CA    | 3:B:322:MET:HB2  | 1.75                     | 1.03              |
| 1:W:29:GLY:HA3   | 3:H:144:THR:CA   | 1.73                     | 1.03              |
| 3:A:121:THR:HG21 | 3:G:48:SER:CB    | 1.76                     | 1.03              |
| 3:H:322:MET:HE1  | 3:D:324:LYS:CA   | 1.86                     | 1.03              |
| 1:T:158:ALA:HB1  | 3:I:1165:VAL:CB  | 1.89                     | 1.03              |
| 3:N:326:VAL:HG21 | 3:E:321:VAL:HG11 | 1.38                     | 1.03              |
| 3:A:1031:MET:CE  | 3:A:1048:PHE:HE2 | 1.71                     | 1.03              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:T:78:ALA:HB3   | 3:I:308:GLU:OE1   | 0.87                     | 1.03              |
| 5:q:172:ARG:HE   | 5:q:200:MET:HE3   | 1.22                     | 1.03              |
| 3:H:98:GLU:OE2   | 3:C:11:TYR:OH     | 1.74                     | 1.03              |
| 3:G:99:VAL:HB    | 3:G:118:ASN:CB    | 1.88                     | 1.03              |
| 3:H:322:MET:HE1  | 3:D:324:LYS:HB3   | 1.40                     | 1.02              |
| 1:W:28:ALA:CB    | 3:H:145:GLY:HA3   | 1.88                     | 1.02              |
| 1:W:29:GLY:CA    | 3:H:144:THR:CA    | 2.36                     | 1.02              |
| 1:l:25:ARG:CB    | 3:D:144:THR:HG22  | 1.90                     | 1.02              |
| 3:G:99:VAL:O     | 3:G:118:ASN:CA    | 2.07                     | 1.02              |
| 3:H:339:MET:HE2  | 3:C:17:MET:HE3    | 1.40                     | 1.02              |
| 3:H:1291:ARG:NE  | 3:C:34:ARG:CB     | 2.14                     | 1.02              |
| 3:B:261:VAL:O    | 3:G:61:TYR:N      | 1.92                     | 1.02              |
| 3:F:54:PHE:HA    | 3:G:323:GLY:O     | 1.58                     | 1.02              |
| 3:F:390:VAL:HG21 | 3:G:104:ILE:HG12  | 1.38                     | 1.02              |
| 2:2:39:ARG:CZ    | 3:N:1085:THR:HG21 | 1.90                     | 1.02              |
| 2:S:2:ILE:HD11   | 3:B:1084:GLU:H    | 1.21                     | 1.01              |
| 1:T:158:ALA:HB1  | 3:I:1165:VAL:HG21 | 1.35                     | 1.01              |
| 3:G:801:ARG:HB3  | 3:G:802:PRO:CD    | 1.89                     | 1.01              |
| 2:2:243:MET:SD   | 3:D:1145:VAL:HG22 | 2.01                     | 1.01              |
| 1:l:158:ALA:HB1  | 3:M:1165:VAL:HG21 | 1.42                     | 1.01              |
| 1:W:28:ALA:CB    | 3:H:148:LEU:HD12  | 1.90                     | 1.00              |
| 3:M:9:PRO:HG3    | 3:D:94:ARG:HH21   | 1.22                     | 1.00              |
| 3:A:1031:MET:CE  | 3:A:1048:PHE:CE2  | 2.43                     | 1.00              |
| 1:Q:44:ARG:HA    | 3:B:322:MET:HE3   | 1.36                     | 1.00              |
| 3:A:329:LEU:HD11 | 3:G:61:TYR:HD2    | 0.84                     | 1.00              |
| 3:D:677:TYR:HD1  | 4:d:95:LYS:NZ     | 1.57                     | 1.00              |
| 1:T:161:TRP:HD1  | 3:I:1166:PHE:CG   | 1.79                     | 1.00              |
| 1:W:349:ARG:CB   | 6:r:14:GLU:CG     | 2.39                     | 1.00              |
| 1:l:257:GLN:OE1  | 3:H:109:PRO:CD    | 2.09                     | 1.00              |
| 3:G:500:ASP:O    | 3:G:504:ARG:HG3   | 1.62                     | 1.00              |
| 1:T:283:ARG:HD2  | 3:H:47:ASN:CB     | 1.90                     | 1.00              |
| 2:X:284:GLN:CG   | 3:H:1166:PHE:HZ   | 1.64                     | 1.00              |
| 2:X:40:GLN:HE22  | 3:H:128:ALA:HB3   | 1.21                     | 1.00              |
| 3:J:469:ILE:HD11 | 3:J:547:PHE:CG    | 1.96                     | 0.99              |
| 3:G:554:ALA:HB2  | 3:G:568:PRO:O     | 0.82                     | 0.99              |
| 2:S:300:PHE:CE2  | 3:A:111:PRO:N     | 2.30                     | 0.99              |
| 1:w:260:LEU:HD23 | 3:O:1316:GLY:CA   | 1.92                     | 0.99              |
| 1:l:25:ARG:CB    | 3:D:144:THR:CG2   | 2.40                     | 0.99              |
| 3:M:139:ALA:HB2  | 3:C:50:TYR:CE2    | 1.98                     | 0.99              |
| 1:l:141:PRO:HG3  | 3:M:1166:PHE:CB   | 1.93                     | 0.99              |
| 3:G:550:PHE:CD1  | 3:G:998:TYR:CD2   | 2.38                     | 0.99              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 3:G:666:ASN:HB2   | 3:G:938:LEU:HD22 | 1.00                     | 0.99              |
| 3:N:322:MET:HE3   | 3:E:324:LYS:HB2  | 1.43                     | 0.98              |
| 1:1:141:PRO:HG3   | 3:M:1166:PHE:HB3 | 1.43                     | 0.98              |
| 3:J:475:GLY:HA2   | 3:J:478:HIS:CD2  | 1.98                     | 0.98              |
| 3:M:36:PHE:CD2    | 3:D:120:MET:SD   | 2.43                     | 0.98              |
| 3:G:99:VAL:HB     | 3:G:118:ASN:HB3  | 1.42                     | 0.98              |
| 2:R:173:LEU:C     | 5:q:371:GLY:HA3  | 1.76                     | 0.98              |
| 5:q:172:ARG:HG3   | 5:q:200:MET:CE   | 1.91                     | 0.98              |
| 3:G:119:TYR:O     | 3:G:120:MET:HG3  | 1.62                     | 0.98              |
| 3:F:159:LEU:CD1   | 3:G:340:GLN:HA   | 1.93                     | 0.98              |
| 1:1:141:PRO:HG3   | 3:M:1166:PHE:CG  | 1.98                     | 0.98              |
| 1:T:162:GLY:HA2   | 3:I:1166:PHE:CE1 | 1.98                     | 0.98              |
| 2:U:300:PHE:HD2   | 3:I:1083:HIS:CD2 | 1.66                     | 0.98              |
| 3:H:324:LYS:C     | 3:D:322:MET:HE1  | 1.88                     | 0.98              |
| 3:D:42:VAL:HG12   | 3:D:43:ARG:O     | 1.62                     | 0.98              |
| 3:M:12:ARG:N      | 3:D:96:GLN:NE2   | 2.09                     | 0.98              |
| 1:Q:44:ARG:CA     | 3:B:322:MET:HE3  | 1.92                     | 0.97              |
| 3:M:59:GLY:HA2    | 3:C:20:THR:HG21  | 1.43                     | 0.97              |
| 3:C:677:TYR:HD1   | 4:c:95:LYS:HE2   | 1.27                     | 0.97              |
| 1:W:347:PHE:HE1   | 6:r:18:PHE:HD2   | 1.01                     | 0.97              |
| 1:W:28:ALA:HB1    | 3:H:148:LEU:CD1  | 1.95                     | 0.97              |
| 3:M:12:ARG:H      | 3:D:96:GLN:HE22  | 1.03                     | 0.97              |
| 3:H:709:LEU:HD13  | 3:H:710:PRO:N    | 1.80                     | 0.97              |
| 3:G:526:MET:HE1   | 3:G:531:PHE:CD1  | 1.99                     | 0.97              |
| 1:w:259:GLU:OE1   | 3:O:1315:PRO:CA  | 2.12                     | 0.97              |
| 2:x:18:ARG:HG2    | 3:O:7:ASP:OD2    | 1.63                     | 0.97              |
| 3:M:9:PRO:CG      | 3:D:94:ARG:HH21  | 1.78                     | 0.97              |
| 3:M:44:SER:O      | 3:C:168:ASN:ND2  | 1.97                     | 0.96              |
| 2:S:300:PHE:CD2   | 3:A:111:PRO:CG   | 2.39                     | 0.96              |
| 1:T:280:GLY:O     | 3:H:51:ASP:OD1   | 1.83                     | 0.96              |
| 3:H:98:GLU:CD     | 3:C:11:TYR:HH    | 1.72                     | 0.96              |
| 2:3:40:GLN:HE22   | 3:D:128:ALA:CB   | 1.78                     | 0.96              |
| 1:w:259:GLU:OE1   | 3:O:1315:PRO:O   | 1.81                     | 0.96              |
| 1:W:29:GLY:HA2    | 3:H:143:LEU:C    | 1.90                     | 0.96              |
| 1:w:259:GLU:OE1   | 3:O:1315:PRO:C   | 2.08                     | 0.96              |
| 3:E:873:ASN:OD1   | 4:d:92:PHE:HB2   | 1.66                     | 0.96              |
| 3:G:521:VAL:HG21  | 3:G:987:VAL:HG12 | 1.48                     | 0.96              |
| 3:G:505:PHE:CD1   | 3:G:991:PRO:HB3  | 2.00                     | 0.96              |
| 1:W:348:GLY:O     | 6:r:12:VAL:CG1   | 2.13                     | 0.96              |
| 3:G:1165:VAL:HG13 | 3:G:1166:PHE:CD2 | 2.01                     | 0.96              |
| 1:Q:45:ASP:H      | 3:B:322:MET:HB3  | 1.18                     | 0.96              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:X:99:ASN:OD1   | 3:C:1086:GLY:HA2  | 1.66                     | 0.96              |
| 2:X:300:PHE:HB3  | 3:C:1083:HIS:NE2  | 1.76                     | 0.96              |
| 3:A:121:THR:HG21 | 3:G:48:SER:HB3    | 1.45                     | 0.96              |
| 3:G:32:HIS:HB2   | 3:G:51:ASP:O      | 1.64                     | 0.96              |
| 3:G:54:PHE:O     | 3:G:55:ASP:OD1    | 1.83                     | 0.95              |
| 2:2:39:ARG:NH1   | 3:N:1083:HIS:CD2  | 2.33                     | 0.95              |
| 3:O:546:ALA:CA   | 3:O:1031:MET:HE1  | 1.94                     | 0.95              |
| 3:G:526:MET:CE   | 3:G:531:PHE:HD1   | 1.78                     | 0.95              |
| 3:G:697:VAL:HG22 | 3:G:816:LEU:HD11  | 1.46                     | 0.95              |
| 1:T:158:ALA:HB2  | 3:I:1165:VAL:HG11 | 1.49                     | 0.95              |
| 1:T:166:GLU:CG   | 3:I:1262:HIS:NE2  | 2.30                     | 0.95              |
| 3:M:11:TYR:CE2   | 3:D:119:TYR:CB    | 2.15                     | 0.95              |
| 3:M:27:ILE:HG12  | 3:D:256:GLN:NE2   | 1.81                     | 0.95              |
| 3:M:524:CYS:SG   | 3:M:1008:GLN:NE2  | 2.40                     | 0.95              |
| 5:q:257:ASN:HA   | 6:s:90:GLN:HE21   | 1.31                     | 0.95              |
| 2:3:39:ARG:HH12  | 3:D:1081:ALA:HB2  | 1.28                     | 0.95              |
| 3:D:677:TYR:CD1  | 4:d:95:LYS:NZ     | 2.33                     | 0.95              |
| 1:T:165:LEU:HG   | 3:I:1166:PHE:HZ   | 1.03                     | 0.95              |
| 2:U:300:PHE:HD2  | 3:I:1083:HIS:HD2  | 1.03                     | 0.95              |
| 3:O:546:ALA:HA   | 3:O:1031:MET:CE   | 1.95                     | 0.95              |
| 3:F:14:ALA:CB    | 3:G:321:VAL:HG22  | 1.97                     | 0.95              |
| 3:M:9:PRO:HG3    | 3:D:94:ARG:NH2    | 1.80                     | 0.95              |
| 3:H:96:GLN:HB3   | 3:C:11:TYR:HE1    | 1.29                     | 0.95              |
| 3:B:872:ALA:HB2  | 4:g:76:GLN:CG     | 1.95                     | 0.95              |
| 3:G:666:ASN:CB   | 3:G:938:LEU:CD2   | 2.43                     | 0.95              |
| 1:w:282:PRO:CB   | 3:L:138:GLU:OE2   | 2.15                     | 0.94              |
| 3:A:461:VAL:HG11 | 3:A:1036:LEU:HD13 | 1.46                     | 0.94              |
| 1:W:257:GLN:OE1  | 3:D:109:PRO:HD2   | 1.66                     | 0.94              |
| 1:w:282:PRO:C    | 3:L:138:GLU:OE2   | 2.09                     | 0.94              |
| 3:C:677:TYR:CD1  | 4:c:95:LYS:HE2    | 2.01                     | 0.94              |
| 1:w:282:PRO:HB2  | 3:L:138:GLU:OE2   | 1.67                     | 0.94              |
| 3:J:469:ILE:HD11 | 3:J:547:PHE:CZ    | 2.02                     | 0.94              |
| 2:Y:183:GLY:H    | 3:H:1170:GLN:HG3  | 1.33                     | 0.94              |
| 2:Y:238:ASN:ND2  | 3:H:1137:PRO:HB3  | 1.82                     | 0.94              |
| 3:K:524:CYS:SG   | 3:K:1008:GLN:NE2  | 2.40                     | 0.94              |
| 3:F:448:GLN:NE2  | 3:G:1201:ARG:NH2  | 2.16                     | 0.94              |
| 1:T:283:ARG:CD   | 3:H:47:ASN:HB3    | 1.98                     | 0.94              |
| 3:M:160:ARG:CD   | 3:C:49:LEU:O      | 2.14                     | 0.94              |
| 3:E:842:MET:HE1  | 3:E:891:MET:HB3   | 1.47                     | 0.94              |
| 3:E:873:ASN:HA   | 4:d:92:PHE:CD2    | 2.02                     | 0.94              |
| 3:F:55:ASP:H     | 3:G:324:LYS:HA    | 1.32                     | 0.94              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:G:742:LEU:HD22  | 3:G:756:ILE:HD13  | 1.50                     | 0.94              |
| 3:B:677:TYR:HA    | 4:b:95:LYS:HZ3    | 1.28                     | 0.93              |
| 3:J:474:GLY:O     | 3:J:478:HIS:NE2   | 2.01                     | 0.93              |
| 1:Q:345:ARG:NH2   | 3:B:1166:PHE:CE1  | 2.35                     | 0.93              |
| 3:E:752:ARG:HH21  | 3:E:915:ASP:HA    | 1.31                     | 0.93              |
| 3:G:23:ILE:CD1    | 3:G:167:ARG:CD    | 2.46                     | 0.93              |
| 3:H:96:GLN:HE22   | 3:C:12:ARG:HB3    | 1.31                     | 0.93              |
| 1:T:158:ALA:HB1   | 3:I:1165:VAL:HG11 | 1.23                     | 0.93              |
| 3:G:100:HIS:CE1   | 3:G:117:HIS:ND1   | 2.37                     | 0.93              |
| 2:X:18:ARG:HH11   | 2:3:18:ARG:HH12   | 1.01                     | 0.93              |
| 3:P:485:ASN:HD21  | 3:P:516:GLY:H     | 1.16                     | 0.93              |
| 3:E:1257:TYR:HB2  | 3:E:1277:PHE:HD2  | 1.33                     | 0.93              |
| 3:G:1334:ILE:HG22 | 3:G:1335:THR:N    | 1.83                     | 0.93              |
| 1:W:347:PHE:CE1   | 6:r:18:PHE:CD2    | 2.57                     | 0.93              |
| 3:N:94:ARG:HH21   | 3:D:9:PRO:HG3     | 1.33                     | 0.93              |
| 3:G:1233:ASP:HB3  | 3:G:1236:ARG:O    | 1.69                     | 0.93              |
| 2:Y:238:ASN:HD22  | 3:H:1137:PRO:HG3  | 0.83                     | 0.92              |
| 3:F:134:SER:CB    | 3:G:114:GLN:NE2   | 2.32                     | 0.92              |
| 5:q:172:ARG:HE    | 5:q:200:MET:HE1   | 1.11                     | 0.92              |
| 3:F:448:GLN:HG2   | 3:G:1201:ARG:CZ   | 1.99                     | 0.92              |
| 3:G:99:VAL:C      | 3:G:118:ASN:HB2   | 1.94                     | 0.92              |
| 1:W:344:GLU:OE1   | 6:r:13:TRP:CZ3    | 2.23                     | 0.92              |
| 3:H:322:MET:CE    | 3:D:324:LYS:CB    | 1.90                     | 0.92              |
| 3:G:103:LEU:HD23  | 3:G:113:GLU:HG3   | 1.52                     | 0.92              |
| 2:X:99:ASN:CG     | 3:C:1086:GLY:HA2  | 1.93                     | 0.92              |
| 3:M:29:VAL:HG11   | 3:D:120:MET:HE1   | 1.45                     | 0.92              |
| 3:P:769:CYS:SG    | 3:P:786:ASN:ND2   | 2.42                     | 0.92              |
| 3:G:505:PHE:HE1   | 3:G:991:PRO:HA    | 1.28                     | 0.92              |
| 2:R:174:PRO:HA    | 5:q:370:GLY:C     | 1.95                     | 0.92              |
| 3:F:52:VAL:HG13   | 3:G:320:LEU:HD23  | 1.49                     | 0.92              |
| 2:3:300:PHE:HD2   | 3:M:1083:HIS:HD2  | 1.03                     | 0.92              |
| 3:G:742:LEU:CD2   | 3:G:756:ILE:HD13  | 2.00                     | 0.92              |
| 1:W:328:TYR:CE1   | 6:r:18:PHE:HZ     | 1.76                     | 0.92              |
| 1:1:257:GLN:CD    | 3:H:109:PRO:HD2   | 1.94                     | 0.92              |
| 3:N:96:GLN:HE22   | 3:D:12:ARG:H      | 1.12                     | 0.92              |
| 2:R:37:ILE:HG21   | 3:A:109:PRO:HG2   | 1.51                     | 0.91              |
| 3:G:829:GLY:O     | 3:G:956:TYR:CD1   | 2.23                     | 0.91              |
| 1:W:259:GLU:OE2   | 3:C:1313:ARG:NH2  | 2.02                     | 0.91              |
| 3:G:554:ALA:HB2   | 3:G:568:PRO:C     | 1.95                     | 0.91              |
| 3:M:12:ARG:N      | 3:D:96:GLN:HE22   | 1.68                     | 0.91              |
| 3:K:826:CYS:HB3   | 3:K:966:GLY:H     | 1.32                     | 0.91              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:N:322:MET:CE    | 3:E:324:LYS:CB    | 1.93                     | 0.91              |
| 1:w:260:LEU:CD2   | 3:O:1316:GLY:HA3  | 2.00                     | 0.91              |
| 3:E:621:ARG:O     | 3:E:943:GLN:NE2   | 2.04                     | 0.91              |
| 3:G:524:CYS:CB    | 3:G:1008:GLN:OE1  | 2.18                     | 0.91              |
| 3:H:120:MET:CB    | 3:C:36:PHE:CD2    | 2.53                     | 0.91              |
| 3:N:123:VAL:HG23  | 3:D:37:ASP:OD2    | 1.69                     | 0.91              |
| 3:D:646:ARG:HD2   | 4:d:98:TYR:O      | 1.70                     | 0.91              |
| 3:H:1291:ARG:NH1  | 3:C:35:LEU:HD12   | 1.86                     | 0.91              |
| 1:W:194:CYS:C     | 1:W:198:TYR:HE2   | 1.78                     | 0.91              |
| 2:X:38:ARG:HH22   | 3:I:109:PRO:C     | 1.78                     | 0.91              |
| 3:G:23:ILE:CD1    | 3:G:167:ARG:HD3   | 2.01                     | 0.91              |
| 1:T:162:GLY:N     | 3:I:1166:PHE:HD1  | 1.51                     | 0.90              |
| 3:M:21:GLY:HA2    | 3:D:350:THR:HG21  | 1.51                     | 0.90              |
| 3:D:1257:TYR:HB2  | 3:D:1277:PHE:HD2  | 1.35                     | 0.90              |
| 3:G:410:ASN:OD1   | 3:G:1196:ILE:HD11 | 1.70                     | 0.90              |
| 2:2:233:GLN:O     | 3:D:1136:PRO:HB3  | 1.71                     | 0.90              |
| 3:A:121:THR:CG2   | 3:G:48:SER:CB     | 2.40                     | 0.90              |
| 3:B:103:LEU:O     | 3:G:175:ALA:HB2   | 1.72                     | 0.90              |
| 3:G:99:VAL:CB     | 3:G:118:ASN:HB2   | 2.01                     | 0.90              |
| 3:G:552:GLY:O     | 3:G:569:GLY:HA3   | 1.72                     | 0.90              |
| 3:N:94:ARG:NH2    | 3:D:9:PRO:HG3     | 1.86                     | 0.90              |
| 1:W:328:TYR:CZ    | 6:r:18:PHE:CE2    | 2.59                     | 0.90              |
| 2:3:300:PHE:CD2   | 3:M:1083:HIS:CG   | 2.60                     | 0.90              |
| 3:B:1296:THR:HG21 | 3:B:1327:LEU:HG   | 1.52                     | 0.90              |
| 3:A:966:GLY:HA3   | 3:A:969:HIS:HB2   | 1.53                     | 0.90              |
| 2:3:39:ARG:HH12   | 3:D:1081:ALA:CB   | 1.84                     | 0.90              |
| 3:M:61:TYR:CD1    | 3:C:21:GLY:O      | 2.23                     | 0.90              |
| 3:N:89:TYR:HE1    | 3:D:157:ARG:HH22  | 0.98                     | 0.90              |
| 3:F:842:MET:HE1   | 3:F:891:MET:HB3   | 1.54                     | 0.90              |
| 3:I:410:ASN:ND2   | 3:I:1359:THR:O    | 2.06                     | 0.89              |
| 1:W:350:LEU:CD2   | 6:r:20:VAL:HG12   | 2.00                     | 0.89              |
| 2:S:260:MET:SD    | 5:q:412:ARG:NH1   | 2.46                     | 0.89              |
| 3:G:452:LEU:HD12  | 3:G:456:ASN:HD22  | 1.37                     | 0.89              |
| 3:B:677:TYR:HD1   | 4:b:95:LYS:HZ3    | 1.14                     | 0.89              |
| 3:G:505:PHE:HD2   | 3:G:506:LEU:HD23  | 1.38                     | 0.89              |
| 3:H:339:MET:CE    | 3:C:17:MET:HE3    | 1.91                     | 0.89              |
| 3:B:261:VAL:O     | 3:G:60:SER:CA     | 2.21                     | 0.89              |
| 3:F:448:GLN:HE21  | 3:G:1201:ARG:NH2  | 1.69                     | 0.89              |
| 3:G:550:PHE:CD1   | 3:G:998:TYR:CD1   | 2.36                     | 0.89              |
| 3:F:55:ASP:O      | 3:G:325:ALA:N     | 2.05                     | 0.89              |
| 3:M:180:THR:HG22  | 3:M:1097:ARG:HH12 | 1.39                     | 0.88              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:A:1037:TYR:O   | 3:A:1041:LYS:HG2  | 1.73                     | 0.88              |
| 1:W:25:ARG:CA    | 3:H:145:GLY:O     | 2.21                     | 0.88              |
| 1:I:138:THR:O    | 3:M:1166:PHE:CE2  | 2.27                     | 0.88              |
| 1:w:78:ALA:CB    | 3:O:308:GLU:OE1   | 2.21                     | 0.88              |
| 3:N:120:MET:SD   | 3:D:36:PHE:CE2    | 2.66                     | 0.88              |
| 3:D:621:ARG:O    | 3:D:943:GLN:NE2   | 2.07                     | 0.88              |
| 3:J:841:ASN:OD1  | 4:j:57:GLN:NE2    | 2.07                     | 0.88              |
| 3:O:524:CYS:SG   | 3:O:1008:GLN:NE2  | 2.45                     | 0.88              |
| 1:T:161:TRP:HE1  | 3:I:1166:PHE:HE2  | 1.13                     | 0.88              |
| 3:B:261:VAL:CG2  | 3:G:61:TYR:O      | 2.20                     | 0.88              |
| 1:W:29:GLY:CA    | 3:H:144:THR:HA    | 2.01                     | 0.88              |
| 1:w:260:LEU:HD23 | 3:O:1316:GLY:HA3  | 1.53                     | 0.88              |
| 2:Y:248:ARG:CD   | 3:H:1141:ASN:ND2  | 2.37                     | 0.88              |
| 1:I:141:PRO:CB   | 3:M:1165:VAL:HG13 | 2.04                     | 0.88              |
| 3:E:677:TYR:HD1  | 4:e:95:LYS:NZ     | 1.72                     | 0.88              |
| 1:T:165:LEU:CG   | 3:I:1166:PHE:HZ   | 1.62                     | 0.88              |
| 1:Q:345:ARG:NH2  | 3:B:1166:PHE:CZ   | 2.42                     | 0.88              |
| 2:S:300:PHE:CD2  | 3:A:111:PRO:HD3   | 2.07                     | 0.88              |
| 3:F:485:ASN:ND2  | 3:F:516:GLY:H     | 1.71                     | 0.88              |
| 3:B:225:ARG:CZ   | 3:G:447:HIS:NE2   | 2.36                     | 0.87              |
| 3:F:52:VAL:CG1   | 3:G:320:LEU:HD23  | 2.04                     | 0.87              |
| 1:Q:45:ASP:CA    | 3:B:322:MET:C     | 2.47                     | 0.87              |
| 3:N:120:MET:HG2  | 3:D:39:PHE:HD1    | 1.37                     | 0.87              |
| 3:N:350:THR:HG21 | 3:D:21:GLY:HA2    | 0.94                     | 0.87              |
| 3:G:103:LEU:HD23 | 3:G:113:GLU:O     | 1.74                     | 0.87              |
| 1:W:350:LEU:CD2  | 6:r:20:VAL:CG1    | 2.51                     | 0.87              |
| 2:S:300:PHE:HE2  | 3:A:111:PRO:HA    | 0.70                     | 0.87              |
| 1:T:141:PRO:HB3  | 3:I:1165:VAL:CG1  | 2.03                     | 0.87              |
| 3:G:469:ILE:HD11 | 3:G:547:PHE:CG    | 2.08                     | 0.87              |
| 1:w:272:GLU:CB   | 1:w:283:ARG:HH21  | 1.88                     | 0.87              |
| 3:M:24:LEU:HD11  | 3:D:260:ALA:HB2   | 1.57                     | 0.87              |
| 3:N:123:VAL:CG2  | 3:D:37:ASP:OD2    | 2.23                     | 0.87              |
| 3:F:448:GLN:HE21 | 3:G:1201:ARG:HH22 | 0.94                     | 0.87              |
| 3:G:103:LEU:HD21 | 3:G:113:GLU:O     | 1.73                     | 0.87              |
| 1:T:170:LEU:HD11 | 3:I:1262:HIS:HB2  | 0.88                     | 0.87              |
| 3:M:157:ARG:NH2  | 3:D:89:TYR:HE1    | 1.72                     | 0.87              |
| 3:P:621:ARG:O    | 3:P:943:GLN:NE2   | 2.08                     | 0.87              |
| 2:S:2:ILE:HD11   | 3:B:1084:GLU:N    | 1.89                     | 0.86              |
| 2:X:300:PHE:CB   | 3:C:1083:HIS:NE2  | 2.30                     | 0.86              |
| 3:D:634:ILE:HA   | 3:D:640:VAL:HG11  | 1.56                     | 0.86              |
| 3:G:524:CYS:HB3  | 3:G:1008:GLN:HE22 | 1.08                     | 0.86              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:L:755:ARG:NH1  | 3:L:911:SER:OG    | 2.07                     | 0.86              |
| 3:H:339:MET:HE1  | 3:C:17:MET:CE     | 2.04                     | 0.86              |
| 3:C:873:ASN:HA   | 4:b:92:PHE:CD2    | 2.09                     | 0.86              |
| 3:G:829:GLY:O    | 3:G:956:TYR:CE1   | 2.27                     | 0.86              |
| 3:J:475:GLY:O    | 3:J:478:HIS:HD2   | 1.56                     | 0.86              |
| 3:I:485:ASN:HD21 | 3:I:516:GLY:H     | 1.17                     | 0.86              |
| 3:B:896:VAL:HA   | 3:B:899:HIS:HD2   | 1.40                     | 0.86              |
| 2:Y:238:ASN:CG   | 3:H:1137:PRO:HG3  | 2.00                     | 0.86              |
| 3:E:863:HIS:HE1  | 3:E:887:ASP:HA    | 1.39                     | 0.86              |
| 3:A:769:CYS:HB2  | 3:A:786:ASN:HD21  | 1.40                     | 0.86              |
| 3:E:873:ASN:OD1  | 4:d:92:PHE:N      | 2.07                     | 0.86              |
| 3:H:1291:ARG:NE  | 3:C:34:ARG:HB3    | 1.90                     | 0.86              |
| 3:D:646:ARG:HB2  | 4:d:97:THR:HA     | 1.58                     | 0.86              |
| 1:I:141:PRO:CB   | 3:M:1165:VAL:CG1  | 2.54                     | 0.86              |
| 3:A:461:VAL:HG11 | 3:A:1036:LEU:CD1  | 2.06                     | 0.86              |
| 5:q:172:ARG:CG   | 5:q:200:MET:HE1   | 2.03                     | 0.86              |
| 3:D:410:ASN:O    | 3:D:415:ARG:NH1   | 2.08                     | 0.86              |
| 3:L:950:GLN:HB2  | 3:L:953:GLU:HG3   | 1.57                     | 0.86              |
| 3:E:677:TYR:HD1  | 4:e:95:LYS:HZ3    | 0.86                     | 0.86              |
| 3:M:27:ILE:HG12  | 3:D:256:GLN:HE22  | 1.38                     | 0.85              |
| 3:H:1000:SER:O   | 3:H:1003:ARG:NH1  | 2.09                     | 0.85              |
| 3:O:896:VAL:HA   | 3:O:899:HIS:HD2   | 1.41                     | 0.85              |
| 3:C:752:ARG:NH2  | 3:C:915:ASP:OD1   | 2.08                     | 0.85              |
| 3:G:524:CYS:HB3  | 3:G:1008:GLN:OE1  | 1.75                     | 0.85              |
| 3:B:728:ASP:O    | 3:B:810:LYS:NZ    | 2.09                     | 0.85              |
| 1:W:166:GLU:CD   | 3:C:1262:HIS:NE2  | 2.34                     | 0.85              |
| 3:L:1215:ALA:O   | 3:L:1287:ARG:NH2  | 2.09                     | 0.85              |
| 3:P:819:ALA:O    | 3:P:822:ARG:NH1   | 2.10                     | 0.85              |
| 3:L:947:HIS:O    | 4:k:80:ALA:N      | 2.09                     | 0.85              |
| 3:L:1176:GLY:HA3 | 3:M:1225:LEU:HD21 | 1.58                     | 0.85              |
| 3:D:880:HIS:HD2  | 4:c:94:LEU:HD22   | 1.38                     | 0.85              |
| 2:S:2:ILE:CD1    | 3:B:1084:GLU:C    | 2.50                     | 0.85              |
| 2:Y:248:ARG:CD   | 3:H:1141:ASN:HD22 | 1.87                     | 0.85              |
| 3:I:485:ASN:HD21 | 3:I:516:GLY:N     | 1.74                     | 0.85              |
| 3:A:94:ARG:HH12  | 3:G:47:ASN:HB3    | 1.41                     | 0.85              |
| 2:X:40:GLN:HE21  | 3:H:128:ALA:HB3   | 1.41                     | 0.85              |
| 1:W:194:CYS:O    | 1:W:198:TYR:HE2   | 1.58                     | 0.85              |
| 1:I:79:THR:CB    | 3:M:308:GLU:OE2   | 2.23                     | 0.85              |
| 3:H:861:PRO:O    | 3:H:869:ASN:ND2   | 2.10                     | 0.85              |
| 3:F:615:ARG:HH21 | 3:F:1017:GLU:HG2  | 1.42                     | 0.85              |
| 3:M:865:LEU:HD11 | 3:M:886:VAL:H     | 1.40                     | 0.85              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:N:89:TYR:HE1   | 3:D:157:ARG:HH21  | 1.23                     | 0.85              |
| 2:R:172:GLU:N    | 5:q:372:ASP:OD1   | 2.10                     | 0.84              |
| 2:S:300:PHE:HD2  | 3:A:111:PRO:HD3   | 1.38                     | 0.84              |
| 1:T:165:LEU:HD11 | 3:I:1166:PHE:HE2  | 1.39                     | 0.84              |
| 3:I:873:ASN:HB3  | 4:h:89:ARG:HH12   | 1.41                     | 0.84              |
| 3:I:1257:TYR:HB2 | 3:I:1277:PHE:HD2  | 1.42                     | 0.84              |
| 3:L:238:GLY:HA2  | 3:L:244:ILE:HD11  | 1.58                     | 0.84              |
| 3:I:484:ALA:O    | 3:I:486:PRO:HD3   | 1.77                     | 0.84              |
| 3:H:709:LEU:HD22 | 3:H:710:PRO:HD2   | 1.59                     | 0.84              |
| 3:G:434:ALA:O    | 3:G:1359:THR:CG2  | 2.24                     | 0.84              |
| 3:J:697:VAL:HG22 | 3:J:816:LEU:HD12  | 1.56                     | 0.84              |
| 3:O:843:VAL:O    | 3:O:876:ASN:ND2   | 2.09                     | 0.84              |
| 3:D:639:HIS:HA   | 4:d:79:PHE:HE2    | 1.40                     | 0.84              |
| 3:B:103:LEU:O    | 3:G:175:ALA:CB    | 2.25                     | 0.84              |
| 2:X:18:ARG:HH12  | 2:3:18:ARG:NH1    | 1.74                     | 0.84              |
| 3:E:896:VAL:HA   | 3:E:899:HIS:HD2   | 1.41                     | 0.84              |
| 3:D:42:VAL:CG1   | 3:D:43:ARG:O      | 2.26                     | 0.84              |
| 3:B:312:ASN:O    | 3:G:54:PHE:HB2    | 1.77                     | 0.84              |
| 3:B:877:ALA:HB1  | 4:g:94:LEU:HD21   | 1.60                     | 0.84              |
| 3:F:432:PRO:O    | 3:G:413:MET:CE    | 2.25                     | 0.84              |
| 3:L:548:ASP:OD1  | 3:L:576:ARG:NE    | 2.10                     | 0.84              |
| 3:C:896:VAL:HA   | 3:C:899:HIS:HD2   | 1.43                     | 0.84              |
| 3:E:521:VAL:HG21 | 3:E:987:VAL:HG12  | 1.60                     | 0.84              |
| 3:M:29:VAL:CG1   | 3:D:120:MET:CE    | 2.47                     | 0.84              |
| 3:L:1029:PHE:HB3 | 3:L:1039:GLN:HE21 | 1.40                     | 0.84              |
| 1:W:198:TYR:O    | 1:W:201:ARG:HD2   | 1.78                     | 0.83              |
| 3:L:621:ARG:O    | 3:L:943:GLN:NE2   | 2.10                     | 0.83              |
| 3:A:119:TYR:CD2  | 3:G:44:SER:HB3    | 2.12                     | 0.83              |
| 3:F:746:ALA:HA   | 3:F:754:CYS:HB3   | 1.58                     | 0.83              |
| 2:Y:238:ASN:HD21 | 3:H:1137:PRO:CB   | 1.88                     | 0.83              |
| 3:I:945:LEU:HD12 | 3:H:676:THR:HG21  | 1.60                     | 0.83              |
| 6:r:80:ILE:HA    | 6:r:83:ARG:HB2    | 1.60                     | 0.83              |
| 1:W:25:ARG:HA    | 3:H:145:GLY:O     | 1.78                     | 0.83              |
| 1:w:260:LEU:HD23 | 3:O:1316:GLY:HA2  | 1.57                     | 0.83              |
| 3:E:966:GLY:HA3  | 3:E:969:HIS:HB2   | 1.60                     | 0.83              |
| 1:W:28:ALA:CB    | 3:H:145:GLY:CA    | 2.51                     | 0.83              |
| 2:3:80:PRO:HG2   | 3:C:53:GLU:OE2    | 1.77                     | 0.83              |
| 3:I:843:VAL:O    | 3:I:876:ASN:ND2   | 2.12                     | 0.83              |
| 3:E:548:ASP:OD1  | 3:E:576:ARG:NE    | 2.11                     | 0.83              |
| 3:G:524:CYS:HB2  | 3:G:1008:GLN:CD   | 2.03                     | 0.83              |
| 3:J:1217:ASP:OD1 | 3:J:1287:ARG:NH1  | 2.10                     | 0.83              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:B:262:PRO:C    | 3:G:59:GLY:O      | 2.20                     | 0.83              |
| 3:J:410:ASN:ND2  | 3:J:1359:THR:O    | 2.12                     | 0.83              |
| 3:D:133:PHE:HB3  | 3:D:1091:PHE:HB2  | 1.61                     | 0.83              |
| 3:E:638:GLU:HB2  | 3:E:789:ALA:HA    | 1.60                     | 0.83              |
| 3:E:873:ASN:HA   | 4:d:92:PHE:HD2    | 1.41                     | 0.83              |
| 3:F:485:ASN:HD21 | 3:F:516:GLY:N     | 1.76                     | 0.83              |
| 3:G:505:PHE:CE1  | 3:G:991:PRO:CA    | 2.61                     | 0.83              |
| 2:R:173:LEU:HA   | 5:q:372:ASP:H     | 1.41                     | 0.83              |
| 3:K:106:ARG:HH21 | 3:K:110:HIS:HB3   | 1.44                     | 0.83              |
| 3:L:742:LEU:HD22 | 3:L:756:ILE:HD11  | 1.61                     | 0.83              |
| 3:H:946:ASP:HB3  | 3:H:949:ILE:H     | 1.43                     | 0.83              |
| 3:G:496:GLY:C    | 3:G:504:ARG:HH22  | 1.87                     | 0.83              |
| 1:T:158:ALA:CB   | 3:I:1165:VAL:CG1  | 2.36                     | 0.82              |
| 1:w:283:ARG:HD3  | 1:w:284:SER:H     | 1.45                     | 0.82              |
| 3:J:475:GLY:C    | 3:J:478:HIS:HD2   | 1.86                     | 0.82              |
| 3:K:440:LEU:HD22 | 3:K:1336:CYS:SG   | 2.19                     | 0.82              |
| 2:S:261:LEU:HD11 | 5:q:378:TRP:CH2   | 2.14                     | 0.82              |
| 1:w:78:ALA:HB1   | 3:O:308:GLU:OE1   | 1.77                     | 0.82              |
| 3:N:728:ASP:O    | 3:N:810:LYS:NZ    | 2.11                     | 0.82              |
| 3:B:262:PRO:HA   | 3:G:59:GLY:O      | 1.78                     | 0.82              |
| 3:D:873:ASN:HA   | 4:c:92:PHE:HD2    | 1.44                     | 0.82              |
| 3:F:159:LEU:HD11 | 3:G:340:GLN:CA    | 2.02                     | 0.82              |
| 3:M:876:ASN:HA   | 3:M:879:PHE:HD2   | 1.42                     | 0.82              |
| 3:B:263:ARG:HB2  | 3:G:59:GLY:HA2    | 1.59                     | 0.82              |
| 5:q:38:VAL:HG13  | 5:q:136:TRP:HZ2   | 1.44                     | 0.82              |
| 3:G:469:ILE:CD1  | 3:G:547:PHE:CD2   | 2.61                     | 0.82              |
| 3:J:842:MET:HE1  | 3:J:891:MET:HB3   | 1.60                     | 0.82              |
| 3:D:580:GLY:HA2  | 3:D:592:ARG:HH12  | 1.44                     | 0.82              |
| 3:G:983:LEU:HD23 | 3:G:983:LEU:O     | 1.79                     | 0.82              |
| 1:W:349:ARG:CB   | 6:r:14:GLU:CB     | 2.57                     | 0.82              |
| 3:K:946:ASP:HB3  | 3:K:949:ILE:H     | 1.45                     | 0.82              |
| 3:C:532:MET:HE1  | 3:C:1244:PRO:HD3  | 1.60                     | 0.82              |
| 3:G:505:PHE:CD2  | 3:G:506:LEU:HD23  | 2.14                     | 0.82              |
| 3:G:1233:ASP:O   | 3:G:1237:PRO:HA   | 1.80                     | 0.82              |
| 2:S:300:PHE:CD2  | 3:A:111:PRO:N     | 2.46                     | 0.82              |
| 3:L:766:ALA:HB3  | 3:L:784:LEU:HA    | 1.62                     | 0.82              |
| 3:D:728:ASP:O    | 3:D:810:LYS:NZ    | 2.11                     | 0.82              |
| 1:T:158:ALA:HB3  | 3:I:1165:VAL:HG21 | 1.61                     | 0.82              |
| 1:T:162:GLY:CA   | 3:I:1166:PHE:CE1  | 2.61                     | 0.82              |
| 2:x:300:PHE:CB   | 3:O:1083:HIS:NE2  | 2.41                     | 0.82              |
| 3:L:843:VAL:O    | 3:L:876:ASN:ND2   | 2.11                     | 0.82              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 3:C:524:CYS:SG    | 3:C:1008:GLN:NE2 | 2.52                     | 0.82              |
| 1:T:161:TRP:NE1   | 3:I:1166:PHE:CZ  | 2.41                     | 0.81              |
| 1:w:283:ARG:HH12  | 3:L:137:THR:CG2  | 1.93                     | 0.81              |
| 3:I:1217:ASP:OD1  | 3:I:1287:ARG:NH1 | 2.13                     | 0.81              |
| 3:J:881:ASN:OD1   | 4:i:95:LYS:NZ    | 2.13                     | 0.81              |
| 3:P:1296:THR:HG21 | 3:P:1327:LEU:HG  | 1.61                     | 0.81              |
| 3:F:132:ALA:HB2   | 3:G:112:VAL:HG11 | 1.60                     | 0.81              |
| 3:A:329:LEU:CG    | 3:G:61:TYR:CE2   | 2.58                     | 0.81              |
| 3:N:950:GLN:HB2   | 3:N:953:GLU:HG3  | 1.62                     | 0.81              |
| 3:K:777:ASN:HA    | 3:K:904:ARG:HD3  | 1.61                     | 0.81              |
| 3:D:1365:ASP:O    | 3:D:1370:LYS:NZ  | 2.14                     | 0.81              |
| 3:G:507:ASN:HA    | 3:G:510:ARG:NE   | 1.94                     | 0.81              |
| 3:G:472:ALA:O     | 3:G:476:VAL:CG2  | 2.28                     | 0.81              |
| 3:G:742:LEU:HD22  | 3:G:756:ILE:CD1  | 2.10                     | 0.81              |
| 3:A:728:ASP:O     | 3:A:810:LYS:NZ   | 2.14                     | 0.81              |
| 3:F:134:SER:CB    | 3:G:114:GLN:HE21 | 1.93                     | 0.81              |
| 1:W:345:ARG:CG    | 6:s:13:TRP:CE3   | 2.60                     | 0.81              |
| 3:M:20:THR:O      | 3:D:350:THR:HG22 | 1.78                     | 0.81              |
| 3:M:152:GLY:O     | 3:H:340:GLN:NE2  | 2.14                     | 0.81              |
| 3:B:846:GLU:HA    | 4:b:68:HIS:HE1   | 1.46                     | 0.81              |
| 3:E:1029:PHE:HB3  | 3:E:1039:GLN:NE2 | 1.95                     | 0.81              |
| 3:F:106:ARG:HH21  | 3:F:110:HIS:HB3  | 1.44                     | 0.81              |
| 3:L:895:GLN:HE21  | 4:l:62:THR:HA    | 1.45                     | 0.81              |
| 3:D:873:ASN:OD1   | 4:c:92:PHE:CB    | 2.29                     | 0.81              |
| 3:I:1296:THR:HG21 | 3:I:1327:LEU:HG  | 1.63                     | 0.81              |
| 3:M:27:ILE:CD1    | 3:D:256:GLN:OE1  | 2.29                     | 0.81              |
| 3:N:326:VAL:CG2   | 3:E:321:VAL:CG1  | 2.55                     | 0.81              |
| 3:E:843:VAL:O     | 3:E:876:ASN:ND2  | 2.15                     | 0.81              |
| 3:G:495:ALA:C     | 3:G:504:ARG:NH1  | 2.38                     | 0.80              |
| 3:H:260:ALA:HB2   | 3:C:24:LEU:HD11  | 1.61                     | 0.80              |
| 3:O:788:GLN:HE22  | 3:O:794:ALA:HA   | 1.46                     | 0.80              |
| 3:E:766:ALA:N     | 3:E:783:LEU:O    | 2.14                     | 0.80              |
| 3:F:754:CYS:O     | 3:F:756:ILE:HG13 | 1.82                     | 0.80              |
| 3:N:1286:HIS:HB2  | 3:D:34:ARG:HH22  | 1.45                     | 0.80              |
| 3:M:12:ARG:H      | 3:D:96:GLN:HE21  | 1.25                     | 0.80              |
| 3:J:485:ASN:ND2   | 3:J:516:GLY:O    | 2.15                     | 0.80              |
| 3:H:324:LYS:O     | 3:D:322:MET:CE   | 2.28                     | 0.80              |
| 3:C:752:ARG:HH21  | 3:C:915:ASP:HA   | 1.47                     | 0.80              |
| 3:C:1217:ASP:OD1  | 3:C:1287:ARG:NH1 | 2.15                     | 0.80              |
| 3:G:99:VAL:N      | 3:G:118:ASN:O    | 2.14                     | 0.80              |
| 1:W:349:ARG:HA    | 6:r:12:VAL:HG12  | 1.62                     | 0.80              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:J:698:GLU:OE2   | 3:K:621:ARG:NH2   | 2.15                     | 0.80              |
| 3:L:122:LYS:NZ    | 3:L:1101:ASP:O    | 2.13                     | 0.80              |
| 3:O:960:VAL:HA    | 3:O:994:LEU:HD13  | 1.63                     | 0.80              |
| 3:E:448:GLN:HE21  | 3:F:1201:ARG:HH12 | 1.29                     | 0.80              |
| 3:E:752:ARG:NH2   | 3:E:915:ASP:OD1   | 2.15                     | 0.80              |
| 2:R:173:LEU:O     | 5:q:371:GLY:HA2   | 1.81                     | 0.80              |
| 3:A:119:TYR:HD2   | 3:G:44:SER:HB3    | 1.47                     | 0.80              |
| 3:F:448:GLN:CD    | 3:G:1201:ARG:HH22 | 1.88                     | 0.80              |
| 3:G:524:CYS:SG    | 3:G:1008:GLN:NE2  | 2.55                     | 0.80              |
| 3:H:96:GLN:HB3    | 3:C:11:TYR:CE1    | 2.16                     | 0.80              |
| 3:N:180:THR:HG22  | 3:N:1097:ARG:HH12 | 1.46                     | 0.80              |
| 1:T:165:LEU:HG    | 3:I:1166:PHE:CE1  | 2.17                     | 0.79              |
| 1:T:165:LEU:HD12  | 3:I:1166:PHE:CE1  | 2.17                     | 0.79              |
| 3:J:742:LEU:HD13  | 3:J:783:LEU:HD13  | 1.64                     | 0.79              |
| 3:B:96:GLN:HG2    | 3:B:121:THR:HG22  | 1.65                     | 0.79              |
| 3:D:742:LEU:HD22  | 3:D:756:ILE:HD13  | 1.64                     | 0.79              |
| 1:W:166:GLU:HG2   | 3:C:1262:HIS:CE1  | 2.16                     | 0.79              |
| 3:I:819:ALA:O     | 3:I:822:ARG:NH1   | 2.15                     | 0.79              |
| 3:A:272:ARG:NH2   | 3:A:372:ASP:O     | 2.15                     | 0.79              |
| 3:A:461:VAL:CG1   | 3:A:1036:LEU:CD1  | 2.60                     | 0.79              |
| 3:B:658:ASN:O     | 3:G:684:GLU:CB    | 2.30                     | 0.79              |
| 3:D:1215:ALA:HB1  | 3:D:1221:ASP:HB3  | 1.63                     | 0.79              |
| 3:E:1120:THR:HG22 | 3:E:1181:GLN:HE21 | 1.46                     | 0.79              |
| 3:M:29:VAL:HG11   | 3:D:120:MET:HE3   | 1.64                     | 0.79              |
| 3:M:923:THR:HA    | 3:M:926:MET:HE3   | 1.63                     | 0.79              |
| 3:D:745:HIS:NE2   | 3:D:754:CYS:SG    | 2.54                     | 0.79              |
| 3:F:1270:LEU:HD22 | 3:F:1303:ALA:HB2  | 1.62                     | 0.79              |
| 1:T:280:GLY:O     | 3:H:51:ASP:HB3    | 1.80                     | 0.79              |
| 3:L:1217:ASP:OD1  | 3:L:1287:ARG:NH1  | 2.16                     | 0.79              |
| 3:G:234:LEU:CD2   | 3:G:244:ILE:HD13  | 2.13                     | 0.79              |
| 1:T:259:GLU:OE1   | 3:I:1315:PRO:CA   | 2.30                     | 0.79              |
| 1:w:282:PRO:CA    | 3:L:138:GLU:OE2   | 2.30                     | 0.79              |
| 3:L:728:ASP:O     | 3:L:810:LYS:NZ    | 2.16                     | 0.79              |
| 3:L:771:VAL:HG23  | 3:L:898:ALA:HA    | 1.63                     | 0.79              |
| 3:H:324:LYS:O     | 3:D:322:MET:HE1   | 1.82                     | 0.79              |
| 3:C:580:GLY:HA2   | 3:C:592:ARG:HH12  | 1.47                     | 0.79              |
| 2:R:173:LEU:O     | 5:q:370:GLY:O     | 2.00                     | 0.79              |
| 3:G:32:HIS:CB     | 3:G:51:ASP:O      | 2.31                     | 0.79              |
| 1:W:344:GLU:O     | 6:r:13:TRP:CD2    | 2.33                     | 0.79              |
| 3:A:461:VAL:CG1   | 3:A:1036:LEU:HD12 | 2.13                     | 0.79              |
| 3:H:709:LEU:HB3   | 3:H:1038:HIS:CE1  | 2.18                     | 0.79              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:F:877:ALA:HB1  | 4:e:94:LEU:HD21  | 1.65                     | 0.79              |
| 3:G:99:VAL:HG12  | 3:G:118:ASN:HD22 | 1.47                     | 0.79              |
| 2:Y:302:GLY:O    | 3:I:111:PRO:HB3  | 1.82                     | 0.79              |
| 3:J:452:LEU:HD12 | 3:J:456:ASN:HD22 | 1.47                     | 0.79              |
| 3:J:475:GLY:CA   | 3:J:478:HIS:CD2  | 2.66                     | 0.79              |
| 3:K:1257:TYR:HB2 | 3:K:1277:PHE:HD2 | 1.47                     | 0.79              |
| 3:H:89:TYR:HE1   | 3:C:157:ARG:HH22 | 0.80                     | 0.79              |
| 4:i:76:GLN:O     | 4:i:96:ARG:NH2   | 2.16                     | 0.79              |
| 4:o:95:LYS:HE3   | 3:P:948:THR:HG21 | 1.64                     | 0.79              |
| 3:O:1217:ASP:OD1 | 3:O:1287:ARG:NH1 | 2.15                     | 0.79              |
| 5:q:65:HIS:HE1   | 5:q:470:PHE:H    | 1.31                     | 0.79              |
| 3:G:119:TYR:O    | 3:G:120:MET:CG   | 2.30                     | 0.79              |
| 2:3:40:GLN:NE2   | 3:D:128:ALA:HB3  | 1.93                     | 0.79              |
| 3:I:524:CYS:SG   | 3:I:1008:GLN:NE2 | 2.56                     | 0.79              |
| 3:G:33:ARG:CD    | 3:G:53:GLU:OE1   | 2.14                     | 0.79              |
| 3:G:1131:LEU:O   | 3:G:1163:LEU:CD1 | 2.31                     | 0.79              |
| 1:W:347:PHE:HE1  | 6:r:18:PHE:CD2   | 1.94                     | 0.79              |
| 3:F:1124:ASN:O   | 3:F:1156:ARG:NH1 | 2.15                     | 0.79              |
| 3:G:410:ASN:OD1  | 3:G:1196:ILE:CD1 | 2.31                     | 0.79              |
| 1:T:170:LEU:HD13 | 3:I:1262:HIS:HB2 | 1.60                     | 0.78              |
| 1:l:138:THR:O    | 3:M:1166:PHE:CZ  | 2.35                     | 0.78              |
| 3:H:324:LYS:CB   | 3:D:322:MET:CE   | 2.59                     | 0.78              |
| 4:l:77:PRO:O     | 4:l:94:LEU:N     | 2.16                     | 0.78              |
| 3:F:1257:TYR:HB2 | 3:F:1277:PHE:HD2 | 1.47                     | 0.78              |
| 3:G:505:PHE:CD1  | 3:G:991:PRO:CB   | 2.67                     | 0.78              |
| 4:j:60:ALA:O     | 4:j:64:LEU:N     | 2.16                     | 0.78              |
| 3:P:950:GLN:HB2  | 3:P:953:GLU:HG3  | 1.66                     | 0.78              |
| 3:E:755:ARG:NH1  | 3:E:911:SER:OG   | 2.14                     | 0.78              |
| 2:X:99:ASN:ND2   | 3:C:1086:GLY:CA  | 2.47                     | 0.78              |
| 3:B:780:ASP:O    | 3:B:904:ARG:NH2  | 2.15                     | 0.78              |
| 6:r:91:VAL:HG22  | 7:u:3093:GLN:HB3 | 1.63                     | 0.78              |
| 3:F:873:ASN:CG   | 4:e:92:PHE:H     | 1.90                     | 0.78              |
| 3:K:646:ARG:HH11 | 3:K:890:ALA:HB2  | 1.48                     | 0.78              |
| 3:N:256:GLN:OE1  | 3:D:27:ILE:HD13  | 1.81                     | 0.78              |
| 3:F:982:ASP:OD1  | 3:F:985:ARG:NH1  | 2.16                     | 0.78              |
| 3:K:778:ARG:O    | 3:K:904:ARG:NH2  | 2.17                     | 0.78              |
| 3:M:63:ASN:HD21  | 3:H:99:VAL:HG13  | 1.49                     | 0.78              |
| 3:F:863:HIS:HE1  | 3:F:887:ASP:HA   | 1.48                     | 0.78              |
| 3:I:580:GLY:HA2  | 3:I:592:ARG:HH12 | 1.47                     | 0.78              |
| 3:P:896:VAL:HA   | 3:P:899:HIS:HD2  | 1.48                     | 0.78              |
| 3:C:842:MET:HE1  | 3:C:891:MET:HB3  | 1.65                     | 0.78              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:G:830:VAL:N     | 3:G:956:TYR:CE1   | 2.52                     | 0.78              |
| 3:G:1334:ILE:CG2  | 3:G:1335:THR:N    | 2.46                     | 0.78              |
| 4:n:57:GLN:NE2    | 3:N:841:ASN:OD1   | 2.16                     | 0.78              |
| 3:C:947:HIS:HB2   | 4:b:79:PHE:CD1    | 2.19                     | 0.78              |
| 3:F:263:ARG:NH2   | 3:F:306:TYR:O     | 2.17                     | 0.78              |
| 3:M:157:ARG:NH2   | 3:D:89:TYR:CE1    | 2.51                     | 0.78              |
| 3:H:324:LYS:CB    | 3:D:322:MET:HE1   | 2.14                     | 0.78              |
| 3:D:950:GLN:HG3   | 4:c:80:ALA:CB     | 2.14                     | 0.78              |
| 5:q:172:ARG:HG3   | 5:q:200:MET:HE1   | 1.60                     | 0.78              |
| 5:q:172:ARG:CD    | 5:q:200:MET:HE1   | 2.13                     | 0.78              |
| 3:E:1217:ASP:OD1  | 3:E:1287:ARG:NH1  | 2.16                     | 0.78              |
| 3:G:469:ILE:CD1   | 3:G:547:PHE:CG    | 2.67                     | 0.78              |
| 3:G:506:LEU:O     | 3:G:510:ARG:HG3   | 1.84                     | 0.78              |
| 3:G:708:THR:HG22  | 3:G:723:ASN:HD22  | 1.49                     | 0.78              |
| 3:I:485:ASN:ND2   | 3:I:516:GLY:H     | 1.80                     | 0.78              |
| 3:F:14:ALA:HB3    | 3:G:321:VAL:CG2   | 2.11                     | 0.78              |
| 2:3:284:GLN:CG    | 3:D:1166:PHE:CZ   | 2.66                     | 0.77              |
| 3:J:1296:THR:HG21 | 3:J:1327:LEU:HG   | 1.67                     | 0.77              |
| 3:F:390:VAL:HG21  | 3:G:104:ILE:CD1   | 2.12                     | 0.77              |
| 3:F:448:GLN:HG2   | 3:G:1201:ARG:NH2  | 1.98                     | 0.77              |
| 3:L:485:ASN:ND2   | 3:L:516:GLY:O     | 2.18                     | 0.77              |
| 3:H:730:ALA:HB2   | 3:H:752:ARG:HH11  | 1.49                     | 0.77              |
| 3:G:52:VAL:HG12   | 3:G:54:PHE:CE2    | 2.18                     | 0.77              |
| 3:E:846:GLU:HA    | 4:e:68:HIS:CE1    | 2.20                     | 0.77              |
| 1:1:141:PRO:HG2   | 3:M:1166:PHE:CE2  | 2.19                     | 0.77              |
| 3:K:1279:ALA:O    | 3:K:1283:THR:HG23 | 1.84                     | 0.77              |
| 3:H:881:ASN:OD1   | 4:m:95:LYS:NZ     | 2.15                     | 0.77              |
| 3:F:1365:ASP:O    | 3:F:1370:LYS:NZ   | 2.18                     | 0.77              |
| 3:K:1190:THR:HG22 | 3:K:1243:ASN:HD21 | 1.49                     | 0.77              |
| 3:O:122:LYS:NZ    | 3:O:1101:ASP:O    | 2.17                     | 0.77              |
| 3:O:1124:ASN:O    | 3:O:1156:ARG:NH1  | 2.17                     | 0.77              |
| 3:I:1270:LEU:HD22 | 3:I:1303:ALA:HB2  | 1.65                     | 0.77              |
| 4:h:76:GLN:HB2    | 4:h:94:LEU:HD12   | 1.66                     | 0.77              |
| 3:M:259:VAL:HG22  | 3:M:1102:LEU:HD13 | 1.66                     | 0.77              |
| 3:N:755:ARG:NH1   | 3:N:911:SER:OG    | 2.17                     | 0.77              |
| 3:F:742:LEU:HD22  | 3:F:756:ILE:HD11  | 1.67                     | 0.77              |
| 2:X:38:ARG:HH22   | 3:I:110:HIS:N     | 1.83                     | 0.77              |
| 1:1:283:ARG:CB    | 3:L:47:ASN:ND2    | 2.48                     | 0.77              |
| 3:O:1346:ALA:HB2  | 3:O:1362:LEU:HD11 | 1.67                     | 0.77              |
| 3:B:1124:ASN:O    | 3:B:1156:ARG:NH1  | 2.17                     | 0.77              |
| 2:R:174:PRO:HD3   | 5:q:371:GLY:C     | 2.10                     | 0.77              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:3:300:PHE:HB3   | 3:M:1083:HIS:NE2  | 2.00                     | 0.77              |
| 3:J:697:VAL:CG2   | 3:J:816:LEU:HD12  | 2.15                     | 0.77              |
| 3:J:879:PHE:O     | 3:J:883:ARG:N     | 2.18                     | 0.77              |
| 3:M:1296:THR:HG21 | 3:M:1327:LEU:HG   | 1.67                     | 0.77              |
| 5:q:172:ARG:CD    | 5:q:200:MET:CE    | 2.62                     | 0.77              |
| 2:S:2:ILE:HD11    | 3:B:1084:GLU:O    | 1.81                     | 0.77              |
| 1:W:328:TYR:HE1   | 6:r:18:PHE:CE1    | 1.99                     | 0.77              |
| 3:B:198:LEU:O     | 3:B:201:MET:N     | 2.18                     | 0.77              |
| 3:D:873:ASN:HA    | 4:c:92:PHE:CD2    | 2.19                     | 0.77              |
| 3:L:840:GLN:HG2   | 4:l:61:LEU:HD11   | 1.66                     | 0.76              |
| 3:P:180:THR:HG22  | 3:P:1097:ARG:HH12 | 1.50                     | 0.76              |
| 3:E:12:ARG:NH1    | 3:F:321:VAL:O     | 2.17                     | 0.76              |
| 1:T:141:PRO:HB3   | 3:I:1165:VAL:HG11 | 1.66                     | 0.76              |
| 3:J:1124:ASN:O    | 3:J:1156:ARG:NH1  | 2.18                     | 0.76              |
| 3:A:119:TYR:O     | 3:G:45:ASP:CG     | 2.28                     | 0.76              |
| 3:N:876:ASN:HA    | 3:N:879:PHE:HD2   | 1.48                     | 0.76              |
| 3:P:466:LEU:HD12  | 3:P:467:MET:HG3   | 1.67                     | 0.76              |
| 3:H:1105:GLY:HA2  | 3:C:32:HIS:NE2    | 2.01                     | 0.76              |
| 3:B:521:VAL:HG11  | 3:B:987:VAL:HG12  | 1.67                     | 0.76              |
| 3:B:677:TYR:HA    | 4:b:95:LYS:HZ2    | 1.50                     | 0.76              |
| 3:F:634:ILE:HG22  | 3:F:636:GLY:H     | 1.50                     | 0.76              |
| 3:F:756:ILE:HB    | 3:F:763:PRO:HD3   | 1.67                     | 0.76              |
| 3:F:853:CYS:HB2   | 4:f:101:PHE:CE1   | 2.20                     | 0.76              |
| 3:G:433:ARG:HG2   | 3:G:433:ARG:HH11  | 1.48                     | 0.76              |
| 1:W:198:TYR:O     | 1:W:201:ARG:CG    | 2.33                     | 0.76              |
| 3:I:229:ASP:O     | 3:I:236:LYS:NZ    | 2.18                     | 0.76              |
| 3:K:63:ASN:HD21   | 3:L:99:VAL:HG13   | 1.51                     | 0.76              |
| 3:M:38:PHE:O      | 3:D:120:MET:HA    | 1.86                     | 0.76              |
| 3:H:709:LEU:HD13  | 3:H:710:PRO:CD    | 2.16                     | 0.76              |
| 3:N:865:LEU:HD11  | 3:N:886:VAL:H     | 1.51                     | 0.76              |
| 3:C:677:TYR:HA    | 4:c:95:LYS:NZ     | 1.99                     | 0.76              |
| 3:C:766:ALA:N     | 3:C:783:LEU:O     | 2.17                     | 0.76              |
| 3:D:406:LEU:HD12  | 3:D:1050:PHE:HB2  | 1.68                     | 0.76              |
| 3:G:23:ILE:HD13   | 3:G:167:ARG:HD3   | 1.59                     | 0.76              |
| 1:W:344:GLU:OE1   | 6:r:13:TRP:CZ2    | 2.38                     | 0.76              |
| 1:l:141:PRO:CG    | 3:M:1166:PHE:HB3  | 2.16                     | 0.76              |
| 3:D:351:LEU:O     | 3:D:351:LEU:HD23  | 1.84                     | 0.76              |
| 5:q:123:VAL:HG22  | 5:q:419:SER:HB3   | 1.67                     | 0.76              |
| 3:E:576:ARG:HH11  | 3:E:582:LEU:HD23  | 1.50                     | 0.76              |
| 3:F:448:GLN:CD    | 3:G:1201:ARG:HH12 | 1.94                     | 0.76              |
| 1:W:25:ARG:O      | 3:H:144:THR:C     | 2.29                     | 0.76              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:P:1000:SER:O    | 3:P:1003:ARG:NH1  | 2.19                     | 0.76              |
| 3:B:677:TYR:CA    | 4:b:95:LYS:NZ     | 2.48                     | 0.76              |
| 1:W:199:ASP:CB    | 6:r:17:ARG:CB     | 2.63                     | 0.76              |
| 3:M:840:GLN:HG2   | 4:m:61:LEU:HD11   | 1.67                     | 0.76              |
| 4:h:22:MET:HG2    | 4:h:64:LEU:HD22   | 1.66                     | 0.76              |
| 3:I:827:THR:OG1   | 3:I:958:LEU:O     | 2.04                     | 0.76              |
| 3:K:293:LEU:HD13  | 3:K:368:VAL:HG11  | 1.67                     | 0.76              |
| 3:O:410:ASN:O     | 3:O:415:ARG:NH1   | 2.18                     | 0.76              |
| 3:O:1257:TYR:HB2  | 3:O:1277:PHE:HD2  | 1.50                     | 0.76              |
| 3:B:261:VAL:HG23  | 3:G:61:TYR:O      | 1.85                     | 0.76              |
| 3:B:490:TYR:OH    | 3:B:560:GLY:O     | 2.03                     | 0.76              |
| 3:C:677:TYR:HA    | 4:c:95:LYS:HZ1    | 1.49                     | 0.76              |
| 3:C:873:ASN:HA    | 4:b:92:PHE:HD2    | 1.49                     | 0.76              |
| 1:T:158:ALA:CB    | 3:I:1165:VAL:CG2  | 2.47                     | 0.76              |
| 3:K:1225:LEU:HD22 | 3:K:1234:PRO:HG3  | 1.68                     | 0.76              |
| 3:H:98:GLU:CG     | 3:C:11:TYR:OH     | 2.33                     | 0.76              |
| 3:P:213:ARG:HH12  | 3:P:1216:GLY:HA3  | 1.50                     | 0.76              |
| 3:B:1342:LEU:HD21 | 3:B:1362:LEU:HB2  | 1.68                     | 0.76              |
| 3:H:1217:ASP:OD1  | 3:H:1287:ARG:NH1  | 2.18                     | 0.76              |
| 3:F:1296:THR:HG21 | 3:F:1327:LEU:HG   | 1.66                     | 0.76              |
| 3:G:497:PRO:N     | 3:G:504:ARG:HH22  | 1.83                     | 0.76              |
| 1:Q:45:ASP:CA     | 3:B:322:MET:O     | 2.32                     | 0.75              |
| 3:M:119:TYR:HB3   | 3:N:11:TYR:HE2    | 1.50                     | 0.75              |
| 3:H:98:GLU:CD     | 3:C:11:TYR:OH     | 2.23                     | 0.75              |
| 3:O:1215:ALA:O    | 3:O:1287:ARG:NH2  | 2.18                     | 0.75              |
| 3:B:452:LEU:HD12  | 3:B:456:ASN:HD22  | 1.50                     | 0.75              |
| 1:W:166:GLU:CD    | 3:C:1262:HIS:CD2  | 2.64                     | 0.75              |
| 3:J:390:VAL:HG11  | 3:K:104:ILE:HD11  | 1.67                     | 0.75              |
| 3:K:1206:ARG:NH1  | 3:K:1208:ARG:O    | 2.19                     | 0.75              |
| 3:L:1054:ARG:NH1  | 3:L:1122:MET:O    | 2.19                     | 0.75              |
| 3:P:133:PHE:HB3   | 3:P:1091:PHE:HB2  | 1.68                     | 0.75              |
| 1:w:260:LEU:CD2   | 3:O:1316:GLY:CA   | 2.61                     | 0.75              |
| 3:I:842:MET:HE1   | 3:I:891:MET:HB3   | 1.67                     | 0.75              |
| 3:J:469:ILE:HD12  | 3:J:547:PHE:CE1   | 2.20                     | 0.75              |
| 3:M:1072:ALA:HB2  | 3:M:1102:LEU:HD23 | 1.67                     | 0.75              |
| 3:E:753:ASP:HB3   | 3:E:755:ARG:HH22  | 1.50                     | 0.75              |
| 3:F:638:GLU:HB2   | 3:F:789:ALA:HA    | 1.69                     | 0.75              |
| 1:w:259:GLU:OE1   | 3:O:1315:PRO:HA   | 1.87                     | 0.75              |
| 3:A:293:LEU:HD13  | 3:A:368:VAL:HG11  | 1.66                     | 0.75              |
| 3:H:1291:ARG:HE   | 3:C:34:ARG:HB3    | 1.51                     | 0.75              |
| 3:O:390:VAL:HG21  | 3:P:104:ILE:HD11  | 1.67                     | 0.75              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:O:1296:THR:HG21 | 3:O:1327:LEU:HG   | 1.67                     | 0.75              |
| 3:F:745:HIS:CE1   | 3:F:754:CYS:HA    | 2.21                     | 0.75              |
| 3:F:842:MET:HE1   | 3:F:891:MET:HE3   | 1.68                     | 0.75              |
| 3:O:1029:PHE:HB3  | 3:O:1039:GLN:NE2  | 2.02                     | 0.75              |
| 3:I:406:LEU:HD12  | 3:I:1050:PHE:HB2  | 1.69                     | 0.75              |
| 3:J:754:CYS:O     | 3:J:756:ILE:HG13  | 1.85                     | 0.75              |
| 3:D:404:LEU:HB2   | 3:D:1052:VAL:HB   | 1.67                     | 0.75              |
| 3:E:488:GLY:HA2   | 3:E:996:ALA:HB1   | 1.68                     | 0.75              |
| 1:I:141:PRO:CG    | 3:M:1166:PHE:CG   | 2.60                     | 0.75              |
| 3:I:752:ARG:HH21  | 3:I:915:ASP:HA    | 1.52                     | 0.75              |
| 3:J:521:VAL:HG21  | 3:J:987:VAL:HG12  | 1.69                     | 0.75              |
| 3:M:41:ARG:NH2    | 3:D:116:VAL:HG11  | 2.02                     | 0.75              |
| 3:B:861:PRO:O     | 3:B:869:ASN:ND2   | 2.19                     | 0.75              |
| 3:F:448:GLN:CG    | 3:G:1201:ARG:NH1  | 2.50                     | 0.75              |
| 3:G:31:SER:O      | 3:G:53:GLU:N      | 2.20                     | 0.75              |
| 3:G:1198:TYR:CD1  | 3:G:1236:ARG:NH1  | 2.53                     | 0.75              |
| 3:J:1191:PRO:HG2  | 3:J:1194:THR:HG23 | 1.69                     | 0.75              |
| 3:L:1000:SER:O    | 3:L:1003:ARG:NH1  | 2.19                     | 0.75              |
| 3:M:1073:TYR:OH   | 3:M:1097:ARG:NH1  | 2.20                     | 0.75              |
| 3:A:626:VAL:HG22  | 3:A:878:MET:HG3   | 1.69                     | 0.75              |
| 3:A:1031:MET:HE2  | 3:A:1048:PHE:CZ   | 2.22                     | 0.75              |
| 3:N:1286:HIS:CD2  | 3:D:34:ARG:NH1    | 2.54                     | 0.75              |
| 3:O:946:ASP:HB3   | 3:O:949:ILE:H     | 1.51                     | 0.75              |
| 3:F:52:VAL:CG1    | 3:G:320:LEU:CD2   | 2.63                     | 0.75              |
| 2:S:263:GLN:HB2   | 5:q:9:VAL:HG11    | 1.67                     | 0.75              |
| 3:J:889:PRO:HB2   | 4:j:100:PRO:HG2   | 1.68                     | 0.75              |
| 3:D:756:ILE:HD12  | 3:D:763:PRO:HG3   | 1.67                     | 0.75              |
| 3:D:1217:ASP:OD1  | 3:D:1287:ARG:NH1  | 2.19                     | 0.75              |
| 3:G:524:CYS:HB2   | 3:G:1008:GLN:OE1  | 1.86                     | 0.75              |
| 6:s:91:VAL:HG11   | 7:t:3092:ILE:HB   | 1.69                     | 0.74              |
| 3:A:119:TYR:HD2   | 3:G:44:SER:CB     | 2.00                     | 0.74              |
| 3:B:532:MET:HE1   | 3:B:1194:THR:HG22 | 1.67                     | 0.74              |
| 3:G:985:ARG:NH1   | 3:G:985:ARG:HB3   | 2.02                     | 0.74              |
| 3:H:133:PHE:HB3   | 3:H:1091:PHE:HB2  | 1.68                     | 0.74              |
| 3:H:1120:THR:HG22 | 3:H:1181:GLN:HE21 | 1.52                     | 0.74              |
| 3:O:133:PHE:HB3   | 3:O:1091:PHE:HB2  | 1.68                     | 0.74              |
| 3:C:873:ASN:HA    | 4:b:92:PHE:HB2    | 1.67                     | 0.74              |
| 3:G:524:CYS:CB    | 3:G:1008:GLN:HE22 | 1.87                     | 0.74              |
| 3:J:475:GLY:O     | 3:J:478:HIS:CD2   | 2.41                     | 0.74              |
| 3:A:1000:SER:O    | 3:A:1003:ARG:NH1  | 2.19                     | 0.74              |
| 3:H:966:GLY:HA3   | 3:H:969:HIS:HB2   | 1.69                     | 0.74              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:n:80:ALA:N      | 3:O:947:HIS:O     | 2.20                     | 0.74              |
| 3:D:646:ARG:NH1   | 4:d:99:SER:CA     | 2.49                     | 0.74              |
| 1:T:282:PRO:HD3   | 3:H:51:ASP:OD1    | 1.87                     | 0.74              |
| 3:K:795:ALA:HB3   | 3:K:798:ARG:HG2   | 1.68                     | 0.74              |
| 3:L:1296:THR:HG21 | 3:L:1327:LEU:HG   | 1.69                     | 0.74              |
| 3:A:305:THR:HG21  | 3:A:357:ALA:HB1   | 1.67                     | 0.74              |
| 3:A:357:ALA:O     | 3:A:359:GLN:NE2   | 2.20                     | 0.74              |
| 3:N:1257:TYR:HB2  | 3:N:1277:PHE:HD2  | 1.51                     | 0.74              |
| 3:C:548:ASP:OD1   | 3:C:576:ARG:NE    | 2.21                     | 0.74              |
| 3:C:827:THR:OG1   | 3:C:958:LEU:O     | 2.05                     | 0.74              |
| 3:D:639:HIS:HA    | 4:d:79:PHE:CE2    | 2.22                     | 0.74              |
| 3:F:1217:ASP:OD1  | 3:F:1287:ARG:NH1  | 2.20                     | 0.74              |
| 1:W:257:GLN:OE1   | 3:D:109:PRO:CD    | 2.36                     | 0.74              |
| 1:w:13:TRP:O      | 3:L:1082:ARG:NH1  | 2.21                     | 0.74              |
| 3:I:752:ARG:NH2   | 3:I:915:ASP:OD1   | 2.20                     | 0.74              |
| 3:I:1174:ARG:O    | 3:J:213:ARG:NH2   | 2.21                     | 0.74              |
| 3:M:756:ILE:HG12  | 3:M:910:CYS:HB3   | 1.70                     | 0.74              |
| 3:A:701:ALA:O     | 3:A:727:ARG:NH2   | 2.21                     | 0.74              |
| 3:N:621:ARG:O     | 3:N:943:GLN:NE2   | 2.16                     | 0.74              |
| 3:O:452:LEU:HD12  | 3:O:456:ASN:HD22  | 1.52                     | 0.74              |
| 3:C:1342:LEU:HD21 | 3:C:1362:LEU:HB2  | 1.67                     | 0.74              |
| 1:T:161:TRP:CD1   | 3:I:1166:PHE:CE1  | 2.76                     | 0.74              |
| 1:T:165:LEU:CD1   | 3:I:1166:PHE:CE1  | 2.69                     | 0.74              |
| 1:I:158:ALA:HB1   | 3:M:1165:VAL:HG22 | 1.68                     | 0.74              |
| 3:J:512:ARG:HA    | 3:J:515:HIS:HD2   | 1.51                     | 0.74              |
| 3:L:580:GLY:HA2   | 3:L:592:ARG:HH12  | 1.52                     | 0.74              |
| 3:A:755:ARG:NH1   | 3:A:911:SER:OG    | 2.20                     | 0.74              |
| 3:G:469:ILE:HG22  | 3:G:469:ILE:O     | 1.87                     | 0.74              |
| 2:S:313:PRO:HG3   | 3:A:111:PRO:HB2   | 1.69                     | 0.74              |
| 1:W:344:GLU:C     | 6:r:13:TRP:CZ3    | 2.21                     | 0.74              |
| 3:J:752:ARG:HH21  | 3:J:915:ASP:HA    | 1.51                     | 0.74              |
| 3:O:580:GLY:HA2   | 3:O:592:ARG:HH12  | 1.53                     | 0.74              |
| 3:P:548:ASP:OD1   | 3:P:576:ARG:NE    | 2.17                     | 0.74              |
| 1:T:259:GLU:OE1   | 3:I:1315:PRO:HA   | 1.86                     | 0.74              |
| 1:W:347:PHE:CZ    | 6:r:18:PHE:CD2    | 2.76                     | 0.74              |
| 3:J:451:ARG:NH1   | 3:K:529:GLU:OE2   | 2.20                     | 0.74              |
| 3:K:863:HIS:HE1   | 3:K:887:ASP:HA    | 1.52                     | 0.74              |
| 3:C:390:VAL:HG21  | 3:D:104:ILE:HD11  | 1.69                     | 0.74              |
| 3:N:258:SER:O     | 3:D:24:LEU:HD12   | 1.88                     | 0.74              |
| 3:O:710:PRO:HG2   | 3:P:517:ARG:HH11  | 1.53                     | 0.74              |
| 3:P:896:VAL:HA    | 3:P:899:HIS:CD2   | 2.22                     | 0.74              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:G:1334:ILE:HG22 | 3:G:1335:THR:H    | 1.53                     | 0.74              |
| 3:D:1131:LEU:HD23 | 3:D:1159:PRO:HG3  | 1.70                     | 0.73              |
| 3:E:106:ARG:HH21  | 3:E:110:HIS:HB3   | 1.53                     | 0.73              |
| 3:A:736:VAL:HG12  | 3:A:738:ASP:H     | 1.53                     | 0.73              |
| 3:B:896:VAL:HA    | 3:B:899:HIS:CD2   | 2.24                     | 0.73              |
| 3:D:1245:TRP:O    | 3:D:1251:SER:HB3  | 1.86                     | 0.73              |
| 3:G:1334:ILE:CG2  | 3:G:1335:THR:H    | 2.01                     | 0.73              |
| 2:R:37:ILE:CG2    | 3:A:109:PRO:HG2   | 2.18                     | 0.73              |
| 1:T:165:LEU:HD12  | 3:I:1166:PHE:CE2  | 2.16                     | 0.73              |
| 3:I:746:ALA:HA    | 3:I:754:CYS:HB3   | 1.69                     | 0.73              |
| 3:K:519:ARG:NH1   | 3:K:998:TYR:OH    | 2.22                     | 0.73              |
| 1:w:113:GLN:O     | 1:w:115:THR:HG23  | 1.89                     | 0.73              |
| 3:M:9:PRO:CG      | 3:D:94:ARG:NH2    | 2.45                     | 0.73              |
| 3:H:709:LEU:CD2   | 3:H:710:PRO:HD2   | 2.19                     | 0.73              |
| 3:B:163:GLN:HE22  | 3:C:348:ARG:NH2   | 1.87                     | 0.73              |
| 3:B:262:PRO:CA    | 3:G:59:GLY:O      | 2.37                     | 0.73              |
| 3:C:1051:THR:HG23 | 3:C:1190:THR:HG21 | 1.69                     | 0.73              |
| 3:E:643:ALA:HB2   | 4:e:78:MET:HE1    | 1.69                     | 0.73              |
| 3:G:827:THR:O     | 3:G:958:LEU:O     | 2.06                     | 0.73              |
| 3:I:1365:ASP:O    | 3:I:1370:LYS:NZ   | 2.20                     | 0.73              |
| 3:H:320:LEU:HD13  | 3:C:156:HIS:CD2   | 2.23                     | 0.73              |
| 3:H:548:ASP:OD1   | 3:H:576:ARG:NE    | 2.20                     | 0.73              |
| 3:H:840:GLN:HG2   | 4:h:61:LEU:HD11   | 1.69                     | 0.73              |
| 3:N:1217:ASP:OD1  | 3:N:1287:ARG:NH1  | 2.21                     | 0.73              |
| 3:B:631:GLN:NE2   | 3:B:666:ASN:OD1   | 2.18                     | 0.73              |
| 3:E:524:CYS:SG    | 3:E:1008:GLN:NE2  | 2.61                     | 0.73              |
| 3:F:789:ALA:O     | 4:f:79:PHE:CE2    | 2.42                     | 0.73              |
| 3:M:548:ASP:OD1   | 3:M:576:ARG:NE    | 2.16                     | 0.73              |
| 3:A:819:ALA:O     | 3:A:822:ARG:NH1   | 2.21                     | 0.73              |
| 3:O:219:LEU:O     | 3:O:222:GLU:N     | 2.15                     | 0.73              |
| 3:B:842:MET:HE1   | 3:B:891:MET:HB3   | 1.69                     | 0.73              |
| 3:D:736:VAL:HG12  | 3:D:738:ASP:H     | 1.52                     | 0.73              |
| 5:q:643:GLY:N     | 5:q:650:CYS:SG    | 2.60                     | 0.73              |
| 3:E:107:ASP:OD1   | 3:E:108:GLY:N     | 2.22                     | 0.73              |
| 3:E:983:LEU:HD21  | 3:E:987:VAL:HG21  | 1.70                     | 0.73              |
| 1:W:352:ILE:CB    | 6:r:12:VAL:HG22   | 2.13                     | 0.73              |
| 1:1:25:ARG:O      | 3:D:144:THR:HG23  | 1.89                     | 0.73              |
| 3:O:1365:ASP:O    | 3:O:1370:LYS:NZ   | 2.21                     | 0.73              |
| 3:C:159:LEU:HD11  | 3:D:340:GLN:HA    | 1.69                     | 0.73              |
| 3:C:708:THR:HG22  | 3:C:723:ASN:HD22  | 1.51                     | 0.73              |
| 3:E:846:GLU:HA    | 4:e:68:HIS:HE1    | 1.52                     | 0.73              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:I:736:VAL:HG12  | 3:I:738:ASP:H     | 1.54                     | 0.73              |
| 3:K:406:LEU:HD12  | 3:K:1050:PHE:HB2  | 1.71                     | 0.73              |
| 3:B:756:ILE:HB    | 3:B:763:PRO:HD3   | 1.70                     | 0.73              |
| 3:J:1257:TYR:HB2  | 3:J:1277:PHE:HD2  | 1.53                     | 0.73              |
| 3:K:512:ARG:HA    | 3:K:515:HIS:CD2   | 2.23                     | 0.73              |
| 3:D:135:LEU:HD21  | 3:D:165:LEU:HD21  | 1.71                     | 0.73              |
| 3:D:512:ARG:HA    | 3:D:515:HIS:CD2   | 2.24                     | 0.73              |
| 3:E:410:ASN:O     | 3:E:415:ARG:NH1   | 2.21                     | 0.73              |
| 3:F:14:ALA:CB     | 3:G:321:VAL:CG2   | 2.67                     | 0.73              |
| 3:A:507:ASN:OD1   | 3:A:510:ARG:NH2   | 2.21                     | 0.73              |
| 3:B:1133:ARG:HD3  | 3:B:1163:LEU:HD13 | 1.71                     | 0.73              |
| 3:E:69:ARG:HB2    | 3:E:72:GLU:HG2    | 1.69                     | 0.73              |
| 3:F:1342:LEU:HD21 | 3:F:1362:LEU:HB2  | 1.69                     | 0.73              |
| 2:R:174:PRO:CD    | 5:q:371:GLY:CA    | 2.55                     | 0.72              |
| 1:1:158:ALA:CB    | 3:M:1165:VAL:HG21 | 2.18                     | 0.72              |
| 3:C:1257:TYR:HB2  | 3:C:1277:PHE:HD2  | 1.54                     | 0.72              |
| 3:D:766:ALA:N     | 3:D:783:LEU:O     | 2.22                     | 0.72              |
| 3:E:873:ASN:OD1   | 4:d:92:PHE:CB     | 2.37                     | 0.72              |
| 3:J:728:ASP:O     | 3:J:810:LYS:NZ    | 2.22                     | 0.72              |
| 3:J:1029:PHE:HB3  | 3:J:1039:GLN:NE2  | 2.04                     | 0.72              |
| 3:M:134:SER:C     | 3:C:44:SER:HG     | 1.90                     | 0.72              |
| 3:M:164:GLN:NE2   | 3:C:49:LEU:HD13   | 2.04                     | 0.72              |
| 3:B:512:ARG:HA    | 3:B:515:HIS:CD2   | 2.24                     | 0.72              |
| 2:R:174:PRO:CA    | 5:q:371:GLY:CA    | 2.55                     | 0.72              |
| 3:I:152:GLY:O     | 3:J:340:GLN:NE2   | 2.21                     | 0.72              |
| 3:J:503:GLN:HE21  | 3:J:507:ASN:HD21  | 1.35                     | 0.72              |
| 3:L:766:ALA:N     | 3:L:783:LEU:O     | 2.20                     | 0.72              |
| 3:H:122:LYS:NZ    | 3:H:1101:ASP:O    | 2.20                     | 0.72              |
| 3:F:755:ARG:NH1   | 3:F:911:SER:OG    | 2.21                     | 0.72              |
| 3:G:697:VAL:CG2   | 3:G:816:LEU:HD11  | 2.19                     | 0.72              |
| 3:J:1008:GLN:HG2  | 3:J:1011:ARG:HH21 | 1.53                     | 0.72              |
| 3:A:950:GLN:HB2   | 3:A:953:GLU:HG3   | 1.71                     | 0.72              |
| 3:O:923:THR:HA    | 3:O:926:MET:HE3   | 1.71                     | 0.72              |
| 3:P:1029:PHE:HB3  | 3:P:1039:GLN:NE2  | 2.04                     | 0.72              |
| 3:E:677:TYR:CD1   | 4:e:95:LYS:NZ     | 2.52                     | 0.72              |
| 3:F:873:ASN:HA    | 4:e:92:PHE:CB     | 2.15                     | 0.72              |
| 3:H:879:PHE:O     | 3:H:883:ARG:N     | 2.21                     | 0.72              |
| 3:N:843:VAL:O     | 3:N:876:ASN:ND2   | 2.22                     | 0.72              |
| 3:P:512:ARG:HA    | 3:P:515:HIS:CD2   | 2.24                     | 0.72              |
| 3:B:63:ASN:OD1    | 3:B:64:THR:N      | 2.22                     | 0.72              |
| 3:B:728:ASP:OD2   | 3:B:1030:LYS:NZ   | 2.17                     | 0.72              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 3:B:863:HIS:HE1   | 3:B:887:ASP:HA   | 1.55                     | 0.72              |
| 3:E:713:GLU:HG2   | 3:E:718:ALA:HA   | 1.70                     | 0.72              |
| 3:G:1161:GLN:HG3  | 3:G:1162:PRO:HD2 | 1.70                     | 0.72              |
| 1:1:281:ARG:CZ    | 3:L:51:ASP:OD2   | 2.37                     | 0.72              |
| 3:J:163:GLN:HE22  | 3:K:348:ARG:HH22 | 1.36                     | 0.72              |
| 3:J:475:GLY:CA    | 3:J:478:HIS:HD2  | 2.02                     | 0.72              |
| 3:K:1029:PHE:HB3  | 3:K:1039:GLN:NE2 | 2.04                     | 0.72              |
| 3:A:752:ARG:HH21  | 3:A:915:ASP:HA   | 1.55                     | 0.72              |
| 3:O:1073:TYR:OH   | 3:O:1097:ARG:NH1 | 2.22                     | 0.72              |
| 3:P:1222:VAL:HG11 | 3:P:1283:THR:HA  | 1.72                     | 0.72              |
| 3:D:834:ARG:NH1   | 3:D:953:GLU:O    | 2.22                     | 0.72              |
| 2:3:40:GLN:NE2    | 3:D:128:ALA:CB   | 2.51                     | 0.72              |
| 2:2:39:ARG:HH22   | 3:N:1085:THR:CB  | 2.00                     | 0.72              |
| 3:M:843:VAL:O     | 3:M:876:ASN:ND2  | 2.22                     | 0.72              |
| 4:j:76:GLN:O      | 4:j:96:ARG:NH2   | 2.16                     | 0.72              |
| 3:N:463:HIS:HD2   | 3:N:465:SER:HB3  | 1.54                     | 0.72              |
| 3:D:827:THR:OG1   | 3:D:958:LEU:O    | 2.05                     | 0.72              |
| 3:D:873:ASN:CG    | 4:c:92:PHE:H     | 1.97                     | 0.72              |
| 3:F:621:ARG:C     | 3:F:943:GLN:HE21 | 1.97                     | 0.72              |
| 3:F:793:ASP:OD2   | 3:F:800:HIS:ND1  | 2.23                     | 0.72              |
| 3:G:938:LEU:HD23  | 3:G:938:LEU:C    | 2.15                     | 0.72              |
| 1:w:79:THR:N      | 3:O:308:GLU:CD   | 2.48                     | 0.72              |
| 3:J:475:GLY:HA2   | 3:J:478:HIS:HD2  | 1.55                     | 0.72              |
| 5:q:569:LEU:HD22  | 5:q:694:GLY:HA2  | 1.71                     | 0.72              |
| 3:P:842:MET:HE1   | 3:P:891:MET:HB3  | 1.72                     | 0.72              |
| 3:E:1115:VAL:HG12 | 3:E:1116:ARG:O   | 1.89                     | 0.72              |
| 3:F:1000:SER:O    | 3:F:1003:ARG:NH1 | 2.23                     | 0.72              |
| 3:G:666:ASN:HD22  | 3:G:938:LEU:HD23 | 1.55                     | 0.72              |
| 3:J:504:ARG:NH2   | 3:J:562:GLU:OE2  | 2.22                     | 0.72              |
| 3:M:728:ASP:O     | 3:M:810:LYS:NZ   | 2.21                     | 0.72              |
| 3:P:410:ASN:ND2   | 3:P:1359:THR:O   | 2.22                     | 0.72              |
| 3:P:1257:TYR:HB2  | 3:P:1277:PHE:HD2 | 1.55                     | 0.72              |
| 3:C:873:ASN:OD1   | 4:b:92:PHE:HB2   | 1.90                     | 0.72              |
| 3:E:158:GLN:O     | 3:E:161:ALA:N    | 2.23                     | 0.72              |
| 3:G:575:TRP:HZ2   | 3:G:1031:MET:O   | 1.73                     | 0.72              |
| 1:1:431:ASP:OD1   | 2:2:39:ARG:HG3   | 1.90                     | 0.71              |
| 3:J:469:ILE:HD11  | 3:J:547:PHE:CD2  | 2.25                     | 0.71              |
| 3:L:433:ARG:O     | 3:L:1360:GLN:NE2 | 2.23                     | 0.71              |
| 3:M:161:ALA:HA    | 3:C:50:TYR:CE1   | 2.24                     | 0.71              |
| 3:N:350:THR:CG2   | 3:D:21:GLY:CA    | 2.54                     | 0.71              |
| 3:D:532:MET:HE1   | 3:D:1244:PRO:HD3 | 1.71                     | 0.71              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:1209:ALA:HB3  | 3:D:1234:PRO:HG2  | 1.71                     | 0.71              |
| 3:I:99:VAL:HB     | 3:I:118:ASN:HB2   | 1.73                     | 0.71              |
| 3:I:728:ASP:O     | 3:I:810:LYS:NZ    | 2.23                     | 0.71              |
| 3:K:728:ASP:O     | 3:K:810:LYS:NZ    | 2.23                     | 0.71              |
| 4:i:51:ARG:O      | 4:i:55:ARG:NH1    | 2.23                     | 0.71              |
| 3:N:896:VAL:HA    | 3:N:899:HIS:HD2   | 1.55                     | 0.71              |
| 3:B:158:GLN:O     | 3:B:161:ALA:N     | 2.23                     | 0.71              |
| 3:B:677:TYR:CD1   | 4:b:95:LYS:HE2    | 2.24                     | 0.71              |
| 3:C:842:MET:HE1   | 3:C:891:MET:HE3   | 1.71                     | 0.71              |
| 3:C:846:GLU:HA    | 4:c:68:HIS:HE1    | 1.55                     | 0.71              |
| 3:E:1082:ARG:HG2  | 3:E:1091:PHE:HE1  | 1.55                     | 0.71              |
| 3:F:133:PHE:HB3   | 3:F:1091:PHE:HB2  | 1.72                     | 0.71              |
| 3:F:1117:ASN:OD1  | 3:G:222:GLU:CD    | 2.33                     | 0.71              |
| 3:I:766:ALA:N     | 3:I:783:LEU:O     | 2.23                     | 0.71              |
| 3:K:142:LEU:O     | 3:K:158:GLN:NE2   | 2.23                     | 0.71              |
| 3:N:1029:PHE:HB3  | 3:N:1039:GLN:NE2  | 2.04                     | 0.71              |
| 3:P:1131:LEU:HD23 | 3:P:1159:PRO:HG3  | 1.72                     | 0.71              |
| 3:D:1215:ALA:O    | 3:D:1287:ARG:NH2  | 2.23                     | 0.71              |
| 3:F:448:GLN:HG2   | 3:G:1201:ARG:NH1  | 2.05                     | 0.71              |
| 3:F:728:ASP:O     | 3:F:810:LYS:NZ    | 2.23                     | 0.71              |
| 3:I:107:ASP:OD1   | 3:I:108:GLY:N     | 2.23                     | 0.71              |
| 3:J:841:ASN:O     | 3:J:875:VAL:HG23  | 1.90                     | 0.71              |
| 3:L:684:GLU:HB3   | 3:M:658:ASN:O     | 1.90                     | 0.71              |
| 3:A:280:THR:HG22  | 3:A:1063:VAL:HG22 | 1.71                     | 0.71              |
| 3:D:198:LEU:O     | 3:D:201:MET:N     | 2.20                     | 0.71              |
| 3:D:219:LEU:O     | 3:D:222:GLU:N     | 2.22                     | 0.71              |
| 3:I:133:PHE:HB3   | 3:I:1091:PHE:HB2  | 1.70                     | 0.71              |
| 3:J:863:HIS:O     | 3:J:869:ASN:ND2   | 2.22                     | 0.71              |
| 3:K:512:ARG:HA    | 3:K:515:HIS:HD2   | 1.56                     | 0.71              |
| 3:M:11:TYR:HB3    | 3:D:121:THR:CG2   | 2.20                     | 0.71              |
| 3:A:1208:ARG:NH1  | 3:A:1240:ALA:O    | 2.24                     | 0.71              |
| 3:E:983:LEU:HD23  | 3:E:983:LEU:C     | 2.14                     | 0.71              |
| 3:F:485:ASN:HD21  | 3:F:516:GLY:H     | 1.33                     | 0.71              |
| 3:G:33:ARG:HD3    | 3:G:53:GLU:OE1    | 1.88                     | 0.71              |
| 3:G:1198:TYR:HD1  | 3:G:1236:ARG:HH11 | 1.36                     | 0.71              |
| 2:R:6:PHE:CZ      | 3:A:109:PRO:HD3   | 2.26                     | 0.71              |
| 2:X:99:ASN:HD21   | 3:C:1086:GLY:CA   | 2.03                     | 0.71              |
| 3:K:881:ASN:OD1   | 4:j:95:LYS:NZ     | 2.24                     | 0.71              |
| 3:H:692:ASP:O     | 3:H:696:HIS:N     | 2.23                     | 0.71              |
| 3:O:819:ALA:O     | 3:O:822:ARG:NH1   | 2.24                     | 0.71              |
| 3:B:827:THR:OG1   | 3:B:958:LEU:O     | 2.05                     | 0.71              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:S:300:PHE:CZ   | 3:A:111:PRO:HA    | 2.23                     | 0.71              |
| 3:I:700:LEU:HD22 | 3:I:1025:MET:HG3  | 1.71                     | 0.71              |
| 3:J:548:ASP:OD1  | 3:J:576:ARG:NE    | 2.21                     | 0.71              |
| 3:K:770:ASN:H    | 3:K:773:THR:HB    | 1.55                     | 0.71              |
| 3:A:829:GLY:N    | 3:A:956:TYR:O     | 2.22                     | 0.71              |
| 3:P:842:MET:HE1  | 3:P:891:MET:HE3   | 1.72                     | 0.71              |
| 3:C:1029:PHE:HB3 | 3:C:1039:GLN:NE2  | 2.05                     | 0.71              |
| 3:E:615:ARG:HH21 | 3:E:1017:GLU:HG2  | 1.53                     | 0.71              |
| 3:E:758:ALA:N    | 3:E:761:HIS:O     | 2.20                     | 0.71              |
| 3:F:107:ASP:OD1  | 3:F:108:GLY:N     | 2.22                     | 0.71              |
| 3:G:481:VAL:HG11 | 3:G:571:ILE:HD11  | 1.72                     | 0.71              |
| 2:2:298:CYS:HB2  | 2:2:315:ILE:HD13  | 1.72                     | 0.71              |
| 3:I:740:ASP:OD2  | 3:I:801:ARG:NH1   | 2.23                     | 0.71              |
| 3:L:1072:ALA:HB2 | 3:L:1102:LEU:HD23 | 1.73                     | 0.71              |
| 3:M:351:LEU:HB3  | 3:N:20:THR:HA     | 1.73                     | 0.71              |
| 3:H:90:MET:HG2   | 3:H:91:ASN:O      | 1.91                     | 0.71              |
| 3:H:198:LEU:O    | 3:H:201:MET:N     | 2.23                     | 0.71              |
| 5:q:257:ASN:OD1  | 6:s:90:GLN:NE2    | 2.23                     | 0.71              |
| 3:F:241:ARG:NE   | 3:F:245:GLU:OE2   | 2.15                     | 0.71              |
| 2:R:174:PRO:HA   | 5:q:370:GLY:O     | 1.90                     | 0.71              |
| 1:T:260:LEU:HD23 | 3:I:1316:GLY:HA2  | 1.72                     | 0.71              |
| 1:W:25:ARG:O     | 3:H:145:GLY:HA3   | 1.91                     | 0.71              |
| 2:3:38:ARG:NH2   | 3:E:110:HIS:O     | 2.24                     | 0.71              |
| 1:w:282:PRO:O    | 3:L:138:GLU:OE2   | 2.08                     | 0.71              |
| 3:I:841:ASN:OD1  | 4:i:57:GLN:NE2    | 2.24                     | 0.71              |
| 3:J:133:PHE:HB3  | 3:J:1091:PHE:HB2  | 1.73                     | 0.71              |
| 3:J:836:TYR:HE1  | 3:J:897:LEU:HD22  | 1.56                     | 0.71              |
| 3:P:580:GLY:HA2  | 3:P:592:ARG:HH12  | 1.54                     | 0.71              |
| 3:C:677:TYR:HD1  | 4:c:95:LYS:CE     | 2.04                     | 0.71              |
| 3:J:793:ASP:OD1  | 3:J:798:ARG:NH2   | 2.23                     | 0.70              |
| 3:K:1174:ARG:O   | 3:L:213:ARG:NH2   | 2.23                     | 0.70              |
| 3:A:587:CYS:SG   | 3:A:592:ARG:NH2   | 2.64                     | 0.70              |
| 3:A:606:MET:HE3  | 3:A:611:ILE:HG12  | 1.72                     | 0.70              |
| 3:H:709:LEU:HD22 | 3:H:710:PRO:CD    | 2.20                     | 0.70              |
| 3:C:873:ASN:OD1  | 4:b:92:PHE:N      | 2.23                     | 0.70              |
| 3:J:484:ALA:O    | 3:J:486:PRO:HD3   | 1.90                     | 0.70              |
| 3:L:34:ARG:HH12  | 3:O:1286:HIS:HB2  | 1.55                     | 0.70              |
| 3:A:452:LEU:HD12 | 3:A:456:ASN:HD22  | 1.56                     | 0.70              |
| 5:q:428:GLU:HA   | 5:q:431:ALA:HB3   | 1.72                     | 0.70              |
| 2:S:260:MET:CG   | 5:q:412:ARG:NH1   | 2.54                     | 0.70              |
| 2:2:39:ARG:CZ    | 3:N:1083:HIS:CD2  | 2.73                     | 0.70              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:w:78:ALA:C      | 3:O:308:GLU:OE1   | 2.35                     | 0.70              |
| 3:J:1245:TRP:O    | 3:J:1251:SER:HB3  | 1.91                     | 0.70              |
| 3:L:907:ALA:HB1   | 3:L:994:LEU:HD21  | 1.71                     | 0.70              |
| 3:M:134:SER:O     | 3:C:44:SER:CB     | 2.40                     | 0.70              |
| 3:A:94:ARG:NH1    | 3:G:47:ASN:HB3    | 2.05                     | 0.70              |
| 4:o:57:GLN:NE2    | 3:O:841:ASN:OD1   | 2.23                     | 0.70              |
| 4:o:61:LEU:HB3    | 3:O:895:GLN:HG2   | 1.73                     | 0.70              |
| 3:J:615:ARG:HH21  | 3:J:1017:GLU:HG2  | 1.56                     | 0.70              |
| 3:K:548:ASP:OD1   | 3:K:576:ARG:NE    | 2.22                     | 0.70              |
| 3:M:133:PHE:HB3   | 3:M:1091:PHE:HB2  | 1.73                     | 0.70              |
| 4:o:61:LEU:HD11   | 3:O:840:GLN:HG2   | 1.72                     | 0.70              |
| 3:D:69:ARG:HB2    | 3:D:72:GLU:HG2    | 1.73                     | 0.70              |
| 3:J:1190:THR:HG22 | 3:J:1243:ASN:HD21 | 1.57                     | 0.70              |
| 3:K:776:PHE:O     | 3:K:904:ARG:NH1   | 2.22                     | 0.70              |
| 3:A:329:LEU:HD12  | 3:G:61:TYR:CD2    | 2.20                     | 0.70              |
| 3:H:1029:PHE:HB3  | 3:H:1039:GLN:NE2  | 2.06                     | 0.70              |
| 3:N:1286:HIS:CD2  | 3:D:34:ARG:HH12   | 2.10                     | 0.70              |
| 3:D:780:ASP:O     | 3:D:904:ARG:NH2   | 2.23                     | 0.70              |
| 2:2:183:GLY:H     | 3:D:1170:GLN:HG3  | 1.56                     | 0.70              |
| 3:J:947:HIS:O     | 4:i:80:ALA:N      | 2.22                     | 0.70              |
| 3:M:1000:SER:O    | 3:M:1003:ARG:NH1  | 2.24                     | 0.70              |
| 3:A:494:PRO:HD3   | 3:A:909:LEU:HD12  | 1.74                     | 0.70              |
| 3:H:1291:ARG:NH1  | 3:C:35:LEU:CD1    | 2.54                     | 0.70              |
| 3:N:326:VAL:HG21  | 3:E:321:VAL:HG12  | 1.67                     | 0.70              |
| 3:D:42:VAL:HG13   | 3:D:46:GLU:HG3    | 1.71                     | 0.70              |
| 5:q:577:PRO:HG2   | 5:q:580:PHE:HB2   | 1.72                     | 0.70              |
| 3:F:512:ARG:HA    | 3:F:515:HIS:CD2   | 2.26                     | 0.70              |
| 3:L:107:ASP:OD1   | 3:L:108:GLY:N     | 2.24                     | 0.70              |
| 3:M:59:GLY:HA2    | 3:C:20:THR:CG2    | 2.19                     | 0.70              |
| 3:O:800:HIS:O     | 3:O:801:ARG:HG3   | 1.91                     | 0.70              |
| 3:C:107:ASP:OD1   | 3:C:108:GLY:N     | 2.25                     | 0.70              |
| 3:F:548:ASP:OD1   | 3:F:576:ARG:NE    | 2.25                     | 0.70              |
| 3:F:750:ARG:HA    | 3:F:753:ASP:HB3   | 1.72                     | 0.70              |
| 3:F:923:THR:HA    | 3:F:926:MET:HE3   | 1.74                     | 0.70              |
| 3:G:23:ILE:HG21   | 3:G:167:ARG:CZ    | 2.22                     | 0.70              |
| 3:G:704:VAL:O     | 3:G:708:THR:HG23  | 1.91                     | 0.70              |
| 1:l:141:PRO:HB3   | 3:M:1165:VAL:HG13 | 1.74                     | 0.70              |
| 2:3:39:ARG:NH1    | 3:D:1081:ALA:CB   | 2.55                     | 0.70              |
| 1:w:272:GLU:HB3   | 1:w:283:ARG:HH21  | 1.44                     | 0.70              |
| 3:M:157:ARG:HH22  | 3:D:89:TYR:HE1    | 1.38                     | 0.70              |
| 3:P:788:GLN:HE22  | 3:P:794:ALA:HA    | 1.55                     | 0.70              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:426:ALA:HB3   | 3:D:429:HIS:HD2   | 1.57                     | 0.70              |
| 3:D:1120:THR:HG22 | 3:D:1181:GLN:HE21 | 1.56                     | 0.70              |
| 3:F:52:VAL:HG11   | 3:G:320:LEU:CD2   | 2.21                     | 0.70              |
| 3:I:410:ASN:O     | 3:I:415:ARG:NH1   | 2.25                     | 0.70              |
| 3:I:923:THR:HA    | 3:I:926:MET:HE3   | 1.73                     | 0.70              |
| 3:M:1029:PHE:HB3  | 3:M:1039:GLN:NE2  | 2.06                     | 0.70              |
| 3:N:1245:TRP:O    | 3:N:1251:SER:HB3  | 1.91                     | 0.70              |
| 3:B:915:ASP:OD2   | 3:B:1030:LYS:NZ   | 2.24                     | 0.70              |
| 3:G:1161:GLN:CG   | 3:G:1162:PRO:HD2  | 2.22                     | 0.70              |
| 2:Y:248:ARG:NE    | 3:H:1141:ASN:ND2  | 2.39                     | 0.70              |
| 3:J:1029:PHE:HB3  | 3:J:1039:GLN:HE22 | 1.55                     | 0.70              |
| 3:H:466:LEU:HD12  | 3:H:467:MET:HG3   | 1.73                     | 0.70              |
| 3:H:512:ARG:HA    | 3:H:515:HIS:CD2   | 2.27                     | 0.70              |
| 3:F:56:ALA:HA     | 3:G:325:ALA:O     | 1.92                     | 0.70              |
| 3:F:1029:PHE:HB3  | 3:F:1039:GLN:NE2  | 2.07                     | 0.70              |
| 3:G:949:ILE:CG2   | 3:G:953:GLU:OE1   | 2.33                     | 0.70              |
| 3:I:484:ALA:O     | 3:I:486:PRO:CD    | 2.40                     | 0.69              |
| 3:K:1217:ASP:OD1  | 3:K:1287:ARG:NH1  | 2.25                     | 0.69              |
| 3:P:77:VAL:HG22   | 3:P:266:HIS:CD2   | 2.27                     | 0.69              |
| 3:B:843:VAL:O     | 3:B:876:ASN:ND2   | 2.25                     | 0.69              |
| 3:C:198:LEU:O     | 3:C:201:MET:N     | 2.24                     | 0.69              |
| 3:D:90:MET:HG2    | 3:D:91:ASN:O      | 1.91                     | 0.69              |
| 5:q:365:TRP:CD1   | 5:q:380:ARG:HD3   | 2.27                     | 0.69              |
| 3:F:406:LEU:HD12  | 3:F:1050:PHE:HB2  | 1.72                     | 0.69              |
| 3:F:896:VAL:HA    | 3:F:899:HIS:HD2   | 1.56                     | 0.69              |
| 3:I:615:ARG:HH21  | 3:I:1017:GLU:HG2  | 1.57                     | 0.69              |
| 3:J:469:ILE:HD11  | 3:J:547:PHE:CE2   | 2.27                     | 0.69              |
| 3:J:475:GLY:C     | 3:J:478:HIS:CD2   | 2.70                     | 0.69              |
| 3:A:1054:ARG:NH1  | 3:A:1123:GLY:O    | 2.25                     | 0.69              |
| 3:H:621:ARG:O     | 3:H:943:GLN:NE2   | 2.24                     | 0.69              |
| 3:B:724:HIS:CE1   | 3:B:1028:TYR:HB2  | 2.27                     | 0.69              |
| 3:D:745:HIS:CD2   | 3:D:754:CYS:HG    | 2.10                     | 0.69              |
| 3:J:603:ARG:NH1   | 3:J:706:ASP:OD2   | 2.18                     | 0.69              |
| 3:L:877:ALA:HB1   | 4:k:94:LEU:HD21   | 1.74                     | 0.69              |
| 3:M:164:GLN:O     | 3:M:168:ASN:ND2   | 2.24                     | 0.69              |
| 3:M:861:PRO:O     | 3:M:869:ASN:ND2   | 2.23                     | 0.69              |
| 3:H:827:THR:OG1   | 3:H:958:LEU:O     | 2.10                     | 0.69              |
| 3:O:728:ASP:O     | 3:O:810:LYS:NZ    | 2.26                     | 0.69              |
| 3:C:90:MET:HG2    | 3:C:91:ASN:O      | 1.92                     | 0.69              |
| 3:G:234:LEU:HD23  | 3:G:244:ILE:HD13  | 1.74                     | 0.69              |
| 2:Y:183:GLY:N     | 3:H:1170:GLN:HG3  | 2.07                     | 0.69              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:J:770:ASN:H    | 3:J:773:THR:HB   | 1.57                     | 0.69              |
| 3:K:69:ARG:HB2   | 3:K:72:GLU:HG2   | 1.72                     | 0.69              |
| 4:n:72:THR:HA    | 4:n:100:PRO:HB2  | 1.73                     | 0.69              |
| 3:O:676:THR:HG21 | 3:P:945:LEU:HD12 | 1.73                     | 0.69              |
| 2:X:284:GLN:CG   | 3:H:1166:PHE:CE1 | 2.59                     | 0.69              |
| 3:N:422:ASP:OD1  | 3:N:1354:ARG:NH2 | 2.26                     | 0.69              |
| 3:D:677:TYR:HA   | 4:d:95:LYS:NZ    | 2.07                     | 0.69              |
| 3:D:1029:PHE:HB3 | 3:D:1039:GLN:NE2 | 2.07                     | 0.69              |
| 2:X:99:ASN:OD1   | 3:C:1086:GLY:CA  | 2.40                     | 0.69              |
| 1:w:79:THR:N     | 3:O:308:GLU:OE2  | 2.25                     | 0.69              |
| 3:J:876:ASN:HA   | 3:J:879:PHE:HD2  | 1.56                     | 0.69              |
| 3:M:639:HIS:HA   | 4:m:79:PHE:CE2   | 2.28                     | 0.69              |
| 3:M:1257:TYR:HB2 | 3:M:1277:PHE:CD2 | 2.28                     | 0.69              |
| 3:N:96:GLN:HE22  | 3:D:12:ARG:N     | 1.89                     | 0.69              |
| 3:O:488:GLY:H    | 3:O:520:TRP:HH2  | 1.40                     | 0.69              |
| 3:D:107:ASP:OD1  | 3:D:108:GLY:N    | 2.25                     | 0.69              |
| 3:F:521:VAL:HG21 | 3:F:987:VAL:HG12 | 1.73                     | 0.69              |
| 1:w:282:PRO:HD2  | 3:L:138:GLU:CD   | 2.16                     | 0.69              |
| 3:A:491:VAL:HG21 | 3:A:929:PHE:HD2  | 1.57                     | 0.69              |
| 3:H:766:ALA:N    | 3:H:783:LEU:O    | 2.23                     | 0.69              |
| 3:E:854:PRO:HG3  | 3:E:862:ALA:HB3  | 1.73                     | 0.69              |
| 3:F:229:ASP:O    | 3:F:236:LYS:NZ   | 2.17                     | 0.69              |
| 1:w:283:ARG:HE   | 3:N:47:ASN:HD21  | 1.33                     | 0.69              |
| 3:I:1197:ASN:OD1 | 3:I:1200:ARG:NH1 | 2.26                     | 0.69              |
| 3:K:484:ALA:O    | 3:K:486:PRO:HD3  | 1.93                     | 0.69              |
| 3:K:1257:TYR:HB2 | 3:K:1277:PHE:CD2 | 2.27                     | 0.69              |
| 3:O:620:ASP:OD2  | 3:O:655:TYR:OH   | 2.11                     | 0.69              |
| 3:O:889:PRO:HA   | 3:O:892:LEU:HD12 | 1.75                     | 0.69              |
| 3:P:158:GLN:O    | 3:P:161:ALA:N    | 2.25                     | 0.69              |
| 3:B:69:ARG:HB2   | 3:B:72:GLU:HG2   | 1.75                     | 0.69              |
| 3:E:829:GLY:N    | 3:E:956:TYR:O    | 2.25                     | 0.69              |
| 3:F:58:LEU:HA    | 3:G:327:ARG:HB2  | 1.73                     | 0.69              |
| 3:G:23:ILE:CD1   | 3:G:167:ARG:HD2  | 2.23                     | 0.69              |
| 3:J:697:VAL:CG2  | 3:J:816:LEU:CD1  | 2.71                     | 0.69              |
| 3:L:756:ILE:HD12 | 3:L:763:PRO:HB3  | 1.75                     | 0.69              |
| 3:M:139:ALA:HB2  | 3:C:50:TYR:HE2   | 1.57                     | 0.69              |
| 3:P:669:SER:O    | 3:P:672:SER:OG   | 2.11                     | 0.69              |
| 3:B:274:VAL:HG11 | 3:B:376:PHE:CD2  | 2.28                     | 0.69              |
| 3:C:1000:SER:O   | 3:C:1003:ARG:NH1 | 2.26                     | 0.69              |
| 3:D:103:LEU:HD11 | 3:D:115:PRO:HA   | 1.75                     | 0.69              |
| 3:D:819:ALA:O    | 3:D:822:ARG:NH1  | 2.25                     | 0.69              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:G:54:PHE:O      | 3:G:55:ASP:CG     | 2.35                     | 0.69              |
| 1:Q:44:ARG:CA     | 3:B:322:MET:HE2   | 2.11                     | 0.69              |
| 3:J:697:VAL:HG22  | 3:J:816:LEU:CD1   | 2.23                     | 0.69              |
| 3:J:785:HIS:HD2   | 3:J:788:GLN:HE21  | 1.39                     | 0.69              |
| 3:K:1357:HIS:O    | 3:K:1360:GLN:N    | 2.26                     | 0.69              |
| 3:M:23:ILE:HA     | 3:D:259:VAL:HG12  | 1.75                     | 0.69              |
| 3:N:133:PHE:HB3   | 3:N:1091:PHE:HB2  | 1.73                     | 0.69              |
| 3:N:842:MET:HE1   | 3:N:891:MET:HB3   | 1.73                     | 0.69              |
| 3:D:861:PRO:O     | 3:D:869:ASN:ND2   | 2.25                     | 0.69              |
| 2:S:298:CYS:HB2   | 2:S:315:ILE:HD13  | 1.75                     | 0.68              |
| 1:W:25:ARG:CA     | 3:H:145:GLY:C     | 2.47                     | 0.68              |
| 3:A:1076:GLY:HA3  | 3:A:1096:PRO:HG2  | 1.75                     | 0.68              |
| 3:O:180:THR:HG22  | 3:O:1097:ARG:HH12 | 1.57                     | 0.68              |
| 3:P:90:MET:HG2    | 3:P:91:ASN:O      | 1.92                     | 0.68              |
| 3:P:879:PHE:O     | 3:P:883:ARG:N     | 2.19                     | 0.68              |
| 3:G:1131:LEU:O    | 3:G:1163:LEU:HD11 | 1.92                     | 0.68              |
| 3:L:180:THR:HG22  | 3:L:1097:ARG:HH12 | 1.58                     | 0.68              |
| 3:M:639:HIS:HA    | 4:m:79:PHE:HE2    | 1.58                     | 0.68              |
| 3:M:1257:TYR:HB2  | 3:M:1277:PHE:HD2  | 1.58                     | 0.68              |
| 3:A:231:SER:O     | 3:A:1112:THR:OG1  | 2.10                     | 0.68              |
| 4:o:62:THR:O      | 4:o:66:VAL:N      | 2.27                     | 0.68              |
| 3:D:708:THR:HG22  | 3:D:723:ASN:HD22  | 1.57                     | 0.68              |
| 3:D:880:HIS:NE2   | 4:c:98:TYR:HD2    | 1.90                     | 0.68              |
| 3:G:519:ARG:NE    | 3:G:523:GLU:OE2   | 2.15                     | 0.68              |
| 3:G:550:PHE:HD1   | 3:G:998:TYR:CD1   | 1.73                     | 0.68              |
| 1:W:25:ARG:O      | 3:H:145:GLY:CA    | 2.41                     | 0.68              |
| 3:M:491:VAL:HG21  | 3:M:929:PHE:HD2   | 1.58                     | 0.68              |
| 3:M:700:LEU:HD22  | 3:M:1025:MET:HG3  | 1.73                     | 0.68              |
| 3:O:898:ALA:HA    | 3:O:901:MET:HE2   | 1.74                     | 0.68              |
| 3:D:802:PRO:HG3   | 3:E:945:LEU:HD21  | 1.73                     | 0.68              |
| 3:D:1191:PRO:HG2  | 3:D:1194:THR:HG23 | 1.74                     | 0.68              |
| 3:E:133:PHE:HB3   | 3:E:1091:PHE:HB2  | 1.75                     | 0.68              |
| 3:E:195:LEU:O     | 3:E:198:LEU:N     | 2.24                     | 0.68              |
| 3:E:800:HIS:O     | 3:E:801:ARG:HG3   | 1.92                     | 0.68              |
| 3:G:99:VAL:HB     | 3:G:118:ASN:HB2   | 1.61                     | 0.68              |
| 3:I:621:ARG:NH2   | 3:H:698:GLU:OE1   | 2.26                     | 0.68              |
| 3:K:1296:THR:HG21 | 3:K:1327:LEU:HG   | 1.73                     | 0.68              |
| 3:A:843:VAL:O     | 3:A:876:ASN:ND2   | 2.26                     | 0.68              |
| 3:N:485:ASN:HD22  | 3:N:516:GLY:H     | 1.41                     | 0.68              |
| 3:P:1073:TYR:OH   | 3:P:1097:ARG:NH1  | 2.27                     | 0.68              |
| 3:B:863:HIS:CE1   | 3:B:887:ASP:HA    | 2.29                     | 0.68              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:E:293:LEU:HD13  | 3:E:368:VAL:HG11  | 1.74                     | 0.68              |
| 3:E:896:VAL:HA    | 3:E:899:HIS:CD2   | 2.27                     | 0.68              |
| 3:F:426:ALA:HA    | 3:G:1358:PHE:CE1  | 2.28                     | 0.68              |
| 1:W:328:TYR:HE1   | 6:r:18:PHE:CZ     | 2.00                     | 0.68              |
| 3:L:452:LEU:HD12  | 3:L:456:ASN:HD22  | 1.56                     | 0.68              |
| 3:M:620:ASP:OD2   | 3:M:655:TYR:OH    | 2.10                     | 0.68              |
| 3:M:1163:LEU:HD23 | 3:M:1169:ALA:HB2  | 1.76                     | 0.68              |
| 3:A:119:TYR:O     | 3:G:45:ASP:OD2    | 2.11                     | 0.68              |
| 3:H:495:ALA:O     | 3:H:504:ARG:NH1   | 2.27                     | 0.68              |
| 3:H:605:ALA:HA    | 3:H:1018:ASN:HD21 | 1.59                     | 0.68              |
| 3:B:1334:ILE:HA   | 3:B:1365:ASP:HB3  | 1.76                     | 0.68              |
| 3:K:198:LEU:O     | 3:K:201:MET:N     | 2.27                     | 0.68              |
| 3:K:485:ASN:HD21  | 3:K:516:GLY:N     | 1.91                     | 0.68              |
| 3:K:621:ARG:O     | 3:K:943:GLN:NE2   | 2.26                     | 0.68              |
| 3:H:1270:LEU:HD22 | 3:H:1303:ALA:HB2  | 1.75                     | 0.68              |
| 3:N:466:LEU:HD12  | 3:N:467:MET:HG3   | 1.76                     | 0.68              |
| 3:C:263:ARG:NH2   | 3:C:306:TYR:O     | 2.25                     | 0.68              |
| 3:D:351:LEU:HD23  | 3:D:351:LEU:C     | 2.19                     | 0.68              |
| 3:E:907:ALA:HB1   | 3:E:994:LEU:HD21  | 1.75                     | 0.68              |
| 3:F:766:ALA:N     | 3:F:783:LEU:O     | 2.26                     | 0.68              |
| 1:T:158:ALA:O     | 3:I:1165:VAL:HG22 | 1.93                     | 0.68              |
| 2:X:99:ASN:CG     | 3:C:1086:GLY:CA   | 2.65                     | 0.68              |
| 2:x:18:ARG:HG2    | 3:O:7:ASP:CG      | 2.19                     | 0.68              |
| 3:L:638:GLU:OE1   | 3:L:677:TYR:OH    | 2.11                     | 0.68              |
| 3:L:639:HIS:HA    | 4:l:79:PHE:CE2    | 2.29                     | 0.68              |
| 3:D:1177:MET:HE1  | 3:E:214:VAL:HG22  | 1.75                     | 0.68              |
| 3:E:1208:ARG:NH1  | 3:E:1240:ALA:O    | 2.26                     | 0.68              |
| 3:F:512:ARG:HD3   | 3:F:515:HIS:HD2   | 1.59                     | 0.68              |
| 3:I:106:ARG:HH21  | 3:I:110:HIS:HB3   | 1.59                     | 0.68              |
| 3:M:738:ASP:OD1   | 3:M:787:THR:OG1   | 2.12                     | 0.68              |
| 3:A:631:GLN:NE2   | 3:A:666:ASN:OD1   | 2.19                     | 0.68              |
| 3:O:512:ARG:HA    | 3:O:515:HIS:CD2   | 2.29                     | 0.68              |
| 3:B:752:ARG:NH2   | 3:B:915:ASP:HA    | 2.09                     | 0.68              |
| 3:I:948:THR:HA    | 4:h:79:PHE:HA     | 1.74                     | 0.68              |
| 3:J:801:ARG:HB3   | 3:J:802:PRO:HD2   | 1.75                     | 0.68              |
| 3:K:631:GLN:NE2   | 3:K:666:ASN:OD1   | 2.25                     | 0.68              |
| 3:L:876:ASN:HA    | 3:L:879:PHE:HD2   | 1.59                     | 0.68              |
| 3:O:1120:THR:HG22 | 3:O:1181:GLN:HE21 | 1.58                     | 0.68              |
| 3:B:1000:SER:O    | 3:B:1003:ARG:NH1  | 2.27                     | 0.68              |
| 3:C:843:VAL:O     | 3:C:876:ASN:ND2   | 2.26                     | 0.68              |
| 5:q:504:ILE:HG23  | 5:q:669:PHE:HB3   | 1.75                     | 0.68              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:F:829:GLY:N    | 3:F:956:TYR:O     | 2.27                     | 0.68              |
| 1:T:161:TRP:CD1  | 3:I:1166:PHE:CG   | 2.66                     | 0.68              |
| 3:M:466:LEU:HD12 | 3:M:467:MET:HG3   | 1.76                     | 0.68              |
| 3:A:329:LEU:C    | 3:G:61:TYR:HE2    | 1.97                     | 0.68              |
| 3:H:1257:TYR:HB2 | 3:H:1277:PHE:HD2  | 1.57                     | 0.68              |
| 3:D:460:THR:HA   | 3:D:1129:PHE:CD2  | 2.29                     | 0.68              |
| 3:E:736:VAL:HG12 | 3:E:738:ASP:H     | 1.59                     | 0.68              |
| 3:E:873:ASN:CG   | 4:d:92:PHE:H      | 2.02                     | 0.68              |
| 1:Q:45:ASP:N     | 3:B:322:MET:HE3   | 2.10                     | 0.67              |
| 3:K:793:ASP:OD1  | 3:K:798:ARG:NH2   | 2.27                     | 0.67              |
| 3:L:795:ALA:HB3  | 3:L:798:ARG:HG2   | 1.74                     | 0.67              |
| 4:k:59:ALA:O     | 4:k:62:THR:OG1    | 2.07                     | 0.67              |
| 3:B:639:HIS:HA   | 4:b:79:PHE:CE2    | 2.29                     | 0.67              |
| 3:B:837:ALA:HB2  | 4:b:54:LEU:HD21   | 1.75                     | 0.67              |
| 5:q:486:CYS:HB3  | 5:q:551:TYR:HE2   | 1.59                     | 0.67              |
| 3:E:198:LEU:O    | 3:E:201:MET:N     | 2.26                     | 0.67              |
| 3:G:52:VAL:CG1   | 3:G:54:PHE:CE2    | 2.78                     | 0.67              |
| 3:G:550:PHE:HD1  | 3:G:998:TYR:CE1   | 2.12                     | 0.67              |
| 3:J:350:THR:HG22 | 3:J:352:ASP:H     | 1.58                     | 0.67              |
| 4:o:90:PRO:HD3   | 3:P:834:ARG:HD3   | 1.75                     | 0.67              |
| 3:N:439:GLN:NE2  | 3:N:451:ARG:HH21  | 1.91                     | 0.67              |
| 3:O:548:ASP:OD1  | 3:O:576:ARG:NE    | 2.19                     | 0.67              |
| 3:C:766:ALA:O    | 3:C:785:HIS:N     | 2.24                     | 0.67              |
| 3:E:802:PRO:HD3  | 3:F:945:LEU:HD21  | 1.76                     | 0.67              |
| 3:F:466:LEU:HD12 | 3:F:467:MET:HG3   | 1.76                     | 0.67              |
| 3:F:524:CYS:SG   | 3:F:1008:GLN:NE2  | 2.68                     | 0.67              |
| 3:I:842:MET:HB2  | 4:i:22:MET:HG2    | 1.77                     | 0.67              |
| 3:K:410:ASN:O    | 3:K:415:ARG:NH1   | 2.27                     | 0.67              |
| 3:M:841:ASN:OD1  | 4:m:57:GLN:NE2    | 2.27                     | 0.67              |
| 3:H:1291:ARG:CZ  | 3:C:35:LEU:HD12   | 2.24                     | 0.67              |
| 4:p:33:GLN:HG2   | 4:p:35:ILE:H      | 1.59                     | 0.67              |
| 3:P:728:ASP:O    | 3:P:810:LYS:NZ    | 2.28                     | 0.67              |
| 3:P:1054:ARG:NH1 | 3:P:1123:GLY:O    | 2.27                     | 0.67              |
| 3:B:77:VAL:HG22  | 3:B:266:HIS:CD2   | 2.29                     | 0.67              |
| 3:B:738:ASP:OD1  | 3:B:787:THR:OG1   | 2.11                     | 0.67              |
| 3:D:397:ALA:HB3  | 3:D:1321:VAL:HG22 | 1.75                     | 0.67              |
| 5:q:61:GLN:HE21  | 5:q:63:ARG:HE     | 1.40                     | 0.67              |
| 3:G:950:GLN:HB2  | 3:G:953:GLU:HG3   | 1.75                     | 0.67              |
| 1:w:282:PRO:CD   | 3:L:138:GLU:OE2   | 2.43                     | 0.67              |
| 3:M:874:THR:H    | 3:M:877:ALA:HB3   | 1.57                     | 0.67              |
| 3:A:766:ALA:N    | 3:A:783:LEU:O     | 2.26                     | 0.67              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:H:907:ALA:HB1   | 3:H:994:LEU:HD21  | 1.76                     | 0.67              |
| 4:p:61:LEU:HD11   | 3:P:840:GLN:HG2   | 1.74                     | 0.67              |
| 3:N:1148:ARG:HH22 | 3:N:1163:LEU:HG   | 1.59                     | 0.67              |
| 3:O:633:ALA:O     | 3:O:635:HIS:ND1   | 2.24                     | 0.67              |
| 3:B:1217:ASP:OD1  | 3:B:1287:ARG:NH1  | 2.27                     | 0.67              |
| 3:D:195:LEU:O     | 3:D:198:LEU:N     | 2.27                     | 0.67              |
| 3:D:677:TYR:CD1   | 4:d:95:LYS:CE     | 2.77                     | 0.67              |
| 5:q:650:CYS:HB2   | 5:q:662:VAL:HB    | 1.76                     | 0.67              |
| 3:E:485:ASN:HD21  | 3:E:516:GLY:H     | 1.41                     | 0.67              |
| 3:F:843:VAL:O     | 3:F:876:ASN:ND2   | 2.21                     | 0.67              |
| 2:3:99:ASN:HD21   | 3:M:1086:GLY:HA3  | 1.60                     | 0.67              |
| 3:K:57:LEU:HD23   | 3:L:94:ARG:HG3    | 1.76                     | 0.67              |
| 3:M:451:ARG:O     | 3:M:1124:ASN:ND2  | 2.28                     | 0.67              |
| 3:M:452:LEU:HD12  | 3:M:456:ASN:HD22  | 1.59                     | 0.67              |
| 3:A:725:LEU:HG    | 3:A:731:LEU:HD11  | 1.76                     | 0.67              |
| 3:A:976:PHE:HE2   | 3:A:981:ARG:HG2   | 1.60                     | 0.67              |
| 3:H:923:THR:HA    | 3:H:926:MET:HE3   | 1.77                     | 0.67              |
| 4:o:64:LEU:HD11   | 3:O:844:VAL:HB    | 1.75                     | 0.67              |
| 3:N:1191:PRO:HG2  | 3:N:1194:THR:HG23 | 1.76                     | 0.67              |
| 3:P:728:ASP:OD2   | 3:P:1030:LYS:NZ   | 2.27                     | 0.67              |
| 3:C:469:ILE:HG23  | 3:C:472:ALA:HB3   | 1.77                     | 0.67              |
| 3:D:718:ALA:HB1   | 3:E:982:ASP:OD2   | 1.95                     | 0.67              |
| 3:D:1128:ASN:HD21 | 3:D:1155:ASN:ND2  | 1.92                     | 0.67              |
| 5:q:125:ASP:O     | 5:q:128:THR:OG1   | 2.11                     | 0.67              |
| 3:L:466:LEU:HD12  | 3:L:467:MET:HG3   | 1.76                     | 0.67              |
| 3:M:739:CYS:HA    | 3:M:742:LEU:HD12  | 1.77                     | 0.67              |
| 3:A:865:LEU:HD21  | 3:A:879:PHE:HB2   | 1.75                     | 0.67              |
| 3:H:896:VAL:HA    | 3:H:899:HIS:HD2   | 1.59                     | 0.67              |
| 3:O:63:ASN:HD21   | 3:P:99:VAL:HG13   | 1.59                     | 0.67              |
| 3:P:259:VAL:HG22  | 3:P:1102:LEU:HD13 | 1.76                     | 0.67              |
| 3:P:843:VAL:O     | 3:P:876:ASN:ND2   | 2.28                     | 0.67              |
| 3:P:844:VAL:HG11  | 3:P:892:LEU:HD21  | 1.77                     | 0.67              |
| 3:B:838:THR:O     | 3:B:875:VAL:HG22  | 1.95                     | 0.67              |
| 3:D:745:HIS:CE1   | 3:D:754:CYS:HG    | 2.12                     | 0.67              |
| 3:E:827:THR:OG1   | 3:E:958:LEU:O     | 2.11                     | 0.67              |
| 3:F:662:ALA:HB2   | 3:F:689:VAL:HG11  | 1.77                     | 0.67              |
| 3:F:873:ASN:HA    | 4:e:92:PHE:CD2    | 2.30                     | 0.67              |
| 3:J:766:ALA:N     | 3:J:783:LEU:O     | 2.26                     | 0.67              |
| 3:M:213:ARG:HH12  | 3:M:1216:GLY:HA3  | 1.59                     | 0.67              |
| 3:A:595:ARG:HD3   | 3:A:1026:ALA:HB1  | 1.77                     | 0.67              |
| 3:A:1031:MET:HE2  | 3:A:1048:PHE:CE2  | 2.26                     | 0.67              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:B:1120:THR:HG22 | 3:B:1181:GLN:HE21 | 1.59                     | 0.67              |
| 3:C:614:VAL:HG21  | 3:C:693:LEU:HD11  | 1.76                     | 0.67              |
| 3:E:1054:ARG:NH1  | 3:E:1123:GLY:O    | 2.27                     | 0.67              |
| 3:F:749:ASP:OD1   | 3:F:752:ARG:HB3   | 1.95                     | 0.67              |
| 3:G:404:LEU:HB2   | 3:G:1052:VAL:HB   | 1.76                     | 0.67              |
| 3:I:1000:SER:O    | 3:I:1003:ARG:NH1  | 2.28                     | 0.67              |
| 3:J:580:GLY:HA2   | 3:J:592:ARG:HH12  | 1.60                     | 0.67              |
| 3:A:433:ARG:O     | 3:A:1359:THR:OG1  | 2.10                     | 0.67              |
| 3:A:752:ARG:HA    | 3:A:913:ALA:HB3   | 1.76                     | 0.67              |
| 3:A:1031:MET:CE   | 3:A:1048:PHE:CZ   | 2.77                     | 0.67              |
| 3:H:98:GLU:OE2    | 3:C:11:TYR:CZ     | 2.47                     | 0.67              |
| 3:H:120:MET:HA    | 3:C:38:PHE:O      | 1.94                     | 0.67              |
| 3:N:870:LEU:HD22  | 3:N:877:ALA:HA    | 1.77                     | 0.67              |
| 3:O:546:ALA:CB    | 3:O:1031:MET:HE3  | 2.25                     | 0.67              |
| 3:O:625:ALA:HA    | 3:O:628:TYR:HD2   | 1.59                     | 0.67              |
| 3:P:1270:LEU:HD22 | 3:P:1303:ALA:HB2  | 1.76                     | 0.67              |
| 3:B:263:ARG:HD2   | 3:G:58:LEU:O      | 1.95                     | 0.67              |
| 5:q:654:ASN:OD1   | 5:q:655:ARG:N     | 2.27                     | 0.67              |
| 1:W:45:ASP:C      | 3:I:345:GLU:CG    | 2.66                     | 0.67              |
| 3:J:1225:LEU:HD22 | 3:J:1234:PRO:HG3  | 1.77                     | 0.67              |
| 3:K:843:VAL:O     | 3:K:876:ASN:ND2   | 2.27                     | 0.67              |
| 3:N:93:GLY:HA3    | 3:N:124:ILE:HD12  | 1.75                     | 0.67              |
| 3:C:947:HIS:HB2   | 4:b:79:PHE:HD1    | 1.60                     | 0.67              |
| 3:E:752:ARG:NH2   | 3:E:915:ASP:HA    | 2.08                     | 0.67              |
| 3:F:802:PRO:HG3   | 3:G:945:LEU:HD21  | 1.77                     | 0.67              |
| 3:F:1120:THR:HG22 | 3:F:1181:GLN:HE21 | 1.59                     | 0.67              |
| 3:F:1333:PRO:HG2  | 3:F:1366:ALA:H    | 1.59                     | 0.67              |
| 1:W:195:ALA:HA    | 1:W:198:TYR:CD2   | 2.30                     | 0.67              |
| 1:I:141:PRO:HG2   | 3:M:1166:PHE:HD2  | 1.08                     | 0.67              |
| 3:I:485:ASN:ND2   | 3:I:516:GLY:O     | 2.27                     | 0.67              |
| 3:I:1020:LEU:O    | 3:I:1023:ALA:N    | 2.28                     | 0.67              |
| 3:A:316:LEU:HD21  | 3:B:312:ASN:HD22  | 1.60                     | 0.67              |
| 4:k:61:LEU:O      | 4:k:65:GLY:N      | 2.28                     | 0.67              |
| 4:n:89:ARG:NH2    | 4:o:30:ASN:OD1    | 2.28                     | 0.67              |
| 3:N:1296:THR:HG21 | 3:N:1327:LEU:HG   | 1.77                     | 0.67              |
| 3:O:451:ARG:O     | 3:O:1124:ASN:ND2  | 2.28                     | 0.67              |
| 3:P:1225:LEU:HD22 | 3:P:1234:PRO:HG3  | 1.76                     | 0.67              |
| 3:B:621:ARG:O     | 3:B:943:GLN:NE2   | 2.27                     | 0.67              |
| 3:F:263:ARG:NH2   | 3:F:305:THR:OG1   | 2.27                     | 0.67              |
| 3:G:526:MET:CE    | 3:G:531:PHE:CD1   | 2.69                     | 0.67              |
| 1:T:78:ALA:CA     | 3:I:308:GLU:OE1   | 2.42                     | 0.66              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:Y:243:MET:SD    | 3:H:1145:VAL:HG22 | 2.35                     | 0.66              |
| 3:I:231:SER:O     | 3:I:1112:THR:OG1  | 2.13                     | 0.66              |
| 3:J:896:VAL:HA    | 3:J:899:HIS:HD2   | 1.59                     | 0.66              |
| 3:L:865:LEU:HD11  | 3:L:886:VAL:H     | 1.61                     | 0.66              |
| 3:B:238:GLY:HA2   | 3:B:244:ILE:HD11  | 1.76                     | 0.66              |
| 3:D:677:TYR:CD1   | 4:d:95:LYS:HE2    | 2.31                     | 0.66              |
| 5:q:65:HIS:CE1    | 5:q:470:PHE:H     | 2.13                     | 0.66              |
| 2:Y:241:LEU:HD12  | 2:Y:248:ARG:HH21  | 1.59                     | 0.66              |
| 3:I:451:ARG:NH1   | 3:J:529:GLU:OE2   | 2.27                     | 0.66              |
| 4:p:22:MET:HA     | 4:p:25:LEU:HB3    | 1.77                     | 0.66              |
| 3:O:469:ILE:HD11  | 3:O:547:PHE:CE1   | 2.30                     | 0.66              |
| 3:P:227:PHE:O     | 3:P:231:SER:OG    | 2.11                     | 0.66              |
| 3:B:219:LEU:O     | 3:B:222:GLU:N     | 2.28                     | 0.66              |
| 3:B:548:ASP:OD1   | 3:B:576:ARG:NE    | 2.27                     | 0.66              |
| 3:C:1225:LEU:HD22 | 3:C:1234:PRO:HG3  | 1.77                     | 0.66              |
| 3:D:730:ALA:HB2   | 3:D:752:ARG:HH11  | 1.60                     | 0.66              |
| 2:X:99:ASN:HD21   | 3:C:1086:GLY:HA3  | 1.59                     | 0.66              |
| 3:J:485:ASN:HD21  | 3:J:516:GLY:N     | 1.93                     | 0.66              |
| 3:J:827:THR:OG1   | 3:J:958:LEU:O     | 2.10                     | 0.66              |
| 3:K:1049:GLY:O    | 3:K:1190:THR:N    | 2.25                     | 0.66              |
| 3:K:1191:PRO:HG2  | 3:K:1194:THR:HG23 | 1.78                     | 0.66              |
| 3:L:896:VAL:HA    | 3:L:899:HIS:HD2   | 1.60                     | 0.66              |
| 3:M:161:ALA:CA    | 3:C:50:TYR:CE1    | 2.78                     | 0.66              |
| 3:E:180:THR:HG22  | 3:E:1097:ARG:NH1  | 2.11                     | 0.66              |
| 3:F:108:GLY:HA2   | 3:F:110:HIS:H     | 1.60                     | 0.66              |
| 2:R:174:PRO:HD3   | 5:q:371:GLY:HA3   | 1.76                     | 0.66              |
| 1:T:165:LEU:CG    | 3:I:1166:PHE:CE1  | 2.78                     | 0.66              |
| 1:T:259:GLU:OE1   | 3:I:1315:PRO:HB3  | 1.95                     | 0.66              |
| 3:K:90:MET:HG2    | 3:K:91:ASN:O      | 1.95                     | 0.66              |
| 3:K:756:ILE:HB    | 3:K:763:PRO:HD3   | 1.75                     | 0.66              |
| 3:K:1120:THR:HG22 | 3:K:1181:GLN:HE21 | 1.61                     | 0.66              |
| 3:M:1128:ASN:OD1  | 3:M:1155:ASN:ND2  | 2.28                     | 0.66              |
| 3:B:107:ASP:OD1   | 3:G:128:ALA:O     | 2.13                     | 0.66              |
| 3:B:263:ARG:CB    | 3:G:59:GLY:HA2    | 2.25                     | 0.66              |
| 3:B:1257:TYR:HB2  | 3:B:1277:PHE:HD2  | 1.59                     | 0.66              |
| 3:D:548:ASP:OD1   | 3:D:576:ARG:NE    | 2.25                     | 0.66              |
| 3:G:829:GLY:HA3   | 3:G:956:TYR:CZ    | 2.31                     | 0.66              |
| 3:K:133:PHE:HB3   | 3:K:1091:PHE:HB2  | 1.77                     | 0.66              |
| 4:o:72:THR:HA     | 4:o:100:PRO:HB2   | 1.78                     | 0.66              |
| 3:P:310:VAL:HG12  | 3:P:312:ASN:H     | 1.59                     | 0.66              |
| 3:B:580:GLY:HA2   | 3:B:592:ARG:HH12  | 1.60                     | 0.66              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:C:615:ARG:HH21  | 3:C:1017:GLU:HG2  | 1.61                     | 0.66              |
| 1:Q:45:ASP:H      | 3:B:322:MET:HE3   | 1.61                     | 0.66              |
| 1:1:112:ARG:HG2   | 1:1:264:THR:HG22  | 1.76                     | 0.66              |
| 3:I:698:GLU:OE2   | 3:J:621:ARG:NH2   | 2.29                     | 0.66              |
| 3:K:840:GLN:HG2   | 4:k:61:LEU:HD11   | 1.78                     | 0.66              |
| 3:H:322:MET:HE1   | 3:D:324:LYS:C     | 2.21                     | 0.66              |
| 3:N:467:MET:O     | 3:N:922:SER:OG    | 2.13                     | 0.66              |
| 3:O:546:ALA:CB    | 3:O:1031:MET:CE   | 2.73                     | 0.66              |
| 3:B:261:VAL:N     | 3:G:61:TYR:O      | 2.28                     | 0.66              |
| 3:B:351:LEU:HD23  | 3:G:58:LEU:HD13   | 1.77                     | 0.66              |
| 3:C:310:VAL:HG12  | 3:C:312:ASN:H     | 1.59                     | 0.66              |
| 3:C:947:HIS:O     | 4:b:80:ALA:N      | 2.18                     | 0.66              |
| 3:C:1129:PHE:O    | 3:C:1132:GLY:N    | 2.28                     | 0.66              |
| 3:D:638:GLU:HB2   | 3:D:789:ALA:HA    | 1.76                     | 0.66              |
| 5:q:259:GLU:HA    | 5:q:262:ALA:HB3   | 1.77                     | 0.66              |
| 1:W:352:ILE:CB    | 6:r:12:VAL:HG11   | 2.25                     | 0.66              |
| 3:L:494:PRO:HD3   | 3:L:909:LEU:HD12  | 1.77                     | 0.66              |
| 3:M:512:ARG:HA    | 3:M:515:HIS:HD2   | 1.60                     | 0.66              |
| 3:A:607:ALA:O     | 3:A:610:THR:OG1   | 2.13                     | 0.66              |
| 3:N:421:GLY:HA3   | 3:O:420:ALA:HB2   | 1.77                     | 0.66              |
| 3:P:231:SER:O     | 3:P:1112:THR:OG1  | 2.14                     | 0.66              |
| 3:B:638:GLU:HB2   | 3:B:789:ALA:HA    | 1.76                     | 0.66              |
| 5:q:584:ASP:O     | 5:q:654:ASN:ND2   | 2.29                     | 0.66              |
| 3:F:426:ALA:HA    | 3:G:1358:PHE:CD1  | 2.31                     | 0.66              |
| 3:G:742:LEU:CD2   | 3:G:756:ILE:CD1   | 2.69                     | 0.66              |
| 3:G:1282:ILE:HD12 | 3:G:1282:ILE:N    | 2.11                     | 0.66              |
| 3:J:836:TYR:HD1   | 3:J:897:LEU:HD13  | 1.59                     | 0.66              |
| 3:J:1321:VAL:HG12 | 3:J:1322:GLU:H    | 1.58                     | 0.66              |
| 3:K:227:PHE:O     | 3:K:231:SER:OG    | 2.09                     | 0.66              |
| 3:M:410:ASN:O     | 3:M:415:ARG:NH1   | 2.27                     | 0.66              |
| 3:A:767:ALA:HA    | 3:A:785:HIS:HB3   | 1.77                     | 0.66              |
| 3:H:485:ASN:ND2   | 3:H:516:GLY:O     | 2.28                     | 0.66              |
| 3:N:293:LEU:HD13  | 3:N:368:VAL:HG11  | 1.78                     | 0.66              |
| 3:O:259:VAL:HG22  | 3:O:1102:LEU:HD13 | 1.77                     | 0.66              |
| 3:P:229:ASP:O     | 3:P:236:LYS:NZ    | 2.22                     | 0.66              |
| 3:D:122:LYS:NZ    | 3:D:1101:ASP:O    | 2.25                     | 0.66              |
| 3:F:134:SER:HB3   | 3:G:114:GLN:NE2   | 2.09                     | 0.66              |
| 3:G:100:HIS:HA    | 3:G:117:HIS:HA    | 1.77                     | 0.66              |
| 1:W:283:ARG:HD2   | 3:B:47:ASN:HB3    | 1.78                     | 0.66              |
| 2:3:300:PHE:CE2   | 3:M:1083:HIS:CG   | 2.83                     | 0.66              |
| 3:K:898:ALA:HB2   | 4:k:58:ALA:HB1    | 1.78                     | 0.66              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:N:714:LEU:HD12  | 3:N:722:LEU:HD22  | 1.78                     | 0.66              |
| 3:N:863:HIS:HE1   | 3:N:887:ASP:HA    | 1.61                     | 0.66              |
| 3:C:631:GLN:NE2   | 3:C:666:ASN:OD1   | 2.26                     | 0.66              |
| 3:E:877:ALA:HB1   | 4:d:94:LEU:HD21   | 1.78                     | 0.66              |
| 3:G:234:LEU:HD23  | 3:G:244:ILE:CD1   | 2.26                     | 0.66              |
| 3:G:451:ARG:HE    | 3:G:453:SER:HB3   | 1.59                     | 0.66              |
| 2:2:302:GLY:O     | 3:E:111:PRO:HB3   | 1.95                     | 0.66              |
| 3:I:90:MET:HG2    | 3:I:91:ASN:O      | 1.96                     | 0.66              |
| 3:K:736:VAL:HG12  | 3:K:738:ASP:H     | 1.61                     | 0.66              |
| 3:L:620:ASP:OD2   | 3:L:655:TYR:OH    | 2.14                     | 0.66              |
| 3:H:1058:PHE:CE2  | 3:H:1369:LEU:HD11 | 2.31                     | 0.66              |
| 4:l:61:LEU:O      | 4:l:65:GLY:N      | 2.28                     | 0.66              |
| 3:O:107:ASP:OD1   | 3:O:108:GLY:N     | 2.28                     | 0.66              |
| 3:O:753:ASP:O     | 3:O:911:SER:OG    | 2.11                     | 0.66              |
| 3:B:90:MET:O      | 3:B:126:ARG:NH1   | 2.28                     | 0.66              |
| 3:B:196:ALA:HB1   | 3:B:227:PHE:HA    | 1.77                     | 0.66              |
| 3:C:896:VAL:HA    | 3:C:899:HIS:CD2   | 2.30                     | 0.66              |
| 3:F:448:GLN:CG    | 3:G:1201:ARG:HH12 | 2.08                     | 0.66              |
| 3:G:1232:SER:HB2  | 3:G:1237:PRO:O    | 1.96                     | 0.66              |
| 2:U:99:ASN:OD1    | 3:I:1086:GLY:HA2  | 1.95                     | 0.65              |
| 2:V:298:CYS:HB2   | 2:V:315:ILE:HD13  | 1.77                     | 0.65              |
| 2:X:40:GLN:NE2    | 3:H:128:ALA:CB    | 2.45                     | 0.65              |
| 2:X:99:ASN:ND2    | 3:C:1086:GLY:O    | 2.28                     | 0.65              |
| 3:I:512:ARG:HA    | 3:I:515:HIS:HD2   | 1.60                     | 0.65              |
| 3:I:1029:PHE:HB3  | 3:I:1039:GLN:NE2  | 2.11                     | 0.65              |
| 3:K:1131:LEU:HD23 | 3:K:1159:PRO:HG3  | 1.77                     | 0.65              |
| 3:L:1365:ASP:O    | 3:L:1370:LYS:NZ   | 2.26                     | 0.65              |
| 3:M:410:ASN:ND2   | 3:M:1359:THR:O    | 2.29                     | 0.65              |
| 3:M:1058:PHE:CE2  | 3:M:1369:LEU:HD11 | 2.31                     | 0.65              |
| 3:A:439:GLN:HE22  | 3:A:451:ARG:HH21  | 1.43                     | 0.65              |
| 3:H:728:ASP:O     | 3:H:810:LYS:NZ    | 2.29                     | 0.65              |
| 3:N:96:GLN:NE2    | 3:D:12:ARG:N      | 2.36                     | 0.65              |
| 3:P:103:LEU:HD11  | 3:P:115:PRO:HA    | 1.76                     | 0.65              |
| 3:B:752:ARG:NH2   | 3:B:915:ASP:OD1   | 2.26                     | 0.65              |
| 2:Y:248:ARG:CZ    | 3:H:1141:ASN:ND2  | 2.59                     | 0.65              |
| 3:J:433:ARG:NH1   | 3:J:1339:ASP:OD2  | 2.28                     | 0.65              |
| 3:A:201:MET:HE1   | 3:A:1293:ILE:HA   | 1.79                     | 0.65              |
| 3:P:274:VAL:HG11  | 3:P:376:PHE:CD2   | 2.31                     | 0.65              |
| 3:P:788:GLN:NE2   | 3:P:794:ALA:HA    | 2.11                     | 0.65              |
| 3:B:225:ARG:HH22  | 3:G:447:HIS:CE1   | 2.14                     | 0.65              |
| 3:B:752:ARG:HA    | 3:B:913:ALA:HB3   | 1.77                     | 0.65              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 3:B:1163:LEU:HD23 | 3:B:1169:ALA:HB2 | 1.78                     | 0.65              |
| 3:C:950:GLN:HB2   | 3:C:953:GLU:HG3  | 1.77                     | 0.65              |
| 3:E:1000:SER:O    | 3:E:1003:ARG:NH1 | 2.29                     | 0.65              |
| 1:w:79:THR:HB     | 3:O:308:GLU:CD   | 2.21                     | 0.65              |
| 3:H:398:MET:HB2   | 3:H:1058:PHE:HB2 | 1.79                     | 0.65              |
| 3:N:736:VAL:HG12  | 3:N:738:ASP:H    | 1.62                     | 0.65              |
| 3:P:717:GLN:HE22  | 3:P:752:ARG:HH12 | 1.42                     | 0.65              |
| 3:B:89:TYR:CZ     | 3:G:35:LEU:HD13  | 2.31                     | 0.65              |
| 3:E:753:ASP:HB3   | 3:E:755:ARG:NH2  | 2.11                     | 0.65              |
| 6:s:79:ASP:OD1    | 6:s:82:ARG:NH2   | 2.26                     | 0.65              |
| 3:J:469:ILE:CD1   | 3:J:547:PHE:CZ   | 2.73                     | 0.65              |
| 3:A:512:ARG:HA    | 3:A:515:HIS:CD2  | 2.31                     | 0.65              |
| 3:A:717:GLN:HE22  | 3:A:752:ARG:CZ   | 2.10                     | 0.65              |
| 3:N:180:THR:HG22  | 3:N:1097:ARG:NH1 | 2.11                     | 0.65              |
| 3:O:543:LEU:HB2   | 3:O:549:PHE:HE2  | 1.60                     | 0.65              |
| 3:O:724:HIS:CE1   | 3:O:1028:TYR:HB2 | 2.31                     | 0.65              |
| 3:E:512:ARG:HA    | 3:E:515:HIS:CD2  | 2.32                     | 0.65              |
| 3:G:697:VAL:HG22  | 3:G:816:LEU:CD1  | 2.24                     | 0.65              |
| 3:J:638:GLU:HB2   | 3:J:789:ALA:HA   | 1.78                     | 0.65              |
| 3:K:107:ASP:OD1   | 3:K:108:GLY:N    | 2.30                     | 0.65              |
| 3:K:738:ASP:OD2   | 3:K:801:ARG:NH1  | 2.30                     | 0.65              |
| 3:M:46:GLU:CD     | 3:M:48:SER:H     | 2.04                     | 0.65              |
| 3:A:718:ALA:HB3   | 3:A:721:GLU:HG3  | 1.79                     | 0.65              |
| 3:O:426:ALA:HB3   | 3:O:429:HIS:HD2  | 1.62                     | 0.65              |
| 3:D:756:ILE:HB    | 3:D:763:PRO:HD3  | 1.77                     | 0.65              |
| 3:D:839:LEU:HB3   | 3:D:894:LEU:HD11 | 1.79                     | 0.65              |
| 2:V:100:LEU:HD13  | 2:V:314:VAL:HG21 | 1.78                     | 0.65              |
| 2:3:284:GLN:HG2   | 3:D:1166:PHE:HZ  | 1.56                     | 0.65              |
| 3:M:180:THR:HG22  | 3:M:1097:ARG:NH1 | 2.12                     | 0.65              |
| 3:A:87:LEU:HD21   | 3:A:126:ARG:HG2  | 1.78                     | 0.65              |
| 3:A:548:ASP:OD1   | 3:A:576:ARG:NE   | 2.17                     | 0.65              |
| 3:H:227:PHE:O     | 3:H:231:SER:OG   | 2.15                     | 0.65              |
| 3:B:105:ALA:HB2   | 3:G:176:PHE:CE1  | 2.32                     | 0.65              |
| 3:B:133:PHE:HB3   | 3:B:1091:PHE:HB2 | 1.78                     | 0.65              |
| 3:C:293:LEU:HD13  | 3:C:368:VAL:HG11 | 1.79                     | 0.65              |
| 3:C:1344:ARG:O    | 3:C:1347:ARG:HG2 | 1.97                     | 0.65              |
| 3:D:745:HIS:CD2   | 3:D:754:CYS:SG   | 2.88                     | 0.65              |
| 3:F:827:THR:OG1   | 3:F:958:LEU:O    | 2.13                     | 0.65              |
| 3:F:873:ASN:CA    | 4:e:92:PHE:HB2   | 2.19                     | 0.65              |
| 3:G:99:VAL:CG1    | 3:G:118:ASN:HD22 | 2.08                     | 0.65              |
| 3:G:827:THR:OG1   | 3:G:958:LEU:O    | 2.13                     | 0.65              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:G:1148:ARG:HH22 | 3:G:1162:PRO:HA   | 1.62                     | 0.65              |
| 1:W:352:ILE:CB    | 6:r:12:VAL:CG1    | 2.75                     | 0.65              |
| 1:w:259:GLU:OE1   | 3:O:1315:PRO:CB   | 2.45                     | 0.65              |
| 3:I:1342:LEU:HD21 | 3:I:1362:LEU:HB2  | 1.79                     | 0.65              |
| 3:K:455:GLU:OE1   | 3:L:530:GLN:NE2   | 2.29                     | 0.65              |
| 3:L:778:ARG:O     | 3:L:904:ARG:NH2   | 2.28                     | 0.65              |
| 3:H:98:GLU:HG3    | 3:C:11:TYR:OH     | 1.96                     | 0.65              |
| 3:H:721:GLU:O     | 3:H:1030:LYS:NZ   | 2.27                     | 0.65              |
| 3:O:90:MET:HG2    | 3:O:91:ASN:O      | 1.96                     | 0.65              |
| 3:O:842:MET:HE1   | 3:O:891:MET:HE3   | 1.78                     | 0.65              |
| 3:P:315:ASN:ND2   | 3:P:326:VAL:O     | 2.28                     | 0.65              |
| 3:B:742:LEU:HD22  | 3:B:756:ILE:HD13  | 1.77                     | 0.65              |
| 3:I:1072:ALA:HB2  | 3:I:1102:LEU:HD23 | 1.79                     | 0.65              |
| 3:L:1034:VAL:HG22 | 3:L:1147:LEU:HD21 | 1.78                     | 0.65              |
| 3:M:16:ALA:HB2    | 3:D:96:GLN:OE1    | 1.97                     | 0.65              |
| 3:O:463:HIS:ND1   | 3:O:464:PRO:HD2   | 2.12                     | 0.65              |
| 3:O:546:ALA:CA    | 3:O:1031:MET:CE   | 2.66                     | 0.65              |
| 1:W:347:PHE:HZ    | 6:r:18:PHE:CE2    | 2.15                     | 0.65              |
| 3:J:843:VAL:O     | 3:J:876:ASN:ND2   | 2.30                     | 0.65              |
| 3:L:42:VAL:HG13   | 3:L:46:GLU:HG3    | 1.79                     | 0.65              |
| 3:L:576:ARG:HH11  | 3:L:582:LEU:HD23  | 1.62                     | 0.65              |
| 3:L:1120:THR:HG22 | 3:L:1181:GLN:HE21 | 1.62                     | 0.65              |
| 3:A:335:HIS:NE2   | 3:A:339:MET:SD    | 2.69                     | 0.65              |
| 4:i:62:THR:O      | 4:i:66:VAL:N      | 2.29                     | 0.65              |
| 3:O:103:LEU:HD11  | 3:O:115:PRO:HA    | 1.78                     | 0.65              |
| 3:O:631:GLN:NE2   | 3:O:666:ASN:OD1   | 2.26                     | 0.65              |
| 3:C:800:HIS:O     | 3:C:801:ARG:HG3   | 1.97                     | 0.65              |
| 3:D:163:GLN:HE22  | 3:E:348:ARG:HH22  | 1.45                     | 0.65              |
| 5:q:260:ILE:H     | 5:q:261:LEU:HB2   | 1.60                     | 0.65              |
| 5:q:495:ARG:HA    | 6:s:36:TRP:HZ3    | 1.61                     | 0.65              |
| 6:r:80:ILE:HB     | 7:u:3104:PHE:CE2  | 2.32                     | 0.65              |
| 3:F:1054:ARG:NH2  | 3:F:1122:MET:HB3  | 2.11                     | 0.65              |
| 3:G:103:LEU:HD11  | 3:G:115:PRO:CA    | 2.15                     | 0.65              |
| 1:W:112:ARG:HG2   | 1:W:264:THR:HG22  | 1.79                     | 0.65              |
| 1:w:283:ARG:CZ    | 3:N:47:ASN:ND2    | 2.57                     | 0.65              |
| 2:x:300:PHE:HB3   | 3:O:1083:HIS:NE2  | 2.10                     | 0.65              |
| 3:J:752:ARG:NH2   | 3:J:915:ASP:OD1   | 2.30                     | 0.65              |
| 3:K:1237:PRO:HD2  | 3:K:1238:PHE:N    | 2.12                     | 0.65              |
| 3:M:50:TYR:CE1    | 3:C:161:ALA:HA    | 2.31                     | 0.65              |
| 3:M:766:ALA:N     | 3:M:783:LEU:O     | 2.30                     | 0.65              |
| 4:m:60:ALA:HA     | 4:m:63:ASP:HB2    | 1.78                     | 0.65              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:N:620:ASP:OD2  | 3:N:655:TYR:OH    | 2.15                     | 0.65              |
| 3:O:644:LEU:HD22 | 3:O:647:LEU:HD12  | 1.79                     | 0.65              |
| 3:O:1000:SER:O   | 3:O:1003:ARG:NH1  | 2.30                     | 0.65              |
| 3:O:1248:GLN:O   | 3:O:1251:SER:OG   | 2.12                     | 0.65              |
| 3:D:180:THR:HG22 | 3:D:1097:ARG:HH12 | 1.61                     | 0.65              |
| 3:D:293:LEU:HD13 | 3:D:368:VAL:HG11  | 1.78                     | 0.65              |
| 3:D:906:THR:OG1  | 3:D:934:HIS:HB3   | 1.96                     | 0.65              |
| 3:F:745:HIS:HE1  | 3:F:754:CYS:HA    | 1.61                     | 0.65              |
| 3:F:756:ILE:HD12 | 3:F:763:PRO:HG3   | 1.79                     | 0.65              |
| 3:F:896:VAL:HA   | 3:F:899:HIS:CD2   | 2.32                     | 0.65              |
| 3:J:497:PRO:HG2  | 3:J:500:ASP:HB2   | 1.79                     | 0.64              |
| 3:L:135:LEU:HD21 | 3:L:165:LEU:HD21  | 1.79                     | 0.64              |
| 3:B:752:ARG:HH22 | 3:B:915:ASP:HA    | 1.63                     | 0.64              |
| 3:B:1292:LEU:HB3 | 3:B:1327:LEU:HD21 | 1.78                     | 0.64              |
| 5:q:89:ILE:HG22  | 5:q:383:ILE:HD13  | 1.78                     | 0.64              |
| 3:E:178:ARG:HB3  | 3:F:104:ILE:HG22  | 1.77                     | 0.64              |
| 3:G:550:PHE:HD2  | 3:G:550:PHE:O     | 1.80                     | 0.64              |
| 1:I:141:PRO:HB2  | 3:M:1165:VAL:HG11 | 1.77                     | 0.64              |
| 3:L:800:HIS:O    | 3:L:801:ARG:HG2   | 1.97                     | 0.64              |
| 3:H:866:HIS:O    | 3:H:870:LEU:N     | 2.24                     | 0.64              |
| 3:P:827:THR:OG1  | 3:P:958:LEU:O     | 2.15                     | 0.64              |
| 5:q:530:LEU:HD23 | 5:q:649:LEU:HD12  | 1.79                     | 0.64              |
| 3:F:390:VAL:CG2  | 3:G:104:ILE:HG12  | 2.22                     | 0.64              |
| 3:F:829:GLY:HA2  | 3:F:905:THR:HG21  | 1.78                     | 0.64              |
| 3:G:469:ILE:HD11 | 3:G:547:PHE:CE2   | 2.30                     | 0.64              |
| 3:I:548:ASP:OD1  | 3:I:576:ARG:NE    | 2.23                     | 0.64              |
| 3:L:861:PRO:O    | 3:L:869:ASN:ND2   | 2.28                     | 0.64              |
| 3:M:838:THR:O    | 3:M:875:VAL:HG22  | 1.97                     | 0.64              |
| 3:H:324:LYS:O    | 3:D:322:MET:HE2   | 1.97                     | 0.64              |
| 3:H:770:ASN:H    | 3:H:773:THR:HB    | 1.61                     | 0.64              |
| 3:O:838:THR:O    | 3:O:875:VAL:HG22  | 1.97                     | 0.64              |
| 3:B:107:ASP:OD1  | 3:B:108:GLY:N     | 2.31                     | 0.64              |
| 3:D:740:ASP:OD2  | 3:D:801:ARG:NH1   | 2.29                     | 0.64              |
| 3:F:634:ILE:HA   | 3:F:640:VAL:HG11  | 1.78                     | 0.64              |
| 3:I:873:ASN:O    | 4:h:89:ARG:NH1    | 2.31                     | 0.64              |
| 3:I:1201:ARG:NH2 | 3:H:446:ASP:OD2   | 2.30                     | 0.64              |
| 3:K:764:VAL:O    | 3:K:783:LEU:N     | 2.30                     | 0.64              |
| 3:D:1072:ALA:HB2 | 3:D:1102:LEU:HD23 | 1.80                     | 0.64              |
| 3:E:714:LEU:HD12 | 3:E:722:LEU:HD22  | 1.79                     | 0.64              |
| 3:F:432:PRO:HB2  | 3:G:413:MET:SD    | 2.38                     | 0.64              |
| 3:F:914:PRO:HG3  | 3:F:923:THR:HG22  | 1.79                     | 0.64              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:F:1197:ASN:OD1  | 3:F:1200:ARG:NH1  | 2.29                     | 0.64              |
| 3:G:497:PRO:HD2   | 3:G:504:ARG:NH2   | 2.12                     | 0.64              |
| 1:I:141:PRO:HG3   | 3:M:1166:PHE:HD2  | 1.17                     | 0.64              |
| 3:J:69:ARG:HB2    | 3:J:72:GLU:HG2    | 1.80                     | 0.64              |
| 3:K:1270:LEU:HD22 | 3:K:1303:ALA:HB2  | 1.79                     | 0.64              |
| 3:M:631:GLN:NE2   | 3:M:666:ASN:OD1   | 2.26                     | 0.64              |
| 3:M:878:MET:O     | 3:M:882:GLY:N     | 2.29                     | 0.64              |
| 3:B:261:VAL:HB    | 3:G:61:TYR:C      | 2.20                     | 0.64              |
| 3:B:467:MET:O     | 3:B:922:SER:OG    | 2.15                     | 0.64              |
| 3:D:1257:TYR:HB2  | 3:D:1277:PHE:CD2  | 2.26                     | 0.64              |
| 5:q:89:ILE:CG2    | 5:q:383:ILE:HD13  | 2.28                     | 0.64              |
| 5:q:402:TYR:HB2   | 5:q:405:SER:HB3   | 1.79                     | 0.64              |
| 3:F:52:VAL:HG11   | 3:G:320:LEU:HD21  | 1.79                     | 0.64              |
| 3:F:866:HIS:ND1   | 3:F:867:PRO:HD2   | 2.12                     | 0.64              |
| 3:G:507:ASN:HA    | 3:G:510:ARG:HE    | 1.62                     | 0.64              |
| 3:I:1347:ARG:NH1  | 3:J:1350:GLU:OE2  | 2.29                     | 0.64              |
| 3:K:651:CYS:O     | 3:K:654:SER:OG    | 2.12                     | 0.64              |
| 3:L:29:VAL:HG11   | 3:O:120:MET:SD    | 2.37                     | 0.64              |
| 3:L:895:GLN:NE2   | 4:l:62:THR:HA     | 2.12                     | 0.64              |
| 3:M:577:VAL:HG12  | 3:M:578:VAL:HG13  | 1.79                     | 0.64              |
| 3:A:822:ARG:NH1   | 3:A:1017:GLU:OE2  | 2.31                     | 0.64              |
| 3:H:765:TYR:HD1   | 3:H:783:LEU:HB2   | 1.62                     | 0.64              |
| 3:N:827:THR:OG1   | 3:N:958:LEU:O     | 2.15                     | 0.64              |
| 3:D:786:ASN:ND2   | 3:D:901:MET:O     | 2.31                     | 0.64              |
| 3:D:845:PRO:HG3   | 3:D:869:ASN:ND2   | 2.13                     | 0.64              |
| 3:E:863:HIS:CE1   | 3:E:887:ASP:HA    | 2.29                     | 0.64              |
| 3:G:830:VAL:N     | 3:G:956:TYR:HE1   | 1.96                     | 0.64              |
| 3:I:914:PRO:HG3   | 3:I:923:THR:HG22  | 1.80                     | 0.64              |
| 3:J:214:VAL:O     | 3:J:217:ALA:N     | 2.30                     | 0.64              |
| 3:L:90:MET:HG2    | 3:L:91:ASN:O      | 1.98                     | 0.64              |
| 3:L:684:GLU:OE1   | 3:M:660:ARG:HG2   | 1.98                     | 0.64              |
| 3:L:840:GLN:HB3   | 4:l:57:GLN:HB3    | 1.78                     | 0.64              |
| 3:M:90:MET:HG2    | 3:M:91:ASN:O      | 1.98                     | 0.64              |
| 3:M:769:CYS:HB2   | 3:M:786:ASN:HD21  | 1.62                     | 0.64              |
| 3:M:1125:LEU:HD22 | 3:M:1184:VAL:HG22 | 1.79                     | 0.64              |
| 3:H:108:GLY:HA2   | 3:H:110:HIS:H     | 1.63                     | 0.64              |
| 3:B:155:LEU:HD22  | 3:C:340:GLN:HG3   | 1.79                     | 0.64              |
| 3:F:1292:LEU:HB3  | 3:F:1327:LEU:HD21 | 1.78                     | 0.64              |
| 2:R:174:PRO:HA    | 5:q:371:GLY:N     | 2.12                     | 0.64              |
| 3:K:231:SER:O     | 3:K:1112:THR:OG1  | 2.14                     | 0.64              |
| 3:M:161:ALA:HA    | 3:C:50:TYR:HE1    | 1.62                     | 0.64              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:M:1221:ASP:O    | 3:M:1224:ALA:N    | 2.30                     | 0.64              |
| 3:H:898:ALA:HA    | 3:H:901:MET:HE2   | 1.80                     | 0.64              |
| 3:C:180:THR:HG22  | 3:C:1097:ARG:HH12 | 1.63                     | 0.64              |
| 5:q:504:ILE:HB    | 6:s:26:PHE:CE1    | 2.33                     | 0.64              |
| 3:E:639:HIS:HA    | 4:e:79:PHE:CE2    | 2.33                     | 0.64              |
| 3:E:1059:VAL:HG11 | 3:E:1116:ARG:HD3  | 1.80                     | 0.64              |
| 3:F:390:VAL:HG21  | 3:G:104:ILE:HD11  | 1.77                     | 0.64              |
| 3:F:853:CYS:HB2   | 4:f:101:PHE:CD1   | 2.33                     | 0.64              |
| 3:G:99:VAL:CB     | 3:G:118:ASN:CB    | 2.61                     | 0.64              |
| 1:w:282:PRO:HD2   | 3:L:138:GLU:OE2   | 1.98                     | 0.64              |
| 3:K:887:ASP:HB3   | 3:K:889:PRO:HD2   | 1.80                     | 0.64              |
| 3:L:77:VAL:HG22   | 3:L:266:HIS:CD2   | 2.33                     | 0.64              |
| 3:L:244:ILE:HD13  | 3:L:292:PHE:CE2   | 2.32                     | 0.64              |
| 3:A:334:ARG:NH2   | 3:B:355:GLU:OE1   | 2.30                     | 0.64              |
| 3:A:1340:PRO:O    | 3:A:1344:ARG:N    | 2.28                     | 0.64              |
| 3:C:512:ARG:HA    | 3:C:515:HIS:HD2   | 1.63                     | 0.64              |
| 3:D:649:THR:HG21  | 3:D:681:ASP:HB3   | 1.80                     | 0.64              |
| 3:D:651:CYS:O     | 3:D:654:SER:OG    | 2.16                     | 0.64              |
| 3:E:1301:SER:HB3  | 3:E:1321:VAL:HG21 | 1.79                     | 0.64              |
| 3:F:485:ASN:ND2   | 3:F:516:GLY:N     | 2.37                     | 0.64              |
| 3:F:752:ARG:NH1   | 3:F:913:ALA:O     | 2.31                     | 0.64              |
| 3:F:1245:TRP:O    | 3:F:1251:SER:HB3  | 1.98                     | 0.64              |
| 3:G:783:LEU:HB3   | 3:G:934:HIS:CE1   | 2.33                     | 0.64              |
| 2:R:174:PRO:HD3   | 5:q:371:GLY:CA    | 2.28                     | 0.64              |
| 1:W:194:CYS:O     | 1:W:198:TYR:CD2   | 2.50                     | 0.64              |
| 3:I:340:GLN:HA    | 3:H:159:LEU:HD13  | 1.80                     | 0.64              |
| 3:A:227:PHE:O     | 3:A:231:SER:OG    | 2.11                     | 0.64              |
| 3:P:870:LEU:HD22  | 3:P:877:ALA:HA    | 1.80                     | 0.64              |
| 3:B:677:TYR:CD1   | 4:b:95:LYS:NZ     | 2.66                     | 0.64              |
| 3:C:776:PHE:O     | 3:C:904:ARG:HB3   | 1.96                     | 0.64              |
| 3:F:507:ASN:OD1   | 3:F:510:ARG:NH2   | 2.29                     | 0.64              |
| 3:G:99:VAL:CA     | 3:G:118:ASN:HB2   | 2.27                     | 0.64              |
| 3:I:485:ASN:ND2   | 3:I:516:GLY:N     | 2.44                     | 0.63              |
| 3:I:623:TYR:H     | 3:I:943:GLN:HE22  | 1.46                     | 0.63              |
| 3:I:1225:LEU:HD22 | 3:I:1234:PRO:HG3  | 1.80                     | 0.63              |
| 3:K:1034:VAL:HA   | 3:K:1147:LEU:HD21 | 1.81                     | 0.63              |
| 3:L:858:VAL:O     | 3:L:866:HIS:ND1   | 2.24                     | 0.63              |
| 3:A:84:PHE:HD2    | 3:A:87:LEU:HD12   | 1.63                     | 0.63              |
| 3:H:310:VAL:HG12  | 3:H:312:ASN:H     | 1.63                     | 0.63              |
| 3:H:452:LEU:HD12  | 3:H:456:ASN:HD22  | 1.63                     | 0.63              |
| 3:N:256:GLN:CD    | 3:D:27:ILE:HD11   | 2.10                     | 0.63              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:C:77:VAL:HG22   | 3:C:266:HIS:CD2   | 2.33                     | 0.63              |
| 3:C:133:PHE:HB3   | 3:C:1091:PHE:HB2  | 1.79                     | 0.63              |
| 3:F:132:ALA:HB2   | 3:G:112:VAL:CG1   | 2.28                     | 0.63              |
| 3:I:840:GLN:HB3   | 4:i:57:GLN:HB3    | 1.79                     | 0.63              |
| 3:I:854:PRO:HG3   | 3:I:862:ALA:HB3   | 1.81                     | 0.63              |
| 3:K:1182:ASP:HB2  | 3:K:1309:VAL:HG13 | 1.78                     | 0.63              |
| 3:L:838:THR:O     | 3:L:875:VAL:HG22  | 1.98                     | 0.63              |
| 4:n:61:LEU:HD11   | 3:N:840:GLN:HG2   | 1.79                     | 0.63              |
| 4:p:79:PHE:CE2    | 3:P:639:HIS:HA    | 2.34                     | 0.63              |
| 3:P:107:ASP:OD1   | 3:P:108:GLY:N     | 2.32                     | 0.63              |
| 3:E:12:ARG:HH12   | 3:F:322:MET:C     | 2.06                     | 0.63              |
| 3:I:838:THR:O     | 3:I:875:VAL:HG22  | 1.98                     | 0.63              |
| 3:J:1083:HIS:O    | 3:J:1090:ASN:N    | 2.29                     | 0.63              |
| 3:J:1257:TYR:HB2  | 3:J:1277:PHE:CD2  | 2.34                     | 0.63              |
| 3:M:752:ARG:HA    | 3:M:913:ALA:HB3   | 1.80                     | 0.63              |
| 4:k:56:GLY:O      | 4:k:60:ALA:N      | 2.26                     | 0.63              |
| 3:N:1072:ALA:HB2  | 3:N:1102:LEU:HD23 | 1.81                     | 0.63              |
| 3:P:764:VAL:O     | 3:P:783:LEU:N     | 2.29                     | 0.63              |
| 3:B:1344:ARG:NH2  | 3:C:414:GLU:OE2   | 2.31                     | 0.63              |
| 5:q:163:ASP:OD1   | 5:q:166:ARG:NE    | 2.27                     | 0.63              |
| 6:r:84:ILE:O      | 6:r:88:GLU:N      | 2.29                     | 0.63              |
| 3:F:863:HIS:CE1   | 3:F:887:ASP:HA    | 2.32                     | 0.63              |
| 3:G:589:VAL:HG11  | 3:G:1012:GLU:O    | 1.98                     | 0.63              |
| 3:J:198:LEU:O     | 3:J:201:MET:N     | 2.29                     | 0.63              |
| 3:J:485:ASN:HD21  | 3:J:516:GLY:H     | 1.45                     | 0.63              |
| 3:J:752:ARG:HG3   | 3:J:912:ALA:HB1   | 1.80                     | 0.63              |
| 3:J:997:ASN:O     | 3:J:1000:SER:OG   | 2.17                     | 0.63              |
| 3:J:1270:LEU:HD22 | 3:J:1303:ALA:HB2  | 1.79                     | 0.63              |
| 3:L:892:LEU:HD22  | 4:l:65:GLY:HA2    | 1.80                     | 0.63              |
| 3:H:914:PRO:HG3   | 3:H:923:THR:HG22  | 1.81                     | 0.63              |
| 3:O:198:LEU:O     | 3:O:201:MET:N     | 2.32                     | 0.63              |
| 3:O:826:CYS:HB3   | 3:O:966:GLY:H     | 1.61                     | 0.63              |
| 3:P:730:ALA:HB2   | 3:P:752:ARG:HH11  | 1.64                     | 0.63              |
| 3:B:1029:PHE:HB3  | 3:B:1039:GLN:NE2  | 2.13                     | 0.63              |
| 3:E:1131:LEU:HD23 | 3:E:1159:PRO:HG3  | 1.81                     | 0.63              |
| 3:G:23:ILE:HG21   | 3:G:167:ARG:NH1   | 2.13                     | 0.63              |
| 3:K:863:HIS:CE1   | 3:K:887:ASP:HA    | 2.33                     | 0.63              |
| 3:L:1161:GLN:OE1  | 3:L:1170:GLN:NE2  | 2.31                     | 0.63              |
| 3:B:625:ALA:HA    | 3:B:628:TYR:HD2   | 1.63                     | 0.63              |
| 3:B:753:ASP:OD2   | 3:B:927:ARG:NH2   | 2.31                     | 0.63              |
| 5:q:365:TRP:O     | 5:q:369:ALA:N     | 2.31                     | 0.63              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:E:728:ASP:O     | 3:E:810:LYS:NZ    | 2.31                     | 0.63              |
| 3:E:776:PHE:O     | 3:E:904:ARG:HB3   | 1.99                     | 0.63              |
| 3:F:122:LYS:NZ    | 3:F:1101:ASP:O    | 2.26                     | 0.63              |
| 3:F:1125:LEU:HD22 | 3:F:1184:VAL:HG22 | 1.81                     | 0.63              |
| 3:H:1291:ARG:NE   | 3:C:34:ARG:HB2    | 1.62                     | 0.63              |
| 4:o:79:PHE:CE2    | 3:O:639:HIS:HA    | 2.33                     | 0.63              |
| 3:B:1131:LEU:HD23 | 3:B:1159:PRO:HG3  | 1.81                     | 0.63              |
| 3:C:1131:LEU:HD23 | 3:C:1159:PRO:HG3  | 1.81                     | 0.63              |
| 3:D:638:GLU:HB3   | 4:d:79:PHE:CZ     | 2.34                     | 0.63              |
| 3:D:752:ARG:HA    | 3:D:913:ALA:HB3   | 1.80                     | 0.63              |
| 3:E:135:LEU:HD21  | 3:E:165:LEU:HD21  | 1.78                     | 0.63              |
| 3:E:1245:TRP:O    | 3:E:1251:SER:HB3  | 1.98                     | 0.63              |
| 3:F:188:LEU:HD23  | 3:F:191:LYS:HD3   | 1.79                     | 0.63              |
| 3:I:691:ARG:NH1   | 3:J:620:ASP:OD1   | 2.32                     | 0.63              |
| 3:J:474:GLY:O     | 3:J:478:HIS:CD2   | 2.52                     | 0.63              |
| 3:J:646:ARG:HH11  | 4:j:100:PRO:HD2   | 1.62                     | 0.63              |
| 3:K:959:PRO:HG2   | 3:K:991:PRO:HD3   | 1.79                     | 0.63              |
| 3:M:32:HIS:NE2    | 3:D:1105:GLY:HA2  | 2.13                     | 0.63              |
| 4:n:5:GLN:H       | 4:n:11:THR:HG21   | 1.62                     | 0.63              |
| 3:N:278:LEU:HG    | 3:N:375:VAL:HG11  | 1.81                     | 0.63              |
| 3:C:521:VAL:HG21  | 3:C:987:VAL:HG12  | 1.81                     | 0.63              |
| 3:E:865:LEU:HA    | 3:E:870:LEU:HD21  | 1.80                     | 0.63              |
| 3:F:651:CYS:O     | 3:F:654:SER:OG    | 2.16                     | 0.63              |
| 3:I:734:PRO:HG3   | 3:I:964:PHE:HE2   | 1.63                     | 0.63              |
| 3:I:985:ARG:HD2   | 3:H:705:ASP:OD2   | 1.98                     | 0.63              |
| 3:J:840:GLN:HG2   | 4:j:61:LEU:HD11   | 1.81                     | 0.63              |
| 3:J:966:GLY:HA3   | 3:J:969:HIS:HB2   | 1.80                     | 0.63              |
| 3:K:77:VAL:HG22   | 3:K:266:HIS:CD2   | 2.34                     | 0.63              |
| 3:L:58:LEU:HD12   | 3:M:124:ILE:HD11  | 1.80                     | 0.63              |
| 3:L:841:ASN:OD1   | 4:l:57:GLN:NE2    | 2.32                     | 0.63              |
| 3:M:33:ARG:NH1    | 3:M:39:PHE:HB3    | 2.14                     | 0.63              |
| 3:H:1296:THR:HG21 | 3:H:1327:LEU:HG   | 1.81                     | 0.63              |
| 3:N:213:ARG:HH12  | 3:N:1216:GLY:HA3  | 1.64                     | 0.63              |
| 3:C:402:PHE:HA    | 3:C:1332:TYR:O    | 1.99                     | 0.63              |
| 3:D:706:ASP:O     | 3:E:525:GLN:NE2   | 2.31                     | 0.63              |
| 3:F:406:LEU:O     | 3:F:1361:TYR:OH   | 2.17                     | 0.63              |
| 3:G:37:ASP:N      | 3:G:37:ASP:OD1    | 2.32                     | 0.63              |
| 1:T:141:PRO:CB    | 3:I:1165:VAL:CG1  | 2.77                     | 0.63              |
| 3:I:874:THR:HG21  | 4:i:26:VAL:HG13   | 1.81                     | 0.63              |
| 3:J:350:THR:HB    | 3:J:353:GLU:HG3   | 1.79                     | 0.63              |
| 3:J:639:HIS:HA    | 4:j:79:PHE:HE2    | 1.64                     | 0.63              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:J:738:ASP:OD1  | 3:J:787:THR:OG1   | 2.17                     | 0.63              |
| 3:L:108:GLY:HA2  | 3:L:110:HIS:H     | 1.63                     | 0.63              |
| 3:L:512:ARG:HA   | 3:L:515:HIS:HD2   | 1.64                     | 0.63              |
| 3:H:180:THR:HG22 | 3:H:1097:ARG:NH1  | 2.13                     | 0.63              |
| 3:C:700:LEU:HD22 | 3:C:1025:MET:HG3  | 1.79                     | 0.63              |
| 3:D:279:VAL:HG12 | 3:D:394:LEU:HD22  | 1.81                     | 0.63              |
| 3:E:55:ASP:OD1   | 3:F:91:ASN:HB2    | 1.99                     | 0.63              |
| 3:F:162:ILE:HG22 | 3:G:344:LEU:CD1   | 2.29                     | 0.63              |
| 3:G:103:LEU:HD21 | 3:G:113:GLU:C     | 2.24                     | 0.63              |
| 3:G:736:VAL:HG12 | 3:G:738:ASP:H     | 1.64                     | 0.63              |
| 2:U:300:PHE:HB3  | 3:I:1083:HIS:NE2  | 2.14                     | 0.62              |
| 2:Y:299:THR:HG22 | 2:Y:313:PRO:HD2   | 1.81                     | 0.62              |
| 3:J:439:GLN:HE22 | 3:J:451:ARG:HH21  | 1.46                     | 0.62              |
| 3:J:471:ALA:O    | 3:J:475:GLY:N     | 2.32                     | 0.62              |
| 3:H:107:ASP:OD1  | 3:H:108:GLY:N     | 2.32                     | 0.62              |
| 3:N:90:MET:HG2   | 3:N:91:ASN:O      | 1.99                     | 0.62              |
| 3:B:863:HIS:O    | 3:B:869:ASN:ND2   | 2.25                     | 0.62              |
| 3:C:621:ARG:O    | 3:C:943:GLN:NE2   | 2.20                     | 0.62              |
| 3:C:889:PRO:HA   | 3:C:892:LEU:HD12  | 1.79                     | 0.62              |
| 3:E:756:ILE:HG12 | 3:E:910:CYS:HB3   | 1.80                     | 0.62              |
| 3:E:946:ASP:HB3  | 3:E:949:ILE:H     | 1.64                     | 0.62              |
| 3:G:35:LEU:HD12  | 3:G:35:LEU:O      | 1.99                     | 0.62              |
| 2:S:313:PRO:CG   | 3:A:111:PRO:HB2   | 2.29                     | 0.62              |
| 4:k:76:GLN:HG2   | 4:k:94:LEU:HD12   | 1.80                     | 0.62              |
| 4:l:76:GLN:HG2   | 4:l:94:LEU:HD12   | 1.81                     | 0.62              |
| 3:N:178:ARG:HB3  | 3:O:104:ILE:HG22  | 1.81                     | 0.62              |
| 3:O:263:ARG:NH2  | 3:O:305:THR:O     | 2.32                     | 0.62              |
| 3:B:462:CYS:SG   | 3:B:1147:LEU:HD22 | 2.39                     | 0.62              |
| 3:B:736:VAL:HG12 | 3:B:738:ASP:H     | 1.63                     | 0.62              |
| 3:D:460:THR:HA   | 3:D:1129:PHE:HD2  | 1.64                     | 0.62              |
| 5:q:659:GLY:N    | 5:q:671:ILE:O     | 2.31                     | 0.62              |
| 3:E:315:ASN:ND2  | 3:E:326:VAL:O     | 2.32                     | 0.62              |
| 3:F:800:HIS:O    | 3:F:801:ARG:HG3   | 1.99                     | 0.62              |
| 3:J:776:PHE:O    | 3:J:904:ARG:HD3   | 1.99                     | 0.62              |
| 3:M:800:HIS:O    | 3:M:801:ARG:HG3   | 1.99                     | 0.62              |
| 3:N:879:PHE:O    | 3:N:883:ARG:N     | 2.32                     | 0.62              |
| 3:D:426:ALA:HB3  | 3:D:429:HIS:CD2   | 2.34                     | 0.62              |
| 3:D:646:ARG:HH12 | 4:d:99:SER:HA     | 1.61                     | 0.62              |
| 5:q:90:LEU:HD12  | 5:q:234:PRO:HB3   | 1.80                     | 0.62              |
| 3:E:219:LEU:O    | 3:E:222:GLU:N     | 2.32                     | 0.62              |
| 3:E:507:ASN:OD1  | 3:E:510:ARG:NH2   | 2.29                     | 0.62              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:E:1082:ARG:HG2  | 3:E:1091:PHE:CE1  | 2.34                     | 0.62              |
| 3:F:45:ASP:OD1    | 3:F:46:GLU:N      | 2.33                     | 0.62              |
| 1:W:89:LYS:HD3    | 3:C:1077:GLN:HE22 | 1.63                     | 0.62              |
| 3:I:517:ARG:HH11  | 3:H:710:PRO:HG2   | 1.64                     | 0.62              |
| 3:I:795:ALA:HB3   | 3:I:798:ARG:HG2   | 1.82                     | 0.62              |
| 3:K:826:CYS:HB3   | 3:K:966:GLY:N     | 2.11                     | 0.62              |
| 3:K:861:PRO:O     | 3:K:869:ASN:ND2   | 2.31                     | 0.62              |
| 3:L:1029:PHE:CB   | 3:L:1039:GLN:HE21 | 2.12                     | 0.62              |
| 3:M:1206:ARG:NH2  | 3:M:1208:ARG:O    | 2.31                     | 0.62              |
| 3:A:857:PRO:HA    | 3:A:863:HIS:CD2   | 2.34                     | 0.62              |
| 3:H:98:GLU:OE2    | 3:C:11:TYR:CE2    | 2.52                     | 0.62              |
| 4:o:57:GLN:HB3    | 3:O:840:GLN:HB3   | 1.82                     | 0.62              |
| 3:C:742:LEU:HD13  | 3:C:783:LEU:HD13  | 1.81                     | 0.62              |
| 3:D:950:GLN:HG3   | 4:c:80:ALA:HB1    | 1.81                     | 0.62              |
| 1:W:349:ARG:CA    | 6:r:14:GLU:HG2    | 2.29                     | 0.62              |
| 3:I:293:LEU:HD13  | 3:I:368:VAL:HG11  | 1.81                     | 0.62              |
| 3:L:752:ARG:HH22  | 3:L:915:ASP:CG    | 2.08                     | 0.62              |
| 3:L:1342:LEU:HD21 | 3:L:1362:LEU:HB2  | 1.80                     | 0.62              |
| 3:O:507:ASN:OD1   | 3:O:510:ARG:NH2   | 2.32                     | 0.62              |
| 3:B:607:ALA:O     | 3:B:610:THR:OG1   | 2.14                     | 0.62              |
| 3:G:626:VAL:HG22  | 3:G:878:MET:HG3   | 1.80                     | 0.62              |
| 1:w:283:ARG:NH1   | 3:L:137:THR:HG1   | 1.93                     | 0.62              |
| 3:I:950:GLN:N     | 3:I:953:GLU:OE2   | 2.31                     | 0.62              |
| 3:J:745:HIS:HB3   | 3:J:754:CYS:HA    | 1.80                     | 0.62              |
| 3:K:274:VAL:HG11  | 3:K:376:PHE:CD2   | 2.34                     | 0.62              |
| 3:K:390:VAL:HG11  | 3:L:104:ILE:HD11  | 1.81                     | 0.62              |
| 3:A:355:GLU:OE1   | 3:B:334:ARG:NH2   | 2.33                     | 0.62              |
| 3:O:213:ARG:NH1   | 3:O:1216:GLY:HA3  | 2.14                     | 0.62              |
| 3:O:752:ARG:NH2   | 3:O:915:ASP:HA    | 2.15                     | 0.62              |
| 3:P:752:ARG:HA    | 3:P:913:ALA:HB3   | 1.80                     | 0.62              |
| 3:P:755:ARG:NH1   | 3:P:911:SER:OG    | 2.33                     | 0.62              |
| 3:B:677:TYR:HD1   | 4:b:95:LYS:NZ     | 1.95                     | 0.62              |
| 3:E:259:VAL:HG22  | 3:E:1102:LEU:HD13 | 1.81                     | 0.62              |
| 3:E:765:TYR:HE1   | 3:E:783:LEU:HD12  | 1.63                     | 0.62              |
| 3:E:887:ASP:O     | 3:E:891:MET:HG2   | 1.99                     | 0.62              |
| 3:F:1128:ASN:HD21 | 3:F:1155:ASN:ND2  | 1.97                     | 0.62              |
| 3:K:580:GLY:HA2   | 3:K:592:ARG:HH12  | 1.65                     | 0.62              |
| 3:K:749:ASP:O     | 3:K:752:ARG:N     | 2.32                     | 0.62              |
| 3:L:834:ARG:HH11  | 3:L:953:GLU:HA    | 1.63                     | 0.62              |
| 3:M:819:ALA:O     | 3:M:822:ARG:NH1   | 2.33                     | 0.62              |
| 3:M:1365:ASP:O    | 3:M:1370:LYS:NZ   | 2.30                     | 0.62              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:A:1325:CYS:O    | 3:A:1329:GLN:N    | 2.33                     | 0.62              |
| 3:N:322:MET:HE3   | 3:E:324:LYS:HD2   | 1.80                     | 0.62              |
| 3:N:1105:GLY:HA2  | 3:D:32:HIS:NE2    | 2.15                     | 0.62              |
| 3:B:766:ALA:N     | 3:B:783:LEU:O     | 2.32                     | 0.62              |
| 3:C:488:GLY:HA2   | 3:C:996:ALA:HB1   | 1.80                     | 0.62              |
| 3:D:440:LEU:HD22  | 3:D:1336:CYS:SG   | 2.38                     | 0.62              |
| 3:D:698:GLU:OE1   | 3:E:621:ARG:NH2   | 2.32                     | 0.62              |
| 3:F:1032:SER:O    | 3:F:1035:ALA:N    | 2.32                     | 0.62              |
| 3:G:829:GLY:C     | 3:G:956:TYR:CZ    | 2.78                     | 0.62              |
| 2:X:38:ARG:NH2    | 3:I:109:PRO:C     | 2.53                     | 0.62              |
| 3:I:521:VAL:HG21  | 3:I:987:VAL:HG12  | 1.82                     | 0.62              |
| 3:J:475:GLY:HA2   | 3:J:478:HIS:NE2   | 2.13                     | 0.62              |
| 3:K:838:THR:O     | 3:K:875:VAL:HG22  | 1.99                     | 0.62              |
| 3:L:914:PRO:HG3   | 3:L:923:THR:HG22  | 1.80                     | 0.62              |
| 3:H:426:ALA:HB3   | 3:H:429:HIS:HD2   | 1.64                     | 0.62              |
| 3:H:742:LEU:HD13  | 3:H:783:LEU:HD13  | 1.81                     | 0.62              |
| 3:H:896:VAL:HA    | 3:H:899:HIS:CD2   | 2.34                     | 0.62              |
| 3:O:709:LEU:HD12  | 3:O:1037:TYR:HE1  | 1.65                     | 0.62              |
| 3:E:730:ALA:HB2   | 3:E:752:ARG:HH11  | 1.65                     | 0.62              |
| 3:E:908:LEU:HD12  | 3:E:932:ALA:HB3   | 1.82                     | 0.62              |
| 3:G:812:TYR:HD1   | 3:G:816:LEU:HD12  | 1.64                     | 0.62              |
| 2:S:100:LEU:HD13  | 2:S:314:VAL:HG21  | 1.82                     | 0.62              |
| 3:M:11:TYR:HB2    | 3:D:96:GLN:NE2    | 2.15                     | 0.62              |
| 3:O:227:PHE:O     | 3:O:231:SER:OG    | 2.13                     | 0.62              |
| 3:O:339:MET:HE1   | 3:O:348:ARG:HE    | 1.65                     | 0.62              |
| 3:O:606:MET:HE3   | 3:O:611:ILE:HG12  | 1.80                     | 0.62              |
| 3:C:914:PRO:HG3   | 3:C:923:THR:HG22  | 1.80                     | 0.62              |
| 3:D:258:SER:OG    | 3:D:259:VAL:N     | 2.32                     | 0.62              |
| 3:F:819:ALA:O     | 3:F:822:ARG:NH1   | 2.32                     | 0.62              |
| 3:F:875:VAL:HG12  | 3:F:879:PHE:HE2   | 1.64                     | 0.62              |
| 1:T:259:GLU:OE1   | 3:I:1315:PRO:CB   | 2.47                     | 0.62              |
| 3:L:1270:LEU:HD22 | 3:L:1303:ALA:HB2  | 1.82                     | 0.62              |
| 3:M:1120:THR:HG22 | 3:M:1181:GLN:HE21 | 1.64                     | 0.62              |
| 3:H:213:ARG:HH12  | 3:H:1216:GLY:HA3  | 1.65                     | 0.62              |
| 3:O:1125:LEU:HD22 | 3:O:1184:VAL:HG22 | 1.81                     | 0.62              |
| 3:C:755:ARG:NH1   | 3:C:911:SER:OG    | 2.33                     | 0.62              |
| 3:C:959:PRO:HG2   | 3:C:991:PRO:HD3   | 1.80                     | 0.62              |
| 3:D:272:ARG:NH2   | 3:D:372:ASP:O     | 2.32                     | 0.62              |
| 3:D:880:HIS:CD2   | 4:c:94:LEU:HD22   | 2.28                     | 0.62              |
| 3:E:752:ARG:HA    | 3:E:913:ALA:HB3   | 1.82                     | 0.62              |
| 6:r:84:ILE:HG12   | 6:r:87:ILE:HD12   | 1.82                     | 0.62              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:F:448:GLN:CG    | 3:G:1201:ARG:NH2  | 2.63                     | 0.62              |
| 3:G:1198:TYR:HB2  | 3:G:1236:ARG:HH12 | 1.63                     | 0.62              |
| 1:1:208:ARG:NH2   | 1:1:225:ASP:OD1   | 2.33                     | 0.61              |
| 3:J:774:ALA:HB1   | 3:J:776:PHE:CE1   | 2.35                     | 0.61              |
| 3:L:870:LEU:HD22  | 3:L:877:ALA:HA    | 1.81                     | 0.61              |
| 3:L:982:ASP:OD1   | 3:L:985:ARG:NH1   | 2.32                     | 0.61              |
| 3:A:486:PRO:HD2   | 3:A:512:ARG:HD2   | 1.81                     | 0.61              |
| 3:H:485:ASN:HD21  | 3:H:516:GLY:H     | 1.45                     | 0.61              |
| 3:N:120:MET:HG2   | 3:D:39:PHE:CD1    | 2.28                     | 0.61              |
| 3:N:227:PHE:O     | 3:N:231:SER:OG    | 2.15                     | 0.61              |
| 3:N:326:VAL:HG21  | 3:E:321:VAL:HG13  | 1.77                     | 0.61              |
| 3:P:766:ALA:HB3   | 3:P:784:LEU:HA    | 1.81                     | 0.61              |
| 3:C:1181:GLN:OE1  | 3:C:1307:SER:OG   | 2.19                     | 0.61              |
| 5:q:69:ASP:OD2    | 5:q:685:ARG:NH2   | 2.33                     | 0.61              |
| 3:F:871:VAL:HB    | 3:F:874:THR:HG21  | 1.82                     | 0.61              |
| 3:G:454:MET:O     | 3:G:457:ALA:N     | 2.26                     | 0.61              |
| 2:3:300:PHE:CD2   | 3:M:1083:HIS:NE2  | 2.64                     | 0.61              |
| 1:w:283:ARG:HH12  | 3:L:137:THR:CB    | 2.13                     | 0.61              |
| 3:I:861:PRO:O     | 3:I:869:ASN:ND2   | 2.33                     | 0.61              |
| 3:J:45:ASP:OD1    | 3:J:46:GLU:N      | 2.33                     | 0.61              |
| 3:J:392:TYR:CE2   | 3:J:394:LEU:HB3   | 2.35                     | 0.61              |
| 3:J:457:ALA:O     | 3:J:460:THR:OG1   | 2.17                     | 0.61              |
| 3:K:439:GLN:HE21  | 3:K:451:ARG:NH2   | 1.98                     | 0.61              |
| 3:M:293:LEU:HD13  | 3:M:368:VAL:HG11  | 1.82                     | 0.61              |
| 3:H:764:VAL:O     | 3:H:782:ARG:HA    | 1.99                     | 0.61              |
| 3:N:469:ILE:O     | 3:N:472:ALA:N     | 2.22                     | 0.61              |
| 3:N:879:PHE:HD1   | 3:N:884:VAL:HB    | 1.65                     | 0.61              |
| 3:N:1131:LEU:HD23 | 3:N:1159:PRO:HG3  | 1.80                     | 0.61              |
| 3:P:172:VAL:HG11  | 3:P:1093:LEU:HD12 | 1.81                     | 0.61              |
| 3:B:261:VAL:O     | 3:G:60:SER:C      | 2.42                     | 0.61              |
| 3:C:879:PHE:O     | 3:C:883:ARG:N     | 2.33                     | 0.61              |
| 3:D:925:ASN:O     | 3:D:927:ARG:NH1   | 2.33                     | 0.61              |
| 3:E:238:GLY:HA2   | 3:E:244:ILE:HD11  | 1.82                     | 0.61              |
| 3:F:433:ARG:O     | 3:F:1360:GLN:NE2  | 2.34                     | 0.61              |
| 1:w:79:THR:N      | 3:O:308:GLU:OE1   | 2.33                     | 0.61              |
| 3:I:729:PRO:HB2   | 3:I:748:LEU:HD11  | 1.82                     | 0.61              |
| 3:J:392:TYR:HE2   | 3:J:394:LEU:HB3   | 1.65                     | 0.61              |
| 3:L:79:CYS:HB3    | 3:L:81:CYS:SG     | 2.40                     | 0.61              |
| 3:D:1208:ARG:NE   | 3:D:1225:LEU:O    | 2.29                     | 0.61              |
| 3:I:452:LEU:HD12  | 3:I:456:ASN:HD22  | 1.66                     | 0.61              |
| 3:I:871:VAL:O     | 3:I:874:THR:OG1   | 2.16                     | 0.61              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:K:768:ALA:HA    | 3:K:786:ASN:HA    | 1.82                     | 0.61              |
| 3:K:819:ALA:O     | 3:K:822:ARG:NH1   | 2.34                     | 0.61              |
| 3:L:1225:LEU:HD22 | 3:L:1234:PRO:HG3  | 1.81                     | 0.61              |
| 3:M:161:ALA:HB2   | 3:C:50:TYR:CE1    | 2.35                     | 0.61              |
| 3:H:756:ILE:HD12  | 3:H:763:PRO:HG3   | 1.82                     | 0.61              |
| 3:B:857:PRO:HB3   | 3:B:865:LEU:HB2   | 1.82                     | 0.61              |
| 3:E:87:LEU:O      | 3:E:90:MET:N      | 2.31                     | 0.61              |
| 3:G:99:VAL:H      | 3:G:118:ASN:C     | 2.08                     | 0.61              |
| 2:Y:300:PHE:CE2   | 3:H:1085:THR:HG21 | 2.36                     | 0.61              |
| 3:I:493:ALA:HB2   | 3:I:559:PRO:HB2   | 1.83                     | 0.61              |
| 3:J:714:LEU:HD12  | 3:J:722:LEU:HD22  | 1.81                     | 0.61              |
| 3:L:836:TYR:HE1   | 3:L:897:LEU:HD22  | 1.65                     | 0.61              |
| 3:H:96:GLN:NE2    | 3:C:12:ARG:HB3    | 2.12                     | 0.61              |
| 4:p:60:ALA:O      | 4:p:64:LEU:N      | 2.30                     | 0.61              |
| 3:N:691:ARG:NH2   | 3:O:620:ASP:OD1   | 2.34                     | 0.61              |
| 3:N:801:ARG:HB3   | 3:N:802:PRO:HD2   | 1.83                     | 0.61              |
| 3:P:788:GLN:HE21  | 3:P:800:HIS:HE1   | 1.49                     | 0.61              |
| 3:P:950:GLN:H     | 3:P:953:GLU:CD    | 2.09                     | 0.61              |
| 3:D:605:ALA:HA    | 3:D:1018:ASN:HD21 | 1.66                     | 0.61              |
| 3:G:23:ILE:HD13   | 3:G:167:ARG:NE    | 2.14                     | 0.61              |
| 3:G:819:ALA:O     | 3:G:822:ARG:NH1   | 2.34                     | 0.61              |
| 3:I:639:HIS:HA    | 4:i:79:PHE:HE2    | 1.66                     | 0.61              |
| 3:K:1072:ALA:HB2  | 3:K:1102:LEU:HD23 | 1.82                     | 0.61              |
| 3:H:98:GLU:OE2    | 3:C:16:ALA:CB     | 2.49                     | 0.61              |
| 3:H:1355:GLU:OE1  | 3:H:1355:GLU:N    | 2.32                     | 0.61              |
| 3:N:752:ARG:NH2   | 3:N:915:ASP:HA    | 2.16                     | 0.61              |
| 3:B:299:GLU:HB3   | 3:B:362:ARG:HD2   | 1.83                     | 0.61              |
| 3:C:1125:LEU:HD22 | 3:C:1184:VAL:HG22 | 1.82                     | 0.61              |
| 3:D:33:ARG:HD3    | 3:D:39:PHE:CD2    | 2.35                     | 0.61              |
| 3:E:274:VAL:HG11  | 3:E:376:PHE:CD2   | 2.34                     | 0.61              |
| 3:E:639:HIS:HA    | 4:e:79:PHE:HE2    | 1.65                     | 0.61              |
| 3:F:683:PRO:HD2   | 3:F:686:CYS:HB3   | 1.81                     | 0.61              |
| 3:F:765:TYR:HD1   | 3:F:783:LEU:HB2   | 1.64                     | 0.61              |
| 3:F:865:LEU:HD11  | 3:F:886:VAL:H     | 1.65                     | 0.61              |
| 3:I:1147:LEU:O    | 3:I:1150:ALA:N    | 2.34                     | 0.61              |
| 3:L:519:ARG:NH1   | 3:L:998:TYR:OH    | 2.32                     | 0.61              |
| 3:M:77:VAL:HG22   | 3:M:266:HIS:CD2   | 2.35                     | 0.61              |
| 3:M:889:PRO:HA    | 3:M:892:LEU:HD12  | 1.82                     | 0.61              |
| 3:A:96:GLN:HG2    | 3:A:121:THR:HG22  | 1.81                     | 0.61              |
| 3:H:201:MET:O     | 3:H:204:TYR:N     | 2.32                     | 0.61              |
| 3:H:397:ALA:HB3   | 3:H:1321:VAL:HG22 | 1.83                     | 0.61              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:m:60:ALA:O      | 4:m:64:LEU:N      | 2.33                     | 0.61              |
| 4:o:89:ARG:HH12   | 3:P:873:ASN:ND2   | 1.99                     | 0.61              |
| 3:C:756:ILE:HB    | 3:C:763:PRO:HD3   | 1.81                     | 0.61              |
| 3:D:180:THR:HG22  | 3:D:1097:ARG:NH1  | 2.15                     | 0.61              |
| 3:G:24:LEU:CD2    | 3:G:62:CYS:O      | 2.49                     | 0.61              |
| 3:A:863:HIS:O     | 3:A:869:ASN:ND2   | 2.33                     | 0.61              |
| 3:N:631:GLN:NE2   | 3:N:666:ASN:OD1   | 2.29                     | 0.61              |
| 3:B:524:CYS:HA    | 3:B:1008:GLN:HE22 | 1.65                     | 0.61              |
| 3:C:623:TYR:H     | 3:C:943:GLN:HE22  | 1.47                     | 0.61              |
| 3:C:1128:ASN:HD21 | 3:C:1155:ASN:ND2  | 1.99                     | 0.61              |
| 3:E:631:GLN:NE2   | 3:E:666:ASN:OD1   | 2.32                     | 0.61              |
| 3:F:778:ARG:O     | 3:F:904:ARG:NE    | 2.33                     | 0.61              |
| 3:G:985:ARG:HB3   | 3:G:985:ARG:HH11  | 1.64                     | 0.61              |
| 1:Q:134:LEU:HD11  | 1:Q:185:VAL:HG23  | 1.81                     | 0.61              |
| 1:w:283:ARG:NH1   | 3:L:137:THR:CB    | 2.63                     | 0.61              |
| 3:J:646:ARG:NH1   | 4:j:100:PRO:HD2   | 2.16                     | 0.61              |
| 3:K:708:THR:HG22  | 3:K:723:ASN:HD22  | 1.66                     | 0.61              |
| 3:L:180:THR:HG22  | 3:L:1097:ARG:NH1  | 2.15                     | 0.61              |
| 3:A:769:CYS:N     | 3:A:786:ASN:OD1   | 2.33                     | 0.61              |
| 3:N:1365:ASP:O    | 3:N:1370:LYS:NZ   | 2.31                     | 0.61              |
| 3:P:180:THR:HG22  | 3:P:1097:ARG:NH1  | 2.15                     | 0.61              |
| 3:B:82:THR:HG21   | 3:G:57:LEU:HD22   | 1.82                     | 0.61              |
| 3:D:473:VAL:HG21  | 3:D:573:ALA:HB2   | 1.82                     | 0.61              |
| 3:D:875:VAL:HG12  | 3:D:879:PHE:CE2   | 2.36                     | 0.61              |
| 3:D:876:ASN:HA    | 3:D:879:PHE:HD2   | 1.66                     | 0.61              |
| 5:q:471:ASP:HB2   | 5:q:474:ALA:HB2   | 1.82                     | 0.61              |
| 3:F:746:ALA:HA    | 3:F:754:CYS:CB    | 2.31                     | 0.61              |
| 3:F:1344:ARG:O    | 3:F:1347:ARG:HG2  | 2.01                     | 0.61              |
| 3:G:950:GLN:H     | 3:G:953:GLU:CD    | 2.08                     | 0.61              |
| 2:U:12:ILE:HD11   | 2:U:83:ILE:HG13   | 1.83                     | 0.61              |
| 3:L:742:LEU:HD13  | 3:L:783:LEU:HD13  | 1.82                     | 0.61              |
| 3:M:27:ILE:HD13   | 3:D:256:GLN:OE1   | 1.99                     | 0.61              |
| 3:M:512:ARG:HA    | 3:M:515:HIS:CD2   | 2.35                     | 0.61              |
| 3:H:948:THR:HA    | 4:m:79:PHE:HA     | 1.83                     | 0.61              |
| 3:N:676:THR:HG21  | 3:O:945:LEU:HD12  | 1.81                     | 0.61              |
| 3:C:69:ARG:HB2    | 3:C:72:GLU:HG2    | 1.83                     | 0.61              |
| 5:q:438:PRO:O     | 5:q:446:GLN:NE2   | 2.27                     | 0.61              |
| 3:E:864:PRO:HG3   | 3:E:888:GLY:HA2   | 1.83                     | 0.61              |
| 3:G:745:HIS:CE1   | 3:G:754:CYS:HB3   | 2.34                     | 0.61              |
| 3:K:266:HIS:CE1   | 3:K:302:VAL:HG13  | 2.35                     | 0.60              |
| 3:M:653:THR:HG22  | 3:M:683:PRO:HD3   | 1.81                     | 0.60              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:O:521:VAL:HG11  | 3:O:987:VAL:HG12  | 1.83                     | 0.60              |
| 3:O:634:ILE:HG22  | 3:O:636:GLY:H     | 1.66                     | 0.60              |
| 3:B:846:GLU:HG3   | 4:b:68:HIS:CE1    | 2.36                     | 0.60              |
| 3:C:793:ASP:OD2   | 3:C:800:HIS:ND1   | 2.34                     | 0.60              |
| 3:C:1304:THR:HG21 | 3:C:1314:PRO:HD2  | 1.82                     | 0.60              |
| 3:D:172:VAL:HG11  | 3:D:1093:LEU:HD12 | 1.81                     | 0.60              |
| 3:D:263:ARG:NH2   | 3:D:306:TYR:O     | 2.34                     | 0.60              |
| 3:D:519:ARG:NH1   | 3:D:998:TYR:OH    | 2.34                     | 0.60              |
| 5:q:36:ALA:HB1    | 5:q:146:LEU:HD21  | 1.81                     | 0.60              |
| 3:E:778:ARG:HH11  | 3:E:782:ARG:HD2   | 1.66                     | 0.60              |
| 3:F:12:ARG:HG2    | 3:G:321:VAL:O     | 2.00                     | 0.60              |
| 3:G:938:LEU:HD23  | 3:G:938:LEU:O     | 2.00                     | 0.60              |
| 3:J:1058:PHE:CE2  | 3:J:1369:LEU:HD11 | 2.36                     | 0.60              |
| 3:M:1054:ARG:NH1  | 3:M:1123:GLY:O    | 2.33                     | 0.60              |
| 3:H:709:LEU:HD13  | 3:H:709:LEU:C     | 2.26                     | 0.60              |
| 4:n:60:ALA:HA     | 4:n:63:ASP:HB2    | 1.82                     | 0.60              |
| 4:o:22:MET:HG2    | 4:o:64:LEU:HD13   | 1.83                     | 0.60              |
| 4:o:100:PRO:HD2   | 3:O:646:ARG:NH1   | 2.16                     | 0.60              |
| 3:O:874:THR:H     | 3:O:877:ALA:HB3   | 1.66                     | 0.60              |
| 3:O:1225:LEU:HD22 | 3:O:1234:PRO:HG3  | 1.82                     | 0.60              |
| 3:P:638:GLU:HB2   | 3:P:789:ALA:HA    | 1.82                     | 0.60              |
| 3:C:764:VAL:O     | 3:C:783:LEU:N     | 2.19                     | 0.60              |
| 3:C:876:ASN:HA    | 3:C:879:PHE:HD2   | 1.65                     | 0.60              |
| 1:w:112:ARG:HG2   | 1:w:264:THR:HG22  | 1.82                     | 0.60              |
| 3:I:947:HIS:O     | 4:h:80:ALA:N      | 2.34                     | 0.60              |
| 3:J:158:GLN:O     | 3:J:161:ALA:N     | 2.34                     | 0.60              |
| 3:M:711:GLY:HA3   | 3:M:719:GLN:HE21  | 1.67                     | 0.60              |
| 3:H:189:LEU:HD23  | 3:H:1064:LEU:HD21 | 1.82                     | 0.60              |
| 3:B:755:ARG:HG2   | 3:B:911:SER:OG    | 2.00                     | 0.60              |
| 3:C:241:ARG:NE    | 3:C:245:GLU:OE2   | 2.31                     | 0.60              |
| 5:q:584:ASP:HB3   | 5:q:654:ASN:HD21  | 1.66                     | 0.60              |
| 3:E:1233:ASP:HB3  | 3:E:1236:ARG:O    | 2.02                     | 0.60              |
| 1:W:345:ARG:O     | 6:r:13:TRP:HB3    | 2.00                     | 0.60              |
| 2:X:39:ARG:HH12   | 3:H:1081:ALA:CB   | 2.15                     | 0.60              |
| 3:J:503:GLN:O     | 3:J:507:ASN:ND2   | 2.33                     | 0.60              |
| 3:J:896:VAL:HA    | 3:J:899:HIS:CD2   | 2.35                     | 0.60              |
| 3:K:830:VAL:HG13  | 3:K:955:PHE:HE1   | 1.66                     | 0.60              |
| 3:A:266:HIS:CE1   | 3:A:303:PRO:HD2   | 2.35                     | 0.60              |
| 3:A:539:LEU:C     | 3:A:1248:GLN:HE22 | 2.09                     | 0.60              |
| 3:N:923:THR:HA    | 3:N:926:MET:HE3   | 1.83                     | 0.60              |
| 3:N:1120:THR:HG22 | 3:N:1181:GLN:HE21 | 1.66                     | 0.60              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:P:463:HIS:ND1   | 3:P:464:PRO:HD2   | 2.17                     | 0.60              |
| 3:P:942:PRO:HA    | 3:P:969:HIS:CE1   | 2.37                     | 0.60              |
| 3:D:390:VAL:HG11  | 3:E:104:ILE:HD11  | 1.84                     | 0.60              |
| 5:q:403:GLU:HG3   | 5:q:411:ARG:HD2   | 1.84                     | 0.60              |
| 3:F:195:LEU:O     | 3:F:198:LEU:N     | 2.27                     | 0.60              |
| 3:G:82:THR:HG22   | 3:G:307:GLY:HA3   | 1.83                     | 0.60              |
| 3:G:1197:ASN:OD1  | 3:G:1200:ARG:NH1  | 2.34                     | 0.60              |
| 3:I:327:ARG:HB2   | 3:H:58:LEU:HA     | 1.84                     | 0.60              |
| 3:I:1131:LEU:HD23 | 3:I:1159:PRO:HG3  | 1.82                     | 0.60              |
| 3:K:769:CYS:O     | 3:K:901:MET:N     | 2.24                     | 0.60              |
| 3:L:784:LEU:HD23  | 3:L:903:GLU:HG2   | 1.82                     | 0.60              |
| 3:A:576:ARG:HH11  | 3:A:582:LEU:HD23  | 1.64                     | 0.60              |
| 3:O:108:GLY:HA2   | 3:O:110:HIS:H     | 1.65                     | 0.60              |
| 3:P:1257:TYR:HB2  | 3:P:1277:PHE:CD2  | 2.35                     | 0.60              |
| 3:B:677:TYR:CA    | 4:b:95:LYS:HZ2    | 2.10                     | 0.60              |
| 3:C:122:LYS:NZ    | 3:C:1101:ASP:O    | 2.33                     | 0.60              |
| 3:C:710:PRO:HG2   | 3:D:517:ARG:HH11  | 1.66                     | 0.60              |
| 3:D:485:ASN:HD21  | 3:D:516:GLY:H     | 1.49                     | 0.60              |
| 3:D:1344:ARG:O    | 3:D:1347:ARG:HG2  | 2.00                     | 0.60              |
| 5:q:159:ARG:NH1   | 5:q:240:ALA:O     | 2.34                     | 0.60              |
| 5:q:439:HIS:NE2   | 5:q:469:PRO:HG2   | 2.17                     | 0.60              |
| 3:G:521:VAL:HG21  | 3:G:987:VAL:CG1   | 2.28                     | 0.60              |
| 3:G:666:ASN:HD22  | 3:G:938:LEU:CD2   | 2.14                     | 0.60              |
| 2:Y:158:ARG:HH21  | 2:Y:193:GLN:HE21  | 1.49                     | 0.60              |
| 3:I:896:VAL:HA    | 3:I:899:HIS:HD2   | 1.66                     | 0.60              |
| 3:I:1292:LEU:HB3  | 3:I:1327:LEU:HD21 | 1.82                     | 0.60              |
| 3:J:790:ARG:HG3   | 3:J:792:ALA:H     | 1.67                     | 0.60              |
| 3:L:729:PRO:HB2   | 3:L:748:LEU:HD11  | 1.82                     | 0.60              |
| 3:M:107:ASP:OD1   | 3:M:108:GLY:N     | 2.35                     | 0.60              |
| 3:N:439:GLN:HE22  | 3:N:451:ARG:HH21  | 1.48                     | 0.60              |
| 3:O:488:GLY:HA2   | 3:O:996:ALA:HB1   | 1.83                     | 0.60              |
| 3:O:1131:LEU:HD23 | 3:O:1159:PRO:HG3  | 1.84                     | 0.60              |
| 3:P:462:CYS:SG    | 3:P:1147:LEU:HD22 | 2.42                     | 0.60              |
| 3:P:1128:ASN:HD21 | 3:P:1155:ASN:ND2  | 1.99                     | 0.60              |
| 3:C:604:HIS:HD2   | 3:C:696:HIS:CD2   | 2.19                     | 0.60              |
| 3:C:925:ASN:O     | 3:C:927:ARG:NH1   | 2.34                     | 0.60              |
| 5:q:133:ARG:HH12  | 5:q:572:LEU:HB3   | 1.67                     | 0.60              |
| 3:E:682:LEU:HB2   | 3:E:687:MET:HG2   | 1.84                     | 0.60              |
| 3:G:842:MET:HE1   | 3:G:891:MET:HB3   | 1.83                     | 0.60              |
| 1:W:116:LEU:HD23  | 1:W:260:LEU:HB3   | 1.83                     | 0.60              |
| 3:I:310:VAL:HG12  | 3:I:312:ASN:H     | 1.65                     | 0.60              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:I:621:ARG:O     | 3:I:943:GLN:NE2   | 2.34                     | 0.60              |
| 3:M:198:LEU:O     | 3:M:201:MET:N     | 2.32                     | 0.60              |
| 3:M:631:GLN:HE22  | 3:M:666:ASN:CG    | 2.08                     | 0.60              |
| 3:M:1131:LEU:HD23 | 3:M:1159:PRO:HG3  | 1.82                     | 0.60              |
| 3:A:438:ARG:HG3   | 3:A:439:GLN:HG3   | 1.84                     | 0.60              |
| 4:o:95:LYS:O      | 3:P:880:HIS:NE2   | 2.35                     | 0.60              |
| 3:O:180:THR:HG22  | 3:O:1097:ARG:NH1  | 2.16                     | 0.60              |
| 3:O:1072:ALA:HB2  | 3:O:1102:LEU:HD23 | 1.82                     | 0.60              |
| 3:P:854:PRO:HG3   | 3:P:862:ALA:HB3   | 1.83                     | 0.60              |
| 3:B:163:GLN:HE22  | 3:C:348:ARG:HH22  | 1.48                     | 0.60              |
| 3:B:351:LEU:HD23  | 3:G:58:LEU:CD1    | 2.32                     | 0.60              |
| 2:x:300:PHE:CE2   | 3:O:1083:HIS:CB   | 2.80                     | 0.60              |
| 3:K:439:GLN:HG2   | 3:K:451:ARG:HH21  | 1.67                     | 0.60              |
| 3:H:875:VAL:HG12  | 3:H:879:PHE:CE2   | 2.37                     | 0.60              |
| 4:l:60:ALA:HA     | 4:l:63:ASP:HB2    | 1.84                     | 0.60              |
| 3:B:135:LEU:HD21  | 3:B:165:LEU:HD21  | 1.83                     | 0.60              |
| 3:B:469:ILE:HD11  | 3:B:547:PHE:CE1   | 2.37                     | 0.60              |
| 3:C:838:THR:O     | 3:C:875:VAL:HG22  | 2.01                     | 0.60              |
| 2:Y:238:ASN:HD21  | 3:H:1137:PRO:HB2  | 1.65                     | 0.60              |
| 3:J:809:HIS:O     | 3:J:813:TYR:HD2   | 1.84                     | 0.60              |
| 3:L:39:PHE:HD1    | 3:O:120:MET:HG2   | 1.65                     | 0.60              |
| 3:M:260:ALA:HB2   | 3:N:24:LEU:HD11   | 1.83                     | 0.60              |
| 3:A:312:ASN:ND2   | 3:B:315:ASN:O     | 2.34                     | 0.60              |
| 3:H:507:ASN:HA    | 3:H:510:ARG:HE    | 1.66                     | 0.60              |
| 4:o:89:ARG:NH2    | 4:p:30:ASN:OD1    | 2.34                     | 0.60              |
| 3:N:189:LEU:HD23  | 3:N:1064:LEU:HD21 | 1.84                     | 0.60              |
| 3:N:207:ASN:O     | 3:D:28:GLU:OE2    | 2.19                     | 0.60              |
| 3:N:463:HIS:ND1   | 3:N:464:PRO:HD2   | 2.16                     | 0.60              |
| 3:N:1286:HIS:CB   | 3:D:34:ARG:HH22   | 2.14                     | 0.60              |
| 3:O:1157:LEU:HD11 | 3:O:1269:VAL:HG21 | 1.84                     | 0.60              |
| 3:P:745:HIS:NE2   | 3:P:910:CYS:HB2   | 2.17                     | 0.60              |
| 3:C:752:ARG:NH2   | 3:C:915:ASP:HA    | 2.15                     | 0.60              |
| 3:G:35:LEU:HD11   | 3:G:39:PHE:HE2    | 1.66                     | 0.60              |
| 3:G:99:VAL:CG1    | 3:G:118:ASN:HB2   | 2.32                     | 0.60              |
| 2:U:26:ARG:O      | 2:U:101:ARG:NH1   | 2.34                     | 0.60              |
| 2:y:100:LEU:HD13  | 2:y:314:VAL:HG21  | 1.84                     | 0.60              |
| 3:J:410:ASN:O     | 3:J:415:ARG:NH1   | 2.34                     | 0.60              |
| 3:L:45:ASP:OD1    | 3:L:46:GLU:N      | 2.35                     | 0.60              |
| 3:M:27:ILE:HG12   | 3:D:256:GLN:CD    | 2.27                     | 0.60              |
| 3:M:863:HIS:CE1   | 3:M:887:ASP:HA    | 2.37                     | 0.60              |
| 3:N:924:ALA:O     | 3:N:927:ARG:NH1   | 2.32                     | 0.60              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:O:1222:VAL:HG11 | 3:O:1283:THR:HA   | 1.84                     | 0.60              |
| 3:P:1120:THR:HG22 | 3:P:1181:GLN:HE21 | 1.67                     | 0.60              |
| 3:B:524:CYS:SG    | 3:B:1008:GLN:NE2  | 2.74                     | 0.60              |
| 3:B:872:ALA:CB    | 4:g:76:GLN:HG2    | 2.16                     | 0.60              |
| 3:B:914:PRO:HG3   | 3:B:923:THR:HG22  | 1.84                     | 0.60              |
| 3:B:1058:PHE:CE2  | 3:B:1369:LEU:HD11 | 2.37                     | 0.60              |
| 3:C:1125:LEU:HD12 | 3:C:1156:ARG:NH2  | 2.16                     | 0.60              |
| 3:C:1173:ARG:HH21 | 3:D:213:ARG:HH12  | 1.50                     | 0.60              |
| 3:F:742:LEU:HA    | 3:F:745:HIS:HB3   | 1.82                     | 0.60              |
| 3:G:100:HIS:HD1   | 3:G:117:HIS:CG    | 2.15                     | 0.60              |
| 2:R:109:CYS:SG    | 2:R:182:ASN:ND2   | 2.75                     | 0.59              |
| 1:T:210:HIS:HB3   | 1:T:445:VAL:HB    | 1.84                     | 0.59              |
| 1:W:258:ASP:HB3   | 3:C:1318:ARG:HD2  | 1.83                     | 0.59              |
| 1:W:344:GLU:CD    | 6:r:13:TRP:CH2    | 2.74                     | 0.59              |
| 3:I:898:ALA:HB2   | 4:i:58:ALA:HB1    | 1.84                     | 0.59              |
| 3:J:1131:LEU:HD23 | 3:J:1159:PRO:HG3  | 1.83                     | 0.59              |
| 3:M:776:PHE:O     | 3:M:904:ARG:HD3   | 2.02                     | 0.59              |
| 3:H:99:VAL:HB     | 3:H:118:ASN:HB2   | 1.83                     | 0.59              |
| 3:H:180:THR:HG22  | 3:H:1097:ARG:HH12 | 1.65                     | 0.59              |
| 4:p:57:GLN:HB3    | 3:P:840:GLN:HB3   | 1.84                     | 0.59              |
| 3:O:491:VAL:HG21  | 3:O:929:PHE:HD2   | 1.67                     | 0.59              |
| 3:O:539:LEU:O     | 3:O:1248:GLN:NE2  | 2.34                     | 0.59              |
| 3:E:462:CYS:SG    | 3:E:1147:LEU:HD22 | 2.41                     | 0.59              |
| 3:F:621:ARG:O     | 3:F:943:GLN:NE2   | 2.34                     | 0.59              |
| 3:G:506:LEU:O     | 3:G:510:ARG:CG    | 2.50                     | 0.59              |
| 1:w:134:LEU:HD11  | 1:w:185:VAL:HG23  | 1.84                     | 0.59              |
| 3:J:403:VAL:HG22  | 3:J:1053:VAL:HG22 | 1.84                     | 0.59              |
| 3:M:229:ASP:O     | 3:M:236:LYS:NZ    | 2.26                     | 0.59              |
| 3:M:745:HIS:CE1   | 3:M:910:CYS:HB2   | 2.36                     | 0.59              |
| 3:A:881:ASN:HD21  | 3:A:948:THR:HG21  | 1.67                     | 0.59              |
| 3:A:1291:ARG:HH22 | 3:A:1314:PRO:HG2  | 1.67                     | 0.59              |
| 4:m:64:LEU:O      | 4:m:67:THR:OG1    | 2.20                     | 0.59              |
| 3:N:1026:ALA:HA   | 3:N:1029:PHE:CE2  | 2.37                     | 0.59              |
| 3:O:896:VAL:HA    | 3:O:899:HIS:CD2   | 2.30                     | 0.59              |
| 3:P:488:GLY:HA2   | 3:P:996:ALA:HB1   | 1.83                     | 0.59              |
| 3:P:778:ARG:HD3   | 3:P:780:ASP:HB2   | 1.84                     | 0.59              |
| 3:B:220:VAL:HG11  | 3:B:1214:TYR:HE1  | 1.67                     | 0.59              |
| 3:F:244:ILE:O     | 3:F:247:TRP:N     | 2.34                     | 0.59              |
| 3:F:485:ASN:ND2   | 3:F:515:HIS:HB2   | 2.16                     | 0.59              |
| 3:F:838:THR:O     | 3:F:875:VAL:HG22  | 2.01                     | 0.59              |
| 3:G:497:PRO:CD    | 3:G:504:ARG:NH2   | 2.65                     | 0.59              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:3:284:GLN:HG2  | 3:D:1166:PHE:HE1  | 1.61                     | 0.59              |
| 3:J:1155:ASN:OD1 | 3:J:1156:ARG:N    | 2.35                     | 0.59              |
| 3:L:652:ILE:O    | 3:L:655:TYR:N     | 2.35                     | 0.59              |
| 3:M:232:PHE:O    | 3:M:236:LYS:HD3   | 2.02                     | 0.59              |
| 3:M:615:ARG:HH21 | 3:M:1017:GLU:HG2  | 1.68                     | 0.59              |
| 3:M:778:ARG:O    | 3:M:904:ARG:NH2   | 2.34                     | 0.59              |
| 3:M:863:HIS:HE1  | 3:M:887:ASP:HA    | 1.67                     | 0.59              |
| 3:A:521:VAL:HG21 | 3:A:987:VAL:HG12  | 1.84                     | 0.59              |
| 3:A:827:THR:OG1  | 3:A:958:LEU:O     | 2.16                     | 0.59              |
| 3:H:756:ILE:HG12 | 3:H:910:CYS:HB3   | 1.82                     | 0.59              |
| 4:i:22:MET:HE2   | 4:i:60:ALA:HB3    | 1.84                     | 0.59              |
| 3:N:259:VAL:HG22 | 3:N:1102:LEU:HD13 | 1.84                     | 0.59              |
| 3:B:463:HIS:HD2  | 3:B:465:SER:HB3   | 1.67                     | 0.59              |
| 3:D:880:HIS:HE2  | 4:c:98:TYR:HD2    | 1.48                     | 0.59              |
| 3:D:1248:GLN:C   | 3:D:1251:SER:HG   | 2.10                     | 0.59              |
| 3:F:756:ILE:HG12 | 3:F:909:LEU:O     | 2.02                     | 0.59              |
| 3:I:77:VAL:HG22  | 3:I:266:HIS:CD2   | 2.38                     | 0.59              |
| 3:I:463:HIS:HD2  | 3:I:465:SER:HB3   | 1.67                     | 0.59              |
| 3:J:274:VAL:HG11 | 3:J:376:PHE:CD2   | 2.37                     | 0.59              |
| 3:A:77:VAL:HG22  | 3:A:266:HIS:CD2   | 2.36                     | 0.59              |
| 3:A:121:THR:CG2  | 3:G:48:SER:HB3    | 2.20                     | 0.59              |
| 3:H:406:LEU:HD23 | 3:H:440:LEU:HG    | 1.85                     | 0.59              |
| 3:H:745:HIS:CE1  | 3:H:910:CYS:HB2   | 2.37                     | 0.59              |
| 3:H:1208:ARG:NH1 | 3:H:1240:ALA:O    | 2.36                     | 0.59              |
| 3:N:103:LEU:HD11 | 3:N:115:PRO:HB3   | 1.85                     | 0.59              |
| 3:O:189:LEU:HD23 | 3:O:1064:LEU:HD21 | 1.83                     | 0.59              |
| 3:O:200:PRO:HG2  | 3:O:223:LEU:HD23  | 1.85                     | 0.59              |
| 3:B:266:HIS:CE1  | 3:B:302:VAL:HG13  | 2.36                     | 0.59              |
| 3:B:274:VAL:HG11 | 3:B:376:PHE:HD2   | 1.66                     | 0.59              |
| 3:C:87:LEU:O     | 3:C:90:MET:N      | 2.29                     | 0.59              |
| 3:C:163:GLN:HA   | 3:D:344:LEU:HD11  | 1.83                     | 0.59              |
| 3:C:301:ASP:OD1  | 3:C:362:ARG:NE    | 2.36                     | 0.59              |
| 3:D:189:LEU:HD23 | 3:D:1064:LEU:HD21 | 1.84                     | 0.59              |
| 3:D:879:PHE:CE1  | 3:D:886:VAL:HG21  | 2.38                     | 0.59              |
| 5:q:84:ASP:HB3   | 5:q:106:SER:H     | 1.68                     | 0.59              |
| 3:E:1050:PHE:CD1 | 3:E:1187:PHE:HB3  | 2.37                     | 0.59              |
| 3:F:266:HIS:CE1  | 3:F:302:VAL:HG13  | 2.38                     | 0.59              |
| 3:G:1279:ALA:HA  | 3:G:1282:ILE:HD13 | 1.82                     | 0.59              |
| 3:J:631:GLN:NE2  | 3:J:666:ASN:OD1   | 2.31                     | 0.59              |
| 3:M:50:TYR:CZ    | 3:C:161:ALA:HA    | 2.37                     | 0.59              |
| 3:M:646:ARG:HH22 | 3:M:889:PRO:HG2   | 1.67                     | 0.59              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:M:651:CYS:O    | 3:M:654:SER:OG    | 2.20                     | 0.59              |
| 3:M:756:ILE:HD12 | 3:M:763:PRO:HG3   | 1.83                     | 0.59              |
| 3:H:120:MET:CB   | 3:C:36:PHE:CE2    | 2.85                     | 0.59              |
| 3:H:732:LEU:HD21 | 3:H:745:HIS:HB2   | 1.84                     | 0.59              |
| 3:N:638:GLU:HB2  | 3:N:789:ALA:HA    | 1.85                     | 0.59              |
| 3:P:350:THR:HG22 | 3:P:352:ASP:H     | 1.67                     | 0.59              |
| 3:P:1058:PHE:CE2 | 3:P:1369:LEU:HD11 | 2.37                     | 0.59              |
| 3:C:266:HIS:HE1  | 3:C:302:VAL:HG13  | 1.66                     | 0.59              |
| 3:D:108:GLY:HA2  | 3:D:110:HIS:H     | 1.67                     | 0.59              |
| 3:E:853:CYS:HB2  | 4:e:101:PHE:CE1   | 2.38                     | 0.59              |
| 3:F:1117:ASN:OD1 | 3:G:222:GLU:OE2   | 2.20                     | 0.59              |
| 3:G:23:ILE:HD12  | 3:G:167:ARG:HD2   | 1.84                     | 0.59              |
| 1:T:170:LEU:HG   | 3:I:1262:HIS:ND1  | 2.17                     | 0.59              |
| 1:W:283:ARG:HH11 | 3:B:47:ASN:HB3    | 1.67                     | 0.59              |
| 2:3:38:ARG:HH22  | 3:E:110:HIS:N     | 2.01                     | 0.59              |
| 3:I:63:ASN:HD21  | 3:J:99:VAL:HG13   | 1.66                     | 0.59              |
| 3:I:840:GLN:HG2  | 4:i:61:LEU:HD11   | 1.84                     | 0.59              |
| 3:I:944:HIS:CD2  | 3:H:802:PRO:HB3   | 2.38                     | 0.59              |
| 3:L:863:HIS:HE1  | 3:L:887:ASP:HA    | 1.67                     | 0.59              |
| 3:A:183:GLN:OE1  | 3:A:1073:TYR:OH   | 2.16                     | 0.59              |
| 3:A:764:VAL:O    | 3:A:783:LEU:N     | 2.30                     | 0.59              |
| 3:A:1133:ARG:HE  | 3:A:1266:ALA:HB3  | 1.66                     | 0.59              |
| 3:H:42:VAL:HG13  | 3:H:46:GLU:HG3    | 1.84                     | 0.59              |
| 3:H:863:HIS:HE1  | 3:H:887:ASP:HA    | 1.68                     | 0.59              |
| 3:N:1058:PHE:CE2 | 3:N:1369:LEU:HD11 | 2.38                     | 0.59              |
| 3:O:195:LEU:O    | 3:O:198:LEU:N     | 2.25                     | 0.59              |
| 3:B:634:ILE:HA   | 3:B:640:VAL:HG11  | 1.84                     | 0.59              |
| 3:C:740:ASP:HA   | 3:C:799:PRO:HB3   | 1.84                     | 0.59              |
| 5:q:67:THR:HG22  | 5:q:466:VAL:HG22  | 1.83                     | 0.59              |
| 3:E:1191:PRO:HG2 | 3:E:1194:THR:HG23 | 1.84                     | 0.59              |
| 3:G:233:PHE:CE2  | 3:G:244:ILE:CG1   | 2.73                     | 0.59              |
| 2:U:300:PHE:CG   | 3:I:1083:HIS:CD2  | 2.88                     | 0.59              |
| 1:w:283:ARG:HH12 | 3:L:137:THR:HG21  | 1.67                     | 0.59              |
| 3:A:1357:HIS:CE1 | 3:A:1358:PHE:HD2  | 2.19                     | 0.59              |
| 3:H:426:ALA:HB3  | 3:H:429:HIS:CD2   | 2.38                     | 0.59              |
| 3:N:107:ASP:OD1  | 3:N:108:GLY:N     | 2.35                     | 0.59              |
| 3:C:493:ALA:O    | 3:C:495:ALA:N     | 2.35                     | 0.59              |
| 3:D:630:LEU:O    | 3:D:634:ILE:HD12  | 2.03                     | 0.59              |
| 3:G:454:MET:CE   | 3:G:1046:PRO:HD2  | 2.21                     | 0.59              |
| 3:J:90:MET:HG2   | 3:J:91:ASN:O      | 2.03                     | 0.59              |
| 3:L:198:LEU:O    | 3:L:201:MET:N     | 2.31                     | 0.59              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:L:591:PHE:HE2   | 3:L:595:ARG:HH21  | 1.50                     | 0.59              |
| 3:A:1257:TYR:HB2  | 3:A:1277:PHE:HD2  | 1.67                     | 0.59              |
| 3:N:97:PHE:HB2    | 3:N:120:MET:HB2   | 1.84                     | 0.59              |
| 3:N:892:LEU:O     | 3:N:895:GLN:HG3   | 2.03                     | 0.59              |
| 3:B:469:ILE:HD11  | 3:B:547:PHE:CZ    | 2.38                     | 0.59              |
| 3:D:213:ARG:HH12  | 3:D:1216:GLY:HA3  | 1.68                     | 0.59              |
| 3:D:1296:THR:HG21 | 3:D:1327:LEU:HG   | 1.84                     | 0.59              |
| 3:E:718:ALA:N     | 3:E:721:GLU:OE1   | 2.35                     | 0.59              |
| 3:K:280:THR:HG22  | 3:K:1063:VAL:HG22 | 1.84                     | 0.59              |
| 3:K:469:ILE:HD11  | 3:K:547:PHE:CE1   | 2.38                     | 0.59              |
| 3:M:724:HIS:CE1   | 3:M:1028:TYR:HB2  | 2.36                     | 0.59              |
| 3:H:947:HIS:O     | 4:m:80:ALA:N      | 2.25                     | 0.59              |
| 4:j:57:GLN:O      | 4:j:61:LEU:N      | 2.32                     | 0.59              |
| 3:N:326:VAL:CG2   | 3:E:321:VAL:HG12  | 2.30                     | 0.59              |
| 3:N:414:GLU:HG2   | 3:N:1356:THR:HG21 | 1.83                     | 0.59              |
| 3:O:309:MET:SD    | 3:O:327:ARG:HG3   | 2.43                     | 0.59              |
| 3:B:677:TYR:CD1   | 4:b:95:LYS:CE     | 2.86                     | 0.59              |
| 3:B:873:ASN:HA    | 4:g:92:PHE:HB2    | 1.85                     | 0.59              |
| 3:B:1054:ARG:NH2  | 3:B:1122:MET:HB3  | 2.17                     | 0.59              |
| 3:D:714:LEU:HD12  | 3:D:722:LEU:HD22  | 1.84                     | 0.59              |
| 3:D:1083:HIS:O    | 3:D:1090:ASN:N    | 2.35                     | 0.59              |
| 3:E:639:HIS:HB2   | 3:E:789:ALA:O     | 2.02                     | 0.59              |
| 1:Q:113:GLN:O     | 1:Q:115:THR:HG23  | 2.03                     | 0.59              |
| 1:Q:123:ASN:OD1   | 1:Q:254:TRP:NE1   | 2.33                     | 0.59              |
| 2:Y:238:ASN:HD22  | 3:H:1137:PRO:HB3  | 1.49                     | 0.59              |
| 3:I:946:ASP:HB3   | 3:I:949:ILE:H     | 1.68                     | 0.59              |
| 3:J:439:GLN:HE22  | 3:J:451:ARG:NH2   | 2.00                     | 0.59              |
| 3:J:1072:ALA:HB2  | 3:J:1102:LEU:HD23 | 1.85                     | 0.59              |
| 3:K:439:GLN:HG2   | 3:K:451:ARG:NH2   | 2.17                     | 0.59              |
| 3:K:634:ILE:HG22  | 3:K:636:GLY:H     | 1.68                     | 0.59              |
| 3:K:998:TYR:O     | 3:K:1003:ARG:NH2  | 2.36                     | 0.59              |
| 3:A:800:HIS:O     | 3:A:801:ARG:HG3   | 2.03                     | 0.59              |
| 4:i:4:PRO:HD3     | 4:i:16:ASN:HB3    | 1.84                     | 0.59              |
| 3:O:631:GLN:HE22  | 3:O:666:ASN:CG    | 2.11                     | 0.59              |
| 3:C:311:LEU:O     | 3:C:316:LEU:HB2   | 2.03                     | 0.59              |
| 3:F:69:ARG:HB2    | 3:F:72:GLU:HG2    | 1.85                     | 0.59              |
| 1:Q:255:VAL:HB    | 1:Q:262:SER:HB3   | 1.85                     | 0.58              |
| 3:K:399:ASP:OD1   | 3:K:1057:ARG:HG2  | 2.03                     | 0.58              |
| 3:H:266:HIS:CE1   | 3:H:303:PRO:HD2   | 2.38                     | 0.58              |
| 3:N:1260:ALA:O    | 3:N:1262:HIS:HD2  | 1.74                     | 0.58              |
| 3:P:801:ARG:HB3   | 3:P:802:PRO:HD2   | 1.83                     | 0.58              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:B:297:ASP:HB3   | 3:B:367:LEU:HB2   | 1.85                     | 0.58              |
| 3:B:828:ALA:HA    | 3:B:958:LEU:H     | 1.67                     | 0.58              |
| 3:D:1165:VAL:HG13 | 3:D:1166:PHE:H    | 1.67                     | 0.58              |
| 3:E:90:MET:HG2    | 3:E:91:ASN:O      | 2.03                     | 0.58              |
| 3:E:712:PRO:O     | 3:E:719:GLN:NE2   | 2.36                     | 0.58              |
| 3:E:1226:MET:HE2  | 3:E:1279:ALA:HB2  | 1.84                     | 0.58              |
| 3:E:1248:GLN:C    | 3:E:1251:SER:HG   | 2.11                     | 0.58              |
| 3:G:1161:GLN:HG2  | 3:G:1162:PRO:N    | 2.18                     | 0.58              |
| 1:l:113:GLN:O     | 1:l:115:THR:HG23  | 2.03                     | 0.58              |
| 3:I:1058:PHE:CE2  | 3:I:1369:LEU:HD11 | 2.38                     | 0.58              |
| 3:L:274:VAL:HG11  | 3:L:376:PHE:CD2   | 2.38                     | 0.58              |
| 4:n:77:PRO:O      | 4:n:94:LEU:N      | 2.27                     | 0.58              |
| 3:N:338:GLU:OE1   | 3:N:338:GLU:N     | 2.36                     | 0.58              |
| 3:N:875:VAL:HG12  | 3:N:879:PHE:CE2   | 2.38                     | 0.58              |
| 3:O:213:ARG:HH12  | 3:O:1216:GLY:HA3  | 1.68                     | 0.58              |
| 3:B:105:ALA:CB    | 3:G:176:PHE:CE1   | 2.86                     | 0.58              |
| 3:C:721:GLU:O     | 3:C:1030:LYS:NZ   | 2.32                     | 0.58              |
| 3:D:1049:GLY:O    | 3:D:1190:THR:N    | 2.32                     | 0.58              |
| 3:E:873:ASN:OD1   | 4:d:92:PHE:CA     | 2.51                     | 0.58              |
| 3:G:49:LEU:N      | 3:G:49:LEU:HD23   | 2.19                     | 0.58              |
| 3:G:212:THR:HG22  | 3:G:214:VAL:H     | 1.67                     | 0.58              |
| 3:G:552:GLY:O     | 3:G:569:GLY:CA    | 2.48                     | 0.58              |
| 1:w:282:PRO:HD2   | 3:L:138:GLU:OE1   | 2.03                     | 0.58              |
| 3:I:1206:ARG:HH21 | 3:I:1210:ALA:HB2  | 1.68                     | 0.58              |
| 3:I:1225:LEU:HD21 | 3:H:1176:GLY:HA3  | 1.85                     | 0.58              |
| 3:K:182:ASP:OD1   | 3:K:385:TYR:OH    | 2.18                     | 0.58              |
| 3:K:907:ALA:HB1   | 3:K:994:LEU:HD21  | 1.85                     | 0.58              |
| 4:l:33:GLN:HE21   | 4:l:35:ILE:HD13   | 1.68                     | 0.58              |
| 4:o:88:LEU:HD12   | 4:o:89:ARG:HG2    | 1.84                     | 0.58              |
| 3:C:266:HIS:CE1   | 3:C:302:VAL:HG13  | 2.39                     | 0.58              |
| 3:D:466:LEU:HD12  | 3:D:467:MET:HG3   | 1.85                     | 0.58              |
| 3:E:1029:PHE:HB3  | 3:E:1039:GLN:HE22 | 1.69                     | 0.58              |
| 3:F:1082:ARG:HG2  | 3:F:1091:PHE:CE1  | 2.38                     | 0.58              |
| 2:X:80:PRO:HD2    | 3:M:53:GLU:OE2    | 2.04                     | 0.58              |
| 2:x:300:PHE:HE2   | 3:O:1083:HIS:HB3  | 1.68                     | 0.58              |
| 3:J:484:ALA:O     | 3:J:486:PRO:CD    | 2.52                     | 0.58              |
| 3:J:604:HIS:HD2   | 3:J:696:HIS:CD2   | 2.22                     | 0.58              |
| 3:J:611:ILE:HG23  | 3:J:820:PHE:HE1   | 1.65                     | 0.58              |
| 3:L:1008:GLN:HA   | 3:L:1011:ARG:HG2  | 1.84                     | 0.58              |
| 3:M:521:VAL:HG21  | 3:M:987:VAL:HG12  | 1.86                     | 0.58              |
| 3:M:914:PRO:HG3   | 3:M:923:THR:HG22  | 1.85                     | 0.58              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:H:259:VAL:HG22  | 3:H:1102:LEU:HD13 | 1.84                     | 0.58              |
| 3:H:863:HIS:ND1   | 3:H:864:PRO:HD2   | 2.18                     | 0.58              |
| 3:N:176:PHE:O     | 3:N:179:GLY:N     | 2.34                     | 0.58              |
| 3:P:736:VAL:HG12  | 3:P:738:ASP:H     | 1.69                     | 0.58              |
| 3:G:500:ASP:O     | 3:G:504:ARG:CG    | 2.45                     | 0.58              |
| 1:T:170:LEU:CG    | 3:I:1262:HIS:CG   | 2.87                     | 0.58              |
| 2:Y:100:LEU:HD13  | 2:Y:314:VAL:HG21  | 1.84                     | 0.58              |
| 3:I:598:GLU:O     | 3:I:601:VAL:HG23  | 2.03                     | 0.58              |
| 3:J:463:HIS:ND1   | 3:J:464:PRO:HD2   | 2.18                     | 0.58              |
| 3:J:488:GLY:HA2   | 3:J:996:ALA:HB1   | 1.85                     | 0.58              |
| 3:K:961:HIS:O     | 3:K:964:PHE:N     | 2.35                     | 0.58              |
| 3:L:753:ASP:HB3   | 3:L:755:ARG:HH22  | 1.68                     | 0.58              |
| 3:L:923:THR:HA    | 3:L:926:MET:HE3   | 1.85                     | 0.58              |
| 3:N:158:GLN:O     | 3:N:161:ALA:N     | 2.36                     | 0.58              |
| 3:O:710:PRO:HG2   | 3:P:517:ARG:NH1   | 2.18                     | 0.58              |
| 3:P:1248:GLN:O    | 3:P:1251:SER:OG   | 2.21                     | 0.58              |
| 3:B:105:ALA:HB2   | 3:G:176:PHE:HE1   | 1.67                     | 0.58              |
| 3:C:863:HIS:CE1   | 3:C:887:ASP:HA    | 2.39                     | 0.58              |
| 3:E:1225:LEU:HD22 | 3:E:1234:PRO:HG3  | 1.85                     | 0.58              |
| 3:G:801:ARG:CB    | 3:G:802:PRO:CD    | 2.72                     | 0.58              |
| 3:G:905:THR:HB    | 3:G:956:TYR:OH    | 2.02                     | 0.58              |
| 7:u:3078:GLY:O    | 7:u:3082:LEU:N    | 2.32                     | 0.58              |
| 3:J:485:ASN:O     | 3:J:487:TYR:N     | 2.34                     | 0.58              |
| 3:L:523:GLU:OE2   | 3:L:538:ASN:ND2   | 2.37                     | 0.58              |
| 3:L:1011:ARG:HG3  | 3:L:1012:GLU:HG3  | 1.85                     | 0.58              |
| 3:M:278:LEU:HG    | 3:M:375:VAL:HG11  | 1.83                     | 0.58              |
| 3:A:182:ASP:HB3   | 3:A:186:HIS:CD2   | 2.39                     | 0.58              |
| 3:H:266:HIS:CE1   | 3:H:302:VAL:HG13  | 2.39                     | 0.58              |
| 3:H:272:ARG:NH2   | 3:H:372:ASP:O     | 2.36                     | 0.58              |
| 4:o:61:LEU:O      | 3:O:895:GLN:NE2   | 2.31                     | 0.58              |
| 3:N:819:ALA:O     | 3:N:822:ARG:NH1   | 2.37                     | 0.58              |
| 3:B:266:HIS:CE1   | 3:B:303:PRO:HD2   | 2.39                     | 0.58              |
| 3:C:1103:GLY:HA3  | 3:C:1107:THR:HG21 | 1.85                     | 0.58              |
| 3:D:227:PHE:O     | 3:D:231:SER:OG    | 2.17                     | 0.58              |
| 3:F:1054:ARG:HH22 | 3:F:1122:MET:HB3  | 1.68                     | 0.58              |
| 2:R:173:LEU:CA    | 5:q:371:GLY:HA2   | 2.32                     | 0.58              |
| 3:I:318:THR:O     | 3:I:323:GLY:N     | 2.36                     | 0.58              |
| 3:I:620:ASP:OD2   | 3:I:655:TYR:OH    | 2.19                     | 0.58              |
| 3:K:1131:LEU:HD11 | 3:K:1157:LEU:HG   | 1.85                     | 0.58              |
| 3:A:119:TYR:CD2   | 3:G:44:SER:CB     | 2.80                     | 0.58              |
| 3:A:344:LEU:HD21  | 3:B:340:GLN:HB3   | 1.84                     | 0.58              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:A:708:THR:HG22 | 3:A:723:ASN:HD22  | 1.69                     | 0.58              |
| 3:O:73:LEU:HD23  | 3:O:383:ARG:HH11  | 1.69                     | 0.58              |
| 3:O:426:ALA:HB3  | 3:O:429:HIS:CD2   | 2.37                     | 0.58              |
| 3:P:485:ASN:ND2  | 3:P:516:GLY:H     | 1.95                     | 0.58              |
| 3:B:73:LEU:HD11  | 3:B:384:ILE:HD11  | 1.85                     | 0.58              |
| 3:B:310:VAL:O    | 3:G:55:ASP:CA     | 2.42                     | 0.58              |
| 3:B:687:MET:O    | 3:B:690:TYR:N     | 2.33                     | 0.58              |
| 3:C:577:VAL:H    | 3:C:581:ASN:HD22  | 1.49                     | 0.58              |
| 3:E:448:GLN:HE21 | 3:F:1201:ARG:NH1  | 1.99                     | 0.58              |
| 3:E:708:THR:HG22 | 3:E:723:ASN:HD22  | 1.69                     | 0.58              |
| 3:G:469:ILE:HG22 | 3:G:473:VAL:HG23  | 1.84                     | 0.58              |
| 1:Q:112:ARG:HG2  | 1:Q:264:THR:HG22  | 1.85                     | 0.58              |
| 1:W:283:ARG:HH11 | 3:B:47:ASN:CB     | 2.17                     | 0.58              |
| 2:x:87:PRO:HG2   | 2:x:91:GLY:H      | 1.67                     | 0.58              |
| 3:J:756:ILE:HB   | 3:J:763:PRO:HD3   | 1.86                     | 0.58              |
| 3:L:177:GLU:O    | 3:L:180:THR:OG1   | 2.20                     | 0.58              |
| 3:M:29:VAL:HG12  | 3:D:120:MET:HE1   | 1.78                     | 0.58              |
| 3:H:339:MET:SD   | 3:C:17:MET:HE2    | 2.41                     | 0.58              |
| 3:H:532:MET:HE1  | 3:H:1244:PRO:HD3  | 1.85                     | 0.58              |
| 3:N:493:ALA:HB2  | 3:N:559:PRO:HB2   | 1.86                     | 0.58              |
| 3:B:241:ARG:NE   | 3:B:245:GLU:OE2   | 2.37                     | 0.58              |
| 3:B:525:GLN:NE2  | 3:G:706:ASP:O     | 2.36                     | 0.58              |
| 3:D:710:PRO:O    | 3:E:517:ARG:NH1   | 2.37                     | 0.58              |
| 5:q:8:GLU:OE2    | 5:q:25:HIS:NE2    | 2.34                     | 0.58              |
| 3:G:1197:ASN:O   | 3:G:1199:PHE:N    | 2.36                     | 0.58              |
| 2:X:80:PRO:CD    | 3:M:53:GLU:OE2    | 2.52                     | 0.58              |
| 3:I:158:GLN:O    | 3:I:161:ALA:N     | 2.37                     | 0.58              |
| 3:M:834:ARG:HD3  | 4:l:90:PRO:HD3    | 1.86                     | 0.58              |
| 3:M:948:THR:HG23 | 3:M:949:ILE:HG13  | 1.86                     | 0.58              |
| 3:H:339:MET:CE   | 3:C:17:MET:HG2    | 2.21                     | 0.58              |
| 3:H:1206:ARG:NH2 | 3:H:1208:ARG:O    | 2.37                     | 0.58              |
| 3:N:120:MET:SD   | 3:D:36:PHE:HE2    | 2.26                     | 0.58              |
| 3:P:644:LEU:HD22 | 3:P:647:LEU:HD12  | 1.86                     | 0.58              |
| 3:B:776:PHE:O    | 3:B:904:ARG:HB3   | 2.04                     | 0.58              |
| 3:C:132:ALA:HB3  | 3:D:114:GLN:HG2   | 1.84                     | 0.58              |
| 3:C:655:TYR:CD2  | 3:C:663:ALA:HB2   | 2.39                     | 0.58              |
| 3:C:1072:ALA:HB2 | 3:C:1102:LEU:HD23 | 1.86                     | 0.58              |
| 3:E:469:ILE:HD11 | 3:E:547:PHE:CD1   | 2.39                     | 0.58              |
| 3:E:865:LEU:HD22 | 3:E:879:PHE:HB2   | 1.86                     | 0.58              |
| 3:E:1072:ALA:HB2 | 3:E:1102:LEU:HD23 | 1.86                     | 0.58              |
| 6:s:26:PHE:CZ    | 6:s:29:PRO:HD3    | 2.39                     | 0.58              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:G:106:ARG:HH12  | 3:G:113:GLU:CD    | 2.12                     | 0.58              |
| 2:R:173:LEU:HA    | 5:q:372:ASP:N     | 2.16                     | 0.58              |
| 2:3:99:ASN:ND2    | 3:M:1086:GLY:CA   | 2.67                     | 0.58              |
| 2:3:300:PHE:CB    | 3:M:1083:HIS:NE2  | 2.67                     | 0.58              |
| 2:y:299:THR:HG22  | 2:y:313:PRO:HD2   | 1.86                     | 0.58              |
| 3:I:201:MET:O     | 3:I:204:TYR:N     | 2.34                     | 0.58              |
| 3:J:499:ALA:HA    | 3:J:956:TYR:CD1   | 2.39                     | 0.58              |
| 3:L:1209:ALA:HB3  | 3:L:1234:PRO:HG2  | 1.85                     | 0.58              |
| 3:M:28:GLU:HG3    | 3:C:387:ALA:HA    | 1.85                     | 0.58              |
| 3:M:195:LEU:HD21  | 3:M:251:LEU:HD23  | 1.85                     | 0.58              |
| 3:O:414:GLU:HG2   | 3:O:1356:THR:HG21 | 1.86                     | 0.58              |
| 3:B:89:TYR:CE1    | 3:G:35:LEU:HD13   | 2.38                     | 0.58              |
| 3:C:634:ILE:HA    | 3:C:640:VAL:HG11  | 1.85                     | 0.58              |
| 3:D:717:GLN:HE22  | 3:D:752:ARG:NH1   | 2.02                     | 0.58              |
| 3:E:266:HIS:HE1   | 3:E:302:VAL:HG13  | 1.68                     | 0.58              |
| 3:F:829:GLY:HA3   | 3:F:956:TYR:CE1   | 2.39                     | 0.58              |
| 3:G:1209:ALA:HB3  | 3:G:1234:PRO:HG2  | 1.85                     | 0.58              |
| 1:T:161:TRP:CD1   | 3:I:1166:PHE:CD1  | 2.92                     | 0.57              |
| 1:l:138:THR:HA    | 3:M:1166:PHE:CG   | 2.17                     | 0.57              |
| 3:K:309:MET:SD    | 3:K:327:ARG:HG3   | 2.43                     | 0.57              |
| 3:K:1124:ASN:O    | 3:K:1156:ARG:NH1  | 2.37                     | 0.57              |
| 3:M:161:ALA:CA    | 3:C:50:TYR:HE1    | 2.15                     | 0.57              |
| 3:M:265:THR:H     | 3:M:1068:ARG:HH21 | 1.51                     | 0.57              |
| 3:M:577:VAL:H     | 3:M:581:ASN:HD22  | 1.52                     | 0.57              |
| 3:A:120:MET:HA    | 3:G:45:ASP:OD2    | 2.04                     | 0.57              |
| 3:N:634:ILE:HA    | 3:N:640:VAL:HG11  | 1.86                     | 0.57              |
| 3:N:1222:VAL:HG11 | 3:N:1283:THR:HA   | 1.86                     | 0.57              |
| 3:P:193:PRO:HG2   | 3:P:198:LEU:HD11  | 1.85                     | 0.57              |
| 3:D:231:SER:O     | 3:D:1112:THR:OG1  | 2.21                     | 0.57              |
| 3:G:103:LEU:HD13  | 3:G:115:PRO:HA    | 1.77                     | 0.57              |
| 2:X:12:ILE:HD11   | 2:X:83:ILE:HG13   | 1.86                     | 0.57              |
| 2:X:40:GLN:OE1    | 3:I:107:ASP:OD1   | 2.22                     | 0.57              |
| 3:I:802:PRO:HB3   | 3:J:945:LEU:HD21  | 1.85                     | 0.57              |
| 3:J:635:HIS:CE1   | 3:J:640:VAL:HG21  | 2.39                     | 0.57              |
| 3:J:866:HIS:ND1   | 3:J:867:PRO:HD2   | 2.19                     | 0.57              |
| 3:L:896:VAL:HA    | 3:L:899:HIS:CD2   | 2.37                     | 0.57              |
| 3:M:579:ASN:HA    | 3:M:1031:MET:HE3  | 1.87                     | 0.57              |
| 3:H:863:HIS:CE1   | 3:H:887:ASP:HA    | 2.39                     | 0.57              |
| 3:C:108:GLY:HA2   | 3:C:110:HIS:H     | 1.69                     | 0.57              |
| 3:D:38:PHE:CG     | 3:D:38:PHE:O      | 2.57                     | 0.57              |
| 3:E:301:ASP:OD1   | 3:E:362:ARG:NE    | 2.36                     | 0.57              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:G:728:ASP:O     | 3:G:810:LYS:NZ    | 2.37                     | 0.57              |
| 2:2:254:ILE:HG22  | 2:2:256:PRO:HD3   | 1.86                     | 0.57              |
| 2:2:306:VAL:HG11  | 2:2:312:ALA:HB2   | 1.85                     | 0.57              |
| 3:I:93:GLY:HA3    | 3:I:124:ILE:HD12  | 1.85                     | 0.57              |
| 3:K:399:ASP:HB2   | 3:K:1323:ASP:OD1  | 2.04                     | 0.57              |
| 3:L:288:LEU:HB3   | 3:L:293:LEU:HD12  | 1.86                     | 0.57              |
| 3:L:521:VAL:HG11  | 3:L:987:VAL:HG12  | 1.87                     | 0.57              |
| 3:M:21:GLY:O      | 3:C:61:TYR:CD1    | 2.57                     | 0.57              |
| 3:M:61:TYR:HD1    | 3:C:21:GLY:C      | 2.06                     | 0.57              |
| 3:M:227:PHE:O     | 3:M:231:SER:OG    | 2.16                     | 0.57              |
| 3:M:842:MET:HE1   | 3:M:891:MET:HB3   | 1.85                     | 0.57              |
| 3:M:842:MET:HE1   | 3:M:891:MET:HE3   | 1.86                     | 0.57              |
| 3:A:879:PHE:CE1   | 3:A:886:VAL:HG21  | 2.40                     | 0.57              |
| 3:O:406:LEU:HD23  | 3:O:440:LEU:HG    | 1.85                     | 0.57              |
| 3:P:469:ILE:HD11  | 3:P:547:PHE:CD1   | 2.39                     | 0.57              |
| 3:C:887:ASP:O     | 3:C:891:MET:HG2   | 2.04                     | 0.57              |
| 3:E:263:ARG:NH2   | 3:E:305:THR:O     | 2.37                     | 0.57              |
| 3:E:749:ASP:OD2   | 3:E:751:HIS:HB2   | 2.05                     | 0.57              |
| 2:y:68:ARG:NH1    | 2:y:288:ILE:O     | 2.37                     | 0.57              |
| 3:J:778:ARG:HH11  | 3:J:782:ARG:HD2   | 1.69                     | 0.57              |
| 3:K:463:HIS:CG    | 3:K:464:PRO:HD2   | 2.40                     | 0.57              |
| 3:L:1148:ARG:HH22 | 3:L:1163:LEU:HG   | 1.68                     | 0.57              |
| 3:A:924:ALA:O     | 3:A:927:ARG:NH1   | 2.30                     | 0.57              |
| 4:o:89:ARG:HH12   | 3:P:873:ASN:HD22  | 1.51                     | 0.57              |
| 3:N:392:TYR:CE2   | 3:N:394:LEU:HB3   | 2.40                     | 0.57              |
| 3:O:545:PRO:HB2   | 3:O:1048:PHE:HE1  | 1.68                     | 0.57              |
| 3:O:709:LEU:HD12  | 3:O:1037:TYR:CE1  | 2.39                     | 0.57              |
| 3:P:485:ASN:ND2   | 3:P:516:GLY:O     | 2.37                     | 0.57              |
| 3:B:745:HIS:CE1   | 3:B:910:CYS:HB2   | 2.39                     | 0.57              |
| 3:D:841:ASN:O     | 3:D:875:VAL:HG23  | 2.04                     | 0.57              |
| 5:q:152:GLU:OE2   | 5:q:390:HIS:ND1   | 2.34                     | 0.57              |
| 3:E:1257:TYR:HB2  | 3:E:1277:PHE:CD2  | 2.25                     | 0.57              |
| 3:F:439:GLN:HE21  | 3:F:451:ARG:NH2   | 2.02                     | 0.57              |
| 3:F:870:LEU:HD22  | 3:F:877:ALA:HA    | 1.85                     | 0.57              |
| 1:W:198:TYR:O     | 1:W:201:ARG:HG2   | 2.03                     | 0.57              |
| 1:W:348:GLY:HA3   | 6:r:13:TRP:HB2    | 1.87                     | 0.57              |
| 2:X:18:ARG:NH1    | 2:3:18:ARG:HH11   | 1.96                     | 0.57              |
| 3:I:124:ILE:HG12  | 3:I:1100:VAL:HG21 | 1.85                     | 0.57              |
| 3:J:466:LEU:HD12  | 3:J:467:MET:HG3   | 1.87                     | 0.57              |
| 3:A:825:CYS:HB2   | 3:A:938:LEU:HD21  | 1.87                     | 0.57              |
| 3:H:1051:THR:HG23 | 3:H:1190:THR:HG21 | 1.87                     | 0.57              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:N:785:HIS:HD2   | 3:N:788:GLN:HE21  | 1.52                     | 0.57              |
| 3:N:1103:GLY:HA3  | 3:N:1107:THR:HG21 | 1.87                     | 0.57              |
| 3:P:524:CYS:HB3   | 3:P:1008:GLN:OE1  | 2.05                     | 0.57              |
| 3:B:895:GLN:HE22  | 4:b:65:GLY:HA3    | 1.69                     | 0.57              |
| 3:D:752:ARG:NH2   | 3:D:915:ASP:HA    | 2.19                     | 0.57              |
| 3:E:838:THR:O     | 3:E:875:VAL:HG22  | 2.04                     | 0.57              |
| 6:r:80:ILE:HD12   | 7:u:3104:PHE:HE2  | 1.68                     | 0.57              |
| 3:G:52:VAL:HG12   | 3:G:54:PHE:HE2    | 1.66                     | 0.57              |
| 4:d:89:ARG:NH2    | 4:e:30:ASN:OD1    | 2.37                     | 0.57              |
| 3:I:426:ALA:HB3   | 3:I:429:HIS:CD2   | 2.40                     | 0.57              |
| 3:J:847:ILE:HG13  | 3:J:862:ALA:HB1   | 1.87                     | 0.57              |
| 3:J:1204:ASN:HD22 | 3:J:1209:ALA:HA   | 1.69                     | 0.57              |
| 3:L:651:CYS:O     | 3:L:654:SER:OG    | 2.19                     | 0.57              |
| 3:M:27:ILE:HD11   | 3:D:256:GLN:OE1   | 2.03                     | 0.57              |
| 3:M:132:ALA:HB3   | 3:H:114:GLN:HG2   | 1.86                     | 0.57              |
| 3:A:896:VAL:HG13  | 3:A:899:HIS:HD2   | 1.68                     | 0.57              |
| 3:N:406:LEU:HD23  | 3:N:440:LEU:HG    | 1.85                     | 0.57              |
| 3:N:1080:VAL:HG22 | 3:N:1093:LEU:HD22 | 1.87                     | 0.57              |
| 3:O:861:PRO:O     | 3:O:869:ASN:ND2   | 2.37                     | 0.57              |
| 3:O:1209:ALA:HB3  | 3:O:1234:PRO:HG2  | 1.87                     | 0.57              |
| 3:B:488:GLY:HA2   | 3:B:996:ALA:HB1   | 1.85                     | 0.57              |
| 3:B:1128:ASN:HD21 | 3:B:1155:ASN:ND2  | 2.01                     | 0.57              |
| 3:D:424:VAL:HG12  | 3:D:425:PRO:O     | 2.05                     | 0.57              |
| 3:D:866:HIS:HB3   | 3:D:869:ASN:HB2   | 1.86                     | 0.57              |
| 3:F:153:ILE:O     | 3:F:157:ARG:N     | 2.37                     | 0.57              |
| 3:G:725:LEU:HG    | 3:G:731:LEU:HD11  | 1.85                     | 0.57              |
| 3:G:737:TRP:HZ2   | 3:G:937:VAL:HG22  | 1.69                     | 0.57              |
| 2:S:2:ILE:HD12    | 3:B:1084:GLU:O    | 1.93                     | 0.57              |
| 2:U:158:ARG:NH2   | 2:U:177:ASN:OD1   | 2.37                     | 0.57              |
| 2:y:154:ARG:NH1   | 2:y:176:LEU:O     | 2.37                     | 0.57              |
| 3:J:107:ASP:OD1   | 3:J:108:GLY:N     | 2.37                     | 0.57              |
| 3:J:736:VAL:HG12  | 3:J:738:ASP:H     | 1.69                     | 0.57              |
| 3:K:1004:GLN:NE2  | 3:K:1007:VAL:HB   | 2.20                     | 0.57              |
| 3:L:866:HIS:ND1   | 3:L:867:PRO:HD2   | 2.20                     | 0.57              |
| 3:M:948:THR:HA    | 4:l:80:ALA:H      | 1.69                     | 0.57              |
| 4:l:4:PRO:HD3     | 4:l:16:ASN:HB3    | 1.86                     | 0.57              |
| 3:O:163:GLN:OE1   | 3:P:348:ARG:NH2   | 2.38                     | 0.57              |
| 3:O:512:ARG:HA    | 3:O:515:HIS:HD2   | 1.68                     | 0.57              |
| 3:B:105:ALA:CB    | 3:G:176:PHE:HE1   | 2.18                     | 0.57              |
| 5:q:473:ALA:HB3   | 6:s:54:VAL:HG13   | 1.86                     | 0.57              |
| 3:E:51:ASP:OD1    | 3:E:52:VAL:N      | 2.38                     | 0.57              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:E:433:ARG:NH1   | 3:F:413:MET:SD    | 2.78                     | 0.57              |
| 3:G:666:ASN:CB    | 3:G:938:LEU:HD21  | 2.32                     | 0.57              |
| 3:G:1029:PHE:HB3  | 3:G:1039:GLN:HE22 | 1.70                     | 0.57              |
| 7:t:3082:LEU:O    | 7:t:3086:ILE:N    | 2.34                     | 0.57              |
| 2:U:217:THR:HA    | 2:U:220:ILE:HD12  | 1.87                     | 0.57              |
| 2:y:57:SER:O      | 2:y:194:GLN:NE2   | 2.38                     | 0.57              |
| 3:J:194:PRO:HA    | 3:J:1110:ALA:O    | 2.04                     | 0.57              |
| 3:J:1321:VAL:HG12 | 3:J:1322:GLU:N    | 2.19                     | 0.57              |
| 3:K:279:VAL:HG12  | 3:K:394:LEU:HD22  | 1.86                     | 0.57              |
| 3:K:633:ALA:O     | 3:K:635:HIS:ND1   | 2.31                     | 0.57              |
| 3:K:706:ASP:O     | 3:L:525:GLN:NE2   | 2.37                     | 0.57              |
| 3:L:863:HIS:CE1   | 3:L:887:ASP:HA    | 2.40                     | 0.57              |
| 4:h:60:ALA:O      | 4:h:64:LEU:N      | 2.31                     | 0.57              |
| 4:l:5:GLN:HB3     | 4:l:7:HIS:CE1     | 2.39                     | 0.57              |
| 3:N:526:MET:HE2   | 3:N:531:PHE:HA    | 1.87                     | 0.57              |
| 3:N:545:PRO:HB2   | 3:N:1048:PHE:HE1  | 1.70                     | 0.57              |
| 3:N:1286:HIS:CG   | 3:D:34:ARG:HH12   | 2.21                     | 0.57              |
| 3:O:457:ALA:O     | 3:O:460:THR:OG1   | 2.22                     | 0.57              |
| 3:P:414:GLU:OE2   | 3:P:1356:THR:HB   | 2.05                     | 0.57              |
| 3:P:1024:LEU:O    | 3:P:1027:GLY:N    | 2.38                     | 0.57              |
| 3:B:615:ARG:HH21  | 3:B:1017:GLU:HG2  | 1.68                     | 0.57              |
| 3:C:399:ASP:OD1   | 3:C:1057:ARG:HG2  | 2.05                     | 0.57              |
| 2:X:284:GLN:HG2   | 3:H:1166:PHE:HZ   | 0.78                     | 0.57              |
| 2:x:26:ARG:O      | 2:x:101:ARG:NH1   | 2.38                     | 0.57              |
| 3:I:104:ILE:HD11  | 3:H:390:VAL:HG11  | 1.85                     | 0.57              |
| 3:I:866:HIS:ND1   | 3:I:867:PRO:HD2   | 2.19                     | 0.57              |
| 3:K:766:ALA:N     | 3:K:783:LEU:O     | 2.20                     | 0.57              |
| 3:L:752:ARG:NH2   | 3:L:915:ASP:OD1   | 2.36                     | 0.57              |
| 3:A:215:ALA:O     | 3:A:218:THR:OG1   | 2.22                     | 0.57              |
| 3:A:348:ARG:HG2   | 3:B:337:LEU:HD13  | 1.87                     | 0.57              |
| 3:H:339:MET:HE1   | 3:C:17:MET:SD     | 2.45                     | 0.57              |
| 3:H:837:ALA:O     | 4:h:57:GLN:NE2    | 2.32                     | 0.57              |
| 3:H:1248:GLN:O    | 3:H:1251:SER:OG   | 2.18                     | 0.57              |
| 3:N:263:ARG:NH2   | 3:N:306:TYR:O     | 2.37                     | 0.57              |
| 3:N:548:ASP:OD1   | 3:N:576:ARG:NE    | 2.21                     | 0.57              |
| 3:O:278:LEU:HG    | 3:O:375:VAL:HG11  | 1.86                     | 0.57              |
| 3:P:255:THR:OG1   | 3:P:1067:GLU:OE2  | 2.19                     | 0.57              |
| 3:C:414:GLU:HG2   | 3:C:1356:THR:HG21 | 1.86                     | 0.57              |
| 3:C:790:ARG:HG3   | 3:C:792:ALA:H     | 1.69                     | 0.57              |
| 5:q:91:ALA:HB3    | 5:q:103:ARG:HD3   | 1.85                     | 0.57              |
| 3:E:58:LEU:HD12   | 3:F:124:ILE:HD11  | 1.87                     | 0.57              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:E:765:TYR:CE1   | 3:E:783:LEU:HD12  | 2.40                     | 0.57              |
| 3:E:1270:LEU:HD22 | 3:E:1303:ALA:HB2  | 1.87                     | 0.57              |
| 6:r:70:ALA:O      | 6:r:74:ALA:N      | 2.38                     | 0.57              |
| 3:F:631:GLN:NE2   | 3:F:666:ASN:OD1   | 2.29                     | 0.57              |
| 1:Q:149:PRO:HD2   | 1:Q:152:ARG:HD2   | 1.86                     | 0.57              |
| 3:K:876:ASN:HA    | 3:K:879:PHE:HD2   | 1.70                     | 0.57              |
| 3:A:94:ARG:HH12   | 3:G:47:ASN:CB     | 2.14                     | 0.57              |
| 3:A:742:LEU:HD22  | 3:A:756:ILE:HD13  | 1.87                     | 0.57              |
| 3:A:1118:PRO:HD3  | 3:A:1374:LEU:HD21 | 1.87                     | 0.57              |
| 3:H:709:LEU:HD13  | 3:H:710:PRO:HD2   | 1.86                     | 0.57              |
| 4:j:60:ALA:HA     | 4:j:63:ASP:HB2    | 1.87                     | 0.57              |
| 3:P:829:GLY:N     | 3:P:956:TYR:O     | 2.38                     | 0.57              |
| 3:C:841:ASN:OD1   | 4:c:57:GLN:NE2    | 2.37                     | 0.57              |
| 3:D:521:VAL:HG11  | 3:D:987:VAL:HG12  | 1.87                     | 0.57              |
| 3:D:873:ASN:OD1   | 4:c:92:PHE:CA     | 2.53                     | 0.57              |
| 3:E:392:TYR:CE2   | 3:E:394:LEU:HB3   | 2.40                     | 0.57              |
| 6:r:80:ILE:HD11   | 7:t:3103:LEU:HD11 | 1.86                     | 0.57              |
| 3:G:547:PHE:CB    | 3:G:549:PHE:HE2   | 2.18                     | 0.57              |
| 2:S:260:MET:CG    | 5:q:412:ARG:HH11  | 2.18                     | 0.56              |
| 1:T:166:GLU:CD    | 3:I:1262:HIS:CD2  | 2.83                     | 0.56              |
| 1:w:181:ARG:HH22  | 3:O:1167:GLY:HA2  | 1.70                     | 0.56              |
| 2:x:12:ILE:HD11   | 2:x:83:ILE:HG13   | 1.87                     | 0.56              |
| 3:I:706:ASP:O     | 3:J:525:GLN:NE2   | 2.38                     | 0.56              |
| 3:J:639:HIS:HA    | 4:j:79:PHE:CE2    | 2.40                     | 0.56              |
| 3:J:1190:THR:HG22 | 3:J:1243:ASN:ND2  | 2.20                     | 0.56              |
| 3:K:1148:ARG:HH22 | 3:K:1163:LEU:HG   | 1.69                     | 0.56              |
| 3:L:55:ASP:OD1    | 3:M:91:ASN:HB2    | 2.04                     | 0.56              |
| 3:L:826:CYS:HB3   | 3:L:966:GLY:H     | 1.69                     | 0.56              |
| 3:M:45:ASP:OD1    | 3:M:46:GLU:N      | 2.37                     | 0.56              |
| 3:M:119:TYR:HB3   | 3:N:11:TYR:CE2    | 2.37                     | 0.56              |
| 3:M:333:GLY:HA2   | 3:O:317:VAL:HG11  | 1.87                     | 0.56              |
| 4:m:76:GLN:HG2    | 4:m:94:LEU:HD12   | 1.87                     | 0.56              |
| 3:P:651:CYS:O     | 3:P:654:SER:OG    | 2.20                     | 0.56              |
| 3:P:1206:ARG:NH2  | 3:P:1208:ARG:O    | 2.38                     | 0.56              |
| 3:C:426:ALA:HB3   | 3:C:429:HIS:CD2   | 2.40                     | 0.56              |
| 3:C:463:HIS:HD2   | 3:C:465:SER:HB3   | 1.69                     | 0.56              |
| 3:E:947:HIS:HB2   | 4:d:79:PHE:CD1    | 2.40                     | 0.56              |
| 6:r:85:ARG:HE     | 7:u:3100:ARG:NH2  | 2.01                     | 0.56              |
| 3:F:116:VAL:HG12  | 3:F:117:HIS:H     | 1.70                     | 0.56              |
| 3:F:1004:GLN:NE2  | 3:F:1007:VAL:HB   | 2.20                     | 0.56              |
| 2:U:10:ILE:HB     | 2:U:83:ILE:HB     | 1.88                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:W:347:PHE:CZ    | 6:r:18:PHE:CE2    | 2.93                     | 0.56              |
| 2:3:80:PRO:CG     | 3:C:53:GLU:OE2    | 2.50                     | 0.56              |
| 3:I:639:HIS:HA    | 4:i:79:PHE:CE2    | 2.40                     | 0.56              |
| 3:I:724:HIS:CE1   | 3:I:1028:TYR:HB2  | 2.40                     | 0.56              |
| 3:I:1215:ALA:HB3  | 3:I:1287:ARG:HE   | 1.69                     | 0.56              |
| 3:K:213:ARG:HH12  | 3:K:1216:GLY:HA3  | 1.69                     | 0.56              |
| 3:K:621:ARG:C     | 3:K:943:GLN:HE21  | 2.12                     | 0.56              |
| 3:L:611:ILE:HG23  | 3:L:820:PHE:HE1   | 1.69                     | 0.56              |
| 3:M:12:ARG:CA     | 3:D:96:GLN:HE22   | 2.18                     | 0.56              |
| 3:A:446:ASP:O     | 3:A:448:GLN:HG3   | 2.05                     | 0.56              |
| 3:N:866:HIS:ND1   | 3:N:867:PRO:HD2   | 2.20                     | 0.56              |
| 3:O:1191:PRO:HG2  | 3:O:1194:THR:HG23 | 1.86                     | 0.56              |
| 3:P:262:PRO:HG3   | 3:P:353:GLU:HG2   | 1.86                     | 0.56              |
| 3:P:767:ALA:HA    | 3:P:796:ASP:OD1   | 2.05                     | 0.56              |
| 3:B:1222:VAL:HG11 | 3:B:1283:THR:HA   | 1.85                     | 0.56              |
| 3:C:819:ALA:O     | 3:C:822:ARG:NH1   | 2.38                     | 0.56              |
| 3:C:873:ASN:CG    | 4:b:92:PHE:H      | 2.14                     | 0.56              |
| 3:D:1174:ARG:NH1  | 3:E:1232:SER:OG   | 2.25                     | 0.56              |
| 3:E:1080:VAL:HG22 | 3:E:1093:LEU:HD22 | 1.87                     | 0.56              |
| 3:F:12:ARG:CG     | 3:G:321:VAL:HA    | 2.35                     | 0.56              |
| 3:F:961:HIS:O     | 3:F:964:PHE:N     | 2.37                     | 0.56              |
| 3:G:497:PRO:O     | 3:G:504:ARG:NH2   | 2.38                     | 0.56              |
| 3:G:1197:ASN:O    | 3:G:1198:TYR:C    | 2.48                     | 0.56              |
| 1:l:78:ALA:CB     | 3:M:308:GLU:OE1   | 2.53                     | 0.56              |
| 1:w:116:LEU:HD23  | 1:w:260:LEU:HB3   | 1.86                     | 0.56              |
| 1:w:158:ALA:HB1   | 3:O:1165:VAL:CG2  | 2.35                     | 0.56              |
| 2:x:89:ASP:OD2    | 2:y:296:ARG:NH2   | 2.38                     | 0.56              |
| 2:y:241:LEU:HD12  | 2:y:248:ARG:HH21  | 1.69                     | 0.56              |
| 3:I:519:ARG:NH1   | 3:I:998:TYR:OH    | 2.30                     | 0.56              |
| 3:J:63:ASN:HD21   | 3:K:99:VAL:HG13   | 1.70                     | 0.56              |
| 3:J:631:GLN:HE22  | 3:J:666:ASN:CG    | 2.13                     | 0.56              |
| 3:J:802:PRO:HG3   | 3:K:945:LEU:HD11  | 1.86                     | 0.56              |
| 3:K:58:LEU:HD12   | 3:L:124:ILE:HD11  | 1.86                     | 0.56              |
| 3:K:263:ARG:NH2   | 3:K:305:THR:OG1   | 2.39                     | 0.56              |
| 3:K:854:PRO:HB2   | 3:K:863:HIS:HB2   | 1.87                     | 0.56              |
| 3:L:692:ASP:O     | 3:L:696:HIS:N     | 2.36                     | 0.56              |
| 3:L:700:LEU:HD22  | 3:L:1025:MET:HG3  | 1.87                     | 0.56              |
| 3:M:463:HIS:ND1   | 3:M:464:PRO:HD2   | 2.21                     | 0.56              |
| 3:M:960:VAL:HA    | 3:M:994:LEU:HD13  | 1.86                     | 0.56              |
| 3:M:1049:GLY:O    | 3:M:1190:THR:N    | 2.36                     | 0.56              |
| 3:A:506:LEU:O     | 3:A:510:ARG:HG3   | 2.03                     | 0.56              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:A:843:VAL:HB   | 3:A:876:ASN:HD22  | 1.71                     | 0.56              |
| 3:H:758:ALA:HB3  | 3:H:781:GLY:HA2   | 1.87                     | 0.56              |
| 3:H:1181:GLN:HB2 | 3:H:1309:VAL:O    | 2.05                     | 0.56              |
| 4:h:76:GLN:O     | 4:h:96:ARG:NH2    | 2.33                     | 0.56              |
| 4:i:22:MET:HE1   | 4:i:57:GLN:HA     | 1.87                     | 0.56              |
| 3:N:119:TYR:HE2  | 3:D:42:VAL:CG2    | 2.19                     | 0.56              |
| 3:N:301:ASP:OD1  | 3:N:362:ARG:NE    | 2.32                     | 0.56              |
| 3:N:390:VAL:HG21 | 3:O:104:ILE:HD11  | 1.86                     | 0.56              |
| 3:N:959:PRO:HG2  | 3:N:991:PRO:HD3   | 1.86                     | 0.56              |
| 3:O:752:ARG:NH2  | 3:O:915:ASP:OD1   | 2.34                     | 0.56              |
| 3:O:1347:ARG:NH2 | 3:P:1355:GLU:OE2  | 2.38                     | 0.56              |
| 3:P:180:THR:O    | 3:P:183:GLN:N     | 2.38                     | 0.56              |
| 3:P:192:ALA:HB1  | 3:P:1110:ALA:H    | 1.70                     | 0.56              |
| 3:P:631:GLN:NE2  | 3:P:666:ASN:OD1   | 2.39                     | 0.56              |
| 3:B:677:TYR:CA   | 4:b:95:LYS:HZ3    | 2.09                     | 0.56              |
| 3:C:106:ARG:HH21 | 3:C:110:HIS:HB3   | 1.69                     | 0.56              |
| 3:C:677:TYR:CD1  | 4:c:95:LYS:CE     | 2.84                     | 0.56              |
| 3:C:753:ASP:HB2  | 3:C:755:ARG:HH12  | 1.69                     | 0.56              |
| 3:C:846:GLU:HA   | 4:c:68:HIS:CE1    | 2.38                     | 0.56              |
| 3:C:1202:PRO:HB3 | 3:C:1332:TYR:HD1  | 1.70                     | 0.56              |
| 3:D:204:TYR:HB2  | 3:D:219:LEU:HD21  | 1.86                     | 0.56              |
| 3:D:462:CYS:SG   | 3:D:1147:LEU:HD22 | 2.46                     | 0.56              |
| 5:q:260:ILE:N    | 5:q:261:LEU:HB2   | 2.20                     | 0.56              |
| 5:q:594:THR:HB   | 5:q:647:ALA:HA    | 1.86                     | 0.56              |
| 3:E:876:ASN:OD1  | 3:E:891:MET:HE2   | 2.05                     | 0.56              |
| 3:F:213:ARG:HH12 | 3:F:1216:GLY:HA3  | 1.68                     | 0.56              |
| 3:F:721:GLU:O    | 3:F:1030:LYS:NZ   | 2.38                     | 0.56              |
| 3:F:790:ARG:NH1  | 4:f:80:ALA:O      | 2.38                     | 0.56              |
| 2:2:68:ARG:NH1   | 2:2:288:ILE:O     | 2.37                     | 0.56              |
| 2:2:78:VAL:HG13  | 2:2:83:ILE:HG12   | 1.87                     | 0.56              |
| 3:I:214:VAL:HG22 | 3:H:1177:MET:HE1  | 1.87                     | 0.56              |
| 3:I:405:PRO:O    | 3:I:440:LEU:HD11  | 2.04                     | 0.56              |
| 3:I:426:ALA:HB3  | 3:I:429:HIS:HD2   | 1.70                     | 0.56              |
| 3:I:462:CYS:SG   | 3:I:1147:LEU:HD22 | 2.45                     | 0.56              |
| 3:I:728:ASP:HB3  | 3:I:730:ALA:H     | 1.70                     | 0.56              |
| 3:J:452:LEU:HD12 | 3:J:456:ASN:ND2   | 2.18                     | 0.56              |
| 3:J:895:GLN:HG2  | 4:j:61:LEU:HB3    | 1.87                     | 0.56              |
| 3:J:1000:SER:O   | 3:J:1003:ARG:NH1  | 2.39                     | 0.56              |
| 3:K:463:HIS:ND1  | 3:K:464:PRO:HD2   | 2.20                     | 0.56              |
| 3:L:258:SER:OG   | 3:L:259:VAL:N     | 2.38                     | 0.56              |
| 3:H:488:GLY:HA2  | 3:H:996:ALA:HB1   | 1.87                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:N:998:TYR:O     | 3:N:1003:ARG:NH1  | 2.39                     | 0.56              |
| 3:O:1051:THR:HG23 | 3:O:1190:THR:HG21 | 1.87                     | 0.56              |
| 3:P:1080:VAL:HG22 | 3:P:1093:LEU:HD22 | 1.88                     | 0.56              |
| 3:C:738:ASP:OD1   | 3:C:787:THR:OG1   | 2.23                     | 0.56              |
| 3:C:1054:ARG:NH2  | 3:C:1122:MET:HB3  | 2.20                     | 0.56              |
| 3:D:865:LEU:HD21  | 3:D:879:PHE:HB2   | 1.87                     | 0.56              |
| 3:D:1157:LEU:HD11 | 3:D:1269:VAL:HG21 | 1.88                     | 0.56              |
| 3:E:469:ILE:HD11  | 3:E:547:PHE:CG    | 2.41                     | 0.56              |
| 3:F:213:ARG:NH1   | 3:F:1216:GLY:HA3  | 2.21                     | 0.56              |
| 3:F:784:LEU:HD23  | 3:F:903:GLU:HG2   | 1.88                     | 0.56              |
| 3:G:405:PRO:HG3   | 3:G:1363:ILE:HD11 | 1.87                     | 0.56              |
| 3:G:620:ASP:OD2   | 3:G:655:TYR:OH    | 2.24                     | 0.56              |
| 3:G:956:TYR:CD1   | 3:G:956:TYR:N     | 2.72                     | 0.56              |
| 2:V:152:VAL:HG21  | 2:V:290:ALA:HB2   | 1.88                     | 0.56              |
| 3:J:842:MET:HB2   | 4:j:22:MET:SD     | 2.45                     | 0.56              |
| 3:J:1120:THR:HG22 | 3:J:1181:GLN:HE21 | 1.69                     | 0.56              |
| 3:K:638:GLU:HB2   | 3:K:789:ALA:HA    | 1.88                     | 0.56              |
| 3:A:460:THR:HA    | 3:A:1129:PHE:HD2  | 1.70                     | 0.56              |
| 3:H:769:CYS:O     | 3:H:901:MET:N     | 2.35                     | 0.56              |
| 4:j:51:ARG:O      | 4:j:55:ARG:NH1    | 2.38                     | 0.56              |
| 3:O:753:ASP:HB3   | 3:O:755:ARG:HH22  | 1.70                     | 0.56              |
| 3:O:795:ALA:HB3   | 3:O:798:ARG:HG2   | 1.87                     | 0.56              |
| 3:P:452:LEU:HD12  | 3:P:456:ASN:HD22  | 1.69                     | 0.56              |
| 3:B:390:VAL:HG21  | 3:C:104:ILE:HD11  | 1.88                     | 0.56              |
| 3:B:1125:LEU:HD21 | 3:B:1157:LEU:HD22 | 1.88                     | 0.56              |
| 3:C:238:GLY:HA2   | 3:C:244:ILE:HD11  | 1.86                     | 0.56              |
| 3:C:610:THR:HG21  | 3:C:692:ASP:OD2   | 2.06                     | 0.56              |
| 3:D:787:THR:OG1   | 3:D:801:ARG:NH2   | 2.39                     | 0.56              |
| 3:D:867:PRO:HA    | 3:D:870:LEU:HD12  | 1.88                     | 0.56              |
| 3:D:966:GLY:HA3   | 3:D:969:HIS:HB2   | 1.87                     | 0.56              |
| 5:q:360:TRP:O     | 5:q:364:GLY:N     | 2.38                     | 0.56              |
| 3:G:23:ILE:HD12   | 3:G:167:ARG:CD    | 2.35                     | 0.56              |
| 3:G:1233:ASP:OD2  | 3:G:1236:ARG:HG2  | 2.05                     | 0.56              |
| 1:W:29:GLY:HA2    | 3:H:144:THR:CA    | 2.23                     | 0.56              |
| 3:I:785:HIS:HD2   | 3:I:788:GLN:HE21  | 1.54                     | 0.56              |
| 3:I:1206:ARG:NH2  | 3:I:1208:ARG:O    | 2.38                     | 0.56              |
| 3:J:180:THR:HG22  | 3:J:1097:ARG:HH12 | 1.70                     | 0.56              |
| 3:K:721:GLU:HG2   | 3:K:727:ARG:HG3   | 1.88                     | 0.56              |
| 3:L:786:ASN:ND2   | 3:L:901:MET:O     | 2.39                     | 0.56              |
| 3:H:494:PRO:HD3   | 3:H:909:LEU:HD12  | 1.88                     | 0.56              |
| 3:O:1128:ASN:HD21 | 3:O:1155:ASN:ND2  | 2.03                     | 0.56              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:P:738:ASP:OD1  | 3:P:787:THR:OG1   | 2.18                     | 0.56              |
| 3:B:867:PRO:HA   | 3:B:870:LEU:HD12  | 1.85                     | 0.56              |
| 3:B:954:TYR:OH   | 4:g:92:PHE:CZ     | 2.55                     | 0.56              |
| 3:C:63:ASN:ND2   | 3:D:99:VAL:HA     | 2.20                     | 0.56              |
| 3:C:435:PHE:HB3  | 3:C:436:PRO:HD2   | 1.87                     | 0.56              |
| 3:E:677:TYR:CD1  | 4:e:95:LYS:HE2    | 2.40                     | 0.56              |
| 3:G:106:ARG:HD2  | 3:G:110:HIS:ND1   | 2.20                     | 0.56              |
| 3:G:1161:GLN:HG2 | 3:G:1162:PRO:CD   | 2.36                     | 0.56              |
| 1:T:170:LEU:CG   | 3:I:1262:HIS:ND1  | 2.69                     | 0.56              |
| 2:3:300:PHE:CE2  | 3:M:1083:HIS:CD2  | 2.82                     | 0.56              |
| 3:I:1124:ASN:O   | 3:I:1156:ARG:NH1  | 2.39                     | 0.56              |
| 3:J:1008:GLN:HB3 | 3:J:1012:GLU:CD   | 2.31                     | 0.56              |
| 3:L:244:ILE:CD1  | 3:L:292:PHE:CE2   | 2.89                     | 0.56              |
| 3:L:266:HIS:CE1  | 3:L:302:VAL:HG13  | 2.41                     | 0.56              |
| 3:L:724:HIS:CE1  | 3:L:1028:TYR:HB2  | 2.41                     | 0.56              |
| 4:o:80:ALA:H     | 3:P:948:THR:HA    | 1.69                     | 0.56              |
| 3:O:738:ASP:OD2  | 3:O:801:ARG:NH1   | 2.39                     | 0.56              |
| 3:P:293:LEU:HD13 | 3:P:368:VAL:HG11  | 1.87                     | 0.56              |
| 3:P:1198:TYR:HD1 | 3:P:1236:ARG:HH11 | 1.53                     | 0.56              |
| 3:B:879:PHE:CE1  | 3:B:886:VAL:HG21  | 2.41                     | 0.56              |
| 3:C:877:ALA:HB1  | 4:b:94:LEU:HD21   | 1.88                     | 0.56              |
| 3:C:1339:ASP:OD2 | 3:C:1360:GLN:HG3  | 2.05                     | 0.56              |
| 5:q:447:THR:HA   | 5:q:450:LEU:HD12  | 1.87                     | 0.56              |
| 3:E:863:HIS:ND1  | 3:E:864:PRO:HD2   | 2.20                     | 0.56              |
| 3:F:42:VAL:HG12  | 3:F:43:ARG:O      | 2.05                     | 0.56              |
| 3:G:548:ASP:OD1  | 3:G:576:ARG:NE    | 2.38                     | 0.56              |
| 3:G:1279:ALA:O   | 3:G:1283:THR:HG23 | 2.06                     | 0.56              |
| 2:Y:68:ARG:NH1   | 2:Y:288:ILE:O     | 2.39                     | 0.56              |
| 1:1:317:ARG:NH1  | 1:1:322:GLN:O     | 2.39                     | 0.56              |
| 3:I:896:VAL:HA   | 3:I:899:HIS:CD2   | 2.40                     | 0.56              |
| 3:M:756:ILE:HB   | 3:M:763:PRO:HD3   | 1.87                     | 0.56              |
| 3:M:1008:GLN:HB3 | 3:M:1012:GLU:CD   | 2.31                     | 0.56              |
| 3:A:462:CYS:SG   | 3:A:1147:LEU:HD22 | 2.45                     | 0.56              |
| 4:o:94:LEU:HD21  | 3:P:877:ALA:HB1   | 1.87                     | 0.56              |
| 3:N:266:HIS:CE1  | 3:N:303:PRO:HD2   | 2.41                     | 0.56              |
| 3:B:351:LEU:CD2  | 3:G:58:LEU:CD1    | 2.84                     | 0.56              |
| 3:B:1103:GLY:HA3 | 3:B:1107:THR:HG21 | 1.88                     | 0.56              |
| 3:C:1248:GLN:O   | 3:C:1251:SER:OG   | 2.18                     | 0.56              |
| 3:E:580:GLY:HA2  | 3:E:592:ARG:HH12  | 1.70                     | 0.56              |
| 3:F:532:MET:HE3  | 3:F:1241:THR:HG23 | 1.86                     | 0.56              |
| 3:G:677:TYR:HA   | 4:g:95:LYS:NZ     | 2.21                     | 0.56              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:1:118:ASP:O    | 1:1:223:ARG:NH1   | 2.38                     | 0.56              |
| 1:1:259:GLU:OE1  | 3:M:1315:PRO:CB   | 2.53                     | 0.56              |
| 2:3:12:ILE:HD11  | 2:3:83:ILE:HG13   | 1.88                     | 0.56              |
| 3:L:309:MET:SD   | 3:L:327:ARG:HG3   | 2.46                     | 0.56              |
| 3:M:41:ARG:CZ    | 3:D:116:VAL:HG11  | 2.34                     | 0.56              |
| 3:A:1337:ALA:HB3 | 3:A:1343:LEU:HB2  | 1.86                     | 0.56              |
| 3:N:1186:GLU:CD  | 3:N:1272:PRO:HD2  | 2.31                     | 0.56              |
| 3:B:335:HIS:NE2  | 3:B:339:MET:SD    | 2.79                     | 0.56              |
| 3:B:440:LEU:HD22 | 3:B:1336:CYS:SG   | 2.46                     | 0.56              |
| 3:B:819:ALA:O    | 3:B:822:ARG:NH1   | 2.39                     | 0.56              |
| 3:C:771:VAL:HG22 | 3:C:901:MET:HE3   | 1.88                     | 0.56              |
| 3:D:350:THR:HB   | 3:D:353:GLU:HG3   | 1.88                     | 0.56              |
| 3:E:204:TYR:CD2  | 3:E:219:LEU:HD11  | 2.41                     | 0.56              |
| 1:T:282:PRO:CD   | 3:H:51:ASP:OD1    | 2.54                     | 0.56              |
| 1:W:352:ILE:CB   | 6:r:12:VAL:CB     | 2.80                     | 0.56              |
| 2:2:154:ARG:NH1  | 2:2:176:LEU:O     | 2.36                     | 0.56              |
| 3:I:765:TYR:HD1  | 3:I:783:LEU:HB2   | 1.70                     | 0.56              |
| 3:I:1211:GLY:HA2 | 3:I:1282:ILE:HG23 | 1.86                     | 0.56              |
| 3:L:1008:GLN:HB3 | 3:L:1012:GLU:CD   | 2.31                     | 0.56              |
| 3:M:61:TYR:HA    | 3:C:21:GLY:O      | 2.06                     | 0.56              |
| 3:M:93:GLY:HA3   | 3:M:124:ILE:HD12  | 1.88                     | 0.56              |
| 3:M:148:LEU:HD11 | 3:M:158:GLN:NE2   | 2.21                     | 0.56              |
| 3:M:252:THR:O    | 3:M:373:ARG:NH1   | 2.39                     | 0.56              |
| 3:H:604:HIS:HD2  | 3:H:696:HIS:CD2   | 2.24                     | 0.56              |
| 3:H:776:PHE:O    | 3:H:904:ARG:HD3   | 2.06                     | 0.56              |
| 4:l:56:GLY:O     | 4:l:60:ALA:N      | 2.33                     | 0.56              |
| 4:o:4:PRO:HD3    | 4:o:16:ASN:HB3    | 1.87                     | 0.56              |
| 3:N:266:HIS:CE1  | 3:N:302:VAL:HG13  | 2.41                     | 0.56              |
| 3:O:148:LEU:HD11 | 3:O:158:GLN:NE2   | 2.21                     | 0.56              |
| 3:P:224:LYS:NZ   | 3:P:1214:TYR:OH   | 2.24                     | 0.56              |
| 3:B:756:ILE:HD12 | 3:B:763:PRO:HG3   | 1.87                     | 0.56              |
| 3:D:756:ILE:HG12 | 3:D:910:CYS:HB3   | 1.86                     | 0.56              |
| 3:D:1058:PHE:CE2 | 3:D:1369:LEU:HD11 | 2.41                     | 0.56              |
| 5:q:384:SER:OG   | 5:q:401:SER:O     | 2.23                     | 0.56              |
| 3:E:698:GLU:OE1  | 3:F:621:ARG:NH2   | 2.39                     | 0.56              |
| 3:E:1209:ALA:HB3 | 3:E:1234:PRO:HG2  | 1.88                     | 0.56              |
| 3:F:231:SER:O    | 3:F:1112:THR:OG1  | 2.24                     | 0.56              |
| 3:F:752:ARG:HA   | 3:F:913:ALA:H     | 1.70                     | 0.56              |
| 2:R:173:LEU:O    | 5:q:371:GLY:CA    | 2.47                     | 0.55              |
| 1:W:28:ALA:CB    | 3:H:145:GLY:HA2   | 2.35                     | 0.55              |
| 3:I:800:HIS:O    | 3:I:801:ARG:HG3   | 2.06                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:I:863:HIS:O     | 3:I:869:ASN:ND2   | 2.29                     | 0.55              |
| 3:I:1229:HIS:CE1  | 3:I:1248:GLN:HG2  | 2.40                     | 0.55              |
| 3:J:142:LEU:O     | 3:J:158:GLN:NE2   | 2.38                     | 0.55              |
| 3:J:554:ALA:HB3   | 3:J:568:PRO:HG2   | 1.88                     | 0.55              |
| 3:K:620:ASP:OD2   | 3:K:655:TYR:OH    | 2.24                     | 0.55              |
| 3:L:50:TYR:O      | 3:N:157:ARG:HD2   | 2.06                     | 0.55              |
| 3:L:157:ARG:HD3   | 3:N:50:TYR:HB3    | 1.88                     | 0.55              |
| 3:L:615:ARG:HH21  | 3:L:1017:GLU:HG2  | 1.70                     | 0.55              |
| 3:M:66:SER:OG     | 3:M:178:ARG:NH2   | 2.39                     | 0.55              |
| 3:H:400:LEU:HD12  | 3:H:1058:PHE:HE2  | 1.70                     | 0.55              |
| 3:O:866:HIS:ND1   | 3:O:867:PRO:HD2   | 2.21                     | 0.55              |
| 3:B:262:PRO:HA    | 3:G:60:SER:HA     | 1.86                     | 0.55              |
| 3:B:639:HIS:HA    | 4:b:79:PHE:HE2    | 1.69                     | 0.55              |
| 3:B:879:PHE:O     | 3:B:883:ARG:N     | 2.39                     | 0.55              |
| 3:D:84:PHE:HE1    | 3:D:309:MET:SD    | 2.29                     | 0.55              |
| 3:D:392:TYR:CE2   | 3:D:394:LEU:HB3   | 2.42                     | 0.55              |
| 3:E:753:ASP:OD2   | 3:E:927:ARG:NE    | 2.39                     | 0.55              |
| 3:F:86:GLU:N      | 3:F:86:GLU:OE1    | 2.39                     | 0.55              |
| 3:F:172:VAL:HG11  | 3:F:1093:LEU:HD12 | 1.88                     | 0.55              |
| 3:F:448:GLN:CG    | 3:G:1201:ARG:CZ   | 2.78                     | 0.55              |
| 3:G:469:ILE:CD1   | 3:G:547:PHE:CE2   | 2.89                     | 0.55              |
| 2:y:158:ARG:HH21  | 2:y:193:GLN:HE21  | 1.53                     | 0.55              |
| 3:J:621:ARG:O     | 3:J:943:GLN:NE2   | 2.39                     | 0.55              |
| 3:J:743:MET:HE2   | 3:J:797:ASP:HA    | 1.87                     | 0.55              |
| 3:J:866:HIS:HD2   | 3:J:868:ALA:HB3   | 1.71                     | 0.55              |
| 3:M:527:THR:HG22  | 3:M:528:ALA:H     | 1.71                     | 0.55              |
| 3:A:620:ASP:HB2   | 3:A:623:TYR:HB2   | 1.87                     | 0.55              |
| 3:A:700:LEU:HD22  | 3:A:1025:MET:HG3  | 1.87                     | 0.55              |
| 3:A:1124:ASN:HA   | 3:A:1185:CYS:SG   | 2.46                     | 0.55              |
| 3:H:350:THR:HG22  | 3:H:352:ASP:H     | 1.69                     | 0.55              |
| 3:H:1131:LEU:HD23 | 3:H:1159:PRO:HG3  | 1.88                     | 0.55              |
| 3:H:1157:LEU:HD11 | 3:H:1269:VAL:HG21 | 1.89                     | 0.55              |
| 4:p:24:GLY:O      | 4:p:28:ALA:N      | 2.39                     | 0.55              |
| 3:N:43:ARG:O      | 3:N:45:ASP:N      | 2.40                     | 0.55              |
| 3:N:863:HIS:ND1   | 3:N:864:PRO:HD2   | 2.21                     | 0.55              |
| 3:B:948:THR:HG23  | 3:B:949:ILE:HG13  | 1.88                     | 0.55              |
| 3:B:1355:GLU:HB2  | 3:G:1344:ARG:NH1  | 2.21                     | 0.55              |
| 3:C:1173:ARG:HH21 | 3:D:213:ARG:NH1   | 2.03                     | 0.55              |
| 3:E:404:LEU:O     | 3:E:1052:VAL:N    | 2.37                     | 0.55              |
| 3:E:706:ASP:O     | 3:F:525:GLN:NE2   | 2.39                     | 0.55              |
| 3:E:961:HIS:CD2   | 3:E:963:LEU:H     | 2.24                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:E:1342:LEU:HD21 | 3:E:1362:LEU:HB2  | 1.86                     | 0.55              |
| 3:F:107:ASP:O     | 3:F:110:HIS:HD2   | 1.89                     | 0.55              |
| 2:S:28:GLU:HB3    | 2:S:101:ARG:HH21  | 1.71                     | 0.55              |
| 1:w:272:GLU:OE1   | 1:w:283:ARG:HD2   | 2.06                     | 0.55              |
| 3:L:255:THR:OG1   | 3:L:1067:GLU:OE2  | 2.23                     | 0.55              |
| 3:M:21:GLY:CA     | 3:D:350:THR:HG21  | 2.30                     | 0.55              |
| 3:M:387:ALA:HA    | 3:C:28:GLU:HG3    | 1.88                     | 0.55              |
| 3:A:392:TYR:CE2   | 3:A:394:LEU:HB3   | 2.41                     | 0.55              |
| 3:A:896:VAL:HG13  | 3:A:899:HIS:CD2   | 2.41                     | 0.55              |
| 3:A:1106:TYR:OH   | 3:A:1313:ARG:NH2  | 2.39                     | 0.55              |
| 3:H:866:HIS:ND1   | 3:H:867:PRO:HD2   | 2.22                     | 0.55              |
| 3:N:1225:LEU:HD22 | 3:N:1234:PRO:HG3  | 1.88                     | 0.55              |
| 3:B:646:ARG:HH22  | 3:B:889:PRO:HG2   | 1.71                     | 0.55              |
| 5:q:133:ARG:NH1   | 5:q:572:LEU:HB3   | 2.21                     | 0.55              |
| 6:r:80:ILE:HG23   | 6:r:84:ILE:HB     | 1.88                     | 0.55              |
| 3:F:425:PRO:HG3   | 3:F:431:GLU:HB2   | 1.88                     | 0.55              |
| 3:G:196:ALA:HB1   | 3:G:227:PHE:HA    | 1.89                     | 0.55              |
| 3:G:433:ARG:HG2   | 3:G:433:ARG:NH1   | 2.14                     | 0.55              |
| 1:W:117:THR:O     | 1:W:121:GLN:NE2   | 2.38                     | 0.55              |
| 3:J:503:GLN:HE21  | 3:J:507:ASN:ND2   | 2.04                     | 0.55              |
| 3:K:45:ASP:OD1    | 3:K:46:GLU:N      | 2.39                     | 0.55              |
| 3:M:485:ASN:HD21  | 3:M:516:GLY:H     | 1.53                     | 0.55              |
| 3:A:182:ASP:HB3   | 3:A:186:HIS:HD2   | 1.71                     | 0.55              |
| 3:A:329:LEU:O     | 3:G:61:TYR:CZ     | 2.52                     | 0.55              |
| 3:H:755:ARG:NH1   | 3:H:911:SER:OG    | 2.40                     | 0.55              |
| 3:N:97:PHE:HD1    | 3:D:23:ILE:HD11   | 1.72                     | 0.55              |
| 3:O:769:CYS:HB2   | 3:O:786:ASN:ND2   | 2.22                     | 0.55              |
| 3:B:257:PRO:HA    | 3:B:1067:GLU:OE1  | 2.06                     | 0.55              |
| 3:B:737:TRP:HB3   | 3:B:787:THR:HG21  | 1.87                     | 0.55              |
| 3:C:880:HIS:CE1   | 4:b:97:THR:OG1    | 2.59                     | 0.55              |
| 3:D:830:VAL:HG13  | 3:D:955:PHE:HE1   | 1.70                     | 0.55              |
| 3:F:502:GLN:HE22  | 3:F:970:VAL:HG13  | 1.71                     | 0.55              |
| 3:F:873:ASN:OD1   | 4:e:92:PHE:N      | 2.40                     | 0.55              |
| 3:F:1176:GLY:HA3  | 3:G:1225:LEU:HD21 | 1.88                     | 0.55              |
| 3:G:575:TRP:CZ2   | 3:G:1031:MET:O    | 2.56                     | 0.55              |
| 2:R:174:PRO:HA    | 5:q:371:GLY:CA    | 2.35                     | 0.55              |
| 2:S:68:ARG:NH1    | 2:S:288:ILE:O     | 2.39                     | 0.55              |
| 1:w:146:HIS:ND1   | 2:y:267:ARG:O     | 2.39                     | 0.55              |
| 3:I:87:LEU:O      | 3:I:90:MET:N      | 2.35                     | 0.55              |
| 3:L:1191:PRO:HG2  | 3:L:1194:THR:HG23 | 1.88                     | 0.55              |
| 3:L:1248:GLN:O    | 3:L:1251:SER:OG   | 2.23                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:M:490:TYR:OH    | 3:M:561:GLY:N     | 2.39                     | 0.55              |
| 3:H:463:HIS:ND1   | 3:H:464:PRO:HD2   | 2.22                     | 0.55              |
| 3:H:1334:ILE:C    | 3:H:1365:ASP:HB3  | 2.32                     | 0.55              |
| 4:m:57:GLN:O      | 4:m:61:LEU:N      | 2.31                     | 0.55              |
| 3:P:425:PRO:HG3   | 3:P:431:GLU:HG2   | 1.88                     | 0.55              |
| 3:B:948:THR:OG1   | 4:g:93:GLY:O      | 2.25                     | 0.55              |
| 3:B:1257:TYR:HB2  | 3:B:1277:PHE:CD2  | 2.41                     | 0.55              |
| 3:C:441:PHE:CE2   | 3:C:1340:PRO:HD3  | 2.41                     | 0.55              |
| 3:C:866:HIS:ND1   | 3:C:867:PRO:HD2   | 2.21                     | 0.55              |
| 3:C:867:PRO:HA    | 3:C:870:LEU:HB2   | 1.89                     | 0.55              |
| 3:D:42:VAL:HG22   | 3:D:46:GLU:CD     | 2.31                     | 0.55              |
| 5:q:436:VAL:HG13  | 5:q:437:ARG:HG3   | 1.89                     | 0.55              |
| 3:E:403:VAL:HG23  | 3:E:1331:ALA:HB3  | 1.86                     | 0.55              |
| 3:E:507:ASN:HA    | 3:E:510:ARG:NE    | 2.22                     | 0.55              |
| 3:G:802:PRO:HD2   | 3:G:805:TRP:HB2   | 1.87                     | 0.55              |
| 1:Q:275:HIS:HA    | 1:Q:282:PRO:HB3   | 1.89                     | 0.55              |
| 3:K:1190:THR:HG22 | 3:K:1243:ASN:ND2  | 2.20                     | 0.55              |
| 3:L:878:MET:HB2   | 4:k:92:PHE:CE2    | 2.42                     | 0.55              |
| 3:M:24:LEU:CD1    | 3:D:258:SER:O     | 2.43                     | 0.55              |
| 3:H:709:LEU:HB3   | 3:H:1038:HIS:HE1  | 1.71                     | 0.55              |
| 3:H:961:HIS:O     | 3:H:964:PHE:N     | 2.36                     | 0.55              |
| 4:o:22:MET:SD     | 3:O:842:MET:HB2   | 2.47                     | 0.55              |
| 3:N:440:LEU:HD22  | 3:N:1336:CYS:SG   | 2.47                     | 0.55              |
| 3:N:1206:ARG:HH22 | 3:N:1226:MET:C    | 2.14                     | 0.55              |
| 3:N:1344:ARG:NH2  | 3:O:414:GLU:OE2   | 2.40                     | 0.55              |
| 3:B:326:VAL:O     | 3:B:330:ASP:N     | 2.22                     | 0.55              |
| 3:C:785:HIS:CD2   | 3:C:788:GLN:HE21  | 2.24                     | 0.55              |
| 3:D:488:GLY:HA2   | 3:D:996:ALA:HB1   | 1.87                     | 0.55              |
| 3:D:638:GLU:O     | 3:D:641:PHE:N     | 2.39                     | 0.55              |
| 3:D:873:ASN:HA    | 4:c:92:PHE:HB2    | 1.88                     | 0.55              |
| 3:D:920:THR:O     | 3:D:923:THR:N     | 2.36                     | 0.55              |
| 3:D:1270:LEU:HD22 | 3:D:1303:ALA:HB2  | 1.89                     | 0.55              |
| 3:F:142:LEU:O     | 3:F:158:GLN:NE2   | 2.39                     | 0.55              |
| 1:T:278:HIS:HB3   | 1:T:281:ARG:H     | 1.70                     | 0.55              |
| 1:W:349:ARG:HA    | 6:r:12:VAL:CG1    | 2.33                     | 0.55              |
| 2:Y:238:ASN:CB    | 3:H:1137:PRO:HG3  | 2.37                     | 0.55              |
| 3:I:631:GLN:NE2   | 3:I:666:ASN:OD1   | 2.38                     | 0.55              |
| 3:I:1120:THR:HG22 | 3:I:1181:GLN:HE21 | 1.72                     | 0.55              |
| 3:J:77:VAL:HG22   | 3:J:266:HIS:CD2   | 2.42                     | 0.55              |
| 3:J:867:PRO:HA    | 3:J:870:LEU:HB2   | 1.89                     | 0.55              |
| 3:L:410:ASN:O     | 3:L:415:ARG:NH1   | 2.40                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:L:451:ARG:HH21  | 3:L:453:SER:HB3   | 1.72                     | 0.55              |
| 3:L:1257:TYR:HB2  | 3:L:1277:PHE:HD2  | 1.71                     | 0.55              |
| 3:M:635:HIS:CE1   | 3:M:640:VAL:HG21  | 2.42                     | 0.55              |
| 3:M:698:GLU:OE2   | 3:H:621:ARG:NH2   | 2.39                     | 0.55              |
| 3:A:752:ARG:NH2   | 3:A:915:ASP:OD1   | 2.40                     | 0.55              |
| 4:j:59:ALA:O      | 4:j:62:THR:OG1    | 2.19                     | 0.55              |
| 3:N:119:TYR:CE2   | 3:D:42:VAL:CG2    | 2.89                     | 0.55              |
| 3:N:163:GLN:HE22  | 3:O:348:ARG:NH2   | 2.05                     | 0.55              |
| 3:O:86:GLU:HG2    | 3:O:86:GLU:O      | 2.06                     | 0.55              |
| 3:O:499:ALA:HA    | 3:O:956:TYR:CD1   | 2.42                     | 0.55              |
| 3:P:593:ASP:OD1   | 3:P:1009:HIS:HE1  | 1.89                     | 0.55              |
| 3:C:213:ARG:HH12  | 3:C:1216:GLY:HA3  | 1.71                     | 0.55              |
| 3:C:717:GLN:HE22  | 3:C:752:ARG:NH1   | 2.05                     | 0.55              |
| 3:C:1170:GLN:OE1  | 3:C:1170:GLN:N    | 2.40                     | 0.55              |
| 3:D:646:ARG:HH11  | 4:d:99:SER:HA     | 1.64                     | 0.55              |
| 3:D:784:LEU:HD13  | 3:D:786:ASN:HB2   | 1.89                     | 0.55              |
| 3:D:1334:ILE:HG22 | 3:D:1335:THR:N    | 2.22                     | 0.55              |
| 3:E:951:ASN:ND2   | 3:E:972:ASN:O     | 2.39                     | 0.55              |
| 6:r:71:LEU:HA     | 6:r:74:ALA:HB3    | 1.89                     | 0.55              |
| 3:G:783:LEU:HD22  | 3:G:934:HIS:ND1   | 2.22                     | 0.55              |
| 3:G:1232:SER:CB   | 3:G:1237:PRO:O    | 2.54                     | 0.55              |
| 4:c:64:LEU:O      | 4:c:67:THR:OG1    | 2.25                     | 0.55              |
| 1:Q:44:ARG:C      | 3:B:322:MET:HE3   | 2.31                     | 0.55              |
| 2:3:68:ARG:NH2    | 2:2:317:TYR:OH    | 2.40                     | 0.55              |
| 2:2:39:ARG:CZ     | 3:N:1083:HIS:NE2  | 2.69                     | 0.55              |
| 3:I:1342:LEU:CD2  | 3:I:1362:LEU:HB2  | 2.37                     | 0.55              |
| 3:K:923:THR:HA    | 3:K:926:MET:HE3   | 1.89                     | 0.55              |
| 3:L:753:ASP:HB3   | 3:L:755:ARG:NH2   | 2.21                     | 0.55              |
| 3:A:758:ALA:N     | 3:A:761:HIS:O     | 2.27                     | 0.55              |
| 3:A:960:VAL:HA    | 3:A:994:LEU:HD13  | 1.88                     | 0.55              |
| 3:H:521:VAL:HG11  | 3:H:987:VAL:HG12  | 1.89                     | 0.55              |
| 3:H:963:LEU:HD23  | 3:H:1007:VAL:HG22 | 1.89                     | 0.55              |
| 3:O:1179:HIS:NE2  | 3:P:1235:ALA:O    | 2.40                     | 0.55              |
| 3:P:906:THR:OG1   | 3:P:934:HIS:HB3   | 2.07                     | 0.55              |
| 3:P:1191:PRO:HG2  | 3:P:1194:THR:HG23 | 1.89                     | 0.55              |
| 3:B:1024:LEU:O    | 3:B:1027:GLY:N    | 2.38                     | 0.55              |
| 3:C:728:ASP:O     | 3:C:810:LYS:NZ    | 2.40                     | 0.55              |
| 3:D:745:HIS:CD2   | 3:D:745:HIS:C     | 2.85                     | 0.55              |
| 5:q:60:THR:HG22   | 5:q:132:LEU:HD23  | 1.89                     | 0.55              |
| 5:q:495:ARG:NH2   | 6:s:42:ASN:OD1    | 2.39                     | 0.55              |
| 3:E:725:LEU:HD23  | 3:E:1028:TYR:HD1  | 1.71                     | 0.55              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:E:789:ALA:O    | 4:e:79:PHE:CE2    | 2.60                     | 0.55              |
| 3:F:460:THR:HA   | 3:F:1129:PHE:CE2  | 2.42                     | 0.55              |
| 3:F:463:HIS:CD2  | 3:F:465:SER:HB3   | 2.42                     | 0.55              |
| 3:F:1052:VAL:HA  | 3:F:1186:GLU:O    | 2.06                     | 0.55              |
| 1:T:147:ARG:NH1  | 1:T:243:GLU:OE1   | 2.40                     | 0.55              |
| 2:2:233:GLN:O    | 3:D:1136:PRO:CB   | 2.50                     | 0.55              |
| 3:I:634:ILE:HG22 | 3:I:636:GLY:H     | 1.72                     | 0.55              |
| 3:I:877:ALA:HA   | 3:I:880:HIS:HB3   | 1.89                     | 0.55              |
| 3:J:390:VAL:HG22 | 3:K:106:ARG:HH11  | 1.71                     | 0.55              |
| 3:J:390:VAL:HG22 | 3:K:106:ARG:NH1   | 2.21                     | 0.55              |
| 3:J:439:GLN:NE2  | 3:J:451:ARG:HH21  | 2.04                     | 0.55              |
| 3:L:24:LEU:HD11  | 3:O:260:ALA:HB2   | 1.88                     | 0.55              |
| 3:M:335:HIS:HB3  | 3:M:339:MET:SD    | 2.46                     | 0.55              |
| 3:N:95:VAL:HG21  | 3:N:1100:VAL:HG11 | 1.88                     | 0.55              |
| 3:B:107:ASP:CG   | 3:G:128:ALA:O     | 2.50                     | 0.55              |
| 3:B:225:ARG:CZ   | 3:G:447:HIS:CD2   | 2.90                     | 0.55              |
| 3:B:280:THR:HG22 | 3:B:1063:VAL:HG22 | 1.88                     | 0.55              |
| 3:B:978:PRO:HA   | 3:B:981:ARG:NH2   | 2.22                     | 0.55              |
| 3:C:85:PRO:HG3   | 3:C:310:VAL:HG22  | 1.88                     | 0.55              |
| 3:C:180:THR:HG22 | 3:C:1097:ARG:NH1  | 2.21                     | 0.55              |
| 5:q:591:TYR:CE2  | 5:q:606:ILE:HD12  | 2.41                     | 0.55              |
| 3:E:440:LEU:HD22 | 3:E:1336:CYS:SG   | 2.47                     | 0.55              |
| 2:X:68:ARG:NH2   | 2:Y:317:TYR:OH    | 2.40                     | 0.55              |
| 3:I:1296:THR:O   | 3:I:1322:GLU:HA   | 2.07                     | 0.55              |
| 3:J:454:MET:CE   | 3:J:1046:PRO:HD2  | 2.36                     | 0.55              |
| 3:K:477:ASN:OD1  | 3:K:571:ILE:N     | 2.36                     | 0.55              |
| 3:M:274:VAL:HG11 | 3:M:376:PHE:CD2   | 2.42                     | 0.55              |
| 3:M:1177:MET:HE1 | 3:H:214:VAL:HG22  | 1.89                     | 0.55              |
| 4:h:72:THR:HA    | 4:h:100:PRO:HB2   | 1.89                     | 0.55              |
| 3:O:244:ILE:HD12 | 3:O:292:PHE:CZ    | 2.42                     | 0.55              |
| 3:O:1037:TYR:C   | 3:O:1037:TYR:CD1  | 2.85                     | 0.55              |
| 3:P:406:LEU:HD23 | 3:P:440:LEU:HG    | 1.89                     | 0.55              |
| 3:P:784:LEU:HB2  | 3:P:786:ASN:ND2   | 2.22                     | 0.55              |
| 3:C:961:HIS:O    | 3:C:964:PHE:N     | 2.33                     | 0.55              |
| 5:q:600:ARG:NH1  | 5:q:602:THR:O     | 2.38                     | 0.55              |
| 3:E:600:GLY:C    | 3:E:602:GLY:H     | 2.15                     | 0.55              |
| 3:E:1058:PHE:CE2 | 3:E:1369:LEU:HD11 | 2.42                     | 0.55              |
| 3:E:1155:ASN:OD1 | 3:E:1156:ARG:N    | 2.40                     | 0.55              |
| 3:F:448:GLN:CD   | 3:G:1201:ARG:NH2  | 2.61                     | 0.55              |
| 3:F:510:ARG:HA   | 3:F:980:LEU:HD11  | 1.88                     | 0.55              |
| 3:G:53:GLU:C     | 3:G:54:PHE:CD2    | 2.85                     | 0.55              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:S:261:LEU:HD11 | 5:q:378:TRP:HH2   | 1.67                     | 0.54              |
| 1:w:246:ARG:NH1  | 2:x:111:GLY:O     | 2.38                     | 0.54              |
| 3:I:213:ARG:HH12 | 3:I:1216:GLY:HA3  | 1.72                     | 0.54              |
| 3:I:263:ARG:NH2  | 3:I:306:TYR:O     | 2.41                     | 0.54              |
| 3:K:765:TYR:HE1  | 3:K:783:LEU:HD12  | 1.72                     | 0.54              |
| 3:K:879:PHE:CE1  | 3:K:886:VAL:HG21  | 2.42                     | 0.54              |
| 3:L:82:THR:HG22  | 3:L:307:GLY:HA3   | 1.88                     | 0.54              |
| 3:L:318:THR:O    | 3:L:323:GLY:N     | 2.38                     | 0.54              |
| 3:L:1156:ARG:NH2 | 3:M:1237:PRO:HB2  | 2.23                     | 0.54              |
| 3:M:332:VAL:HG22 | 3:N:18:VAL:HB     | 1.89                     | 0.54              |
| 3:A:651:CYS:O    | 3:A:654:SER:OG    | 2.24                     | 0.54              |
| 3:H:578:VAL:HB   | 3:H:1027:GLY:O    | 2.07                     | 0.54              |
| 3:N:123:VAL:HG21 | 3:D:37:ASP:OD2    | 2.02                     | 0.54              |
| 3:N:786:ASN:ND2  | 3:N:902:ALA:HA    | 2.22                     | 0.54              |
| 3:N:906:THR:OG1  | 3:N:934:HIS:HB3   | 2.07                     | 0.54              |
| 3:B:866:HIS:ND1  | 3:B:867:PRO:HD2   | 2.21                     | 0.54              |
| 3:C:646:ARG:HH22 | 3:C:889:PRO:HG2   | 1.72                     | 0.54              |
| 3:C:723:ASN:C    | 3:C:1030:LYS:HZ3  | 2.15                     | 0.54              |
| 3:C:1058:PHE:HE2 | 3:C:1369:LEU:HD11 | 1.71                     | 0.54              |
| 3:C:1178:ASP:O   | 3:D:217:ALA:HB1   | 2.06                     | 0.54              |
| 3:C:1336:CYS:O   | 3:C:1362:LEU:HG   | 2.07                     | 0.54              |
| 3:D:86:GLU:OE1   | 3:D:86:GLU:N      | 2.40                     | 0.54              |
| 3:D:960:VAL:HA   | 3:D:994:LEU:HD13  | 1.88                     | 0.54              |
| 3:E:227:PHE:CE2  | 3:E:1324:PRO:HB3  | 2.41                     | 0.54              |
| 3:E:1339:ASP:OD2 | 3:E:1360:GLN:HG3  | 2.07                     | 0.54              |
| 3:F:829:GLY:O    | 3:F:956:TYR:N     | 2.40                     | 0.54              |
| 3:G:1197:ASN:C   | 3:G:1199:PHE:N    | 2.64                     | 0.54              |
| 4:d:64:LEU:O     | 4:d:67:THR:OG1    | 2.25                     | 0.54              |
| 3:J:264:LEU:HD11 | 3:J:1069:ALA:HB2  | 1.90                     | 0.54              |
| 3:J:944:HIS:HB2  | 3:J:951:ASN:HD21  | 1.72                     | 0.54              |
| 3:L:745:HIS:C    | 3:L:745:HIS:CD2   | 2.85                     | 0.54              |
| 3:L:853:CYS:HB2  | 4:l:101:PHE:CD1   | 2.42                     | 0.54              |
| 3:M:134:SER:C    | 3:C:44:SER:OG     | 2.43                     | 0.54              |
| 3:M:736:VAL:HG12 | 3:M:738:ASP:H     | 1.72                     | 0.54              |
| 3:M:1011:ARG:HG3 | 3:M:1012:GLU:HG3  | 1.89                     | 0.54              |
| 3:A:453:SER:H    | 3:A:456:ASN:ND2   | 2.04                     | 0.54              |
| 3:H:576:ARG:HH11 | 3:H:582:LEU:HD23  | 1.71                     | 0.54              |
| 3:H:724:HIS:CE1  | 3:H:1028:TYR:HB2  | 2.41                     | 0.54              |
| 3:H:1085:THR:OG1 | 3:H:1090:ASN:ND2  | 2.40                     | 0.54              |
| 4:p:64:LEU:HD11  | 3:P:844:VAL:HB    | 1.89                     | 0.54              |
| 3:P:614:VAL:HG21 | 3:P:693:LEU:HD21  | 1.87                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:P:675:VAL:HG21  | 3:P:694:VAL:HG21  | 1.89                     | 0.54              |
| 3:P:742:LEU:HD22  | 3:P:756:ILE:HD13  | 1.88                     | 0.54              |
| 3:B:1125:LEU:HD22 | 3:B:1184:VAL:HG22 | 1.89                     | 0.54              |
| 3:C:1296:THR:HG21 | 3:C:1327:LEU:HG   | 1.89                     | 0.54              |
| 3:D:683:PRO:HD2   | 3:D:686:CYS:HB3   | 1.89                     | 0.54              |
| 3:E:106:ARG:NH2   | 3:E:110:HIS:HB3   | 2.23                     | 0.54              |
| 3:F:278:LEU:HG    | 3:F:375:VAL:HG11  | 1.89                     | 0.54              |
| 3:F:644:LEU:HD22  | 3:F:647:LEU:HD12  | 1.90                     | 0.54              |
| 3:F:880:HIS:NE2   | 4:e:98:TYR:HD2    | 2.05                     | 0.54              |
| 3:G:99:VAL:HG12   | 3:G:118:ASN:HB2   | 1.89                     | 0.54              |
| 3:G:496:GLY:CA    | 3:G:504:ARG:HH22  | 2.20                     | 0.54              |
| 3:G:654:SER:O     | 3:G:658:ASN:ND2   | 2.40                     | 0.54              |
| 3:G:1157:LEU:HD11 | 3:G:1269:VAL:HG21 | 1.90                     | 0.54              |
| 2:S:2:ILE:HD12    | 3:B:1084:GLU:HB2  | 1.88                     | 0.54              |
| 1:W:350:LEU:CD2   | 6:r:20:VAL:HG13   | 2.37                     | 0.54              |
| 3:I:485:ASN:O     | 3:I:487:TYR:N     | 2.35                     | 0.54              |
| 3:I:635:HIS:CE1   | 3:I:640:VAL:HG21  | 2.42                     | 0.54              |
| 3:I:1333:PRO:HG2  | 3:I:1366:ALA:H    | 1.73                     | 0.54              |
| 3:J:180:THR:HG22  | 3:J:1097:ARG:NH1  | 2.23                     | 0.54              |
| 3:J:264:LEU:HB2   | 3:J:1068:ARG:NH2  | 2.23                     | 0.54              |
| 3:J:675:VAL:HG21  | 3:J:694:VAL:HG21  | 1.88                     | 0.54              |
| 3:J:721:GLU:HG2   | 3:J:727:ARG:HG3   | 1.88                     | 0.54              |
| 3:K:525:GLN:CD    | 3:K:525:GLN:H     | 2.15                     | 0.54              |
| 3:L:204:TYR:HB2   | 3:L:219:LEU:HD21  | 1.89                     | 0.54              |
| 3:A:329:LEU:HG    | 3:G:61:TYR:HE2    | 1.57                     | 0.54              |
| 3:A:668:TYR:HD2   | 3:A:809:HIS:CE1   | 2.24                     | 0.54              |
| 3:H:86:GLU:O      | 3:H:86:GLU:HG2    | 2.06                     | 0.54              |
| 3:H:631:GLN:NE2   | 3:H:666:ASN:OD1   | 2.39                     | 0.54              |
| 3:H:1334:ILE:HG22 | 3:H:1335:THR:N    | 2.23                     | 0.54              |
| 4:h:56:GLY:O      | 4:h:60:ALA:N      | 2.38                     | 0.54              |
| 3:O:950:GLN:HB2   | 3:O:953:GLU:HG3   | 1.88                     | 0.54              |
| 3:O:1148:ARG:HH22 | 3:O:1163:LEU:H    | 1.55                     | 0.54              |
| 3:P:204:TYR:CE1   | 3:P:215:ALA:HB1   | 2.41                     | 0.54              |
| 3:P:204:TYR:CD2   | 3:P:219:LEU:HD11  | 2.43                     | 0.54              |
| 3:B:93:GLY:HA3    | 3:B:124:ILE:HD12  | 1.89                     | 0.54              |
| 3:B:1225:LEU:HD22 | 3:B:1234:PRO:HG2  | 1.89                     | 0.54              |
| 3:C:774:ALA:HB1   | 3:C:776:PHE:CE1   | 2.42                     | 0.54              |
| 3:D:677:TYR:HA    | 4:d:95:LYS:HZ3    | 1.70                     | 0.54              |
| 3:E:405:PRO:HB3   | 3:E:1199:PHE:CE2  | 2.43                     | 0.54              |
| 3:F:709:LEU:HD23  | 3:G:525:GLN:OE1   | 2.08                     | 0.54              |
| 3:F:840:GLN:C     | 3:F:842:MET:H     | 2.14                     | 0.54              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 4:e:64:LEU:O      | 4:e:67:THR:OG1   | 2.25                     | 0.54              |
| 2:V:299:THR:HG22  | 2:V:313:PRO:HD2  | 1.89                     | 0.54              |
| 3:I:488:GLY:HA2   | 3:I:996:ALA:HB1  | 1.89                     | 0.54              |
| 3:I:867:PRO:HA    | 3:I:870:LEU:HG   | 1.89                     | 0.54              |
| 3:J:845:PRO:HG3   | 3:J:869:ASN:HD21 | 1.72                     | 0.54              |
| 3:J:875:VAL:HG12  | 3:J:879:PHE:CE2  | 2.41                     | 0.54              |
| 3:J:1073:TYR:OH   | 3:J:1097:ARG:NH1 | 2.40                     | 0.54              |
| 3:J:1222:VAL:HG11 | 3:J:1283:THR:HA  | 1.89                     | 0.54              |
| 3:M:735:LEU:HD11  | 3:M:938:LEU:HB2  | 1.88                     | 0.54              |
| 3:M:906:THR:OG1   | 3:M:934:HIS:HB3  | 2.08                     | 0.54              |
| 3:A:1288:CYS:HA   | 3:A:1291:ARG:HD3 | 1.88                     | 0.54              |
| 4:p:57:GLN:OE1    | 3:P:837:ALA:HA   | 2.08                     | 0.54              |
| 3:N:790:ARG:HG3   | 3:N:792:ALA:H    | 1.72                     | 0.54              |
| 3:O:595:ARG:HG3   | 3:O:596:GLY:N    | 2.23                     | 0.54              |
| 3:O:621:ARG:O     | 3:O:943:GLN:NE2  | 2.40                     | 0.54              |
| 3:P:874:THR:O     | 3:P:878:MET:N    | 2.38                     | 0.54              |
| 3:B:311:LEU:HA    | 3:G:55:ASP:OD1   | 2.07                     | 0.54              |
| 3:B:525:GLN:HE22  | 3:G:706:ASP:HA   | 1.72                     | 0.54              |
| 3:B:1054:ARG:HH22 | 3:B:1122:MET:HB3 | 1.72                     | 0.54              |
| 3:D:163:GLN:NE2   | 3:E:348:ARG:HH22 | 2.05                     | 0.54              |
| 3:D:176:PHE:O     | 3:D:180:THR:HG23 | 2.06                     | 0.54              |
| 3:D:266:HIS:CE1   | 3:D:302:VAL:HG13 | 2.42                     | 0.54              |
| 3:E:865:LEU:HD11  | 3:E:886:VAL:H    | 1.73                     | 0.54              |
| 3:E:961:HIS:HD2   | 3:E:963:LEU:HB2  | 1.71                     | 0.54              |
| 3:F:219:LEU:O     | 3:F:222:GLU:N    | 2.38                     | 0.54              |
| 3:G:983:LEU:HD23  | 3:G:983:LEU:C    | 2.32                     | 0.54              |
| 1:Q:89:LYS:O      | 1:Q:93:GLY:N     | 2.40                     | 0.54              |
| 3:L:182:ASP:OD1   | 3:L:385:TYR:OH   | 2.20                     | 0.54              |
| 3:L:646:ARG:HH12  | 3:L:889:PRO:HG2  | 1.71                     | 0.54              |
| 3:L:867:PRO:HA    | 3:L:870:LEU:HD12 | 1.89                     | 0.54              |
| 3:M:47:ASN:ND2    | 3:C:137:THR:OG1  | 2.40                     | 0.54              |
| 3:M:445:LYS:NZ    | 3:M:1179:HIS:O   | 2.40                     | 0.54              |
| 3:M:1195:ASP:OD1  | 3:M:1195:ASP:N   | 2.37                     | 0.54              |
| 3:A:1029:PHE:HB3  | 3:A:1039:GLN:NE2 | 2.21                     | 0.54              |
| 3:H:339:MET:CE    | 3:C:17:MET:SD    | 2.95                     | 0.54              |
| 3:H:873:ASN:ND2   | 4:m:89:ARG:HH12  | 2.04                     | 0.54              |
| 4:i:77:PRO:O      | 4:i:94:LEU:N     | 2.31                     | 0.54              |
| 4:o:56:GLY:O      | 4:o:60:ALA:N     | 2.35                     | 0.54              |
| 3:O:282:ALA:N     | 3:O:381:GLU:OE2  | 2.32                     | 0.54              |
| 3:C:258:SER:OG    | 3:C:259:VAL:N    | 2.35                     | 0.54              |
| 3:C:606:MET:HE3   | 3:C:611:ILE:HG12 | 1.89                     | 0.54              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:C:861:PRO:O    | 3:C:869:ASN:ND2   | 2.40                     | 0.54              |
| 3:D:441:PHE:CE2  | 3:D:1340:PRO:HD3  | 2.43                     | 0.54              |
| 3:E:172:VAL:O    | 3:E:175:ALA:N     | 2.28                     | 0.54              |
| 3:E:200:PRO:HG2  | 3:E:223:LEU:HD23  | 1.88                     | 0.54              |
| 3:E:227:PHE:O    | 3:E:231:SER:OG    | 2.24                     | 0.54              |
| 3:E:280:THR:HG22 | 3:E:1063:VAL:HG13 | 1.90                     | 0.54              |
| 3:E:663:ALA:N    | 3:E:690:TYR:OH    | 2.40                     | 0.54              |
| 3:E:950:GLN:HB2  | 3:E:953:GLU:HG3   | 1.88                     | 0.54              |
| 3:F:790:ARG:HG3  | 3:F:792:ALA:H     | 1.72                     | 0.54              |
| 1:T:260:LEU:HD11 | 3:J:109:PRO:HG2   | 1.89                     | 0.54              |
| 1:1:436:LEU:HB2  | 1:1:451:ILE:HB    | 1.90                     | 0.54              |
| 2:y:55:GLY:C     | 3:L:1262:HIS:CD2  | 2.73                     | 0.54              |
| 2:y:306:VAL:HG11 | 2:y:312:ALA:HB2   | 1.90                     | 0.54              |
| 3:I:132:ALA:HB3  | 3:J:114:GLN:HG2   | 1.90                     | 0.54              |
| 3:J:493:ALA:HB2  | 3:J:559:PRO:HB2   | 1.90                     | 0.54              |
| 3:J:874:THR:HG22 | 4:j:26:VAL:HG21   | 1.88                     | 0.54              |
| 3:L:257:PRO:HA   | 3:L:1067:GLU:OE1  | 2.08                     | 0.54              |
| 3:L:876:ASN:HA   | 3:L:879:PHE:CD2   | 2.43                     | 0.54              |
| 3:H:158:GLN:O    | 3:H:161:ALA:N     | 2.40                     | 0.54              |
| 3:H:238:GLY:HA2  | 3:H:244:ILE:HD11  | 1.90                     | 0.54              |
| 4:k:83:ALA:HB3   | 4:k:86:GLU:HG2    | 1.89                     | 0.54              |
| 3:B:1366:ALA:HA  | 3:B:1370:LYS:NZ   | 2.23                     | 0.54              |
| 3:D:406:LEU:HD23 | 3:D:440:LEU:HG    | 1.88                     | 0.54              |
| 3:E:463:HIS:HD2  | 3:E:465:SER:HB3   | 1.73                     | 0.54              |
| 3:F:52:VAL:CG2   | 3:G:320:LEU:CD2   | 2.84                     | 0.54              |
| 2:R:173:LEU:CA   | 5:q:372:ASP:H     | 2.17                     | 0.54              |
| 2:U:102:ASN:ND2  | 2:U:307:GLN:O     | 2.41                     | 0.54              |
| 2:V:254:ILE:HG22 | 2:V:256:PRO:HD3   | 1.89                     | 0.54              |
| 3:I:512:ARG:HA   | 3:I:515:HIS:CD2   | 2.41                     | 0.54              |
| 3:I:746:ALA:HA   | 3:I:754:CYS:CB    | 2.38                     | 0.54              |
| 3:J:746:ALA:N    | 3:J:754:CYS:HB3   | 2.22                     | 0.54              |
| 3:J:778:ARG:NH1  | 3:J:782:ARG:HH11  | 2.06                     | 0.54              |
| 3:K:1160:ALA:HB2 | 3:K:1172:PRO:HG3  | 1.90                     | 0.54              |
| 3:L:17:MET:O     | 3:O:348:ARG:NE    | 2.41                     | 0.54              |
| 3:L:148:LEU:HD11 | 3:L:158:GLN:NE2   | 2.23                     | 0.54              |
| 3:M:438:ARG:O    | 3:M:454:MET:HG2   | 2.08                     | 0.54              |
| 3:M:866:HIS:ND1  | 3:M:867:PRO:HD2   | 2.23                     | 0.54              |
| 3:M:1344:ARG:NH2 | 3:H:414:GLU:OE2   | 2.39                     | 0.54              |
| 3:H:700:LEU:HD22 | 3:H:1025:MET:HG3  | 1.89                     | 0.54              |
| 4:n:99:SER:HA    | 3:N:646:ARG:NH1   | 2.23                     | 0.54              |
| 3:N:265:THR:H    | 3:N:1068:ARG:HH21 | 1.53                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:O:827:THR:OG1   | 3:O:958:LEU:O     | 2.24                     | 0.54              |
| 3:P:866:HIS:ND1   | 3:P:867:PRO:HD2   | 2.22                     | 0.54              |
| 3:B:85:PRO:HG2    | 3:B:86:GLU:OE1    | 2.07                     | 0.54              |
| 3:B:214:VAL:HG22  | 3:G:1177:MET:HE1  | 1.88                     | 0.54              |
| 3:B:842:MET:HE1   | 3:B:891:MET:HE3   | 1.88                     | 0.54              |
| 3:C:204:TYR:HB2   | 3:C:219:LEU:HD21  | 1.90                     | 0.54              |
| 3:C:787:THR:C     | 3:C:788:GLN:HG3   | 2.33                     | 0.54              |
| 3:C:1058:PHE:CE2  | 3:C:1369:LEU:HD11 | 2.42                     | 0.54              |
| 3:F:448:GLN:HB3   | 3:G:1201:ARG:NH1  | 2.23                     | 0.54              |
| 3:F:469:ILE:HD11  | 3:F:547:PHE:CE1   | 2.42                     | 0.54              |
| 3:G:677:TYR:HA    | 4:g:95:LYS:HZ3    | 1.72                     | 0.54              |
| 1:T:436:LEU:HB2   | 1:T:451:ILE:HB    | 1.89                     | 0.54              |
| 3:I:469:ILE:O     | 3:I:471:ALA:N     | 2.40                     | 0.54              |
| 3:J:469:ILE:HD13  | 3:J:547:PHE:CD1   | 2.36                     | 0.54              |
| 3:J:785:HIS:CD2   | 3:J:788:GLN:HE21  | 2.21                     | 0.54              |
| 3:J:1177:MET:HE1  | 3:K:214:VAL:HG22  | 1.89                     | 0.54              |
| 3:K:259:VAL:HG22  | 3:K:1102:LEU:HD13 | 1.90                     | 0.54              |
| 3:L:403:VAL:HG22  | 3:L:1053:VAL:HG22 | 1.88                     | 0.54              |
| 3:L:957:VAL:HG12  | 3:L:959:PRO:HD3   | 1.89                     | 0.54              |
| 3:A:403:VAL:HG22  | 3:A:1053:VAL:HG22 | 1.90                     | 0.54              |
| 3:H:507:ASN:HA    | 3:H:510:ARG:NE    | 2.22                     | 0.54              |
| 4:o:65:GLY:HA2    | 4:o:68:HIS:HB2    | 1.89                     | 0.54              |
| 3:N:194:PRO:HA    | 3:N:1110:ALA:O    | 2.08                     | 0.54              |
| 3:N:1026:ALA:HA   | 3:N:1029:PHE:HE2  | 1.72                     | 0.54              |
| 3:O:946:ASP:HB3   | 3:O:949:ILE:N     | 2.23                     | 0.54              |
| 3:C:463:HIS:CG    | 3:C:464:PRO:HD2   | 2.43                     | 0.54              |
| 3:C:675:VAL:HG21  | 3:C:694:VAL:HG21  | 1.90                     | 0.54              |
| 5:q:260:ILE:O     | 5:q:264:VAL:HG23  | 2.08                     | 0.54              |
| 5:q:586:HIS:HD2   | 5:q:625:MET:HE2   | 1.72                     | 0.54              |
| 3:F:1181:GLN:OE1  | 3:F:1307:SER:OG   | 2.25                     | 0.54              |
| 3:F:1225:LEU:HD22 | 3:F:1234:PRO:HG2  | 1.89                     | 0.54              |
| 3:G:505:PHE:CD2   | 3:G:505:PHE:C     | 2.85                     | 0.54              |
| 3:G:775:ASP:HB2   | 3:G:778:ARG:HH21  | 1.73                     | 0.54              |
| 3:I:618:PHE:O     | 3:I:941:ALA:HB2   | 2.06                     | 0.54              |
| 3:J:399:ASP:CG    | 3:J:1321:VAL:HG11 | 2.32                     | 0.54              |
| 3:M:255:THR:OG1   | 3:M:1067:GLU:OE2  | 2.19                     | 0.54              |
| 3:M:405:PRO:HB3   | 3:M:1199:PHE:CE2  | 2.43                     | 0.54              |
| 3:H:1128:ASN:OD1  | 3:H:1155:ASN:ND2  | 2.41                     | 0.54              |
| 4:o:76:GLN:O      | 4:o:96:ARG:NH2    | 2.33                     | 0.54              |
| 3:N:406:LEU:HD12  | 3:N:1050:PHE:HB2  | 1.90                     | 0.54              |
| 3:N:615:ARG:HH21  | 3:N:1017:GLU:HG2  | 1.73                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:O:765:TYR:CE1   | 3:O:783:LEU:HD12  | 2.42                     | 0.54              |
| 3:P:784:LEU:HB2   | 3:P:786:ASN:CG    | 2.33                     | 0.54              |
| 3:B:845:PRO:HG3   | 3:B:869:ASN:ND2   | 2.22                     | 0.54              |
| 5:q:56:PHE:N      | 5:q:78:ALA:O      | 2.40                     | 0.54              |
| 3:E:558:LEU:HD13  | 3:E:929:PHE:HE2   | 1.73                     | 0.54              |
| 3:E:947:HIS:HB2   | 4:d:79:PHE:HD1    | 1.72                     | 0.54              |
| 1:Q:418:THR:H     | 1:Q:465:CYS:HB3   | 1.73                     | 0.54              |
| 1:T:170:LEU:HD21  | 3:I:1262:HIS:HD1  | 1.72                     | 0.54              |
| 2:3:25:GLN:NE2    | 2:3:28:GLU:OE2    | 2.41                     | 0.54              |
| 2:3:99:ASN:ND2    | 3:M:1086:GLY:HA3  | 2.22                     | 0.54              |
| 3:I:1170:GLN:OE1  | 3:I:1170:GLN:N    | 2.40                     | 0.54              |
| 3:J:749:ASP:O     | 3:J:752:ARG:N     | 2.40                     | 0.54              |
| 3:J:827:THR:OG1   | 3:J:960:VAL:HG23  | 2.07                     | 0.54              |
| 3:K:1128:ASN:HD21 | 3:K:1155:ASN:ND2  | 2.06                     | 0.54              |
| 3:M:20:THR:O      | 3:D:352:ASP:N     | 2.39                     | 0.54              |
| 3:M:857:PRO:HB3   | 3:M:865:LEU:HB2   | 1.90                     | 0.54              |
| 3:A:577:VAL:HG12  | 3:A:578:VAL:HG13  | 1.90                     | 0.54              |
| 3:H:1225:LEU:HD22 | 3:H:1234:PRO:HG3  | 1.89                     | 0.54              |
| 4:m:62:THR:O      | 4:m:66:VAL:HG23   | 2.07                     | 0.54              |
| 3:N:69:ARG:HB3    | 3:N:72:GLU:HG2    | 1.90                     | 0.54              |
| 3:B:646:ARG:HH12  | 3:B:889:PRO:HB2   | 1.73                     | 0.54              |
| 3:D:1206:ARG:HH21 | 3:D:1210:ALA:HB2  | 1.73                     | 0.54              |
| 5:q:644:GLU:OE1   | 5:q:645:SER:OG    | 2.23                     | 0.54              |
| 3:F:499:ALA:HA    | 3:F:956:TYR:CD1   | 2.43                     | 0.54              |
| 2:X:40:GLN:HE21   | 3:H:128:ALA:CB    | 2.17                     | 0.53              |
| 2:Y:248:ARG:NE    | 3:H:1141:ASN:HD21 | 2.06                     | 0.53              |
| 1:w:118:ASP:O     | 1:w:223:ARG:NH1   | 2.42                     | 0.53              |
| 3:I:198:LEU:O     | 3:I:201:MET:N     | 2.41                     | 0.53              |
| 3:K:410:ASN:ND2   | 3:K:1359:THR:O    | 2.41                     | 0.53              |
| 3:L:756:ILE:HG21  | 3:L:908:LEU:HD22  | 1.88                     | 0.53              |
| 3:M:266:HIS:CE1   | 3:M:302:VAL:HG13  | 2.42                     | 0.53              |
| 3:H:119:TYR:O     | 3:C:39:PHE:HA     | 2.07                     | 0.53              |
| 3:H:717:GLN:HE22  | 3:H:752:ARG:NH1   | 2.06                     | 0.53              |
| 3:H:890:ALA:O     | 3:H:893:THR:OG1   | 2.25                     | 0.53              |
| 4:n:54:LEU:HD22   | 3:N:836:TYR:HB2   | 1.88                     | 0.53              |
| 3:N:1290:GLU:HB3  | 3:D:32:HIS:HB3    | 1.90                     | 0.53              |
| 3:O:1197:ASN:OD1  | 3:O:1200:ARG:NH1  | 2.41                     | 0.53              |
| 3:P:724:HIS:CE1   | 3:P:1028:TYR:HB2  | 2.44                     | 0.53              |
| 3:P:889:PRO:HA    | 3:P:892:LEU:HD12  | 1.90                     | 0.53              |
| 3:C:1227:TYR:CD1  | 3:C:1249:ARG:HB2  | 2.43                     | 0.53              |
| 3:D:159:LEU:HD13  | 3:E:340:GLN:HA    | 1.89                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:193:PRO:HB2   | 3:D:1293:ILE:HG22 | 1.90                     | 0.53              |
| 3:D:1225:LEU:HD22 | 3:D:1234:PRO:HG3  | 1.89                     | 0.53              |
| 3:E:649:THR:HG22  | 3:E:678:LEU:HD13  | 1.90                     | 0.53              |
| 3:E:677:TYR:CD1   | 4:e:95:LYS:CE     | 2.91                     | 0.53              |
| 2:U:164:ASN:O     | 2:V:226:ARG:NH2   | 2.41                     | 0.53              |
| 2:Y:300:PHE:CE2   | 3:H:1085:THR:CG2  | 2.91                     | 0.53              |
| 1:L:283:ARG:CB    | 3:L:47:ASN:HD21   | 2.20                     | 0.53              |
| 3:I:840:GLN:CB    | 4:i:57:GLN:HB3    | 2.38                     | 0.53              |
| 3:I:863:HIS:CE1   | 3:I:887:ASP:HA    | 2.43                     | 0.53              |
| 3:J:627:PHE:HD1   | 3:J:664:PHE:CE1   | 2.25                     | 0.53              |
| 3:K:193:PRO:HG2   | 3:K:198:LEU:HD11  | 1.90                     | 0.53              |
| 3:K:914:PRO:HG3   | 3:K:923:THR:HG22  | 1.90                     | 0.53              |
| 3:H:778:ARG:HD3   | 3:H:780:ASP:HB2   | 1.90                     | 0.53              |
| 4:j:4:PRO:HA      | 4:j:11:THR:HG22   | 1.89                     | 0.53              |
| 4:j:77:PRO:HB3    | 4:j:82:ASP:HB3    | 1.90                     | 0.53              |
| 3:N:595:ARG:HD3   | 3:N:1026:ALA:HB1  | 1.88                     | 0.53              |
| 3:N:829:GLY:N     | 3:N:956:TYR:O     | 2.40                     | 0.53              |
| 3:P:33:ARG:O      | 3:P:36:PHE:N      | 2.38                     | 0.53              |
| 3:P:521:VAL:HG21  | 3:P:987:VAL:HG12  | 1.90                     | 0.53              |
| 3:B:778:ARG:NH1   | 3:B:782:ARG:HD2   | 2.23                     | 0.53              |
| 5:q:390:HIS:CD2   | 5:q:393:THR:H     | 2.26                     | 0.53              |
| 3:F:532:MET:HE1   | 3:F:1244:PRO:HD3  | 1.91                     | 0.53              |
| 1:T:260:LEU:CD2   | 3:I:1316:GLY:HA2  | 2.36                     | 0.53              |
| 2:3:38:ARG:HH22   | 3:E:109:PRO:C     | 2.15                     | 0.53              |
| 1:w:158:ALA:HB1   | 3:O:1165:VAL:HG21 | 1.91                     | 0.53              |
| 2:y:268:ARG:NH2   | 2:y:273:GLU:OE1   | 2.41                     | 0.53              |
| 3:I:704:VAL:HG11  | 3:I:727:ARG:HG3   | 1.90                     | 0.53              |
| 3:J:1339:ASP:OD2  | 3:J:1360:GLN:HG3  | 2.08                     | 0.53              |
| 3:K:499:ALA:HA    | 3:K:956:TYR:CD1   | 2.43                     | 0.53              |
| 3:K:1029:PHE:HB3  | 3:K:1039:GLN:HE22 | 1.71                     | 0.53              |
| 3:K:1161:GLN:HB3  | 3:K:1170:GLN:NE2  | 2.23                     | 0.53              |
| 3:L:532:MET:HE1   | 3:L:1244:PRO:HD3  | 1.90                     | 0.53              |
| 3:L:1157:LEU:HD11 | 3:L:1269:VAL:HG21 | 1.91                     | 0.53              |
| 3:H:244:ILE:O     | 3:H:247:TRP:N     | 2.35                     | 0.53              |
| 4:n:25:LEU:HD21   | 4:n:57:GLN:HG2    | 1.90                     | 0.53              |
| 3:O:1176:GLY:HA3  | 3:P:1225:LEU:HD21 | 1.90                     | 0.53              |
| 3:P:708:THR:HG22  | 3:P:723:ASN:HD22  | 1.73                     | 0.53              |
| 3:P:867:PRO:HA    | 3:P:870:LEU:HB2   | 1.89                     | 0.53              |
| 3:B:129:LEU:O     | 3:B:1094:THR:HA   | 2.07                     | 0.53              |
| 3:B:392:TYR:CE2   | 3:B:394:LEU:HB3   | 2.43                     | 0.53              |
| 3:B:633:ALA:O     | 3:B:635:HIS:ND1   | 2.33                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:C:873:ASN:CA    | 4:b:92:PHE:HD2    | 2.20                     | 0.53              |
| 5:q:104:VAL:HB    | 5:q:234:PRO:HD2   | 1.89                     | 0.53              |
| 5:q:260:ILE:HG21  | 7:u:3092:ILE:HD11 | 1.90                     | 0.53              |
| 5:q:601:LEU:O     | 5:q:635:ARG:NH1   | 2.41                     | 0.53              |
| 3:E:265:THR:H     | 3:E:1068:ARG:HH21 | 1.57                     | 0.53              |
| 3:E:405:PRO:O     | 3:E:440:LEU:HD11  | 2.09                     | 0.53              |
| 3:G:712:PRO:HD2   | 3:G:1146:TYR:CE1  | 2.43                     | 0.53              |
| 3:G:827:THR:OG1   | 3:G:960:VAL:HG23  | 2.09                     | 0.53              |
| 4:b:64:LEU:O      | 4:b:67:THR:OG1    | 2.25                     | 0.53              |
| 7:u:3095:GLN:HG2  | 7:u:3098:ARG:HH21 | 1.71                     | 0.53              |
| 3:I:56:ALA:HA     | 3:J:325:ALA:O     | 2.08                     | 0.53              |
| 3:I:85:PRO:HG2    | 3:I:86:GLU:OE1    | 2.07                     | 0.53              |
| 3:J:729:PRO:HB2   | 3:J:748:LEU:HD11  | 1.91                     | 0.53              |
| 3:A:399:ASP:OD1   | 3:A:1057:ARG:HG2  | 2.08                     | 0.53              |
| 3:A:1198:TYR:CZ   | 3:A:1203:CYS:HB2  | 2.43                     | 0.53              |
| 3:H:320:LEU:CD1   | 3:C:156:HIS:CD2   | 2.91                     | 0.53              |
| 3:H:819:ALA:O     | 3:H:822:ARG:NH1   | 2.42                     | 0.53              |
| 3:N:1248:GLN:C    | 3:N:1251:SER:HG   | 2.16                     | 0.53              |
| 3:C:85:PRO:HG2    | 3:C:86:GLU:OE1    | 2.08                     | 0.53              |
| 3:C:511:GLN:OE1   | 3:C:511:GLN:N     | 2.38                     | 0.53              |
| 3:C:730:ALA:HB2   | 3:C:752:ARG:NH1   | 2.24                     | 0.53              |
| 3:D:490:TYR:CD1   | 3:D:564:PRO:HB3   | 2.44                     | 0.53              |
| 3:E:866:HIS:ND1   | 3:E:867:PRO:HD2   | 2.23                     | 0.53              |
| 3:E:906:THR:OG1   | 3:E:934:HIS:HB3   | 2.09                     | 0.53              |
| 3:E:914:PRO:HG3   | 3:E:923:THR:HG22  | 1.89                     | 0.53              |
| 6:r:3:PRO:HG2     | 6:r:5:TYR:HE2     | 1.73                     | 0.53              |
| 6:r:77:PRO:HB3    | 7:u:3108:ASN:OD1  | 2.09                     | 0.53              |
| 3:F:57:LEU:O      | 3:G:327:ARG:HB2   | 2.08                     | 0.53              |
| 3:G:344:LEU:O     | 3:G:345:GLU:HG3   | 2.07                     | 0.53              |
| 2:S:299:THR:HG22  | 2:S:313:PRO:HD2   | 1.90                     | 0.53              |
| 2:Y:204:SER:O     | 2:Y:208:ASN:ND2   | 2.42                     | 0.53              |
| 2:Y:268:ARG:NH2   | 2:Y:273:GLU:OE1   | 2.41                     | 0.53              |
| 3:I:950:GLN:HG3   | 4:h:80:ALA:HB1    | 1.90                     | 0.53              |
| 3:J:756:ILE:HD12  | 3:J:763:PRO:HG3   | 1.91                     | 0.53              |
| 3:J:925:ASN:O     | 3:J:927:ARG:NH1   | 2.41                     | 0.53              |
| 3:J:1318:ARG:HH21 | 3:J:1320:LEU:HD21 | 1.73                     | 0.53              |
| 3:A:670:LEU:HA    | 3:A:673:TYR:CD2   | 2.44                     | 0.53              |
| 3:A:709:LEU:H     | 3:A:1038:HIS:CE1  | 2.26                     | 0.53              |
| 3:A:906:THR:OG1   | 3:A:934:HIS:HB3   | 2.09                     | 0.53              |
| 3:H:736:VAL:HG12  | 3:H:738:ASP:H     | 1.73                     | 0.53              |
| 3:H:873:ASN:HA    | 4:m:92:PHE:CD2    | 2.43                     | 0.53              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 3:B:261:VAL:CA    | 3:G:61:TYR:O     | 2.54                     | 0.53              |
| 3:D:512:ARG:HD3   | 3:D:515:HIS:HD2  | 1.73                     | 0.53              |
| 5:q:379:SER:HA    | 5:q:383:ILE:HD11 | 1.89                     | 0.53              |
| 3:E:1190:THR:HG22 | 3:E:1243:ASN:ND2 | 2.24                     | 0.53              |
| 3:F:162:ILE:HG22  | 3:G:344:LEU:HD11 | 1.90                     | 0.53              |
| 3:F:770:ASN:OD1   | 3:F:900:ASN:HA   | 2.08                     | 0.53              |
| 3:J:86:GLU:HG2    | 3:J:86:GLU:O     | 2.08                     | 0.53              |
| 3:K:898:ALA:HA    | 3:K:901:MET:HE2  | 1.91                     | 0.53              |
| 3:L:392:TYR:CE2   | 3:L:394:LEU:HB3  | 2.44                     | 0.53              |
| 3:M:28:GLU:CD     | 3:C:389:ASN:OD1  | 2.49                     | 0.53              |
| 3:M:194:PRO:HA    | 3:M:1110:ALA:O   | 2.08                     | 0.53              |
| 3:M:892:LEU:HD13  | 4:m:68:HIS:CG    | 2.44                     | 0.53              |
| 3:A:637:SER:HB3   | 3:A:640:VAL:HB   | 1.91                     | 0.53              |
| 3:H:709:LEU:CD1   | 3:H:710:PRO:HD2  | 2.38                     | 0.53              |
| 3:H:749:ASP:OD2   | 3:H:751:HIS:HB2  | 2.08                     | 0.53              |
| 4:j:73:PHE:CD2    | 4:j:100:PRO:HA   | 2.44                     | 0.53              |
| 4:o:22:MET:HE3    | 4:o:64:LEU:HD22  | 1.91                     | 0.53              |
| 3:N:204:TYR:CD2   | 3:N:219:LEU:HD11 | 2.44                     | 0.53              |
| 3:N:543:LEU:HB2   | 3:N:549:PHE:CE2  | 2.43                     | 0.53              |
| 3:P:521:VAL:HG11  | 3:P:987:VAL:HG12 | 1.90                     | 0.53              |
| 3:P:595:ARG:NH1   | 3:P:1026:ALA:HB1 | 2.24                     | 0.53              |
| 3:P:876:ASN:HA    | 3:P:879:PHE:HD2  | 1.72                     | 0.53              |
| 3:C:714:LEU:HD12  | 3:C:722:LEU:HD22 | 1.90                     | 0.53              |
| 3:D:784:LEU:HB2   | 3:D:786:ASN:CG   | 2.34                     | 0.53              |
| 3:D:826:CYS:HB3   | 3:D:966:GLY:H    | 1.74                     | 0.53              |
| 3:E:278:LEU:HG    | 3:E:375:VAL:HG11 | 1.89                     | 0.53              |
| 3:E:769:CYS:SG    | 3:E:786:ASN:ND2  | 2.76                     | 0.53              |
| 3:E:1128:ASN:HD21 | 3:E:1155:ASN:ND2 | 2.06                     | 0.53              |
| 3:F:440:LEU:HD22  | 3:F:1336:CYS:SG  | 2.48                     | 0.53              |
| 3:G:227:PHE:O     | 3:G:231:SER:OG   | 2.24                     | 0.53              |
| 3:G:550:PHE:HD1   | 3:G:998:TYR:CD2  | 1.89                     | 0.53              |
| 1:T:208:ARG:NH2   | 1:T:225:ASP:OD2  | 2.41                     | 0.53              |
| 2:X:116:LEU:HB2   | 2:X:140:PRO:HB2  | 1.91                     | 0.53              |
| 3:I:754:CYS:SG    | 3:I:756:ILE:HG13 | 2.49                     | 0.53              |
| 3:J:213:ARG:NH1   | 3:J:1216:GLY:HA3 | 2.24                     | 0.53              |
| 3:J:819:ALA:O     | 3:J:822:ARG:NH1  | 2.41                     | 0.53              |
| 3:J:1201:ARG:HB2  | 3:J:1202:PRO:HD2 | 1.90                     | 0.53              |
| 3:L:634:ILE:HG22  | 3:L:636:GLY:H    | 1.73                     | 0.53              |
| 3:M:193:PRO:HG2   | 3:M:198:LEU:HD11 | 1.89                     | 0.53              |
| 3:M:491:VAL:HG21  | 3:M:929:PHE:CD2  | 2.42                     | 0.53              |
| 3:M:948:THR:HA    | 4:l:79:PHE:HA    | 1.91                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:A:524:CYS:SG    | 3:A:1008:GLN:NE2  | 2.82                     | 0.53              |
| 3:A:744:ARG:HA    | 3:A:747:ALA:HB3   | 1.89                     | 0.53              |
| 3:H:135:LEU:HD21  | 3:H:165:LEU:HD21  | 1.90                     | 0.53              |
| 4:o:68:HIS:HB3    | 3:O:892:LEU:HD13  | 1.91                     | 0.53              |
| 3:B:102:PRO:HB3   | 3:G:178:ARG:HH12  | 1.74                     | 0.53              |
| 3:B:725:LEU:HB3   | 3:B:1028:TYR:HB3  | 1.91                     | 0.53              |
| 3:B:907:ALA:HB1   | 3:B:994:LEU:HD21  | 1.91                     | 0.53              |
| 3:B:1174:ARG:NH1  | 3:C:1232:SER:OG   | 2.42                     | 0.53              |
| 3:B:1178:ASP:O    | 3:C:217:ALA:HB1   | 2.07                     | 0.53              |
| 3:C:610:THR:HG22  | 3:C:689:VAL:HA    | 1.91                     | 0.53              |
| 3:D:600:GLY:C     | 3:D:602:GLY:H     | 2.17                     | 0.53              |
| 3:D:866:HIS:ND1   | 3:D:867:PRO:HD2   | 2.24                     | 0.53              |
| 3:E:898:ALA:HA    | 3:E:901:MET:HE2   | 1.90                     | 0.53              |
| 3:F:512:ARG:HD3   | 3:F:515:HIS:CD2   | 2.41                     | 0.53              |
| 3:F:873:ASN:C     | 4:e:92:PHE:CD2    | 2.87                     | 0.53              |
| 2:X:284:GLN:CD    | 3:H:1166:PHE:CE1  | 2.86                     | 0.53              |
| 3:I:274:VAL:HG11  | 3:I:376:PHE:CE2   | 2.44                     | 0.53              |
| 3:I:785:HIS:CD2   | 3:I:788:GLN:HE21  | 2.26                     | 0.53              |
| 3:J:948:THR:HA    | 4:i:79:PHE:HA     | 1.91                     | 0.53              |
| 3:J:1178:ASP:O    | 3:K:217:ALA:HB1   | 2.09                     | 0.53              |
| 3:L:714:LEU:HD22  | 3:L:1143:ALA:HA   | 1.91                     | 0.53              |
| 3:M:486:PRO:HG2   | 3:M:564:PRO:HG3   | 1.91                     | 0.53              |
| 3:A:638:GLU:HB2   | 3:A:789:ALA:HA    | 1.89                     | 0.53              |
| 3:A:961:HIS:CD2   | 3:A:963:LEU:H     | 2.26                     | 0.53              |
| 3:H:778:ARG:NH1   | 3:H:782:ARG:HD2   | 2.23                     | 0.53              |
| 3:H:880:HIS:NE2   | 4:m:95:LYS:O      | 2.39                     | 0.53              |
| 4:o:89:ARG:HD3    | 3:P:841:ASN:HD21  | 1.73                     | 0.53              |
| 3:O:708:THR:HG22  | 3:O:723:ASN:HD22  | 1.73                     | 0.53              |
| 3:P:775:ASP:OD2   | 3:P:778:ARG:NH2   | 2.38                     | 0.53              |
| 3:B:829:GLY:N     | 3:B:956:TYR:O     | 2.36                     | 0.53              |
| 3:C:738:ASP:OD2   | 3:C:801:ARG:NH1   | 2.41                     | 0.53              |
| 3:D:1300:VAL:HG21 | 3:D:1318:ARG:HH21 | 1.73                     | 0.53              |
| 3:E:677:TYR:HA    | 4:e:95:LYS:NZ     | 2.24                     | 0.53              |
| 3:F:497:PRO:HG2   | 3:F:500:ASP:HB2   | 1.91                     | 0.53              |
| 1:Q:185:VAL:HG21  | 1:Q:245:MET:HE1   | 1.91                     | 0.53              |
| 1:T:259:GLU:OE1   | 3:I:1315:PRO:O    | 2.27                     | 0.53              |
| 1:I:257:GLN:CD    | 3:H:109:PRO:CD    | 2.70                     | 0.53              |
| 3:I:96:GLN:HG2    | 3:I:121:THR:HG22  | 1.90                     | 0.53              |
| 3:I:895:GLN:HA    | 4:i:61:LEU:HD13   | 1.90                     | 0.53              |
| 3:K:837:ALA:HA    | 4:k:57:GLN:HE22   | 1.73                     | 0.53              |
| 3:M:469:ILE:HD11  | 3:M:547:PHE:CE1   | 2.44                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:M:624:PRO:HB3   | 3:M:882:GLY:O     | 2.09                     | 0.53              |
| 3:M:1334:ILE:HG22 | 3:M:1335:THR:H    | 1.74                     | 0.53              |
| 3:H:752:ARG:NH2   | 3:H:915:ASP:HA    | 2.23                     | 0.53              |
| 3:H:919:ASN:ND2   | 3:H:1139:LEU:HD12 | 2.23                     | 0.53              |
| 4:k:89:ARG:NH2    | 4:l:30:ASN:OD1    | 2.42                     | 0.53              |
| 4:o:61:LEU:HD13   | 3:O:895:GLN:HA    | 1.91                     | 0.53              |
| 3:N:63:ASN:ND2    | 3:O:99:VAL:HA     | 2.24                     | 0.53              |
| 3:O:95:VAL:HG21   | 3:O:1100:VAL:HG11 | 1.89                     | 0.53              |
| 3:P:890:ALA:O     | 3:P:893:THR:OG1   | 2.19                     | 0.53              |
| 3:B:463:HIS:ND1   | 3:B:464:PRO:HD2   | 2.23                     | 0.53              |
| 3:D:604:HIS:NE2   | 3:D:605:ALA:O     | 2.42                     | 0.53              |
| 3:E:266:HIS:CE1   | 3:E:302:VAL:HG13  | 2.43                     | 0.53              |
| 1:Q:44:ARG:CB     | 3:B:322:MET:HE3   | 2.39                     | 0.53              |
| 2:R:12:ILE:HD11   | 2:R:83:ILE:HG13   | 1.90                     | 0.53              |
| 1:W:342:ALA:O     | 6:s:13:TRP:HH2    | 1.92                     | 0.53              |
| 2:X:99:ASN:ND2    | 3:C:1086:GLY:C    | 2.67                     | 0.53              |
| 2:X:158:ARG:NH2   | 2:X:177:ASN:OD1   | 2.41                     | 0.53              |
| 1:1:431:ASP:OD2   | 2:2:39:ARG:HD2    | 2.09                     | 0.53              |
| 3:I:91:ASN:HB2    | 3:H:55:ASP:OD1    | 2.09                     | 0.53              |
| 3:I:350:THR:HG22  | 3:I:352:ASP:H     | 1.74                     | 0.53              |
| 3:J:739:CYS:SG    | 3:J:765:TYR:HB3   | 2.49                     | 0.53              |
| 3:K:1017:GLU:O    | 3:K:1021:THR:HG23 | 2.09                     | 0.53              |
| 3:M:58:LEU:HD12   | 3:H:124:ILE:HD11  | 1.91                     | 0.53              |
| 3:M:481:VAL:HG11  | 3:M:571:ILE:HD12  | 1.91                     | 0.53              |
| 3:M:507:ASN:OD1   | 3:M:510:ARG:NH2   | 2.42                     | 0.53              |
| 3:M:957:VAL:HG12  | 3:M:959:PRO:HD3   | 1.91                     | 0.53              |
| 3:N:99:VAL:HG21   | 3:D:29:VAL:HG21   | 1.89                     | 0.53              |
| 3:N:352:ASP:OD1   | 3:D:20:THR:HB     | 2.09                     | 0.53              |
| 3:O:1186:GLU:CD   | 3:O:1272:PRO:HD2  | 2.34                     | 0.53              |
| 3:P:895:GLN:O     | 3:P:898:ALA:N     | 2.39                     | 0.53              |
| 3:B:866:HIS:HD2   | 3:B:868:ALA:HB3   | 1.74                     | 0.53              |
| 3:C:755:ARG:HG2   | 3:C:911:SER:OG    | 2.09                     | 0.53              |
| 3:D:204:TYR:CD2   | 3:D:219:LEU:HD11  | 2.44                     | 0.53              |
| 3:D:259:VAL:HG22  | 3:D:1102:LEU:HD13 | 1.91                     | 0.53              |
| 3:D:265:THR:H     | 3:D:1068:ARG:HH21 | 1.57                     | 0.53              |
| 3:D:1227:TYR:O    | 3:D:1229:HIS:ND1  | 2.41                     | 0.53              |
| 5:q:80:TYR:HA     | 5:q:110:LEU:HA    | 1.91                     | 0.53              |
| 3:F:90:MET:HG2    | 3:F:91:ASN:O      | 2.09                     | 0.53              |
| 3:F:258:SER:OG    | 3:F:259:VAL:N     | 2.40                     | 0.53              |
| 3:F:266:HIS:CE1   | 3:F:303:PRO:HD2   | 2.44                     | 0.53              |
| 3:F:1058:PHE:CE2  | 3:F:1369:LEU:HD11 | 2.44                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:G:723:ASN:OD1   | 3:G:1039:GLN:NE2  | 2.36                     | 0.53              |
| 2:X:24:LEU:HD13   | 2:X:83:ILE:HD11   | 1.91                     | 0.52              |
| 2:3:158:ARG:HH22  | 2:3:188:LEU:HB2   | 1.73                     | 0.52              |
| 3:I:124:ILE:HA    | 3:I:1100:VAL:HG22 | 1.89                     | 0.52              |
| 3:I:148:LEU:HD11  | 3:I:158:GLN:NE2   | 2.25                     | 0.52              |
| 3:L:11:TYR:HE1    | 3:O:96:GLN:HB3    | 1.73                     | 0.52              |
| 3:H:469:ILE:HD11  | 3:H:547:PHE:CE1   | 2.44                     | 0.52              |
| 3:H:639:HIS:HA    | 4:h:79:PHE:CE2    | 2.45                     | 0.52              |
| 3:H:1257:TYR:HB2  | 3:H:1277:PHE:CD2  | 2.43                     | 0.52              |
| 4:o:99:SER:HA     | 3:O:646:ARG:NH1   | 2.24                     | 0.52              |
| 3:O:1148:ARG:HH22 | 3:O:1163:LEU:HG   | 1.74                     | 0.52              |
| 3:P:631:GLN:HE22  | 3:P:666:ASN:CG    | 2.17                     | 0.52              |
| 3:C:204:TYR:CG    | 3:C:219:LEU:HD11  | 2.43                     | 0.52              |
| 3:C:488:GLY:HA3   | 3:C:520:TRP:CH2   | 2.44                     | 0.52              |
| 3:C:684:GLU:HG2   | 3:D:658:ASN:O     | 2.09                     | 0.52              |
| 3:D:866:HIS:O     | 3:D:870:LEU:N     | 2.42                     | 0.52              |
| 3:E:879:PHE:O     | 3:E:883:ARG:N     | 2.42                     | 0.52              |
| 3:E:983:LEU:HD23  | 3:E:983:LEU:O     | 2.09                     | 0.52              |
| 3:F:288:LEU:HD23  | 3:F:292:PHE:HD2   | 1.74                     | 0.52              |
| 3:F:533:GLN:HB3   | 3:F:534:PRO:HD2   | 1.91                     | 0.52              |
| 3:F:753:ASP:OD2   | 3:F:755:ARG:HB3   | 2.08                     | 0.52              |
| 3:F:1115:VAL:HG12 | 3:F:1116:ARG:O    | 2.10                     | 0.52              |
| 3:G:52:VAL:CG1    | 3:G:54:PHE:HE2    | 2.20                     | 0.52              |
| 3:G:985:ARG:CB    | 3:G:985:ARG:CZ    | 2.87                     | 0.52              |
| 2:R:26:ARG:O      | 2:R:101:ARG:NH1   | 2.39                     | 0.52              |
| 3:I:99:VAL:HA     | 3:H:63:ASN:ND2    | 2.23                     | 0.52              |
| 3:K:778:ARG:HH11  | 3:K:782:ARG:HD3   | 1.72                     | 0.52              |
| 3:K:866:HIS:ND1   | 3:K:867:PRO:HD2   | 2.25                     | 0.52              |
| 3:K:1237:PRO:HD2  | 3:K:1238:PHE:H    | 1.75                     | 0.52              |
| 3:L:244:ILE:HD12  | 3:L:292:PHE:CZ    | 2.45                     | 0.52              |
| 3:L:840:GLN:CB    | 4:l:57:GLN:HB3    | 2.39                     | 0.52              |
| 3:M:20:THR:C      | 3:D:350:THR:HG22  | 2.33                     | 0.52              |
| 3:M:630:LEU:O     | 3:M:634:ILE:HD12  | 2.09                     | 0.52              |
| 3:M:740:ASP:OD2   | 3:M:801:ARG:NH1   | 2.42                     | 0.52              |
| 3:M:769:CYS:HB2   | 3:M:786:ASN:ND2   | 2.25                     | 0.52              |
| 3:M:1225:LEU:HD22 | 3:M:1234:PRO:HG3  | 1.89                     | 0.52              |
| 3:M:1248:GLN:O    | 3:M:1251:SER:OG   | 2.27                     | 0.52              |
| 3:A:300:ALA:HB2   | 3:A:367:LEU:HD11  | 1.91                     | 0.52              |
| 3:O:363:VAL:HG12  | 3:O:364:ARG:N     | 2.24                     | 0.52              |
| 3:O:1103:GLY:HA3  | 3:O:1107:THR:HG21 | 1.91                     | 0.52              |
| 3:P:266:HIS:CE1   | 3:P:302:VAL:HG13  | 2.44                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:P:722:LEU:O     | 3:P:1030:LYS:HD2  | 2.09                     | 0.52              |
| 3:C:71:LEU:HD13   | 3:C:304:VAL:O     | 2.09                     | 0.52              |
| 3:C:313:GLY:O     | 3:C:316:LEU:N     | 2.37                     | 0.52              |
| 3:C:638:GLU:HB2   | 3:C:789:ALA:HA    | 1.92                     | 0.52              |
| 3:D:744:ARG:NH1   | 3:D:806:THR:HG23  | 2.23                     | 0.52              |
| 3:D:838:THR:O     | 3:D:875:VAL:HG22  | 2.09                     | 0.52              |
| 3:D:889:PRO:HA    | 3:D:892:LEU:HD12  | 1.91                     | 0.52              |
| 3:D:1129:PHE:O    | 3:D:1132:GLY:N    | 2.36                     | 0.52              |
| 3:E:448:GLN:NE2   | 3:F:1201:ARG:HH12 | 2.03                     | 0.52              |
| 3:E:764:VAL:O     | 3:E:783:LEU:N     | 2.43                     | 0.52              |
| 6:r:22:ASP:OD1    | 6:r:23:SER:N      | 2.42                     | 0.52              |
| 3:F:77:VAL:HG22   | 3:F:266:HIS:CD2   | 2.45                     | 0.52              |
| 3:F:448:GLN:CD    | 3:G:1201:ARG:NH1  | 2.65                     | 0.52              |
| 3:G:780:ASP:O     | 3:G:904:ARG:NH2   | 2.42                     | 0.52              |
| 4:g:64:LEU:O      | 4:g:67:THR:OG1    | 2.25                     | 0.52              |
| 1:Q:117:THR:O     | 1:Q:121:GLN:NE2   | 2.42                     | 0.52              |
| 2:S:120:VAL:HG12  | 2:S:188:LEU:HB2   | 1.90                     | 0.52              |
| 3:I:576:ARG:NH1   | 3:I:582:LEU:HD23  | 2.25                     | 0.52              |
| 3:J:469:ILE:HG22  | 3:J:469:ILE:O     | 2.10                     | 0.52              |
| 3:J:642:CYS:SG    | 4:j:95:LYS:HG2    | 2.50                     | 0.52              |
| 3:K:635:HIS:CE1   | 3:K:640:VAL:HG21  | 2.44                     | 0.52              |
| 3:K:724:HIS:O     | 3:K:1030:LYS:NZ   | 2.42                     | 0.52              |
| 3:K:1186:GLU:CD   | 3:K:1272:PRO:HD2  | 2.34                     | 0.52              |
| 3:L:873:ASN:HA    | 4:k:92:PHE:HB2    | 1.91                     | 0.52              |
| 3:M:752:ARG:NH2   | 3:M:915:ASP:OD1   | 2.21                     | 0.52              |
| 3:A:709:LEU:N     | 3:A:1038:HIS:ND1  | 2.53                     | 0.52              |
| 3:A:783:LEU:HD22  | 3:A:934:HIS:CD2   | 2.44                     | 0.52              |
| 3:A:1106:TYR:HE1  | 3:A:1313:ARG:NH1  | 2.08                     | 0.52              |
| 3:A:1342:LEU:HD21 | 3:A:1362:LEU:HB2  | 1.90                     | 0.52              |
| 3:H:1082:ARG:HG3  | 3:H:1091:PHE:HE1  | 1.73                     | 0.52              |
| 3:N:106:ARG:HE    | 3:N:110:HIS:HB3   | 1.75                     | 0.52              |
| 3:N:600:GLY:C     | 3:N:602:GLY:H     | 2.16                     | 0.52              |
| 3:N:946:ASP:HB3   | 3:N:948:THR:HG22  | 1.89                     | 0.52              |
| 3:O:753:ASP:HB3   | 3:O:755:ARG:NH2   | 2.24                     | 0.52              |
| 3:P:30:ALA:HB2    | 3:P:41:ARG:HD2    | 1.91                     | 0.52              |
| 3:C:837:ALA:O     | 3:C:840:GLN:N     | 2.42                     | 0.52              |
| 3:D:56:ALA:HA     | 3:E:325:ALA:O     | 2.09                     | 0.52              |
| 3:D:643:ALA:HB2   | 4:d:78:MET:HE1    | 1.92                     | 0.52              |
| 6:r:94:ILE:HG23   | 7:t:3085:LEU:HD23 | 1.91                     | 0.52              |
| 3:F:877:ALA:O     | 3:F:881:ASN:HB2   | 2.09                     | 0.52              |
| 3:G:1037:TYR:C    | 3:G:1037:TYR:CD1  | 2.86                     | 0.52              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:Q:112:ARG:NH2  | 1:Q:262:SER:OG    | 2.42                     | 0.52              |
| 3:I:630:LEU:O    | 3:I:634:ILE:HD12  | 2.10                     | 0.52              |
| 3:J:595:ARG:HD3  | 3:J:1026:ALA:HB1  | 1.91                     | 0.52              |
| 3:J:892:LEU:O    | 3:J:895:GLN:HG3   | 2.10                     | 0.52              |
| 3:J:1248:GLN:O   | 3:J:1251:SER:OG   | 2.17                     | 0.52              |
| 3:K:406:LEU:HD23 | 3:K:440:LEU:HG    | 1.90                     | 0.52              |
| 3:L:189:LEU:HD23 | 3:L:1064:LEU:HD21 | 1.92                     | 0.52              |
| 3:A:490:TYR:OH   | 3:A:561:GLY:O     | 2.22                     | 0.52              |
| 3:A:536:ASN:ND2  | 3:A:538:ASN:HB2   | 2.25                     | 0.52              |
| 4:k:60:ALA:O     | 4:k:64:LEU:N      | 2.40                     | 0.52              |
| 3:N:874:THR:O    | 3:N:878:MET:N     | 2.40                     | 0.52              |
| 3:N:1156:ARG:NH2 | 3:N:1182:ASP:OD2  | 2.43                     | 0.52              |
| 3:O:802:PRO:HB3  | 3:P:944:HIS:CD2   | 2.44                     | 0.52              |
| 3:P:739:CYS:HB2  | 3:P:785:HIS:ND1   | 2.24                     | 0.52              |
| 3:C:438:ARG:O    | 3:C:454:MET:HG2   | 2.10                     | 0.52              |
| 3:D:264:LEU:O    | 3:D:265:THR:OG1   | 2.27                     | 0.52              |
| 3:D:756:ILE:HG23 | 3:D:910:CYS:HB3   | 1.92                     | 0.52              |
| 5:q:27:ILE:HD11  | 5:q:89:ILE:HD11   | 1.91                     | 0.52              |
| 5:q:431:ALA:HA   | 7:u:3115:HIS:CD2  | 2.44                     | 0.52              |
| 3:E:424:VAL:HG12 | 3:E:425:PRO:O     | 2.09                     | 0.52              |
| 3:E:543:LEU:HB2  | 3:E:549:PHE:HE2   | 1.72                     | 0.52              |
| 3:E:775:ASP:OD2  | 3:E:778:ARG:NH2   | 2.42                     | 0.52              |
| 3:F:603:ARG:NH1  | 3:F:706:ASP:OD2   | 2.38                     | 0.52              |
| 3:F:784:LEU:CD2  | 3:F:903:GLU:H     | 2.22                     | 0.52              |
| 3:G:752:ARG:HH21 | 3:G:915:ASP:HA    | 1.74                     | 0.52              |
| 2:R:276:VAL:HG11 | 2:S:154:ARG:HE    | 1.74                     | 0.52              |
| 2:x:116:LEU:HB2  | 2:x:140:PRO:HB2   | 1.92                     | 0.52              |
| 3:I:95:VAL:HG22  | 3:H:58:LEU:HB2    | 1.92                     | 0.52              |
| 3:I:399:ASP:CG   | 3:I:1321:VAL:HG11 | 2.35                     | 0.52              |
| 3:I:1248:GLN:HB2 | 3:I:1251:SER:OG   | 2.09                     | 0.52              |
| 3:J:77:VAL:HG12  | 3:J:1068:ARG:O    | 2.10                     | 0.52              |
| 3:J:93:GLY:HA3   | 3:J:124:ILE:HD12  | 1.92                     | 0.52              |
| 3:J:266:HIS:CE1  | 3:J:303:PRO:HD2   | 2.44                     | 0.52              |
| 3:J:545:PRO:O    | 3:J:576:ARG:NH1   | 2.42                     | 0.52              |
| 3:K:469:ILE:HD11 | 3:K:547:PHE:CD1   | 2.44                     | 0.52              |
| 3:M:426:ALA:HB3  | 3:M:429:HIS:CD2   | 2.44                     | 0.52              |
| 3:A:1037:TYR:CD1 | 3:A:1037:TYR:C    | 2.88                     | 0.52              |
| 3:H:194:PRO:HA   | 3:H:1110:ALA:O    | 2.10                     | 0.52              |
| 3:H:324:LYS:CA   | 3:D:322:MET:HE1   | 2.39                     | 0.52              |
| 3:H:469:ILE:HD11 | 3:H:547:PHE:CD1   | 2.45                     | 0.52              |
| 3:H:1083:HIS:O   | 3:H:1090:ASN:N    | 2.33                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:H:1334:ILE:HG22 | 3:H:1335:THR:H    | 1.74                     | 0.52              |
| 4:o:57:GLN:OE1    | 3:O:837:ALA:HA    | 2.09                     | 0.52              |
| 3:O:1270:LEU:HD22 | 3:O:1303:ALA:HB2  | 1.91                     | 0.52              |
| 3:B:58:LEU:HD12   | 3:C:124:ILE:HD11  | 1.91                     | 0.52              |
| 3:B:668:TYR:HD2   | 3:B:809:HIS:ND1   | 2.07                     | 0.52              |
| 3:E:86:GLU:HG2    | 3:E:86:GLU:O      | 2.10                     | 0.52              |
| 3:E:129:LEU:HD11  | 3:E:1097:ARG:NH1  | 2.24                     | 0.52              |
| 3:E:1170:GLN:N    | 3:E:1170:GLN:OE1  | 2.43                     | 0.52              |
| 3:F:134:SER:H     | 3:G:114:GLN:HE21  | 1.57                     | 0.52              |
| 3:F:577:VAL:H     | 3:F:581:ASN:ND2   | 2.06                     | 0.52              |
| 3:F:703:LEU:O     | 3:F:706:ASP:N     | 2.43                     | 0.52              |
| 3:F:1191:PRO:HG2  | 3:F:1194:THR:HG23 | 1.92                     | 0.52              |
| 3:G:278:LEU:HG    | 3:G:375:VAL:HG11  | 1.92                     | 0.52              |
| 3:G:550:PHE:HD1   | 3:G:998:TYR:CE2   | 2.25                     | 0.52              |
| 3:G:571:ILE:N     | 3:G:571:ILE:HD12  | 2.23                     | 0.52              |
| 2:S:180:TYR:OH    | 2:S:185:ARG:NH1   | 2.42                     | 0.52              |
| 2:X:26:ARG:O      | 2:X:101:ARG:NH1   | 2.42                     | 0.52              |
| 1:w:257:GLN:OE1   | 3:P:109:PRO:HG2   | 2.09                     | 0.52              |
| 1:w:283:ARG:HB2   | 3:N:47:ASN:ND2    | 2.24                     | 0.52              |
| 3:I:625:ALA:HA    | 3:I:628:TYR:HD2   | 1.74                     | 0.52              |
| 3:I:742:LEU:HD22  | 3:I:756:ILE:HD11  | 1.92                     | 0.52              |
| 3:I:834:ARG:HB3   | 4:h:90:PRO:HD3    | 1.90                     | 0.52              |
| 3:J:422:ASP:OD1   | 3:J:1354:ARG:NH2  | 2.42                     | 0.52              |
| 3:J:578:VAL:HB    | 3:J:1027:GLY:O    | 2.10                     | 0.52              |
| 3:J:1034:VAL:O    | 3:J:1037:TYR:N    | 2.42                     | 0.52              |
| 3:K:1051:THR:HG23 | 3:K:1190:THR:HG21 | 1.91                     | 0.52              |
| 3:L:575:TRP:CZ3   | 3:L:577:VAL:HG22  | 2.45                     | 0.52              |
| 3:L:895:GLN:NE2   | 4:l:65:GLY:HA3    | 2.25                     | 0.52              |
| 3:L:1036:LEU:HD23 | 3:L:1039:GLN:OE1  | 2.10                     | 0.52              |
| 3:M:440:LEU:HD22  | 3:M:1336:CYS:SG   | 2.49                     | 0.52              |
| 3:A:20:THR:OG1    | 3:A:21:GLY:N      | 2.43                     | 0.52              |
| 3:A:740:ASP:OD2   | 3:A:801:ARG:NH1   | 2.43                     | 0.52              |
| 3:A:1264:ASN:ND2  | 3:A:1271:SER:H    | 2.08                     | 0.52              |
| 3:H:398:MET:O     | 3:H:1057:ARG:HA   | 2.10                     | 0.52              |
| 3:H:704:VAL:O     | 3:H:708:THR:HG23  | 2.10                     | 0.52              |
| 3:H:887:ASP:O     | 3:H:891:MET:HG2   | 2.09                     | 0.52              |
| 3:O:595:ARG:HG3   | 3:O:596:GLY:H     | 1.75                     | 0.52              |
| 3:O:770:ASN:H     | 3:O:773:THR:HB    | 1.75                     | 0.52              |
| 3:D:631:GLN:NE2   | 3:D:666:ASN:OD1   | 2.40                     | 0.52              |
| 3:E:148:LEU:HD11  | 3:E:158:GLN:NE2   | 2.24                     | 0.52              |
| 3:G:404:LEU:HD21  | 3:G:1334:ILE:HD12 | 1.91                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:G:491:VAL:HA    | 3:G:992:PRO:HB2   | 1.91                     | 0.52              |
| 3:G:812:TYR:CD1   | 3:G:816:LEU:HD12  | 2.44                     | 0.52              |
| 2:S:2:ILE:HD11    | 3:B:1084:GLU:CA   | 2.40                     | 0.52              |
| 1:T:141:PRO:CB    | 3:I:1165:VAL:HG12 | 2.40                     | 0.52              |
| 2:X:90:LEU:HD21   | 2:Y:315:ILE:HD12  | 1.90                     | 0.52              |
| 3:I:836:TYR:HE1   | 3:I:897:LEU:HD22  | 1.75                     | 0.52              |
| 3:I:1103:GLY:HA3  | 3:I:1107:THR:HG21 | 1.92                     | 0.52              |
| 3:I:1357:HIS:O    | 3:I:1358:PHE:C    | 2.53                     | 0.52              |
| 3:J:175:ALA:HB2   | 3:K:103:LEU:HB2   | 1.91                     | 0.52              |
| 3:J:213:ARG:HH12  | 3:J:1216:GLY:HA3  | 1.73                     | 0.52              |
| 3:J:784:LEU:HD22  | 3:J:786:ASN:ND2   | 2.25                     | 0.52              |
| 3:J:838:THR:O     | 3:J:875:VAL:HG22  | 2.10                     | 0.52              |
| 3:K:488:GLY:HA2   | 3:K:996:ALA:HB1   | 1.92                     | 0.52              |
| 3:L:32:HIS:NE2    | 3:O:1105:GLY:HA2  | 2.24                     | 0.52              |
| 3:L:646:ARG:NH1   | 4:l:100:PRO:HD2   | 2.25                     | 0.52              |
| 3:A:788:GLN:NE2   | 3:A:793:ASP:O     | 2.42                     | 0.52              |
| 3:H:123:VAL:HG23  | 3:C:37:ASP:CG     | 2.11                     | 0.52              |
| 3:H:611:ILE:O     | 3:H:614:VAL:N     | 2.43                     | 0.52              |
| 4:m:23:ARG:HH12   | 4:m:27:LEU:HD21   | 1.75                     | 0.52              |
| 4:o:59:ALA:O      | 4:o:62:THR:OG1    | 2.26                     | 0.52              |
| 3:O:874:THR:O     | 3:O:878:MET:N     | 2.43                     | 0.52              |
| 3:B:354:LEU:HD12  | 3:G:58:LEU:CD1    | 2.40                     | 0.52              |
| 3:B:643:ALA:HB2   | 4:b:78:MET:HE1    | 1.90                     | 0.52              |
| 3:B:1334:ILE:HG22 | 3:B:1335:THR:N    | 2.25                     | 0.52              |
| 3:C:739:CYS:O     | 3:C:743:MET:HG2   | 2.10                     | 0.52              |
| 3:C:1174:ARG:HH12 | 3:D:1232:SER:HG   | 1.52                     | 0.52              |
| 3:C:1292:LEU:HB3  | 3:C:1327:LEU:HD21 | 1.92                     | 0.52              |
| 3:D:469:ILE:HD11  | 3:D:547:PHE:CZ    | 2.44                     | 0.52              |
| 5:q:139:TRP:CZ2   | 5:q:604:ARG:HD2   | 2.45                     | 0.52              |
| 3:E:842:MET:HE1   | 3:E:891:MET:HE3   | 1.91                     | 0.52              |
| 6:r:84:ILE:HG23   | 6:r:87:ILE:HB     | 1.91                     | 0.52              |
| 3:G:32:HIS:HB2    | 3:G:51:ASP:C      | 2.32                     | 0.52              |
| 4:e:83:ALA:O      | 4:e:86:GLU:HG3    | 2.10                     | 0.52              |
| 2:S:61:LEU:HD12   | 2:S:155:LEU:HB3   | 1.92                     | 0.52              |
| 2:V:204:SER:O     | 2:V:208:ASN:ND2   | 2.42                     | 0.52              |
| 1:W:195:ALA:HA    | 1:W:198:TYR:HD2   | 1.69                     | 0.52              |
| 1:W:436:LEU:HB2   | 1:W:451:ILE:HB    | 1.91                     | 0.52              |
| 2:Y:120:VAL:HG12  | 2:Y:188:LEU:HB2   | 1.92                     | 0.52              |
| 3:I:793:ASP:OD2   | 3:I:800:HIS:ND1   | 2.34                     | 0.52              |
| 3:I:1257:TYR:HB2  | 3:I:1277:PHE:CD2  | 2.33                     | 0.52              |
| 3:K:441:PHE:CE2   | 3:K:1340:PRO:HD3  | 2.43                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:K:1103:GLY:HA3  | 3:K:1107:THR:HG21 | 1.92                     | 0.52              |
| 3:K:1115:VAL:HG12 | 3:K:1116:ARG:O    | 2.10                     | 0.52              |
| 3:K:1161:GLN:HB3  | 3:K:1170:GLN:HE22 | 1.73                     | 0.52              |
| 3:L:445:LYS:NZ    | 3:L:1179:HIS:O    | 2.41                     | 0.52              |
| 3:L:721:GLU:HG2   | 3:L:727:ARG:HB3   | 1.90                     | 0.52              |
| 3:L:1128:ASN:HD21 | 3:L:1155:ASN:ND2  | 2.08                     | 0.52              |
| 3:M:9:PRO:HG2     | 3:D:94:ARG:HH21   | 1.71                     | 0.52              |
| 3:M:263:ARG:NH2   | 3:M:305:THR:O     | 2.43                     | 0.52              |
| 3:M:948:THR:HG21  | 4:l:95:LYS:HE3    | 1.91                     | 0.52              |
| 3:A:452:LEU:HD21  | 3:A:1052:VAL:HG21 | 1.92                     | 0.52              |
| 3:H:717:GLN:HE22  | 3:H:752:ARG:CZ    | 2.23                     | 0.52              |
| 3:H:1115:VAL:HG11 | 3:H:1374:LEU:HD11 | 1.91                     | 0.52              |
| 3:H:1215:ALA:HB3  | 3:H:1287:ARG:HE   | 1.75                     | 0.52              |
| 3:N:214:VAL:O     | 3:N:217:ALA:N     | 2.42                     | 0.52              |
| 3:N:342:GLU:HB3   | 3:N:343:GLN:HG3   | 1.92                     | 0.52              |
| 3:N:863:HIS:CE1   | 3:N:887:ASP:HA    | 2.42                     | 0.52              |
| 3:P:778:ARG:NH1   | 3:P:782:ARG:HD2   | 2.25                     | 0.52              |
| 3:B:1208:ARG:NH1  | 3:B:1240:ALA:O    | 2.43                     | 0.52              |
| 3:C:350:THR:HG22  | 3:C:352:ASP:H     | 1.74                     | 0.52              |
| 3:D:405:PRO:HB3   | 3:D:1199:PHE:CD2  | 2.45                     | 0.52              |
| 5:q:518:GLU:O     | 6:r:33:ARG:NH1    | 2.43                     | 0.52              |
| 3:E:435:PHE:HB3   | 3:E:436:PRO:HD2   | 1.91                     | 0.52              |
| 3:G:469:ILE:CG2   | 3:G:473:VAL:HG23  | 2.40                     | 0.52              |
| 4:b:83:ALA:O      | 4:b:86:GLU:HG3    | 2.10                     | 0.52              |
| 4:c:83:ALA:O      | 4:c:86:GLU:HG3    | 2.10                     | 0.52              |
| 2:3:26:ARG:O      | 2:3:101:ARG:NH1   | 2.42                     | 0.52              |
| 3:I:765:TYR:CE1   | 3:I:783:LEU:HD12  | 2.45                     | 0.52              |
| 3:L:373:ARG:NH1   | 3:L:1067:GLU:OE2  | 2.39                     | 0.52              |
| 3:L:464:PRO:HB3   | 3:L:1138:LEU:HD23 | 1.92                     | 0.52              |
| 3:L:1369:LEU:HD22 | 3:L:1372:LEU:HD12 | 1.91                     | 0.52              |
| 3:M:1186:GLU:CD   | 3:M:1272:PRO:HD2  | 2.35                     | 0.52              |
| 3:A:884:VAL:HG12  | 3:A:886:VAL:HG23  | 1.92                     | 0.52              |
| 3:H:739:CYS:HA    | 3:H:742:LEU:HD12  | 1.92                     | 0.52              |
| 3:H:877:ALA:HB1   | 4:m:94:LEU:HD21   | 1.92                     | 0.52              |
| 3:O:86:GLU:OE1    | 3:O:86:GLU:N      | 2.43                     | 0.52              |
| 3:O:769:CYS:HB2   | 3:O:786:ASN:HD21  | 1.73                     | 0.52              |
| 3:B:502:GLN:O     | 3:B:505:PHE:HB3   | 2.09                     | 0.52              |
| 3:B:1339:ASP:OD2  | 3:B:1360:GLN:HG3  | 2.10                     | 0.52              |
| 3:C:753:ASP:HB3   | 3:C:755:ARG:HH22  | 1.74                     | 0.52              |
| 3:D:467:MET:SD    | 3:D:918:ALA:HB1   | 2.50                     | 0.52              |
| 3:D:802:PRO:HB3   | 3:E:944:HIS:CD2   | 2.45                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:q:490:LEU:O     | 5:q:494:ILE:N     | 2.29                     | 0.52              |
| 3:F:488:GLY:HA3   | 3:F:520:TRP:CH2   | 2.44                     | 0.52              |
| 3:G:103:LEU:HD21  | 3:G:114:GLN:C     | 2.35                     | 0.52              |
| 3:G:1282:ILE:N    | 3:G:1282:ILE:CD1  | 2.73                     | 0.52              |
| 1:W:150:PRO:HA    | 2:Y:267:ARG:HH21  | 1.74                     | 0.52              |
| 1:1:141:PRO:CD    | 3:M:1166:PHE:HB3  | 2.40                     | 0.52              |
| 3:I:432:PRO:HA    | 3:I:435:PHE:CE2   | 2.45                     | 0.52              |
| 3:I:463:HIS:ND1   | 3:I:464:PRO:HD2   | 2.24                     | 0.52              |
| 3:J:682:LEU:HB2   | 3:J:687:MET:HG2   | 1.90                     | 0.52              |
| 3:K:77:VAL:HG22   | 3:K:266:HIS:CG    | 2.45                     | 0.52              |
| 3:L:752:ARG:HA    | 3:L:913:ALA:HB3   | 1.92                     | 0.52              |
| 3:M:161:ALA:CB    | 3:C:50:TYR:CE1    | 2.93                     | 0.52              |
| 3:M:778:ARG:HH11  | 3:M:782:ARG:HD2   | 1.74                     | 0.52              |
| 3:M:1334:ILE:HG22 | 3:M:1335:THR:N    | 2.24                     | 0.52              |
| 3:A:721:GLU:HA    | 3:A:727:ARG:HB2   | 1.91                     | 0.52              |
| 3:H:43:ARG:C      | 3:H:45:ASP:H      | 2.18                     | 0.52              |
| 3:H:867:PRO:HA    | 3:H:870:LEU:HB2   | 1.91                     | 0.52              |
| 4:i:59:ALA:O      | 4:i:62:THR:OG1    | 2.16                     | 0.52              |
| 3:O:914:PRO:HG3   | 3:O:923:THR:HG22  | 1.91                     | 0.52              |
| 3:B:950:GLN:HB2   | 3:B:953:GLU:HG3   | 1.92                     | 0.52              |
| 3:C:753:ASP:O     | 3:C:911:SER:OG    | 2.24                     | 0.52              |
| 3:C:1155:ASN:OD1  | 3:C:1156:ARG:N    | 2.43                     | 0.52              |
| 3:D:178:ARG:HB3   | 3:E:104:ILE:HG22  | 1.92                     | 0.52              |
| 3:D:1208:ARG:NH1  | 3:D:1240:ALA:O    | 2.43                     | 0.52              |
| 3:E:400:LEU:HD12  | 3:E:1058:PHE:HE2  | 1.76                     | 0.52              |
| 3:E:1328:PHE:O    | 3:E:1330:GLU:HG3  | 2.10                     | 0.52              |
| 3:F:421:GLY:HA3   | 3:G:420:ALA:HB2   | 1.91                     | 0.52              |
| 3:F:1176:GLY:CA   | 3:G:1225:LEU:HD21 | 2.40                     | 0.52              |
| 2:U:25:GLN:NE2    | 2:U:28:GLU:OE2    | 2.43                     | 0.51              |
| 2:Y:52:VAL:HG23   | 2:Y:57:SER:HA     | 1.91                     | 0.51              |
| 2:Y:254:ILE:HG22  | 2:Y:256:PRO:HD3   | 1.91                     | 0.51              |
| 2:y:298:CYS:HB2   | 2:y:315:ILE:HD13  | 1.91                     | 0.51              |
| 3:M:310:VAL:HG12  | 3:M:312:ASN:H     | 1.74                     | 0.51              |
| 3:M:841:ASN:O     | 3:M:875:VAL:HG23  | 2.10                     | 0.51              |
| 3:H:227:PHE:CE2   | 3:H:1324:PRO:HB3  | 2.44                     | 0.51              |
| 3:H:895:GLN:NE2   | 4:h:62:THR:HA     | 2.25                     | 0.51              |
| 3:N:433:ARG:NH1   | 3:N:1339:ASP:OD2  | 2.40                     | 0.51              |
| 3:N:643:ALA:HB1   | 3:N:896:VAL:HG21  | 1.91                     | 0.51              |
| 3:O:576:ARG:HH11  | 3:O:582:LEU:HD23  | 1.75                     | 0.51              |
| 3:P:410:ASN:HB3   | 3:P:414:GLU:OE1   | 2.09                     | 0.51              |
| 3:D:842:MET:HE1   | 3:D:891:MET:HB3   | 1.91                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:1334:ILE:HG22 | 3:D:1335:THR:H    | 1.75                     | 0.51              |
| 5:q:169:ARG:O     | 5:q:173:HIS:N     | 2.33                     | 0.51              |
| 3:E:641:PHE:O     | 3:E:644:LEU:N     | 2.43                     | 0.51              |
| 3:F:1257:TYR:HB2  | 3:F:1277:PHE:CD2  | 2.37                     | 0.51              |
| 3:G:233:PHE:HE2   | 3:G:244:ILE:CG1   | 1.98                     | 0.51              |
| 3:G:1165:VAL:CG1  | 3:G:1166:PHE:CD2  | 2.86                     | 0.51              |
| 1:1:255:VAL:HB    | 1:1:262:SER:HB3   | 1.92                     | 0.51              |
| 3:I:98:GLU:HB2    | 3:H:62:CYS:HA     | 1.91                     | 0.51              |
| 3:J:878:MET:HE2   | 4:i:92:PHE:CE1    | 2.46                     | 0.51              |
| 3:K:263:ARG:NH2   | 3:K:306:TYR:O     | 2.43                     | 0.51              |
| 3:K:1177:MET:HE1  | 3:L:214:VAL:HG22  | 1.92                     | 0.51              |
| 3:L:543:LEU:HB2   | 3:L:549:PHE:HE2   | 1.75                     | 0.51              |
| 3:M:1223:ILE:HG23 | 3:M:1227:TYR:HD2  | 1.75                     | 0.51              |
| 3:A:752:ARG:NH2   | 3:A:915:ASP:HA    | 2.24                     | 0.51              |
| 3:N:1337:ALA:HB3  | 3:N:1343:LEU:HB2  | 1.92                     | 0.51              |
| 3:P:165:LEU:O     | 3:P:168:ASN:N     | 2.43                     | 0.51              |
| 3:P:1031:MET:HE3  | 3:P:1048:PHE:HZ   | 1.75                     | 0.51              |
| 3:B:213:ARG:NH2   | 3:G:1176:GLY:HA2  | 2.25                     | 0.51              |
| 3:C:845:PRO:HG3   | 3:C:869:ASN:ND2   | 2.25                     | 0.51              |
| 3:D:724:HIS:CE1   | 3:D:1028:TYR:HB2  | 2.45                     | 0.51              |
| 5:q:30:SER:HB2    | 5:q:40:LEU:HD21   | 1.91                     | 0.51              |
| 5:q:67:THR:HG22   | 5:q:466:VAL:H     | 1.76                     | 0.51              |
| 3:E:717:GLN:HE22  | 3:E:752:ARG:NH1   | 2.07                     | 0.51              |
| 3:E:1171:VAL:HG11 | 3:E:1309:VAL:HG21 | 1.92                     | 0.51              |
| 3:G:23:ILE:CG2    | 3:G:167:ARG:CZ    | 2.87                     | 0.51              |
| 3:G:24:LEU:HD22   | 3:G:62:CYS:O      | 2.10                     | 0.51              |
| 3:G:454:MET:O     | 3:G:456:ASN:N     | 2.43                     | 0.51              |
| 3:G:738:ASP:OD1   | 3:G:787:THR:OG1   | 2.23                     | 0.51              |
| 3:G:1072:ALA:HB3  | 3:G:1100:VAL:HB   | 1.91                     | 0.51              |
| 4:g:83:ALA:O      | 4:g:86:GLU:HG3    | 2.10                     | 0.51              |
| 1:1:258:ASP:CB    | 3:M:1318:ARG:HD2  | 2.39                     | 0.51              |
| 1:1:310:LEU:HD21  | 1:1:428:MET:HE3   | 1.93                     | 0.51              |
| 2:x:272:TYR:OH    | 2:y:164:ASN:ND2   | 2.43                     | 0.51              |
| 3:J:1138:LEU:HD11 | 3:J:1144:ALA:N    | 2.24                     | 0.51              |
| 3:J:1355:GLU:OE1  | 3:J:1355:GLU:N    | 2.37                     | 0.51              |
| 3:K:266:HIS:HE1   | 3:K:302:VAL:HG13  | 1.75                     | 0.51              |
| 3:L:543:LEU:HB2   | 3:L:549:PHE:CE2   | 2.46                     | 0.51              |
| 3:M:7:ASP:O       | 3:M:9:PRO:HD3     | 2.10                     | 0.51              |
| 3:M:189:LEU:HD23  | 3:M:1064:LEU:HD21 | 1.92                     | 0.51              |
| 3:M:861:PRO:HA    | 3:M:866:HIS:CD2   | 2.46                     | 0.51              |
| 3:H:876:ASN:HA    | 3:H:879:PHE:HD2   | 1.74                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:N:85:PRO:HG2    | 3:N:86:GLU:OE1    | 2.10                     | 0.51              |
| 3:B:463:HIS:CD2   | 3:B:465:SER:HB3   | 2.45                     | 0.51              |
| 3:C:42:VAL:HG12   | 3:C:43:ARG:O      | 2.11                     | 0.51              |
| 3:C:274:VAL:HG11  | 3:C:376:PHE:CD2   | 2.45                     | 0.51              |
| 3:C:463:HIS:ND1   | 3:C:464:PRO:HD2   | 2.25                     | 0.51              |
| 3:C:950:GLN:HB2   | 3:C:953:GLU:CG    | 2.38                     | 0.51              |
| 3:D:1052:VAL:HA   | 3:D:1186:GLU:O    | 2.11                     | 0.51              |
| 3:E:700:LEU:HD22  | 3:E:1025:MET:HG3  | 1.92                     | 0.51              |
| 3:E:1304:THR:HG21 | 3:E:1314:PRO:HD2  | 1.91                     | 0.51              |
| 3:F:367:LEU:HD21  | 3:F:376:PHE:HE1   | 1.74                     | 0.51              |
| 3:F:844:VAL:HG11  | 3:F:892:LEU:HD21  | 1.93                     | 0.51              |
| 3:G:497:PRO:N     | 3:G:504:ARG:NH2   | 2.54                     | 0.51              |
| 3:G:961:HIS:O     | 3:G:964:PHE:N     | 2.43                     | 0.51              |
| 1:T:281:ARG:HA    | 3:H:51:ASP:OD2    | 2.10                     | 0.51              |
| 2:X:25:GLN:NE2    | 2:X:28:GLU:OE2    | 2.43                     | 0.51              |
| 2:X:78:VAL:HG13   | 2:X:83:ILE:HG12   | 1.92                     | 0.51              |
| 3:I:57:LEU:HD23   | 3:J:94:ARG:HB2    | 1.92                     | 0.51              |
| 3:I:1073:TYR:OH   | 3:I:1097:ARG:NH1  | 2.43                     | 0.51              |
| 3:J:579:ASN:HA    | 3:J:1031:MET:HE3  | 1.91                     | 0.51              |
| 3:K:411:PRO:O     | 3:K:415:ARG:NH1   | 2.44                     | 0.51              |
| 3:M:398:MET:O     | 3:M:1057:ARG:HA   | 2.11                     | 0.51              |
| 3:A:279:VAL:HA    | 3:A:378:GLU:O     | 2.11                     | 0.51              |
| 3:A:963:LEU:HD23  | 3:A:1007:VAL:HG22 | 1.93                     | 0.51              |
| 4:h:62:THR:O      | 4:h:66:VAL:HG23   | 2.10                     | 0.51              |
| 3:N:274:VAL:HG11  | 3:N:376:PHE:CD2   | 2.45                     | 0.51              |
| 3:N:280:THR:HG22  | 3:N:1063:VAL:HG22 | 1.92                     | 0.51              |
| 3:N:746:ALA:HA    | 3:N:754:CYS:HB3   | 1.91                     | 0.51              |
| 3:P:232:PHE:O     | 3:P:236:LYS:HD3   | 2.10                     | 0.51              |
| 3:P:1072:ALA:HB2  | 3:P:1102:LEU:HD23 | 1.93                     | 0.51              |
| 3:B:762:GLU:HB3   | 3:B:763:PRO:HD2   | 1.91                     | 0.51              |
| 3:D:873:ASN:CG    | 4:c:92:PHE:HB2    | 2.30                     | 0.51              |
| 3:E:392:TYR:HE2   | 3:E:394:LEU:HB3   | 1.75                     | 0.51              |
| 3:F:842:MET:CE    | 3:F:891:MET:HE3   | 2.40                     | 0.51              |
| 3:G:830:VAL:C     | 3:G:956:TYR:HE1   | 2.19                     | 0.51              |
| 4:d:83:ALA:O      | 4:d:86:GLU:HG3    | 2.10                     | 0.51              |
| 3:I:842:MET:HE1   | 3:I:891:MET:HE3   | 1.90                     | 0.51              |
| 3:I:1201:ARG:HB2  | 3:I:1202:PRO:HD2  | 1.91                     | 0.51              |
| 3:J:840:GLN:HE22  | 4:j:58:ALA:HB2    | 1.76                     | 0.51              |
| 3:J:1339:ASP:O    | 3:J:1343:LEU:N    | 2.44                     | 0.51              |
| 3:K:524:CYS:HB2   | 3:K:525:GLN:OE1   | 2.11                     | 0.51              |
| 3:M:20:THR:C      | 3:D:350:THR:CG2   | 2.84                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:M:44:SER:CB     | 3:D:115:PRO:HG2   | 2.40                     | 0.51              |
| 3:M:764:VAL:O     | 3:M:782:ARG:HA    | 2.10                     | 0.51              |
| 3:A:452:LEU:HD12  | 3:A:456:ASN:ND2   | 2.24                     | 0.51              |
| 3:N:279:VAL:HG12  | 3:N:394:LEU:HD22  | 1.92                     | 0.51              |
| 3:B:349:GLU:O     | 3:B:353:GLU:N     | 2.42                     | 0.51              |
| 3:B:683:PRO:HD2   | 3:B:686:CYS:HB3   | 1.92                     | 0.51              |
| 3:D:247:TRP:O     | 3:D:250:ASP:N     | 2.38                     | 0.51              |
| 3:E:753:ASP:HB2   | 3:E:755:ARG:HH12  | 1.76                     | 0.51              |
| 3:E:867:PRO:HA    | 3:E:870:LEU:HD12  | 1.92                     | 0.51              |
| 3:E:1034:VAL:HG22 | 3:E:1147:LEU:HD21 | 1.91                     | 0.51              |
| 3:F:132:ALA:CB    | 3:G:112:VAL:HG11  | 2.38                     | 0.51              |
| 3:F:776:PHE:HD2   | 3:F:833:ASP:OD1   | 1.94                     | 0.51              |
| 3:G:262:PRO:HG3   | 3:G:353:GLU:HG2   | 1.93                     | 0.51              |
| 4:f:64:LEU:O      | 4:f:67:THR:OG1    | 2.25                     | 0.51              |
| 1:T:149:PRO:HD3   | 1:T:238:HIS:HB2   | 1.92                     | 0.51              |
| 1:T:158:ALA:C     | 3:I:1165:VAL:HG22 | 2.36                     | 0.51              |
| 1:W:194:CYS:C     | 1:W:198:TYR:CE2   | 2.62                     | 0.51              |
| 1:W:328:TYR:CE2   | 6:r:18:PHE:CE2    | 2.97                     | 0.51              |
| 1:W:348:GLY:CA    | 6:r:13:TRP:HB2    | 2.41                     | 0.51              |
| 1:l:257:GLN:OE1   | 3:H:109:PRO:CG    | 2.57                     | 0.51              |
| 2:3:249:GLU:O     | 2:3:253:LEU:N     | 2.42                     | 0.51              |
| 1:w:125:GLU:OE2   | 1:w:215:TYR:OH    | 2.28                     | 0.51              |
| 3:I:252:THR:HB    | 3:I:373:ARG:HD2   | 1.92                     | 0.51              |
| 3:K:425:PRO:HG3   | 3:K:431:GLU:HG2   | 1.92                     | 0.51              |
| 3:K:639:HIS:HA    | 4:k:79:PHE:CE2    | 2.45                     | 0.51              |
| 3:M:1301:SER:OG   | 3:M:1319:GLU:HB2  | 2.11                     | 0.51              |
| 3:A:406:LEU:HD12  | 3:A:1050:PHE:HB2  | 1.93                     | 0.51              |
| 3:A:1004:GLN:N    | 3:A:1005:PRO:HD2  | 2.26                     | 0.51              |
| 3:H:400:LEU:HD12  | 3:H:1058:PHE:CE2  | 2.45                     | 0.51              |
| 3:H:438:ARG:HG3   | 3:H:439:GLN:HG3   | 1.92                     | 0.51              |
| 3:H:634:ILE:HA    | 3:H:640:VAL:HG11  | 1.91                     | 0.51              |
| 4:o:65:GLY:HA3    | 3:O:895:GLN:HE22  | 1.75                     | 0.51              |
| 4:p:68:HIS:CE1    | 3:P:847:ILE:HD12  | 2.46                     | 0.51              |
| 3:O:266:HIS:CE1   | 3:O:302:VAL:HG13  | 2.45                     | 0.51              |
| 3:O:318:THR:O     | 3:O:323:GLY:N     | 2.41                     | 0.51              |
| 3:P:509:TRP:CZ2   | 3:P:564:PRO:HD3   | 2.46                     | 0.51              |
| 3:B:745:HIS:NE2   | 3:B:910:CYS:HB2   | 2.25                     | 0.51              |
| 3:C:1344:ARG:NH2  | 3:D:414:GLU:OE2   | 2.37                     | 0.51              |
| 3:E:180:THR:HG22  | 3:E:1097:ARG:HH12 | 1.76                     | 0.51              |
| 3:E:390:VAL:HG11  | 3:F:104:ILE:HD11  | 1.92                     | 0.51              |
| 3:E:502:GLN:O     | 3:E:505:PHE:N     | 2.44                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:E:512:ARG:HD3   | 3:E:515:HIS:HD2   | 1.76                     | 0.51              |
| 3:E:705:ASP:OD2   | 3:F:985:ARG:HD3   | 2.11                     | 0.51              |
| 3:F:873:ASN:C     | 4:e:92:PHE:HD2    | 2.19                     | 0.51              |
| 3:G:829:GLY:CA    | 3:G:956:TYR:CZ    | 2.94                     | 0.51              |
| 2:S:129:ARG:NH2   | 2:S:134:ASP:OD1   | 2.44                     | 0.51              |
| 2:y:93:THR:HB     | 2:y:96:GLY:H      | 1.75                     | 0.51              |
| 3:I:711:GLY:HA3   | 3:I:719:GLN:HE21  | 1.75                     | 0.51              |
| 3:J:398:MET:O     | 3:J:1057:ARG:HA   | 2.11                     | 0.51              |
| 3:J:948:THR:OG1   | 4:i:93:GLY:O      | 2.28                     | 0.51              |
| 3:K:878:MET:O     | 3:K:882:GLY:N     | 2.43                     | 0.51              |
| 3:K:1181:GLN:HB2  | 3:K:1309:VAL:O    | 2.11                     | 0.51              |
| 3:L:63:ASN:OD1    | 3:N:23:ILE:HB     | 2.10                     | 0.51              |
| 3:L:756:ILE:HB    | 3:L:763:PRO:HD3   | 1.93                     | 0.51              |
| 3:L:1186:GLU:CD   | 3:L:1272:PRO:HD2  | 2.35                     | 0.51              |
| 3:L:1334:ILE:HG22 | 3:L:1335:THR:N    | 2.26                     | 0.51              |
| 3:M:488:GLY:HA2   | 3:M:996:ALA:HB1   | 1.91                     | 0.51              |
| 3:A:440:LEU:HD22  | 3:A:1336:CYS:SG   | 2.50                     | 0.51              |
| 3:H:120:MET:CB    | 3:C:36:PHE:CG     | 2.94                     | 0.51              |
| 3:H:241:ARG:HE    | 3:H:245:GLU:CD    | 2.18                     | 0.51              |
| 3:H:339:MET:HE2   | 3:C:17:MET:HE2    | 0.51                     | 0.51              |
| 3:N:163:GLN:HG2   | 3:O:344:LEU:HD21  | 1.93                     | 0.51              |
| 3:N:784:LEU:HD23  | 3:N:903:GLU:HB2   | 1.93                     | 0.51              |
| 3:O:752:ARG:HA    | 3:O:913:ALA:HB3   | 1.91                     | 0.51              |
| 3:P:282:ALA:N     | 3:P:381:GLU:OE2   | 2.42                     | 0.51              |
| 3:B:1304:THR:HG21 | 3:B:1314:PRO:HD2  | 1.93                     | 0.51              |
| 3:C:873:ASN:CA    | 4:b:92:PHE:CD2    | 2.91                     | 0.51              |
| 3:C:1073:TYR:OH   | 3:C:1097:ARG:NH1  | 2.42                     | 0.51              |
| 3:D:1357:HIS:O    | 3:D:1358:PHE:C    | 2.54                     | 0.51              |
| 3:E:1202:PRO:HB3  | 3:E:1332:TYR:HD1  | 1.75                     | 0.51              |
| 3:G:620:ASP:HB2   | 3:G:623:TYR:HB2   | 1.92                     | 0.51              |
| 3:G:1161:GLN:CG   | 3:G:1162:PRO:CD   | 2.88                     | 0.51              |
| 1:W:344:GLU:CD    | 6:r:13:TRP:CZ3    | 2.89                     | 0.51              |
| 1:1:78:ALA:HB1    | 3:M:308:GLU:OE1   | 2.11                     | 0.51              |
| 2:3:300:PHE:CE2   | 3:M:1083:HIS:CB   | 2.94                     | 0.51              |
| 2:x:69:ARG:NH1    | 2:y:112:ASP:OD1   | 2.43                     | 0.51              |
| 2:y:120:VAL:HG12  | 2:y:188:LEU:HB2   | 1.90                     | 0.51              |
| 3:I:623:TYR:H     | 3:I:943:GLN:NE2   | 2.07                     | 0.51              |
| 3:I:1176:GLY:HA3  | 3:J:1225:LEU:HD21 | 1.92                     | 0.51              |
| 3:J:278:LEU:HG    | 3:J:375:VAL:HG11  | 1.93                     | 0.51              |
| 3:J:724:HIS:CE1   | 3:J:1028:TYR:HB2  | 2.45                     | 0.51              |
| 3:K:158:GLN:O     | 3:K:161:ALA:N     | 2.43                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:K:872:ALA:HA    | 4:j:94:LEU:HD11   | 1.92                     | 0.51              |
| 3:L:85:PRO:HG3    | 3:L:310:VAL:HG22  | 1.93                     | 0.51              |
| 3:L:405:PRO:HB3   | 3:L:1199:PHE:CE2  | 2.45                     | 0.51              |
| 3:L:642:CYS:SG    | 4:l:95:LYS:HG2    | 2.51                     | 0.51              |
| 3:L:687:MET:O     | 3:L:690:TYR:N     | 2.43                     | 0.51              |
| 3:H:148:LEU:HD11  | 3:H:158:GLN:NE2   | 2.24                     | 0.51              |
| 4:i:64:LEU:O      | 4:i:67:THR:OG1    | 2.26                     | 0.51              |
| 3:O:130:ASN:OD1   | 3:O:1094:THR:HG22 | 2.10                     | 0.51              |
| 3:P:788:GLN:HG2   | 3:P:800:HIS:ND1   | 2.26                     | 0.51              |
| 3:B:1115:VAL:HG12 | 3:B:1116:ARG:O    | 2.11                     | 0.51              |
| 3:C:280:THR:HG22  | 3:C:1063:VAL:HG13 | 1.93                     | 0.51              |
| 3:D:687:MET:O     | 3:D:690:TYR:N     | 2.44                     | 0.51              |
| 3:E:148:LEU:HD21  | 3:E:158:GLN:HG3   | 1.93                     | 0.51              |
| 3:E:426:ALA:HB3   | 3:E:429:HIS:CD2   | 2.46                     | 0.51              |
| 3:E:829:GLY:HA3   | 3:E:956:TYR:CZ    | 2.45                     | 0.51              |
| 3:E:1357:HIS:O    | 3:E:1360:GLN:N    | 2.44                     | 0.51              |
| 3:F:132:ALA:CB    | 3:G:112:VAL:CG1   | 2.89                     | 0.51              |
| 3:G:481:VAL:HG11  | 3:G:571:ILE:CD1   | 2.40                     | 0.51              |
| 2:Y:306:VAL:HG11  | 2:Y:312:ALA:HB2   | 1.93                     | 0.51              |
| 2:3:38:ARG:NH1    | 3:E:109:PRO:HA    | 2.26                     | 0.51              |
| 3:J:749:ASP:OD1   | 3:J:752:ARG:HB3   | 2.10                     | 0.51              |
| 3:K:652:ILE:O     | 3:K:655:TYR:N     | 2.44                     | 0.51              |
| 3:K:1237:PRO:CD   | 3:K:1238:PHE:N    | 2.74                     | 0.51              |
| 3:L:234:LEU:HD12  | 3:L:1113:ALA:HB1  | 1.91                     | 0.51              |
| 3:M:205:LEU:HD22  | 3:N:31:SER:HB2    | 1.93                     | 0.51              |
| 3:M:840:GLN:HB3   | 4:m:57:GLN:HB3    | 1.93                     | 0.51              |
| 3:M:875:VAL:HG12  | 3:M:879:PHE:CE2   | 2.45                     | 0.51              |
| 3:M:1170:GLN:N    | 3:M:1170:GLN:OE1  | 2.44                     | 0.51              |
| 3:A:216:ARG:HH22  | 3:A:1290:GLU:HA   | 1.75                     | 0.51              |
| 3:A:1342:LEU:O    | 3:A:1345:SER:OG   | 2.29                     | 0.51              |
| 3:H:263:ARG:NH2   | 3:H:306:TYR:O     | 2.43                     | 0.51              |
| 3:H:865:LEU:HD22  | 3:H:879:PHE:HB2   | 1.93                     | 0.51              |
| 3:O:865:LEU:HD22  | 3:O:879:PHE:HB2   | 1.93                     | 0.51              |
| 3:P:778:ARG:O     | 3:P:904:ARG:NE    | 2.43                     | 0.51              |
| 3:B:406:LEU:HD23  | 3:B:440:LEU:HG    | 1.93                     | 0.51              |
| 3:B:577:VAL:HG12  | 3:B:578:VAL:HG13  | 1.92                     | 0.51              |
| 3:C:875:VAL:O     | 3:C:878:MET:HB3   | 2.11                     | 0.51              |
| 3:D:800:HIS:O     | 3:D:801:ARG:HG3   | 2.11                     | 0.51              |
| 3:E:63:ASN:ND2    | 3:F:99:VAL:HG13   | 2.25                     | 0.51              |
| 3:F:399:ASP:CG    | 3:F:1321:VAL:HG11 | 2.35                     | 0.51              |
| 3:F:448:GLN:CG    | 3:G:1201:ARG:HH22 | 2.24                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:F:769:CYS:SG    | 3:F:903:GLU:HG2   | 2.51                     | 0.51              |
| 3:F:1124:ASN:OD1  | 3:F:1124:ASN:N    | 2.43                     | 0.51              |
| 3:G:777:ASN:ND2   | 4:g:47:GLN:OE1    | 2.43                     | 0.51              |
| 7:u:3085:LEU:HA   | 7:u:3088:ALA:HB3  | 1.93                     | 0.51              |
| 1:T:260:LEU:CD1   | 3:J:109:PRO:HG2   | 2.40                     | 0.51              |
| 3:I:601:VAL:O     | 3:I:601:VAL:HG12  | 2.11                     | 0.51              |
| 3:J:440:LEU:HD22  | 3:J:1336:CYS:SG   | 2.52                     | 0.51              |
| 3:J:788:GLN:HE22  | 3:J:794:ALA:HA    | 1.76                     | 0.51              |
| 3:J:840:GLN:HB3   | 4:j:57:GLN:HB3    | 1.93                     | 0.51              |
| 3:K:757:ASP:HB3   | 3:K:760:GLY:HA2   | 1.93                     | 0.51              |
| 3:L:847:ILE:HG21  | 4:l:101:PHE:HE1   | 1.75                     | 0.51              |
| 3:L:1020:LEU:O    | 3:L:1023:ALA:N    | 2.44                     | 0.51              |
| 3:M:280:THR:HG22  | 3:M:1063:VAL:HG22 | 1.92                     | 0.51              |
| 3:A:463:HIS:ND1   | 3:A:464:PRO:HD2   | 2.26                     | 0.51              |
| 3:H:840:GLN:HB3   | 4:h:57:GLN:HB3    | 1.92                     | 0.51              |
| 3:H:847:ILE:HD13  | 4:h:71:ASN:ND2    | 2.26                     | 0.51              |
| 3:H:878:MET:O     | 3:H:882:GLY:N     | 2.44                     | 0.51              |
| 3:H:1034:VAL:HG22 | 3:H:1147:LEU:HD21 | 1.93                     | 0.51              |
| 4:j:78:MET:HE2    | 4:j:96:ARG:NH1    | 2.25                     | 0.51              |
| 4:p:95:LYS:HG2    | 3:P:642:CYS:SG    | 2.51                     | 0.51              |
| 3:N:198:LEU:O     | 3:N:201:MET:N     | 2.43                     | 0.51              |
| 3:N:1227:TYR:CD1  | 3:N:1249:ARG:HB2  | 2.46                     | 0.51              |
| 3:O:604:HIS:HD2   | 3:O:696:HIS:CD2   | 2.29                     | 0.51              |
| 3:P:762:GLU:HB3   | 3:P:763:PRO:HD2   | 1.93                     | 0.51              |
| 3:P:970:VAL:HG11  | 3:P:989:LEU:HD12  | 1.93                     | 0.51              |
| 3:B:56:ALA:HA     | 3:C:325:ALA:O     | 2.11                     | 0.51              |
| 3:B:82:THR:HG22   | 3:B:307:GLY:HA3   | 1.93                     | 0.51              |
| 3:C:865:LEU:HD22  | 3:C:879:PHE:HB2   | 1.92                     | 0.51              |
| 3:D:638:GLU:HB3   | 4:d:79:PHE:CE1    | 2.46                     | 0.51              |
| 3:D:888:GLY:O     | 3:D:892:LEU:HG    | 2.11                     | 0.51              |
| 5:q:160:TYR:OH    | 5:q:409:GLY:O     | 2.22                     | 0.51              |
| 3:E:543:LEU:HB2   | 3:E:549:PHE:CE2   | 2.46                     | 0.51              |
| 3:E:646:ARG:NH1   | 4:e:99:SER:HA     | 2.26                     | 0.51              |
| 3:F:725:LEU:HG    | 3:F:731:LEU:HD11  | 1.93                     | 0.51              |
| 3:F:867:PRO:HA    | 3:F:870:LEU:HB2   | 1.93                     | 0.51              |
| 3:F:1186:GLU:CD   | 3:F:1272:PRO:HD2  | 2.37                     | 0.51              |
| 3:G:454:MET:C     | 3:G:456:ASN:N     | 2.69                     | 0.51              |
| 4:f:83:ALA:O      | 4:f:86:GLU:HG3    | 2.10                     | 0.51              |
| 1:T:112:ARG:HG2   | 1:T:264:THR:HG22  | 1.92                     | 0.50              |
| 2:2:204:SER:O     | 2:2:208:ASN:ND2   | 2.43                     | 0.50              |
| 1:w:78:ALA:HB3    | 3:O:308:GLU:OE1   | 2.08                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:I:426:ALA:HA    | 3:J:1358:PHE:CD1  | 2.46                     | 0.50              |
| 3:J:1058:PHE:HE2  | 3:J:1369:LEU:HD11 | 1.76                     | 0.50              |
| 3:K:438:ARG:HB2   | 3:K:454:MET:HG3   | 1.93                     | 0.50              |
| 3:K:944:HIS:CE1   | 3:K:972:ASN:HD22  | 2.29                     | 0.50              |
| 3:M:469:ILE:HD11  | 3:M:547:PHE:CD1   | 2.47                     | 0.50              |
| 3:A:303:PRO:HA    | 3:A:360:THR:HG22  | 1.93                     | 0.50              |
| 3:H:874:THR:H     | 3:H:877:ALA:HB3   | 1.75                     | 0.50              |
| 4:i:98:TYR:HE1    | 4:i:100:PRO:HB3   | 1.76                     | 0.50              |
| 3:N:311:LEU:O     | 3:N:316:LEU:HB2   | 2.11                     | 0.50              |
| 3:B:293:LEU:HD13  | 3:B:368:VAL:HG11  | 1.92                     | 0.50              |
| 3:D:266:HIS:CE1   | 3:D:303:PRO:HD2   | 2.46                     | 0.50              |
| 3:D:652:ILE:O     | 3:D:655:TYR:N     | 2.43                     | 0.50              |
| 3:D:942:PRO:HA    | 3:D:969:HIS:CE1   | 2.46                     | 0.50              |
| 5:q:506:GLN:HE21  | 5:q:619:GLN:NE2   | 2.09                     | 0.50              |
| 3:F:765:TYR:CE1   | 3:F:783:LEU:HD12  | 2.46                     | 0.50              |
| 3:G:571:ILE:N     | 3:G:571:ILE:CD1   | 2.73                     | 0.50              |
| 3:G:753:ASP:OD2   | 3:G:927:ARG:NH2   | 2.43                     | 0.50              |
| 2:S:2:ILE:CD1     | 3:B:1084:GLU:CA   | 2.89                     | 0.50              |
| 2:S:97:THR:HG21   | 2:S:300:PHE:HZ    | 1.76                     | 0.50              |
| 2:V:12:ILE:HD11   | 2:V:83:ILE:HG13   | 1.93                     | 0.50              |
| 3:K:507:ASN:OD1   | 3:K:510:ARG:NH2   | 2.44                     | 0.50              |
| 3:K:745:HIS:CE1   | 3:K:910:CYS:HB2   | 2.46                     | 0.50              |
| 3:L:1131:LEU:HD23 | 3:L:1159:PRO:HG3  | 1.92                     | 0.50              |
| 3:M:601:VAL:O     | 3:M:601:VAL:HG12  | 2.11                     | 0.50              |
| 3:A:756:ILE:HD12  | 3:A:763:PRO:HG3   | 1.93                     | 0.50              |
| 4:p:79:PHE:HE2    | 3:P:639:HIS:HA    | 1.76                     | 0.50              |
| 3:N:96:GLN:HE21   | 3:D:12:ARG:H      | 1.53                     | 0.50              |
| 3:N:1106:TYR:OH   | 3:N:1290:GLU:O    | 2.28                     | 0.50              |
| 3:B:606:MET:H     | 3:B:1018:ASN:ND2  | 2.09                     | 0.50              |
| 3:B:840:GLN:HB3   | 4:b:61:LEU:HD11   | 1.92                     | 0.50              |
| 5:q:381:ARG:HB3   | 5:q:403:GLU:OE1   | 2.11                     | 0.50              |
| 3:E:596:GLY:O     | 3:E:599:LEU:N     | 2.44                     | 0.50              |
| 3:E:1054:ARG:NH2  | 3:E:1122:MET:HB3  | 2.27                     | 0.50              |
| 3:E:1221:ASP:O    | 3:E:1224:ALA:N    | 2.44                     | 0.50              |
| 3:F:463:HIS:HD2   | 3:F:465:SER:HB3   | 1.74                     | 0.50              |
| 3:G:23:ILE:HD13   | 3:G:167:ARG:HD2   | 1.85                     | 0.50              |
| 1:Q:418:THR:HG1   | 1:Q:465:CYS:HG    | 1.60                     | 0.50              |
| 1:I:79:THR:CA     | 3:M:308:GLU:OE2   | 2.60                     | 0.50              |
| 2:x:217:THR:HA    | 2:x:220:ILE:HD12  | 1.93                     | 0.50              |
| 3:I:425:PRO:HD3   | 3:I:431:GLU:HG2   | 1.93                     | 0.50              |
| 3:I:610:THR:HG21  | 3:I:692:ASP:OD2   | 2.11                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:I:740:ASP:CG    | 3:I:799:PRO:HB3   | 2.36                     | 0.50              |
| 3:J:666:ASN:OD1   | 3:J:666:ASN:N     | 2.44                     | 0.50              |
| 3:J:764:VAL:O     | 3:J:782:ARG:HA    | 2.11                     | 0.50              |
| 3:J:788:GLN:NE2   | 3:J:794:ALA:HA    | 2.26                     | 0.50              |
| 3:K:1208:ARG:NH2  | 3:K:1228:ASP:O    | 2.44                     | 0.50              |
| 3:L:20:THR:O      | 3:O:350:THR:HG22  | 2.10                     | 0.50              |
| 3:L:264:LEU:HD11  | 3:L:1069:ALA:HB2  | 1.93                     | 0.50              |
| 3:M:85:PRO:HG2    | 3:M:86:GLU:OE1    | 2.11                     | 0.50              |
| 3:A:469:ILE:HG22  | 3:A:472:ALA:HB3   | 1.93                     | 0.50              |
| 3:A:668:TYR:HB2   | 3:A:812:TYR:CD2   | 2.46                     | 0.50              |
| 3:A:925:ASN:O     | 3:A:927:ARG:NH1   | 2.44                     | 0.50              |
| 3:A:991:PRO:HD2   | 3:A:994:LEU:HD12  | 1.92                     | 0.50              |
| 3:H:296:GLU:OE1   | 3:H:374:LEU:HD21  | 2.11                     | 0.50              |
| 3:H:873:ASN:HD22  | 4:m:89:ARG:HH12   | 1.59                     | 0.50              |
| 3:H:1128:ASN:HD22 | 3:H:1158:GLY:HA2  | 1.76                     | 0.50              |
| 4:n:61:LEU:C      | 3:N:895:GLN:HG2   | 2.36                     | 0.50              |
| 4:p:59:ALA:O      | 4:p:62:THR:OG1    | 2.22                     | 0.50              |
| 3:N:1190:THR:HG22 | 3:N:1243:ASN:ND2  | 2.26                     | 0.50              |
| 3:P:463:HIS:CG    | 3:P:464:PRO:HD2   | 2.46                     | 0.50              |
| 3:P:1217:ASP:OD1  | 3:P:1287:ARG:NH1  | 2.44                     | 0.50              |
| 3:B:776:PHE:HD2   | 3:B:833:ASP:OD1   | 1.93                     | 0.50              |
| 3:C:580:GLY:HA3   | 3:C:1006:VAL:HG22 | 1.93                     | 0.50              |
| 3:C:874:THR:O     | 3:C:878:MET:N     | 2.43                     | 0.50              |
| 5:q:443:PRO:HA    | 5:q:446:GLN:HB2   | 1.93                     | 0.50              |
| 3:E:84:PHE:HE1    | 3:E:309:MET:SD    | 2.33                     | 0.50              |
| 3:E:1296:THR:HG21 | 3:E:1327:LEU:HG   | 1.93                     | 0.50              |
| 3:F:462:CYS:SG    | 3:F:1147:LEU:HD22 | 2.51                     | 0.50              |
| 3:F:884:VAL:HG12  | 3:F:886:VAL:HG23  | 1.93                     | 0.50              |
| 3:G:1257:TYR:HB2  | 3:G:1277:PHE:HD2  | 1.76                     | 0.50              |
| 4:f:66:VAL:O      | 4:f:66:VAL:HG12   | 2.12                     | 0.50              |
| 1:Q:45:ASP:CB     | 3:B:322:MET:O     | 2.58                     | 0.50              |
| 3:I:651:CYS:O     | 3:I:654:SER:OG    | 2.24                     | 0.50              |
| 3:I:915:ASP:O     | 3:I:919:ASN:N     | 2.45                     | 0.50              |
| 3:I:1321:VAL:HG12 | 3:I:1322:GLU:N    | 2.26                     | 0.50              |
| 3:J:86:GLU:OE1    | 3:J:86:GLU:N      | 2.44                     | 0.50              |
| 3:H:631:GLN:HE22  | 3:H:666:ASN:CG    | 2.18                     | 0.50              |
| 4:n:60:ALA:O      | 4:n:64:LEU:N      | 2.44                     | 0.50              |
| 3:O:142:LEU:HD23  | 3:O:147:ALA:HB3   | 1.93                     | 0.50              |
| 3:P:865:LEU:HD22  | 3:P:879:PHE:HB2   | 1.94                     | 0.50              |
| 3:B:1350:GLU:OE1  | 3:G:1347:ARG:NH1  | 2.44                     | 0.50              |
| 3:C:1191:PRO:HG2  | 3:C:1194:THR:HG23 | 1.93                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:264:LEU:HB2   | 3:D:1068:ARG:NH2  | 2.26                     | 0.50              |
| 3:E:398:MET:O     | 3:E:1057:ARG:HA   | 2.11                     | 0.50              |
| 3:E:766:ALA:HB3   | 3:E:784:LEU:HA    | 1.93                     | 0.50              |
| 3:E:802:PRO:HB3   | 3:F:944:HIS:NE2   | 2.27                     | 0.50              |
| 3:E:1156:ARG:NH2  | 3:E:1182:ASP:OD2  | 2.45                     | 0.50              |
| 3:G:1282:ILE:CD1  | 3:G:1282:ILE:H    | 2.23                     | 0.50              |
| 7:t:3095:GLN:HA   | 7:t:3098:ARG:HH21 | 1.76                     | 0.50              |
| 2:U:300:PHE:CB    | 3:I:1083:HIS:NE2  | 2.74                     | 0.50              |
| 2:y:52:VAL:HG23   | 2:y:57:SER:HA     | 1.93                     | 0.50              |
| 3:I:204:TYR:CD2   | 3:I:219:LEU:HD11  | 2.47                     | 0.50              |
| 3:L:405:PRO:O     | 3:L:440:LEU:HD11  | 2.11                     | 0.50              |
| 3:L:1071:GLU:HG3  | 3:L:1100:VAL:O    | 2.11                     | 0.50              |
| 3:A:575:TRP:CZ3   | 3:A:577:VAL:HG22  | 2.46                     | 0.50              |
| 3:A:1034:VAL:HG22 | 3:A:1147:LEU:HD21 | 1.93                     | 0.50              |
| 3:N:558:LEU:HA    | 3:N:559:PRO:C     | 2.36                     | 0.50              |
| 3:N:1232:SER:HB2  | 3:N:1237:PRO:O    | 2.11                     | 0.50              |
| 3:P:103:LEU:HD11  | 3:P:115:PRO:CA    | 2.42                     | 0.50              |
| 3:P:148:LEU:HD11  | 3:P:158:GLN:NE2   | 2.26                     | 0.50              |
| 3:D:696:HIS:CE1   | 3:D:1021:THR:HG21 | 2.47                     | 0.50              |
| 5:q:430:CYS:SG    | 5:q:441:LEU:HB2   | 2.52                     | 0.50              |
| 3:E:925:ASN:O     | 3:E:927:ARG:NH1   | 2.44                     | 0.50              |
| 3:E:1248:GLN:O    | 3:E:1251:SER:OG   | 2.21                     | 0.50              |
| 6:r:3:PRO:HB3     | 6:s:27:ILE:HB     | 1.93                     | 0.50              |
| 3:F:193:PRO:HD2   | 3:F:1108:ALA:O    | 2.11                     | 0.50              |
| 3:F:195:LEU:O     | 3:F:197:LEU:N     | 2.45                     | 0.50              |
| 3:F:950:GLN:HB2   | 3:F:953:GLU:HG3   | 1.94                     | 0.50              |
| 2:U:300:PHE:CD2   | 3:I:1083:HIS:CG   | 2.93                     | 0.50              |
| 2:3:31:VAL:HG11   | 2:3:116:LEU:HD22  | 1.92                     | 0.50              |
| 3:I:263:ARG:NH1   | 3:I:307:GLY:HA2   | 2.27                     | 0.50              |
| 3:I:878:MET:HB2   | 4:h:92:PHE:CE2    | 2.46                     | 0.50              |
| 3:I:1054:ARG:NH1  | 3:I:1123:GLY:O    | 2.45                     | 0.50              |
| 3:J:129:LEU:O     | 3:J:1094:THR:HA   | 2.11                     | 0.50              |
| 3:J:204:TYR:CG    | 3:J:219:LEU:HD11  | 2.46                     | 0.50              |
| 3:J:771:VAL:HG22  | 3:J:901:MET:HE3   | 1.93                     | 0.50              |
| 3:K:595:ARG:HG3   | 3:K:596:GLY:N     | 2.26                     | 0.50              |
| 3:H:576:ARG:NH1   | 3:H:582:LEU:HD23  | 2.26                     | 0.50              |
| 4:k:58:ALA:HA     | 4:k:61:LEU:HD12   | 1.93                     | 0.50              |
| 4:k:78:MET:HB2    | 4:k:79:PHE:CE2    | 2.47                     | 0.50              |
| 3:N:55:ASP:OD1    | 3:O:91:ASN:HB2    | 2.11                     | 0.50              |
| 3:N:433:ARG:HH11  | 3:N:1339:ASP:CG   | 2.18                     | 0.50              |
| 3:O:491:VAL:H     | 3:O:558:LEU:HD22  | 1.77                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:B:1058:PHE:HE2  | 3:B:1369:LEU:HD11 | 1.75                     | 0.50              |
| 3:C:153:ILE:O     | 3:C:156:HIS:N     | 2.45                     | 0.50              |
| 3:C:440:LEU:HD22  | 3:C:1336:CYS:SG   | 2.52                     | 0.50              |
| 3:C:1241:THR:HG1  | 3:C:1247:SER:HG   | 1.55                     | 0.50              |
| 3:D:523:GLU:OE2   | 3:D:538:ASN:ND2   | 2.45                     | 0.50              |
| 3:D:668:TYR:HD2   | 3:D:809:HIS:CE1   | 2.30                     | 0.50              |
| 3:D:780:ASP:HB3   | 3:D:782:ARG:HG3   | 1.94                     | 0.50              |
| 5:q:506:GLN:HB3   | 5:q:667:PHE:CD1   | 2.47                     | 0.50              |
| 3:F:675:VAL:HG12  | 3:G:621:ARG:HB2   | 1.94                     | 0.50              |
| 6:s:77:PRO:HA     | 6:s:80:ILE:HD12   | 1.93                     | 0.50              |
| 3:G:1198:TYR:HD1  | 3:G:1236:ARG:NH1  | 2.02                     | 0.50              |
| 4:g:66:VAL:HG12   | 4:g:66:VAL:O      | 2.12                     | 0.50              |
| 2:V:306:VAL:HG11  | 2:V:312:ALA:HB2   | 1.93                     | 0.50              |
| 1:w:89:LYS:HA     | 1:w:92:ARG:HE     | 1.77                     | 0.50              |
| 3:I:267:ALA:HB1   | 3:I:272:ARG:H     | 1.76                     | 0.50              |
| 3:J:42:VAL:HG12   | 3:J:43:ARG:O      | 2.12                     | 0.50              |
| 3:J:272:ARG:HE    | 3:J:374:LEU:HD11  | 1.76                     | 0.50              |
| 3:J:1248:GLN:C    | 3:J:1251:SER:HG   | 2.15                     | 0.50              |
| 3:K:452:LEU:HD12  | 3:K:456:ASN:HD22  | 1.77                     | 0.50              |
| 3:K:466:LEU:HD12  | 3:K:467:MET:HG3   | 1.93                     | 0.50              |
| 3:K:628:TYR:HB3   | 3:K:955:PHE:HE2   | 1.75                     | 0.50              |
| 3:L:201:MET:O     | 3:L:204:TYR:N     | 2.43                     | 0.50              |
| 3:M:39:PHE:CD1    | 3:D:120:MET:HE2   | 2.47                     | 0.50              |
| 3:M:1270:LEU:HD22 | 3:M:1303:ALA:HB2  | 1.94                     | 0.50              |
| 3:A:332:VAL:CG1   | 3:G:26:THR:HG22   | 2.41                     | 0.50              |
| 3:A:745:HIS:NE2   | 3:A:910:CYS:HB2   | 2.27                     | 0.50              |
| 3:H:204:TYR:CD2   | 3:H:219:LEU:HD11  | 2.46                     | 0.50              |
| 3:H:844:VAL:HG11  | 3:H:892:LEU:HD11  | 1.94                     | 0.50              |
| 3:H:895:GLN:HE22  | 4:h:65:GLY:HA3    | 1.77                     | 0.50              |
| 4:i:89:ARG:NH2    | 4:j:29:THR:OG1    | 2.45                     | 0.50              |
| 3:B:1124:ASN:OD1  | 3:B:1124:ASN:N    | 2.44                     | 0.50              |
| 3:C:424:VAL:HG12  | 3:C:425:PRO:O     | 2.11                     | 0.50              |
| 3:D:198:LEU:HD21  | 3:D:1106:TYR:CD2  | 2.47                     | 0.50              |
| 3:D:785:HIS:NE2   | 3:D:795:ALA:O     | 2.44                     | 0.50              |
| 3:D:868:ALA:HB2   | 4:c:73:PHE:CE1    | 2.47                     | 0.50              |
| 5:q:646:TYR:CZ    | 6:r:29:PRO:HB3    | 2.47                     | 0.50              |
| 5:q:655:ARG:HG3   | 5:q:656:ARG:N     | 2.27                     | 0.50              |
| 3:G:985:ARG:NH1   | 3:G:985:ARG:CB    | 2.73                     | 0.50              |
| 2:S:263:GLN:CB    | 5:q:9:VAL:HG11    | 2.38                     | 0.50              |
| 1:1:288:ILE:O     | 1:1:450:VAL:N     | 2.42                     | 0.50              |
| 3:J:752:ARG:HA    | 3:J:913:ALA:H     | 1.77                     | 0.50              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:J:854:PRO:HB2  | 3:J:863:HIS:HB2   | 1.93                     | 0.50              |
| 3:J:857:PRO:HG3  | 3:J:885:VAL:HG22  | 1.92                     | 0.50              |
| 3:L:274:VAL:HG11 | 3:L:376:PHE:CE2   | 2.46                     | 0.50              |
| 3:L:1342:LEU:CD2 | 3:L:1362:LEU:HB2  | 2.41                     | 0.50              |
| 3:M:451:ARG:NH1  | 3:H:529:GLU:OE1   | 2.45                     | 0.50              |
| 3:M:739:CYS:O    | 3:M:743:MET:HG2   | 2.11                     | 0.50              |
| 3:A:467:MET:HE2  | 3:A:575:TRP:HE1   | 1.76                     | 0.50              |
| 3:A:1058:PHE:HE2 | 3:A:1369:LEU:HD11 | 1.77                     | 0.50              |
| 3:H:96:GLN:NE2   | 3:C:12:ARG:H      | 2.09                     | 0.50              |
| 3:H:752:ARG:HA   | 3:H:913:ALA:HB3   | 1.93                     | 0.50              |
| 4:o:79:PHE:N     | 4:o:93:GLY:HA3    | 2.27                     | 0.50              |
| 3:N:56:ALA:HA    | 3:O:325:ALA:O     | 2.11                     | 0.50              |
| 3:N:86:GLU:O     | 3:N:86:GLU:HG2    | 2.11                     | 0.50              |
| 3:O:714:LEU:HD12 | 3:O:722:LEU:HD22  | 1.92                     | 0.50              |
| 3:P:717:GLN:HE22 | 3:P:752:ARG:NH1   | 2.09                     | 0.50              |
| 3:D:1004:GLN:NE2 | 3:D:1007:VAL:HB   | 2.27                     | 0.50              |
| 5:q:1:MET:HG3    | 5:q:5:PHE:HE2     | 1.76                     | 0.50              |
| 3:E:576:ARG:NH1  | 3:E:582:LEU:HD23  | 2.21                     | 0.50              |
| 3:F:469:ILE:HD11 | 3:F:547:PHE:CD1   | 2.46                     | 0.50              |
| 3:F:710:PRO:HB3  | 3:G:986:HIS:CE1   | 2.46                     | 0.50              |
| 3:G:193:PRO:HG2  | 3:G:198:LEU:HD21  | 1.94                     | 0.50              |
| 3:G:843:VAL:O    | 3:G:876:ASN:ND2   | 2.43                     | 0.50              |
| 3:G:1197:ASN:C   | 3:G:1199:PHE:H    | 2.20                     | 0.50              |
| 4:c:89:ARG:NH2   | 4:d:30:ASN:OD1    | 2.44                     | 0.50              |
| 1:Q:128:GLY:H    | 1:Q:251:LEU:HB2   | 1.77                     | 0.50              |
| 1:Q:354:ASN:HD21 | 1:Q:419:TYR:HB3   | 1.76                     | 0.50              |
| 2:S:16:ILE:O     | 3:B:92:GLU:OE2    | 2.29                     | 0.50              |
| 1:T:427:VAL:HG21 | 1:T:458:ARG:HH21  | 1.76                     | 0.50              |
| 3:I:278:LEU:HG   | 3:I:375:VAL:HG11  | 1.93                     | 0.50              |
| 3:I:405:PRO:HB3  | 3:I:1199:PHE:CE2  | 2.47                     | 0.50              |
| 3:K:509:TRP:CZ2  | 3:K:564:PRO:HD3   | 2.47                     | 0.50              |
| 3:L:604:HIS:HD2  | 3:L:696:HIS:CD2   | 2.30                     | 0.50              |
| 3:L:892:LEU:O    | 3:L:895:GLN:HG3   | 2.12                     | 0.50              |
| 3:L:1008:GLN:HG2 | 3:L:1011:ARG:HH11 | 1.77                     | 0.50              |
| 3:M:20:THR:OG1   | 3:C:61:TYR:CE1    | 2.65                     | 0.50              |
| 3:M:339:MET:HE2  | 3:N:17:MET:HE2    | 1.94                     | 0.50              |
| 3:M:519:ARG:NH1  | 3:M:998:TYR:OH    | 2.45                     | 0.50              |
| 3:M:786:ASN:ND2  | 3:M:901:MET:O     | 2.45                     | 0.50              |
| 3:A:143:LEU:HD13 | 3:A:165:LEU:HD11  | 1.94                     | 0.50              |
| 3:A:871:VAL:O    | 3:A:874:THR:OG1   | 2.23                     | 0.50              |
| 3:H:790:ARG:HG3  | 3:H:792:ALA:H     | 1.76                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:H:1013:SER:OG   | 3:H:1020:LEU:HD21 | 2.12                     | 0.50              |
| 3:N:86:GLU:OE1    | 3:N:86:GLU:N      | 2.45                     | 0.50              |
| 3:N:148:LEU:HD11  | 3:N:158:GLN:NE2   | 2.27                     | 0.50              |
| 3:N:446:ASP:OD2   | 3:O:1201:ARG:NH2  | 2.45                     | 0.50              |
| 3:N:778:ARG:NH1   | 3:N:782:ARG:HD2   | 2.26                     | 0.50              |
| 3:B:172:VAL:HG11  | 3:B:1093:LEU:HD12 | 1.94                     | 0.50              |
| 3:C:724:HIS:CE1   | 3:C:1028:TYR:HB2  | 2.47                     | 0.50              |
| 3:D:263:ARG:NH2   | 3:D:305:THR:OG1   | 2.44                     | 0.50              |
| 3:D:309:MET:SD    | 3:D:327:ARG:HG3   | 2.51                     | 0.50              |
| 5:q:260:ILE:HG23  | 7:u:3088:ALA:HB1  | 1.92                     | 0.50              |
| 3:E:163:GLN:HG3   | 3:F:344:LEU:HD11  | 1.93                     | 0.50              |
| 3:F:440:LEU:N     | 3:F:452:LEU:O     | 2.45                     | 0.50              |
| 3:F:601:VAL:O     | 3:F:601:VAL:HG12  | 2.12                     | 0.50              |
| 3:G:475:GLY:HA3   | 3:G:1250:PHE:HE2  | 1.77                     | 0.50              |
| 3:G:802:PRO:HD2   | 3:G:805:TRP:CB    | 2.42                     | 0.50              |
| 3:G:1223:ILE:HG22 | 3:G:1223:ILE:O    | 2.10                     | 0.50              |
| 4:b:66:VAL:O      | 4:b:66:VAL:HG12   | 2.12                     | 0.50              |
| 2:R:261:LEU:H     | 2:S:254:ILE:HG12  | 1.77                     | 0.49              |
| 2:V:27:CYS:HA     | 2:V:30:ARG:HE     | 1.76                     | 0.49              |
| 1:w:283:ARG:HD3   | 1:w:284:SER:N     | 2.19                     | 0.49              |
| 2:x:249:GLU:O     | 2:x:253:LEU:N     | 2.43                     | 0.49              |
| 3:I:802:PRO:HG2   | 3:I:805:TRP:HB2   | 1.94                     | 0.49              |
| 3:J:424:VAL:HG12  | 3:J:425:PRO:O     | 2.12                     | 0.49              |
| 3:K:462:CYS:SG    | 3:K:1147:LEU:HD22 | 2.52                     | 0.49              |
| 3:K:763:PRO:HB2   | 3:K:765:TYR:CE1   | 2.46                     | 0.49              |
| 3:L:488:GLY:HA3   | 3:L:520:TRP:CH2   | 2.46                     | 0.49              |
| 3:L:499:ALA:HA    | 3:L:956:TYR:CD1   | 2.47                     | 0.49              |
| 3:L:1206:ARG:HA   | 3:L:1277:PHE:HE1  | 1.77                     | 0.49              |
| 3:M:266:HIS:CE1   | 3:M:303:PRO:HD2   | 2.47                     | 0.49              |
| 3:M:558:LEU:HD13  | 3:M:929:PHE:HZ    | 1.77                     | 0.49              |
| 3:M:863:HIS:ND1   | 3:M:864:PRO:HD2   | 2.28                     | 0.49              |
| 3:A:277:VAL:O     | 3:A:1065:PHE:HA   | 2.12                     | 0.49              |
| 3:A:1320:LEU:HA   | 3:A:1327:LEU:HD11 | 1.94                     | 0.49              |
| 3:A:1344:ARG:O    | 3:A:1347:ARG:HG2  | 2.12                     | 0.49              |
| 3:H:213:ARG:NH1   | 3:H:1216:GLY:HA3  | 2.27                     | 0.49              |
| 3:H:381:GLU:HB3   | 3:H:392:TYR:CD1   | 2.47                     | 0.49              |
| 3:O:299:GLU:HB3   | 3:O:362:ARG:HD2   | 1.93                     | 0.49              |
| 3:O:546:ALA:CB    | 3:O:1031:MET:HE1  | 2.42                     | 0.49              |
| 3:P:888:GLY:O     | 3:P:892:LEU:HG    | 2.12                     | 0.49              |
| 3:B:159:LEU:HD23  | 3:B:162:ILE:HD12  | 1.93                     | 0.49              |
| 3:B:866:HIS:O     | 3:B:870:LEU:N     | 2.40                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:B:954:TYR:OH    | 4:g:92:PHE:HZ     | 1.92                     | 0.49              |
| 3:B:1347:ARG:NH2  | 3:C:1355:GLU:OE2  | 2.34                     | 0.49              |
| 3:D:405:PRO:HB3   | 3:D:1199:PHE:CE2  | 2.45                     | 0.49              |
| 3:D:495:ALA:HB1   | 3:D:504:ARG:NH1   | 2.27                     | 0.49              |
| 3:D:802:PRO:HG2   | 3:D:805:TRP:HB2   | 1.92                     | 0.49              |
| 5:q:591:TYR:HE2   | 5:q:606:ILE:HD12  | 1.76                     | 0.49              |
| 3:E:765:TYR:HD1   | 3:E:783:LEU:HB2   | 1.77                     | 0.49              |
| 3:F:646:ARG:HE    | 3:F:650:GLN:NE2   | 2.10                     | 0.49              |
| 3:F:749:ASP:OD1   | 3:F:749:ASP:N     | 2.43                     | 0.49              |
| 3:F:873:ASN:HA    | 4:e:92:PHE:HD2    | 1.75                     | 0.49              |
| 2:R:162:ASP:OD2   | 2:R:199:ASN:ND2   | 2.45                     | 0.49              |
| 1:T:166:GLU:CG    | 3:I:1262:HIS:CD2  | 2.95                     | 0.49              |
| 2:X:38:ARG:NH2    | 3:I:110:HIS:C     | 2.70                     | 0.49              |
| 2:X:38:ARG:NH2    | 3:I:110:HIS:N     | 2.56                     | 0.49              |
| 2:2:119:PRO:HB2   | 2:2:125:ALA:HA    | 1.94                     | 0.49              |
| 3:J:257:PRO:HA    | 3:J:1067:GLU:OE1  | 2.12                     | 0.49              |
| 3:J:1318:ARG:NH2  | 3:J:1320:LEU:HD21 | 2.27                     | 0.49              |
| 3:L:43:ARG:C      | 3:L:45:ASP:H      | 2.20                     | 0.49              |
| 3:L:126:ARG:HG3   | 3:L:1097:ARG:O    | 2.12                     | 0.49              |
| 3:L:763:PRO:HB2   | 3:L:765:TYR:CE1   | 2.47                     | 0.49              |
| 3:M:441:PHE:CE2   | 3:M:1340:PRO:HD3  | 2.48                     | 0.49              |
| 3:A:95:VAL:O      | 3:A:121:THR:HA    | 2.12                     | 0.49              |
| 3:A:790:ARG:NH2   | 3:A:793:ASP:HB2   | 2.27                     | 0.49              |
| 3:A:843:VAL:HB    | 3:A:876:ASN:ND2   | 2.27                     | 0.49              |
| 3:H:1245:TRP:O    | 3:H:1251:SER:HB3  | 2.11                     | 0.49              |
| 3:N:633:ALA:O     | 3:N:635:HIS:ND1   | 2.39                     | 0.49              |
| 3:N:756:ILE:HD12  | 3:N:763:PRO:HB3   | 1.94                     | 0.49              |
| 3:O:158:GLN:O     | 3:O:161:ALA:N     | 2.44                     | 0.49              |
| 3:P:818:PRO:HB3   | 3:P:963:LEU:HD22  | 1.93                     | 0.49              |
| 3:B:755:ARG:O     | 3:B:910:CYS:HA    | 2.12                     | 0.49              |
| 3:B:1245:TRP:O    | 3:B:1251:SER:HB3  | 2.12                     | 0.49              |
| 3:C:426:ALA:HA    | 3:D:1358:PHE:CE1  | 2.47                     | 0.49              |
| 3:D:137:THR:OG1   | 3:D:138:GLU:N     | 2.46                     | 0.49              |
| 3:D:631:GLN:O     | 3:D:634:ILE:N     | 2.45                     | 0.49              |
| 3:E:268:ASP:HB3   | 3:E:270:ARG:H     | 1.77                     | 0.49              |
| 3:E:1008:GLN:HB3  | 3:E:1012:GLU:CD   | 2.37                     | 0.49              |
| 3:F:134:SER:HB3   | 3:G:114:GLN:HE21  | 1.71                     | 0.49              |
| 3:F:398:MET:O     | 3:F:1057:ARG:HA   | 2.12                     | 0.49              |
| 3:F:1147:LEU:O    | 3:F:1150:ALA:N    | 2.45                     | 0.49              |
| 3:G:1152:VAL:HG13 | 3:G:1159:PRO:HD2  | 1.94                     | 0.49              |
| 7:u:3098:ARG:O    | 7:u:3102:ALA:N    | 2.46                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:I:1058:PHE:HE2  | 3:I:1369:LEU:HD11 | 1.76                     | 0.49              |
| 3:J:895:GLN:HE22  | 4:j:65:GLY:HA3    | 1.77                     | 0.49              |
| 3:K:1164:PRO:HG2  | 3:K:1167:GLY:O    | 2.13                     | 0.49              |
| 3:L:895:GLN:O     | 3:L:898:ALA:N     | 2.36                     | 0.49              |
| 3:L:942:PRO:HA    | 3:L:969:HIS:CE1   | 2.47                     | 0.49              |
| 3:M:878:MET:HB2   | 4:l:92:PHE:CE2    | 2.47                     | 0.49              |
| 3:A:669:SER:O     | 3:A:672:SER:OG    | 2.22                     | 0.49              |
| 3:A:1198:TYR:OH   | 3:A:1204:ASN:O    | 2.30                     | 0.49              |
| 3:H:630:LEU:O     | 3:H:634:ILE:HD12  | 2.12                     | 0.49              |
| 3:H:752:ARG:HG3   | 3:H:913:ALA:H     | 1.76                     | 0.49              |
| 3:H:1222:VAL:HG11 | 3:H:1283:THR:HA   | 1.95                     | 0.49              |
| 4:o:80:ALA:N      | 3:P:947:HIS:O     | 2.42                     | 0.49              |
| 4:o:101:PHE:HE1   | 3:O:847:ILE:HG21  | 1.78                     | 0.49              |
| 3:N:405:PRO:HB3   | 3:N:1199:PHE:CE2  | 2.47                     | 0.49              |
| 3:N:1342:LEU:HD21 | 3:N:1362:LEU:HB2  | 1.94                     | 0.49              |
| 3:O:467:MET:O     | 3:O:922:SER:OG    | 2.28                     | 0.49              |
| 3:P:263:ARG:NH2   | 3:P:306:TYR:O     | 2.45                     | 0.49              |
| 3:D:351:LEU:C     | 3:D:351:LEU:CD2   | 2.86                     | 0.49              |
| 3:D:512:ARG:HD3   | 3:D:515:HIS:CD2   | 2.47                     | 0.49              |
| 3:D:865:LEU:CD2   | 3:D:879:PHE:HB2   | 2.43                     | 0.49              |
| 5:q:610:ILE:HG22  | 5:q:611:ASP:H     | 1.77                     | 0.49              |
| 3:E:839:LEU:O     | 3:E:842:MET:HG2   | 2.12                     | 0.49              |
| 3:E:866:HIS:O     | 3:E:870:LEU:HG    | 2.12                     | 0.49              |
| 3:F:629:LEU:HD22  | 3:F:835:VAL:HG13  | 1.94                     | 0.49              |
| 3:G:35:LEU:CD1    | 3:G:39:PHE:HE2    | 2.24                     | 0.49              |
| 1:Q:44:ARG:C      | 3:B:322:MET:HB3   | 2.17                     | 0.49              |
| 2:Y:205:LEU:HD22  | 2:Y:209:MET:HE3   | 1.94                     | 0.49              |
| 3:I:158:GLN:O     | 3:I:162:ILE:N     | 2.35                     | 0.49              |
| 3:I:159:LEU:HD13  | 3:J:339:MET:O     | 2.12                     | 0.49              |
| 3:I:1347:ARG:NH2  | 3:J:1355:GLU:OE2  | 2.45                     | 0.49              |
| 3:J:390:VAL:HG21  | 3:K:104:ILE:HG13  | 1.94                     | 0.49              |
| 3:J:399:ASP:OD1   | 3:J:1057:ARG:HG2  | 2.12                     | 0.49              |
| 3:J:915:ASP:O     | 3:J:919:ASN:HB2   | 2.12                     | 0.49              |
| 3:K:469:ILE:O     | 3:K:472:ALA:N     | 2.44                     | 0.49              |
| 3:K:863:HIS:ND1   | 3:K:864:PRO:HD2   | 2.27                     | 0.49              |
| 3:L:452:LEU:HD13  | 3:L:1124:ASN:HB2  | 1.94                     | 0.49              |
| 3:L:576:ARG:NH1   | 3:L:582:LEU:HD23  | 2.26                     | 0.49              |
| 3:L:892:LEU:HD21  | 4:l:68:HIS:HD2    | 1.77                     | 0.49              |
| 3:M:1115:VAL:HG12 | 3:M:1116:ARG:O    | 2.13                     | 0.49              |
| 3:A:490:TYR:CE1   | 3:A:564:PRO:HB3   | 2.46                     | 0.49              |
| 3:A:624:PRO:HB2   | 3:A:627:PHE:CE2   | 2.48                     | 0.49              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:A:923:THR:HA   | 3:A:926:MET:HE3   | 1.94                     | 0.49              |
| 4:i:61:LEU:O     | 4:i:65:GLY:N      | 2.43                     | 0.49              |
| 4:n:57:GLN:HB3   | 3:N:840:GLN:HB3   | 1.94                     | 0.49              |
| 3:N:502:GLN:O    | 3:N:505:PHE:N     | 2.45                     | 0.49              |
| 3:O:440:LEU:HD22 | 3:O:1336:CYS:SG   | 2.53                     | 0.49              |
| 3:P:204:TYR:HE1  | 3:P:215:ALA:HB1   | 1.77                     | 0.49              |
| 3:P:485:ASN:HD21 | 3:P:516:GLY:N     | 1.97                     | 0.49              |
| 3:B:775:ASP:HB2  | 3:B:778:ARG:HH21  | 1.78                     | 0.49              |
| 3:C:601:VAL:O    | 3:C:601:VAL:HG12  | 2.12                     | 0.49              |
| 3:C:1254:ASP:HB3 | 3:C:1258:ASN:HD21 | 1.78                     | 0.49              |
| 3:D:198:LEU:HD21 | 3:D:1106:TYR:CE2  | 2.46                     | 0.49              |
| 3:D:744:ARG:O    | 3:D:747:ALA:HB3   | 2.13                     | 0.49              |
| 3:D:950:GLN:HB2  | 3:D:953:GLU:HG3   | 1.94                     | 0.49              |
| 3:D:1208:ARG:NH2 | 3:D:1228:ASP:O    | 2.45                     | 0.49              |
| 3:E:86:GLU:OE1   | 3:E:86:GLU:N      | 2.46                     | 0.49              |
| 3:E:187:VAL:HG11 | 3:E:1071:GLU:OE2  | 2.13                     | 0.49              |
| 3:E:469:ILE:HD11 | 3:E:547:PHE:CE1   | 2.48                     | 0.49              |
| 6:r:79:ASP:O     | 6:r:83:ARG:HG2    | 2.12                     | 0.49              |
| 3:F:54:PHE:HA    | 3:G:323:GLY:C     | 2.34                     | 0.49              |
| 3:F:422:ASP:OD2  | 3:F:1354:ARG:NH2  | 2.45                     | 0.49              |
| 3:F:604:HIS:NE2  | 3:F:605:ALA:O     | 2.45                     | 0.49              |
| 3:F:625:ALA:HA   | 3:F:628:TYR:HD2   | 1.77                     | 0.49              |
| 3:F:731:LEU:HB2  | 3:F:810:LYS:NZ    | 2.26                     | 0.49              |
| 3:F:764:VAL:O    | 3:F:783:LEU:N     | 2.41                     | 0.49              |
| 3:F:825:CYS:HB2  | 3:F:939:LEU:O     | 2.11                     | 0.49              |
| 2:R:114:VAL:HB   | 2:R:295:VAL:HB    | 1.94                     | 0.49              |
| 2:U:158:ARG:HH22 | 2:U:188:LEU:HB2   | 1.77                     | 0.49              |
| 2:X:217:THR:HA   | 2:X:220:ILE:HD12  | 1.94                     | 0.49              |
| 1:1:125:GLU:OE2  | 1:1:215:TYR:OH    | 2.24                     | 0.49              |
| 2:3:99:ASN:CG    | 3:M:1086:GLY:HA2  | 2.37                     | 0.49              |
| 3:I:398:MET:O    | 3:I:1057:ARG:HA   | 2.13                     | 0.49              |
| 3:I:593:ASP:O    | 3:I:597:LEU:N     | 2.29                     | 0.49              |
| 3:I:1178:ASP:O   | 3:J:217:ALA:HB1   | 2.12                     | 0.49              |
| 3:J:610:THR:HG21 | 3:J:692:ASP:OD2   | 2.13                     | 0.49              |
| 3:K:639:HIS:HA   | 4:k:79:PHE:CZ     | 2.47                     | 0.49              |
| 3:L:50:TYR:HE2   | 3:N:139:ALA:HB2   | 1.77                     | 0.49              |
| 3:M:406:LEU:HD11 | 3:M:1187:PHE:HE1  | 1.76                     | 0.49              |
| 3:A:83:LYS:HG2   | 3:A:1075:LEU:HD11 | 1.95                     | 0.49              |
| 3:A:667:ASP:HB2  | 3:A:670:LEU:HD12  | 1.94                     | 0.49              |
| 3:A:770:ASN:H    | 3:A:773:THR:HB    | 1.77                     | 0.49              |
| 3:A:1191:PRO:HG2 | 3:A:1194:THR:HG23 | 1.94                     | 0.49              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:H:266:HIS:HE1  | 3:H:302:VAL:HG13  | 1.76                     | 0.49              |
| 3:H:350:THR:HG22 | 3:C:20:THR:O      | 2.12                     | 0.49              |
| 3:H:866:HIS:CD2  | 3:H:868:ALA:HB3   | 2.48                     | 0.49              |
| 3:O:274:VAL:HG11 | 3:O:376:PHE:CD2   | 2.48                     | 0.49              |
| 3:P:71:LEU:HD11  | 3:P:306:TYR:CE1   | 2.47                     | 0.49              |
| 3:P:861:PRO:HA   | 3:P:866:HIS:CG    | 2.47                     | 0.49              |
| 3:P:923:THR:HG23 | 3:P:926:MET:HE3   | 1.94                     | 0.49              |
| 3:P:1052:VAL:HA  | 3:P:1186:GLU:O    | 2.12                     | 0.49              |
| 3:D:616:GLY:O    | 3:D:620:ASP:N     | 2.45                     | 0.49              |
| 3:D:1319:GLU:N   | 3:D:1319:GLU:OE1  | 2.45                     | 0.49              |
| 3:E:915:ASP:O    | 3:E:919:ASN:HB2   | 2.12                     | 0.49              |
| 3:F:311:LEU:O    | 3:F:316:LEU:HB2   | 2.12                     | 0.49              |
| 3:G:783:LEU:HD22 | 3:G:934:HIS:CG    | 2.48                     | 0.49              |
| 1:W:246:ARG:NH1  | 2:X:111:GLY:O     | 2.45                     | 0.49              |
| 2:x:68:ARG:NH1   | 2:x:287:ASP:O     | 2.45                     | 0.49              |
| 3:I:769:CYS:SG   | 3:I:786:ASN:ND2   | 2.82                     | 0.49              |
| 3:I:857:PRO:HB3  | 3:I:863:HIS:CD2   | 2.48                     | 0.49              |
| 3:I:1177:MET:HE1 | 3:J:214:VAL:HG22  | 1.94                     | 0.49              |
| 3:K:310:VAL:HG12 | 3:K:312:ASN:H     | 1.76                     | 0.49              |
| 3:K:1218:LYS:HB3 | 3:K:1221:ASP:CG   | 2.38                     | 0.49              |
| 3:L:309:MET:HE1  | 3:L:327:ARG:HA    | 1.95                     | 0.49              |
| 3:L:863:HIS:ND1  | 3:L:864:PRO:HD2   | 2.28                     | 0.49              |
| 3:A:1257:TYR:HB2 | 3:A:1277:PHE:CD2  | 2.47                     | 0.49              |
| 3:H:274:VAL:HG11 | 3:H:376:PHE:CD2   | 2.47                     | 0.49              |
| 3:H:280:THR:HG22 | 3:H:1063:VAL:HG13 | 1.93                     | 0.49              |
| 4:i:66:VAL:HA    | 4:i:69:ALA:HB2    | 1.93                     | 0.49              |
| 4:j:73:PHE:HD2   | 4:j:100:PRO:HA    | 1.78                     | 0.49              |
| 4:o:79:PHE:HE2   | 3:O:639:HIS:HD2   | 1.60                     | 0.49              |
| 3:N:85:PRO:HG3   | 3:N:310:VAL:HG22  | 1.95                     | 0.49              |
| 3:N:928:ILE:HG21 | 3:N:1001:SER:HB3  | 1.93                     | 0.49              |
| 3:O:231:SER:O    | 3:O:1112:THR:OG1  | 2.30                     | 0.49              |
| 3:O:266:HIS:HE1  | 3:O:302:VAL:HG13  | 1.77                     | 0.49              |
| 3:O:399:ASP:CG   | 3:O:1321:VAL:HG11 | 2.38                     | 0.49              |
| 3:O:405:PRO:HB3  | 3:O:1199:PHE:CD2  | 2.47                     | 0.49              |
| 3:C:154:SER:O    | 3:C:157:ARG:N     | 2.44                     | 0.49              |
| 3:C:863:HIS:CD2  | 3:C:865:LEU:HB2   | 2.48                     | 0.49              |
| 3:E:533:GLN:C    | 3:E:535:ASP:H     | 2.21                     | 0.49              |
| 3:E:842:MET:SD   | 3:E:891:MET:HE3   | 2.53                     | 0.49              |
| 3:F:116:VAL:HG12 | 3:F:117:HIS:N     | 2.27                     | 0.49              |
| 3:G:467:MET:O    | 3:G:922:SER:OG    | 2.30                     | 0.49              |
| 4:d:66:VAL:O     | 4:d:66:VAL:HG12   | 2.12                     | 0.49              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:T:113:GLN:O    | 1:T:115:THR:HG23  | 2.12                     | 0.49              |
| 1:W:28:ALA:CA    | 3:H:145:GLY:HA3   | 2.41                     | 0.49              |
| 2:2:120:VAL:HG12 | 2:2:188:LEU:HB2   | 1.94                     | 0.49              |
| 3:I:463:HIS:CG   | 3:I:464:PRO:HD2   | 2.48                     | 0.49              |
| 3:I:621:ARG:C    | 3:I:943:GLN:HE21  | 2.21                     | 0.49              |
| 3:I:833:ASP:HA   | 4:i:54:LEU:HD11   | 1.95                     | 0.49              |
| 3:J:116:VAL:HG12 | 3:J:117:HIS:N     | 2.28                     | 0.49              |
| 3:J:652:ILE:O    | 3:J:655:TYR:N     | 2.46                     | 0.49              |
| 3:J:836:TYR:CE1  | 3:J:897:LEU:HD22  | 2.42                     | 0.49              |
| 3:K:424:VAL:HG12 | 3:K:425:PRO:O     | 2.11                     | 0.49              |
| 3:L:108:GLY:HA2  | 3:L:110:HIS:N     | 2.28                     | 0.49              |
| 3:L:1227:TYR:CD1 | 3:L:1249:ARG:HB2  | 2.47                     | 0.49              |
| 3:M:168:ASN:O    | 3:M:171:ALA:N     | 2.46                     | 0.49              |
| 3:M:204:TYR:HB2  | 3:M:219:LEU:HD21  | 1.93                     | 0.49              |
| 3:A:79:CYS:SG    | 3:A:184:MET:HE1   | 2.53                     | 0.49              |
| 3:H:403:VAL:HG22 | 3:H:1053:VAL:HG22 | 1.93                     | 0.49              |
| 3:N:255:THR:OG1  | 3:N:1067:GLU:OE2  | 2.21                     | 0.49              |
| 3:N:463:HIS:CG   | 3:N:464:PRO:HD2   | 2.47                     | 0.49              |
| 3:P:512:ARG:NH1  | 3:P:564:PRO:HD2   | 2.28                     | 0.49              |
| 3:B:863:HIS:CD2  | 3:B:865:LEU:HB2   | 2.47                     | 0.49              |
| 3:C:79:CYS:HB3   | 3:C:81:CYS:SG     | 2.53                     | 0.49              |
| 3:C:126:ARG:HG3  | 3:C:1097:ARG:O    | 2.12                     | 0.49              |
| 3:E:863:HIS:CD2  | 3:E:865:LEU:H     | 2.31                     | 0.49              |
| 3:F:390:VAL:CG2  | 3:G:104:ILE:HD11  | 2.43                     | 0.49              |
| 3:F:595:ARG:HD3  | 3:F:1026:ALA:HB1  | 1.95                     | 0.49              |
| 3:F:668:TYR:HD2  | 3:F:809:HIS:CE1   | 2.30                     | 0.49              |
| 3:G:547:PHE:HB2  | 3:G:549:PHE:HE2   | 1.78                     | 0.49              |
| 1:T:271:GLN:NE2  | 1:T:284:SER:OG    | 2.40                     | 0.49              |
| 2:U:68:ARG:NH2   | 2:V:317:TYR:OH    | 2.46                     | 0.49              |
| 1:W:260:LEU:HD23 | 3:C:1316:GLY:HA2  | 1.95                     | 0.49              |
| 1:I:258:ASP:HB3  | 3:M:1318:ARG:HD2  | 1.94                     | 0.49              |
| 3:I:196:ALA:HB1  | 3:I:227:PHE:HA    | 1.95                     | 0.49              |
| 3:I:529:GLU:OE1  | 3:H:451:ARG:NH1   | 2.46                     | 0.49              |
| 3:I:580:GLY:HA2  | 3:I:592:ARG:NH1   | 2.22                     | 0.49              |
| 3:I:829:GLY:N    | 3:I:956:TYR:O     | 2.46                     | 0.49              |
| 3:J:460:THR:HA   | 3:J:1129:PHE:CD2  | 2.48                     | 0.49              |
| 3:J:642:CYS:HB2  | 4:j:78:MET:HB3    | 1.95                     | 0.49              |
| 3:K:85:PRO:HG2   | 3:K:86:GLU:OE1    | 2.11                     | 0.49              |
| 3:L:866:HIS:O    | 3:L:870:LEU:HG    | 2.12                     | 0.49              |
| 3:L:1181:GLN:HB2 | 3:L:1309:VAL:O    | 2.12                     | 0.49              |
| 3:M:29:VAL:HG13  | 3:D:120:MET:HE1   | 1.85                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:M:438:ARG:HB2   | 3:M:454:MET:HG2   | 1.95                     | 0.49              |
| 3:M:802:PRO:HB3   | 3:H:944:HIS:NE2   | 2.28                     | 0.49              |
| 3:M:1259:GLY:HA3  | 3:M:1274:PHE:HE1  | 1.77                     | 0.49              |
| 3:H:765:TYR:HE1   | 3:H:783:LEU:HD12  | 1.78                     | 0.49              |
| 4:h:88:LEU:HD12   | 4:h:89:ARG:HG2    | 1.95                     | 0.49              |
| 3:N:309:MET:SD    | 3:N:327:ARG:HG3   | 2.53                     | 0.49              |
| 3:O:546:ALA:HB1   | 3:O:1031:MET:HE3  | 1.94                     | 0.49              |
| 3:O:576:ARG:NH1   | 3:O:582:LEU:HD23  | 2.27                     | 0.49              |
| 3:P:318:THR:O     | 3:P:323:GLY:N     | 2.45                     | 0.49              |
| 3:P:440:LEU:HD22  | 3:P:1336:CYS:SG   | 2.52                     | 0.49              |
| 3:P:441:PHE:CE2   | 3:P:1340:PRO:HD3  | 2.48                     | 0.49              |
| 3:P:490:TYR:CD1   | 3:P:564:PRO:HB3   | 2.48                     | 0.49              |
| 3:P:776:PHE:HD2   | 3:P:833:ASP:OD1   | 1.95                     | 0.49              |
| 3:P:961:HIS:O     | 3:P:964:PHE:N     | 2.41                     | 0.49              |
| 3:B:201:MET:O     | 3:B:204:TYR:N     | 2.46                     | 0.49              |
| 3:C:277:VAL:O     | 3:C:1065:PHE:HA   | 2.12                     | 0.49              |
| 3:D:158:GLN:O     | 3:D:161:ALA:N     | 2.46                     | 0.49              |
| 3:D:388:THR:HG23  | 3:E:102:PRO:HG2   | 1.95                     | 0.49              |
| 3:D:485:ASN:HD21  | 3:D:516:GLY:N     | 2.09                     | 0.49              |
| 3:E:607:ALA:O     | 3:E:610:THR:OG1   | 2.26                     | 0.49              |
| 3:E:746:ALA:HA    | 3:E:754:CYS:HB3   | 1.94                     | 0.49              |
| 3:E:961:HIS:O     | 3:E:964:PHE:N     | 2.39                     | 0.49              |
| 3:F:297:ASP:HB3   | 3:F:367:LEU:HD12  | 1.94                     | 0.49              |
| 3:F:653:THR:HG22  | 3:F:683:PRO:HD3   | 1.95                     | 0.49              |
| 3:F:724:HIS:CE1   | 3:F:1028:TYR:HB2  | 2.48                     | 0.49              |
| 3:F:1157:LEU:HD11 | 3:F:1269:VAL:HG21 | 1.95                     | 0.49              |
| 1:Q:45:ASP:H      | 3:B:322:MET:CB    | 1.99                     | 0.49              |
| 1:T:283:ARG:NH2   | 3:H:47:ASN:H      | 2.11                     | 0.49              |
| 1:W:259:GLU:OE2   | 3:C:1313:ARG:CZ   | 2.60                     | 0.49              |
| 3:I:280:THR:HG22  | 3:I:1063:VAL:HG22 | 1.95                     | 0.49              |
| 3:I:340:GLN:HG3   | 3:H:159:LEU:HD11  | 1.94                     | 0.49              |
| 3:J:634:ILE:HG22  | 3:J:636:GLY:N     | 2.27                     | 0.49              |
| 3:L:452:LEU:HD12  | 3:L:456:ASN:ND2   | 2.24                     | 0.49              |
| 3:L:1125:LEU:HD22 | 3:L:1184:VAL:HG22 | 1.93                     | 0.49              |
| 3:M:321:VAL:HG11  | 3:O:326:VAL:HG21  | 1.95                     | 0.49              |
| 3:M:864:PRO:HG3   | 3:M:888:GLY:HA2   | 1.95                     | 0.49              |
| 3:A:380:LEU:HB3   | 3:A:384:ILE:HD13  | 1.95                     | 0.49              |
| 3:A:460:THR:HA    | 3:A:1129:PHE:CD2  | 2.47                     | 0.49              |
| 3:A:790:ARG:HG3   | 3:A:792:ALA:H     | 1.78                     | 0.49              |
| 3:A:866:HIS:ND1   | 3:A:867:PRO:HD2   | 2.28                     | 0.49              |
| 3:H:649:THR:HG22  | 3:H:678:LEU:HD13  | 1.93                     | 0.49              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 3:H:752:ARG:HH21  | 3:H:915:ASP:HA   | 1.77                     | 0.49              |
| 3:H:1304:THR:HG21 | 3:H:1314:PRO:HD2 | 1.95                     | 0.49              |
| 4:n:53:PHE:HE2    | 3:N:837:ALA:HB1  | 1.77                     | 0.49              |
| 4:o:65:GLY:HA3    | 3:O:895:GLN:NE2  | 2.28                     | 0.49              |
| 4:o:80:ALA:N      | 3:P:948:THR:HA   | 2.27                     | 0.49              |
| 4:o:92:PHE:N      | 3:P:873:ASN:OD1  | 2.19                     | 0.49              |
| 4:p:61:LEU:HB3    | 3:P:895:GLN:HG2  | 1.95                     | 0.49              |
| 3:N:321:VAL:HG11  | 3:E:326:VAL:HG21 | 1.93                     | 0.49              |
| 3:N:426:ALA:HB3   | 3:N:429:HIS:CD2  | 2.48                     | 0.49              |
| 3:N:496:GLY:HA3   | 3:N:504:ARG:HH22 | 1.77                     | 0.49              |
| 3:N:811:ILE:O     | 3:N:815:VAL:HB   | 2.12                     | 0.49              |
| 3:O:840:GLN:C     | 3:O:842:MET:HG2  | 2.38                     | 0.49              |
| 3:P:788:GLN:NE2   | 3:P:800:HIS:HE1  | 2.10                     | 0.49              |
| 3:C:227:PHE:O     | 3:C:231:SER:OG   | 2.14                     | 0.49              |
| 3:D:63:ASN:HD21   | 3:E:99:VAL:HG22  | 1.77                     | 0.49              |
| 3:D:913:ALA:HB1   | 3:D:914:PRO:HD2  | 1.95                     | 0.49              |
| 3:D:950:GLN:HG3   | 4:c:80:ALA:HB3   | 1.92                     | 0.49              |
| 5:q:505:PHE:HA    | 6:s:26:PHE:HB2   | 1.95                     | 0.49              |
| 3:E:842:MET:SD    | 3:E:894:LEU:HD13 | 2.53                     | 0.49              |
| 3:F:766:ALA:H     | 3:F:783:LEU:C    | 2.20                     | 0.49              |
| 3:F:827:THR:OG1   | 3:F:960:VAL:HG23 | 2.12                     | 0.49              |
| 3:F:870:LEU:HD23  | 3:F:876:ASN:HB3  | 1.94                     | 0.49              |
| 3:G:550:PHE:HD2   | 3:G:550:PHE:C    | 2.21                     | 0.49              |
| 3:G:700:LEU:HD22  | 3:G:1025:MET:HG3 | 1.95                     | 0.49              |
| 4:c:66:VAL:O      | 4:c:66:VAL:HG12  | 2.12                     | 0.49              |
| 2:R:317:TYR:OH    | 2:S:4:ASP:OD1    | 2.30                     | 0.49              |
| 1:W:345:ARG:HB3   | 6:s:13:TRP:CH2   | 2.44                     | 0.49              |
| 2:2:61:LEU:HD21   | 2:2:201:GLU:HG3  | 1.93                     | 0.49              |
| 2:x:276:VAL:HG11  | 2:y:154:ARG:HE   | 1.77                     | 0.49              |
| 3:I:920:THR:O     | 3:I:924:ALA:N    | 2.45                     | 0.49              |
| 3:I:1074:PHE:CZ   | 3:H:58:LEU:HD13  | 2.48                     | 0.49              |
| 3:I:1339:ASP:HB2  | 3:I:1342:LEU:HB3 | 1.93                     | 0.49              |
| 3:J:790:ARG:HE    | 3:J:792:ALA:HB3  | 1.77                     | 0.49              |
| 3:K:708:THR:HG22  | 3:K:723:ASN:ND2  | 2.28                     | 0.49              |
| 3:M:162:ILE:HG22  | 3:H:344:LEU:HD12 | 1.94                     | 0.49              |
| 3:M:335:HIS:O     | 3:M:339:MET:HB2  | 2.12                     | 0.49              |
| 3:A:510:ARG:HG2   | 3:A:980:LEU:HD11 | 1.93                     | 0.49              |
| 3:A:623:TYR:HB3   | 3:A:943:GLN:NE2  | 2.28                     | 0.49              |
| 3:A:1071:GLU:HG3  | 3:A:1100:VAL:O   | 2.13                     | 0.49              |
| 3:H:840:GLN:HB2   | 4:h:57:GLN:OE1   | 2.13                     | 0.49              |
| 4:k:57:GLN:O      | 4:k:61:LEU:N     | 2.40                     | 0.49              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 4:n:61:LEU:HB3   | 3:N:895:GLN:HG2   | 1.95                     | 0.49              |
| 3:N:402:PHE:HA   | 3:N:1332:TYR:O    | 2.13                     | 0.49              |
| 3:P:600:GLY:C    | 3:P:602:GLY:H     | 2.21                     | 0.49              |
| 3:P:746:ALA:HA   | 3:P:754:CYS:HB3   | 1.95                     | 0.49              |
| 3:B:488:GLY:HA3  | 3:B:520:TRP:CH2   | 2.48                     | 0.49              |
| 3:B:778:ARG:HH12 | 3:B:782:ARG:HH11  | 1.61                     | 0.49              |
| 3:B:1248:GLN:O   | 3:B:1251:SER:OG   | 2.29                     | 0.49              |
| 3:C:1366:ALA:HA  | 3:C:1370:LYS:NZ   | 2.28                     | 0.49              |
| 3:D:86:GLU:O     | 3:D:86:GLU:HG2    | 2.11                     | 0.49              |
| 3:D:607:ALA:O    | 3:D:610:THR:OG1   | 2.29                     | 0.49              |
| 5:q:373:ARG:HG2  | 5:q:376:TRP:CE2   | 2.48                     | 0.49              |
| 5:q:660:LEU:HD23 | 5:q:670:THR:HA    | 1.94                     | 0.49              |
| 3:E:42:VAL:HG12  | 3:E:44:SER:H      | 1.77                     | 0.49              |
| 3:E:1178:ASP:O   | 3:F:217:ALA:HB1   | 2.13                     | 0.49              |
| 3:F:338:GLU:OE1  | 3:F:338:GLU:N     | 2.44                     | 0.49              |
| 3:F:755:ARG:HH11 | 3:F:911:SER:CB    | 2.26                     | 0.49              |
| 3:G:220:VAL:HG11 | 3:G:1214:TYR:HE1  | 1.77                     | 0.49              |
| 3:G:606:MET:HE3  | 3:G:611:ILE:HG12  | 1.95                     | 0.49              |
| 4:e:66:VAL:O     | 4:e:66:VAL:HG12   | 2.12                     | 0.49              |
| 1:T:317:ARG:HH12 | 1:T:322:GLN:HB3   | 1.78                     | 0.48              |
| 1:w:117:THR:O    | 1:w:121:GLN:NE2   | 2.46                     | 0.48              |
| 2:x:287:ASP:OD2  | 2:y:149:ARG:NH1   | 2.38                     | 0.48              |
| 3:I:499:ALA:HA   | 3:I:956:TYR:CD1   | 2.48                     | 0.48              |
| 3:J:172:VAL:O    | 3:J:175:ALA:N     | 2.45                     | 0.48              |
| 3:K:148:LEU:HD11 | 3:K:158:GLN:NE2   | 2.28                     | 0.48              |
| 3:K:195:LEU:O    | 3:K:198:LEU:N     | 2.32                     | 0.48              |
| 3:K:272:ARG:HD3  | 3:K:374:LEU:HD11  | 1.94                     | 0.48              |
| 3:K:804:ASP:HB3  | 3:K:808:HIS:NE2   | 2.28                     | 0.48              |
| 3:L:158:GLN:O    | 3:L:161:ALA:N     | 2.46                     | 0.48              |
| 3:L:244:ILE:HD13 | 3:L:292:PHE:HE2   | 1.78                     | 0.48              |
| 3:M:231:SER:O    | 3:M:1112:THR:OG1  | 2.31                     | 0.48              |
| 3:M:301:ASP:OD1  | 3:M:362:ARG:NE    | 2.45                     | 0.48              |
| 3:M:646:ARG:HD2  | 4:m:98:TYR:O      | 2.13                     | 0.48              |
| 3:A:524:CYS:CB   | 3:A:1008:GLN:HE22 | 2.26                     | 0.48              |
| 3:A:1058:PHE:CE2 | 3:A:1369:LEU:HD11 | 2.47                     | 0.48              |
| 3:H:311:LEU:O    | 3:H:316:LEU:HB2   | 2.13                     | 0.48              |
| 3:N:805:TRP:NE1  | 3:N:809:HIS:HE2   | 2.10                     | 0.48              |
| 3:N:1170:GLN:OE1 | 3:N:1170:GLN:N    | 2.45                     | 0.48              |
| 3:B:872:ALA:HB2  | 4:g:76:GLN:CB     | 2.43                     | 0.48              |
| 3:C:466:LEU:HD12 | 3:C:467:MET:HG3   | 1.94                     | 0.48              |
| 3:C:873:ASN:OD1  | 4:b:92:PHE:CB     | 2.60                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:C:1208:ARG:NE   | 3:C:1225:LEU:O    | 2.46                     | 0.48              |
| 3:D:580:GLY:HA3   | 3:D:1006:VAL:HG22 | 1.94                     | 0.48              |
| 3:D:764:VAL:O     | 3:D:783:LEU:N     | 2.46                     | 0.48              |
| 3:D:1054:ARG:NH1  | 3:D:1123:GLY:O    | 2.46                     | 0.48              |
| 5:q:25:HIS:HB2    | 5:q:400:VAL:O     | 2.12                     | 0.48              |
| 3:E:66:SER:OG     | 3:E:178:ARG:NH2   | 2.46                     | 0.48              |
| 3:E:668:TYR:HD2   | 3:E:809:HIS:CE1   | 2.31                     | 0.48              |
| 3:E:983:LEU:CD2   | 3:E:987:VAL:CG2   | 2.91                     | 0.48              |
| 3:F:487:TYR:OH    | 3:F:990:VAL:O     | 2.25                     | 0.48              |
| 3:F:826:CYS:HB3   | 3:F:966:GLY:H     | 1.78                     | 0.48              |
| 3:G:666:ASN:ND2   | 3:G:938:LEU:CD2   | 2.76                     | 0.48              |
| 1:Q:150:PRO:HA    | 2:S:267:ARG:HH21  | 1.78                     | 0.48              |
| 2:S:61:LEU:HD21   | 2:S:201:GLU:HG3   | 1.95                     | 0.48              |
| 1:W:350:LEU:HD22  | 6:r:20:VAL:CG1    | 2.39                     | 0.48              |
| 2:3:38:ARG:NH2    | 3:E:108:GLY:HA2   | 2.27                     | 0.48              |
| 3:I:440:LEU:HD22  | 3:I:1336:CYS:SG   | 2.53                     | 0.48              |
| 3:I:801:ARG:HB3   | 3:I:802:PRO:HD2   | 1.94                     | 0.48              |
| 3:I:863:HIS:ND1   | 3:I:864:PRO:HD2   | 2.28                     | 0.48              |
| 3:J:172:VAL:HG11  | 3:J:1093:LEU:HD12 | 1.93                     | 0.48              |
| 3:K:802:PRO:HD3   | 3:L:945:LEU:HD21  | 1.94                     | 0.48              |
| 3:L:769:CYS:O     | 3:L:901:MET:N     | 2.46                     | 0.48              |
| 3:L:865:LEU:HD22  | 3:L:879:PHE:HB2   | 1.95                     | 0.48              |
| 3:L:1115:VAL:HG12 | 3:L:1116:ARG:O    | 2.13                     | 0.48              |
| 3:M:646:ARG:NH1   | 4:m:100:PRO:HD2   | 2.28                     | 0.48              |
| 3:M:787:THR:O     | 3:M:788:GLN:HG3   | 2.14                     | 0.48              |
| 3:A:100:HIS:CE1   | 3:A:117:HIS:CE1   | 3.00                     | 0.48              |
| 3:H:324:LYS:C     | 3:D:322:MET:CE    | 2.69                     | 0.48              |
| 3:H:399:ASP:CG    | 3:H:1321:VAL:HG11 | 2.38                     | 0.48              |
| 3:O:646:ARG:HH22  | 3:O:889:PRO:HG2   | 1.77                     | 0.48              |
| 3:P:195:LEU:O     | 3:P:198:LEU:N     | 2.39                     | 0.48              |
| 3:P:740:ASP:OD2   | 3:P:801:ARG:NH1   | 2.46                     | 0.48              |
| 3:P:784:LEU:HG    | 3:P:934:HIS:NE2   | 2.28                     | 0.48              |
| 3:P:866:HIS:CG    | 3:P:867:PRO:HD2   | 2.48                     | 0.48              |
| 3:B:578:VAL:H     | 3:B:581:ASN:ND2   | 2.11                     | 0.48              |
| 3:B:631:GLN:HE22  | 3:B:666:ASN:CG    | 2.17                     | 0.48              |
| 3:B:834:ARG:HD3   | 4:g:90:PRO:HD3    | 1.94                     | 0.48              |
| 3:B:947:HIS:HB2   | 4:g:79:PHE:CD1    | 2.48                     | 0.48              |
| 3:B:1248:GLN:HB2  | 3:B:1251:SER:OG   | 2.13                     | 0.48              |
| 3:C:487:TYR:CD1   | 3:C:513:LEU:HD21  | 2.48                     | 0.48              |
| 3:C:1218:LYS:HB3  | 3:C:1221:ASP:CG   | 2.39                     | 0.48              |
| 3:E:790:ARG:NH2   | 4:e:81:GLY:HA3    | 2.28                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:E:827:THR:OG1   | 3:E:960:VAL:HG23  | 2.13                     | 0.48              |
| 3:E:1195:ASP:N    | 3:E:1195:ASP:OD1  | 2.44                     | 0.48              |
| 3:F:293:LEU:O     | 3:F:294:LYS:HD2   | 2.13                     | 0.48              |
| 3:F:426:ALA:HB3   | 3:F:429:HIS:CD2   | 2.49                     | 0.48              |
| 2:R:172:GLU:N     | 5:q:372:ASP:CG    | 2.70                     | 0.48              |
| 2:U:249:GLU:O     | 2:U:253:LEU:N     | 2.46                     | 0.48              |
| 2:3:217:THR:HA    | 2:3:220:ILE:HD12  | 1.95                     | 0.48              |
| 3:I:633:ALA:O     | 3:I:635:HIS:ND1   | 2.38                     | 0.48              |
| 3:K:963:LEU:HD23  | 3:K:1007:VAL:HG22 | 1.95                     | 0.48              |
| 3:M:176:PHE:O     | 3:M:180:THR:HG23  | 2.13                     | 0.48              |
| 3:M:837:ALA:HA    | 4:m:57:GLN:OE1    | 2.12                     | 0.48              |
| 3:A:262:PRO:HD2   | 3:A:1068:ARG:NH1  | 2.28                     | 0.48              |
| 3:A:1032:SER:HB3  | 3:A:1035:ALA:H    | 1.77                     | 0.48              |
| 3:H:639:HIS:HA    | 4:h:79:PHE:HE2    | 1.78                     | 0.48              |
| 3:H:712:PRO:O     | 3:H:719:GLN:NE2   | 2.46                     | 0.48              |
| 3:H:841:ASN:HB3   | 3:H:874:THR:HG22  | 1.95                     | 0.48              |
| 4:j:88:LEU:HD12   | 4:j:89:ARG:N      | 2.28                     | 0.48              |
| 4:p:65:GLY:O      | 4:p:69:ALA:N      | 2.46                     | 0.48              |
| 3:O:605:ALA:HA    | 3:O:1018:ASN:HD21 | 1.78                     | 0.48              |
| 3:P:879:PHE:HD1   | 3:P:884:VAL:HB    | 1.77                     | 0.48              |
| 3:B:424:VAL:HG12  | 3:B:425:PRO:O     | 2.13                     | 0.48              |
| 3:B:466:LEU:HD12  | 3:B:467:MET:HG3   | 1.95                     | 0.48              |
| 3:B:837:ALA:O     | 3:B:840:GLN:N     | 2.46                     | 0.48              |
| 3:C:204:TYR:CD2   | 3:C:219:LEU:HD11  | 2.49                     | 0.48              |
| 5:q:430:CYS:HB2   | 7:u:3119:MET:HE2  | 1.95                     | 0.48              |
| 5:q:531:LEU:HD21  | 5:q:663:PHE:HZ    | 1.79                     | 0.48              |
| 3:E:198:LEU:O     | 3:E:199:LEU:C     | 2.56                     | 0.48              |
| 3:E:1106:TYR:OH   | 3:E:1290:GLU:O    | 2.28                     | 0.48              |
| 3:F:52:VAL:CG2    | 3:G:320:LEU:HD22  | 2.43                     | 0.48              |
| 3:F:1020:LEU:O    | 3:F:1024:LEU:N    | 2.46                     | 0.48              |
| 3:G:550:PHE:C     | 3:G:550:PHE:CD2   | 2.90                     | 0.48              |
| 3:I:769:CYS:O     | 3:I:901:MET:N     | 2.42                     | 0.48              |
| 3:K:86:GLU:O      | 3:K:86:GLU:HG2    | 2.13                     | 0.48              |
| 3:K:460:THR:HA    | 3:K:1129:PHE:CD2  | 2.47                     | 0.48              |
| 3:K:769:CYS:H     | 3:K:786:ASN:CG    | 2.22                     | 0.48              |
| 3:L:1271:SER:OG   | 3:L:1274:PHE:HB2  | 2.14                     | 0.48              |
| 3:M:274:VAL:HG11  | 3:M:376:PHE:CE2   | 2.48                     | 0.48              |
| 3:M:961:HIS:O     | 3:M:964:PHE:N     | 2.46                     | 0.48              |
| 3:M:1051:THR:HG23 | 3:M:1190:THR:HG21 | 1.94                     | 0.48              |
| 3:A:64:THR:HG22   | 3:A:65:LEU:H      | 1.77                     | 0.48              |
| 3:A:234:LEU:HD12  | 3:A:1113:ALA:HB1  | 1.95                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:A:1186:GLU:CD   | 3:A:1272:PRO:HD2  | 2.39                     | 0.48              |
| 3:H:983:LEU:O     | 3:H:987:VAL:HG22  | 2.13                     | 0.48              |
| 4:i:33:GLN:HE21   | 4:i:35:ILE:HD13   | 1.79                     | 0.48              |
| 4:o:51:ARG:HB3    | 4:o:55:ARG:HH12   | 1.77                     | 0.48              |
| 3:O:316:LEU:O     | 3:O:319:ALA:N     | 2.45                     | 0.48              |
| 3:O:532:MET:HE1   | 3:O:1244:PRO:HD3  | 1.96                     | 0.48              |
| 3:O:778:ARG:O     | 3:O:904:ARG:NE    | 2.46                     | 0.48              |
| 3:O:1208:ARG:NH1  | 3:O:1240:ALA:O    | 2.46                     | 0.48              |
| 3:P:219:LEU:O     | 3:P:222:GLU:N     | 2.46                     | 0.48              |
| 3:B:463:HIS:CG    | 3:B:464:PRO:HD2   | 2.48                     | 0.48              |
| 3:C:384:ILE:HG22  | 3:C:385:TYR:N     | 2.28                     | 0.48              |
| 3:C:778:ARG:NH1   | 3:C:782:ARG:HD2   | 2.28                     | 0.48              |
| 3:D:463:HIS:CG    | 3:D:464:PRO:HD2   | 2.48                     | 0.48              |
| 3:D:469:ILE:HD11  | 3:D:547:PHE:CE1   | 2.48                     | 0.48              |
| 3:D:646:ARG:NH1   | 4:d:99:SER:CB     | 2.76                     | 0.48              |
| 3:E:1181:GLN:HB2  | 3:E:1309:VAL:O    | 2.13                     | 0.48              |
| 6:r:15:HIS:HD1    | 6:s:13:TRP:CD1    | 2.31                     | 0.48              |
| 6:s:66:LEU:O      | 6:s:70:ALA:N      | 2.47                     | 0.48              |
| 3:G:505:PHE:HE1   | 3:G:992:PRO:HD3   | 1.78                     | 0.48              |
| 3:G:830:VAL:CA    | 3:G:956:TYR:HE1   | 2.26                     | 0.48              |
| 3:G:1004:GLN:HE21 | 3:G:1008:GLN:HG3  | 1.78                     | 0.48              |
| 2:x:89:ASP:HB3    | 2:y:315:ILE:HG21  | 1.96                     | 0.48              |
| 3:J:103:LEU:HD11  | 3:J:115:PRO:HA    | 1.95                     | 0.48              |
| 3:J:259:VAL:HG23  | 3:J:261:VAL:HG23  | 1.94                     | 0.48              |
| 3:J:402:PHE:CG    | 3:J:1334:ILE:HD11 | 2.48                     | 0.48              |
| 3:J:512:ARG:HA    | 3:J:515:HIS:CD2   | 2.39                     | 0.48              |
| 3:J:778:ARG:O     | 3:J:904:ARG:CZ    | 2.61                     | 0.48              |
| 3:J:857:PRO:HB3   | 3:J:865:LEU:HB2   | 1.95                     | 0.48              |
| 3:K:683:PRO:HD2   | 3:K:686:CYS:HB3   | 1.94                     | 0.48              |
| 3:K:802:PRO:HG3   | 3:L:944:HIS:NE2   | 2.28                     | 0.48              |
| 3:K:1072:ALA:HB3  | 3:K:1100:VAL:HB   | 1.95                     | 0.48              |
| 3:L:11:TYR:CE1    | 3:O:96:GLN:HB3    | 2.48                     | 0.48              |
| 3:L:390:VAL:HG11  | 3:M:104:ILE:HD11  | 1.94                     | 0.48              |
| 3:M:1174:ARG:O    | 3:H:213:ARG:NH2   | 2.47                     | 0.48              |
| 3:A:337:LEU:HD13  | 3:B:348:ARG:HG2   | 1.95                     | 0.48              |
| 3:H:460:THR:HA    | 3:H:1129:PHE:CD2  | 2.47                     | 0.48              |
| 3:N:90:MET:O      | 3:N:126:ARG:NH2   | 2.43                     | 0.48              |
| 3:O:392:TYR:CE2   | 3:O:394:LEU:HB3   | 2.48                     | 0.48              |
| 3:O:879:PHE:CE1   | 3:O:886:VAL:HG21  | 2.48                     | 0.48              |
| 3:P:875:VAL:HG11  | 3:P:891:MET:HE1   | 1.94                     | 0.48              |
| 3:B:88:ALA:HA     | 3:B:126:ARG:NH2   | 2.29                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:B:261:VAL:C     | 3:G:60:SER:HA     | 2.31                     | 0.48              |
| 3:C:708:THR:CG2   | 3:C:723:ASN:HD22  | 2.20                     | 0.48              |
| 3:C:1050:PHE:HA   | 3:C:1188:ILE:O    | 2.14                     | 0.48              |
| 3:C:1335:THR:N    | 3:C:1365:ASP:HB3  | 2.28                     | 0.48              |
| 3:F:1176:GLY:N    | 3:G:1225:LEU:HD21 | 2.28                     | 0.48              |
| 3:F:1357:HIS:O    | 3:F:1358:PHE:C    | 2.56                     | 0.48              |
| 3:G:496:GLY:HA3   | 3:G:504:ARG:HH22  | 1.79                     | 0.48              |
| 3:G:752:ARG:HA    | 3:G:913:ALA:HB3   | 1.96                     | 0.48              |
| 3:G:802:PRO:CD    | 3:G:805:TRP:HB2   | 2.42                     | 0.48              |
| 7:u:3095:GLN:HG2  | 7:u:3098:ARG:NH2  | 2.28                     | 0.48              |
| 1:T:117:THR:O     | 1:T:121:GLN:NE2   | 2.46                     | 0.48              |
| 1:T:258:ASP:HB3   | 3:I:1318:ARG:HD2  | 1.95                     | 0.48              |
| 1:W:149:PRO:HD2   | 1:W:152:ARG:HD2   | 1.96                     | 0.48              |
| 2:x:18:ARG:CG     | 3:O:7:ASP:OD2     | 2.49                     | 0.48              |
| 3:J:668:TYR:HD2   | 3:J:809:HIS:CE1   | 2.32                     | 0.48              |
| 3:J:873:ASN:HB2   | 4:i:89:ARG:HH12   | 1.77                     | 0.48              |
| 3:K:506:LEU:O     | 3:K:510:ARG:N     | 2.47                     | 0.48              |
| 3:K:812:TYR:CD1   | 3:K:816:LEU:HD12  | 2.48                     | 0.48              |
| 3:K:1011:ARG:HG3  | 3:K:1012:GLU:HG3  | 1.94                     | 0.48              |
| 3:L:279:VAL:HG12  | 3:L:394:LEU:HD22  | 1.96                     | 0.48              |
| 3:L:1128:ASN:HD21 | 3:L:1155:ASN:CG   | 2.22                     | 0.48              |
| 3:L:1129:PHE:O    | 3:L:1132:GLY:N    | 2.47                     | 0.48              |
| 3:M:39:PHE:CE1    | 3:D:120:MET:HE2   | 2.49                     | 0.48              |
| 3:M:122:LYS:NZ    | 3:M:1101:ASP:O    | 2.33                     | 0.48              |
| 3:A:842:MET:HE1   | 3:A:891:MET:HE3   | 1.96                     | 0.48              |
| 3:A:866:HIS:HB3   | 3:A:869:ASN:ND2   | 2.29                     | 0.48              |
| 3:A:1050:PHE:HA   | 3:A:1188:ILE:O    | 2.14                     | 0.48              |
| 3:H:493:ALA:N     | 3:H:559:PRO:HB2   | 2.28                     | 0.48              |
| 3:H:496:GLY:HA3   | 3:H:504:ARG:NH1   | 2.29                     | 0.48              |
| 3:H:505:PHE:CD1   | 3:H:992:PRO:HD2   | 2.48                     | 0.48              |
| 4:j:58:ALA:HA     | 4:j:61:LEU:HD12   | 1.95                     | 0.48              |
| 4:l:58:ALA:HA     | 4:l:61:LEU:HD12   | 1.94                     | 0.48              |
| 3:N:300:ALA:HB2   | 3:N:367:LEU:HD11  | 1.95                     | 0.48              |
| 3:N:634:ILE:HG22  | 3:N:636:GLY:H     | 1.78                     | 0.48              |
| 3:O:399:ASP:OD1   | 3:O:1057:ARG:HG2  | 2.13                     | 0.48              |
| 3:O:870:LEU:HD22  | 3:O:877:ALA:HA    | 1.96                     | 0.48              |
| 3:O:1334:ILE:HG22 | 3:O:1335:THR:N    | 2.29                     | 0.48              |
| 3:P:244:ILE:O     | 3:P:247:TRP:N     | 2.45                     | 0.48              |
| 3:P:708:THR:CG2   | 3:P:723:ASN:HD22  | 2.25                     | 0.48              |
| 3:B:195:LEU:O     | 3:B:198:LEU:N     | 2.36                     | 0.48              |
| 3:B:243:ALA:O     | 3:B:246:ALA:N     | 2.46                     | 0.48              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:B:268:ASP:OD2  | 3:B:272:ARG:HB3   | 2.14                     | 0.48              |
| 3:B:950:GLN:HG3  | 4:g:80:ALA:CB     | 2.44                     | 0.48              |
| 3:C:392:TYR:CE2  | 3:C:394:LEU:HB3   | 2.48                     | 0.48              |
| 3:C:398:MET:O    | 3:C:1057:ARG:HA   | 2.13                     | 0.48              |
| 3:C:668:TYR:HD2  | 3:C:809:HIS:CE1   | 2.31                     | 0.48              |
| 3:E:505:PHE:CD1  | 3:E:992:PRO:HD3   | 2.48                     | 0.48              |
| 3:E:642:CYS:HA   | 3:E:645:ALA:HB2   | 1.94                     | 0.48              |
| 3:E:790:ARG:NH1  | 4:e:80:ALA:O      | 2.46                     | 0.48              |
| 3:F:1262:HIS:CE1 | 3:F:1265:GLY:HA3  | 2.48                     | 0.48              |
| 2:S:306:VAL:HG11 | 2:S:312:ALA:HB2   | 1.93                     | 0.48              |
| 1:W:25:ARG:HA    | 3:H:145:GLY:C     | 2.30                     | 0.48              |
| 2:x:162:ASP:OD2  | 2:x:199:ASN:ND2   | 2.47                     | 0.48              |
| 3:I:86:GLU:O     | 3:I:86:GLU:HG2    | 2.13                     | 0.48              |
| 3:I:166:ALA:HB1  | 3:J:346:ALA:HB2   | 1.96                     | 0.48              |
| 3:J:198:LEU:HD21 | 3:J:1106:TYR:CD2  | 2.49                     | 0.48              |
| 3:J:634:ILE:HG22 | 3:J:636:GLY:H     | 1.79                     | 0.48              |
| 3:K:1170:GLN:OE1 | 3:K:1170:GLN:N    | 2.46                     | 0.48              |
| 3:L:116:VAL:HG12 | 3:L:117:HIS:N     | 2.28                     | 0.48              |
| 3:L:142:LEU:HD23 | 3:L:147:ALA:HB3   | 1.96                     | 0.48              |
| 3:L:512:ARG:HA   | 3:L:515:HIS:CD2   | 2.45                     | 0.48              |
| 3:L:842:MET:HE2  | 3:L:891:MET:HB3   | 1.94                     | 0.48              |
| 3:M:778:ARG:HG2  | 3:M:904:ARG:HH12  | 1.79                     | 0.48              |
| 3:A:182:ASP:O    | 3:A:186:HIS:N     | 2.36                     | 0.48              |
| 3:A:195:LEU:HD21 | 3:A:251:LEU:HD23  | 1.96                     | 0.48              |
| 3:A:603:ARG:HD3  | 3:A:703:LEU:HD21  | 1.96                     | 0.48              |
| 3:A:722:LEU:O    | 3:A:1030:LYS:HD2  | 2.14                     | 0.48              |
| 4:n:80:ALA:H     | 3:O:948:THR:HA    | 1.79                     | 0.48              |
| 3:N:326:VAL:CG2  | 3:E:321:VAL:HG11  | 2.27                     | 0.48              |
| 3:O:600:GLY:C    | 3:O:602:GLY:H     | 2.22                     | 0.48              |
| 3:P:278:LEU:HG   | 3:P:375:VAL:HG11  | 1.95                     | 0.48              |
| 3:P:594:ALA:O    | 3:P:598:GLU:HB2   | 2.14                     | 0.48              |
| 3:C:865:LEU:HD11 | 3:C:886:VAL:H     | 1.79                     | 0.48              |
| 3:C:879:PHE:HD1  | 3:C:884:VAL:HB    | 1.77                     | 0.48              |
| 3:D:677:TYR:HA   | 4:d:95:LYS:HZ2    | 1.78                     | 0.48              |
| 5:q:251:VAL:O    | 5:q:254:THR:OG1   | 2.28                     | 0.48              |
| 3:E:79:CYS:HB3   | 3:E:81:CYS:SG     | 2.54                     | 0.48              |
| 3:E:399:ASP:CG   | 3:E:1321:VAL:HG11 | 2.39                     | 0.48              |
| 3:E:600:GLY:O    | 3:E:602:GLY:N     | 2.47                     | 0.48              |
| 3:E:749:ASP:CG   | 3:E:752:ARG:H     | 2.21                     | 0.48              |
| 3:F:1181:GLN:HB2 | 3:F:1309:VAL:O    | 2.14                     | 0.48              |
| 1:Q:466:ALA:O    | 2:S:281:HIS:NE2   | 2.40                     | 0.48              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:R:219:LEU:HD21 | 2:S:246:VAL:HG21  | 1.95                     | 0.48              |
| 2:Y:57:SER:O     | 2:Y:194:GLN:NE2   | 2.46                     | 0.48              |
| 1:w:181:ARG:NH2  | 3:O:1167:GLY:HA2  | 2.28                     | 0.48              |
| 3:I:834:ARG:HD3  | 4:h:90:PRO:HD3    | 1.96                     | 0.48              |
| 3:I:1206:ARG:NH2 | 3:I:1210:ALA:HB2  | 2.29                     | 0.48              |
| 3:J:86:GLU:HB2   | 3:J:89:TYR:HD2    | 1.79                     | 0.48              |
| 3:J:1342:LEU:CD2 | 3:J:1362:LEU:HB2  | 2.43                     | 0.48              |
| 3:K:392:TYR:CE2  | 3:K:394:LEU:HB3   | 2.49                     | 0.48              |
| 3:K:490:TYR:CD1  | 3:K:564:PRO:HB3   | 2.49                     | 0.48              |
| 3:K:769:CYS:N    | 3:K:786:ASN:OD1   | 2.47                     | 0.48              |
| 3:K:829:GLY:HA3  | 3:K:956:TYR:CZ    | 2.49                     | 0.48              |
| 3:L:682:LEU:HD12 | 3:L:687:MET:SD    | 2.53                     | 0.48              |
| 3:L:1156:ARG:NH2 | 3:L:1182:ASP:OD2  | 2.46                     | 0.48              |
| 3:M:20:THR:O     | 3:D:350:THR:CG2   | 2.56                     | 0.48              |
| 3:M:286:GLN:O    | 3:M:289:LEU:N     | 2.46                     | 0.48              |
| 3:M:861:PRO:HA   | 3:M:866:HIS:CG    | 2.48                     | 0.48              |
| 3:A:121:THR:HG23 | 3:G:48:SER:CB     | 2.38                     | 0.48              |
| 3:A:441:PHE:CE2  | 3:A:1340:PRO:HD3  | 2.49                     | 0.48              |
| 3:H:622:SER:HA   | 3:H:943:GLN:NE2   | 2.28                     | 0.48              |
| 3:H:865:LEU:HD21 | 3:H:879:PHE:CD2   | 2.49                     | 0.48              |
| 3:N:776:PHE:HD2  | 3:N:833:ASP:OD1   | 1.97                     | 0.48              |
| 3:O:621:ARG:C    | 3:O:943:GLN:HE21  | 2.21                     | 0.48              |
| 3:O:675:VAL:HG21 | 3:O:694:VAL:HG21  | 1.94                     | 0.48              |
| 3:O:765:TYR:CD1  | 3:O:783:LEU:HD12  | 2.48                     | 0.48              |
| 3:P:578:VAL:HB   | 3:P:1027:GLY:O    | 2.13                     | 0.48              |
| 3:B:1004:GLN:NE2 | 3:B:1007:VAL:HB   | 2.28                     | 0.48              |
| 3:C:687:MET:O    | 3:C:690:TYR:N     | 2.47                     | 0.48              |
| 3:D:142:LEU:HD23 | 3:D:147:ALA:HB3   | 1.96                     | 0.48              |
| 3:D:963:LEU:HD23 | 3:D:1007:VAL:HG22 | 1.96                     | 0.48              |
| 3:D:1251:SER:O   | 3:D:1255:LEU:HG   | 2.14                     | 0.48              |
| 3:F:189:LEU:HD23 | 3:F:1064:LEU:HD21 | 1.96                     | 0.48              |
| 3:F:637:SER:HA   | 3:F:787:THR:HB    | 1.94                     | 0.48              |
| 3:F:739:CYS:O    | 3:F:743:MET:HG2   | 2.14                     | 0.48              |
| 3:G:497:PRO:CD   | 3:G:504:ARG:HH22  | 2.26                     | 0.48              |
| 3:G:647:LEU:O    | 3:G:651:CYS:N     | 2.45                     | 0.48              |
| 3:G:793:ASP:OD1  | 3:G:798:ARG:NH2   | 2.46                     | 0.48              |
| 1:l:138:THR:C    | 3:M:1166:PHE:CZ   | 2.90                     | 0.48              |
| 1:w:283:ARG:HE   | 3:N:47:ASN:HD22   | 0.49                     | 0.48              |
| 3:I:124:ILE:HD11 | 3:H:58:LEU:HD12   | 1.96                     | 0.48              |
| 3:I:380:LEU:O    | 3:I:383:ARG:N     | 2.47                     | 0.48              |
| 3:I:579:ASN:HD22 | 3:I:595:ARG:HH12  | 1.61                     | 0.48              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:L:524:CYS:CB   | 3:L:1008:GLN:HE22 | 2.27                     | 0.48              |
| 3:M:506:LEU:O    | 3:M:510:ARG:HG3   | 2.13                     | 0.48              |
| 3:H:96:GLN:HE22  | 3:C:12:ARG:CB     | 2.13                     | 0.48              |
| 3:H:204:TYR:CG   | 3:H:219:LEU:HD11  | 2.49                     | 0.48              |
| 3:H:392:TYR:CE2  | 3:H:394:LEU:HB3   | 2.49                     | 0.48              |
| 3:H:544:HIS:CG   | 3:H:545:PRO:HD2   | 2.48                     | 0.48              |
| 3:H:725:LEU:HD23 | 3:H:1028:TYR:HD1  | 1.79                     | 0.48              |
| 3:H:842:MET:HE2  | 3:H:891:MET:HB3   | 1.96                     | 0.48              |
| 3:H:1191:PRO:HG2 | 3:H:1194:THR:HG23 | 1.96                     | 0.48              |
| 4:h:61:LEU:O     | 4:h:65:GLY:N      | 2.43                     | 0.48              |
| 3:N:118:ASN:ND2  | 3:D:29:VAL:HB     | 2.28                     | 0.48              |
| 3:N:729:PRO:HB2  | 3:N:748:LEU:HD11  | 1.96                     | 0.48              |
| 3:N:888:GLY:O    | 3:N:891:MET:HB2   | 2.14                     | 0.48              |
| 3:N:1013:SER:OG  | 3:N:1020:LEU:HD21 | 2.14                     | 0.48              |
| 3:B:492:ALA:H    | 3:B:992:PRO:HB2   | 1.79                     | 0.48              |
| 3:B:601:VAL:O    | 3:B:601:VAL:HG12  | 2.14                     | 0.48              |
| 3:D:42:VAL:C     | 3:D:43:ARG:O      | 2.46                     | 0.48              |
| 5:q:504:ILE:HB   | 6:s:26:PHE:HE1    | 1.77                     | 0.48              |
| 3:E:163:GLN:HE22 | 3:F:339:MET:HE3   | 1.79                     | 0.48              |
| 3:E:675:VAL:HG12 | 3:F:621:ARG:HB2   | 1.96                     | 0.48              |
| 3:F:433:ARG:O    | 3:F:1359:THR:OG1  | 2.32                     | 0.48              |
| 3:G:1241:THR:OG1 | 3:G:1242:ALA:N    | 2.47                     | 0.48              |
| 3:I:424:VAL:HG12 | 3:I:425:PRO:O     | 2.14                     | 0.48              |
| 3:I:784:LEU:HB2  | 3:I:786:ASN:CG    | 2.38                     | 0.48              |
| 3:J:627:PHE:HD1  | 3:J:664:PHE:CZ    | 2.31                     | 0.48              |
| 3:J:853:CYS:HB2  | 4:j:101:PHE:CD1   | 2.49                     | 0.48              |
| 3:J:1248:GLN:N   | 3:J:1251:SER:OG   | 2.47                     | 0.48              |
| 3:K:920:THR:O    | 3:K:923:THR:N     | 2.45                     | 0.48              |
| 3:L:776:PHE:O    | 3:L:904:ARG:HD3   | 2.13                     | 0.48              |
| 3:M:46:GLU:OE1   | 3:M:48:SER:N      | 2.47                     | 0.48              |
| 3:M:452:LEU:HD13 | 3:M:1124:ASN:HB2  | 1.95                     | 0.48              |
| 3:M:463:HIS:CG   | 3:M:464:PRO:HD2   | 2.49                     | 0.48              |
| 3:M:1083:HIS:O   | 3:M:1090:ASN:N    | 2.34                     | 0.48              |
| 3:A:119:TYR:HD2  | 3:G:44:SER:HB2    | 1.79                     | 0.48              |
| 3:A:524:CYS:HB3  | 3:A:1008:GLN:HE22 | 1.79                     | 0.48              |
| 3:A:894:LEU:HG   | 3:A:897:LEU:HD12  | 1.95                     | 0.48              |
| 3:H:77:VAL:HG22  | 3:H:266:HIS:CD2   | 2.48                     | 0.48              |
| 3:H:601:VAL:HG12 | 3:H:601:VAL:O     | 2.13                     | 0.48              |
| 3:H:683:PRO:HD2  | 3:H:686:CYS:HB3   | 1.96                     | 0.48              |
| 3:H:769:CYS:SG   | 3:H:786:ASN:ND2   | 2.80                     | 0.48              |
| 3:O:23:ILE:HG22  | 3:O:25:SER:H      | 1.79                     | 0.48              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:O:85:PRO:HG2   | 3:O:86:GLU:OE1    | 2.13                     | 0.48              |
| 3:O:266:HIS:CE1  | 3:O:303:PRO:HD2   | 2.48                     | 0.48              |
| 3:O:718:ALA:HB3  | 3:O:721:GLU:HG3   | 1.95                     | 0.48              |
| 3:O:887:ASP:O    | 3:O:891:MET:HG2   | 2.13                     | 0.48              |
| 3:P:135:LEU:HD21 | 3:P:165:LEU:HD21  | 1.95                     | 0.48              |
| 3:P:201:MET:O    | 3:P:204:TYR:N     | 2.47                     | 0.48              |
| 3:B:494:PRO:HD3  | 3:B:909:LEU:HD12  | 1.94                     | 0.48              |
| 3:B:605:ALA:HA   | 3:B:1018:ASN:HD21 | 1.78                     | 0.48              |
| 3:B:898:ALA:HA   | 3:B:901:MET:HE2   | 1.96                     | 0.48              |
| 3:B:980:LEU:O    | 3:B:983:LEU:N     | 2.47                     | 0.48              |
| 3:C:326:VAL:HB   | 3:C:329:LEU:HD12  | 1.95                     | 0.48              |
| 3:C:490:TYR:CD1  | 3:C:564:PRO:HB3   | 2.49                     | 0.48              |
| 3:C:873:ASN:OD1  | 4:b:92:PHE:CA     | 2.62                     | 0.48              |
| 3:C:1254:ASP:HB3 | 3:C:1258:ASN:ND2  | 2.29                     | 0.48              |
| 3:D:432:PRO:HA   | 3:D:435:PHE:CE2   | 2.49                     | 0.48              |
| 3:D:769:CYS:O    | 3:D:901:MET:N     | 2.45                     | 0.48              |
| 3:D:950:GLN:HB2  | 3:D:953:GLU:CG    | 2.43                     | 0.48              |
| 3:E:643:ALA:CB   | 4:e:78:MET:HE1    | 2.43                     | 0.48              |
| 3:E:769:CYS:HB2  | 3:E:901:MET:O     | 2.14                     | 0.48              |
| 6:r:79:ASP:CG    | 7:t:3106:ARG:HH11 | 2.22                     | 0.48              |
| 3:F:631:GLN:HE22 | 3:F:666:ASN:CG    | 2.19                     | 0.48              |
| 3:F:1355:GLU:HA  | 3:F:1362:LEU:HB3  | 1.96                     | 0.48              |
| 3:G:488:GLY:HA2  | 3:G:996:ALA:HB1   | 1.95                     | 0.48              |
| 2:Y:154:ARG:NH1  | 2:Y:176:LEU:O     | 2.44                     | 0.47              |
| 2:y:204:SER:O    | 2:y:208:ASN:ND2   | 2.47                     | 0.47              |
| 3:I:749:ASP:O    | 3:I:752:ARG:N     | 2.47                     | 0.47              |
| 3:I:871:VAL:HG11 | 4:i:26:VAL:HG12   | 1.96                     | 0.47              |
| 3:I:1215:ALA:HA  | 3:I:1225:LEU:HD11 | 1.96                     | 0.47              |
| 3:J:463:HIS:HD2  | 3:J:465:SER:HB3   | 1.79                     | 0.47              |
| 3:K:56:ALA:HA    | 3:L:325:ALA:O     | 2.14                     | 0.47              |
| 3:K:426:ALA:HB3  | 3:K:429:HIS:CD2   | 2.49                     | 0.47              |
| 3:L:469:ILE:O    | 3:L:472:ALA:N     | 2.45                     | 0.47              |
| 3:L:469:ILE:HD11 | 3:L:547:PHE:CE2   | 2.49                     | 0.47              |
| 3:L:884:VAL:HG12 | 3:L:886:VAL:HG23  | 1.95                     | 0.47              |
| 3:M:44:SER:HB2   | 3:D:115:PRO:HG2   | 1.96                     | 0.47              |
| 3:M:1191:PRO:HG2 | 3:M:1194:THR:HG23 | 1.96                     | 0.47              |
| 3:H:829:GLY:HA3  | 3:H:956:TYR:CZ    | 2.48                     | 0.47              |
| 3:H:954:TYR:CE1  | 4:m:90:PRO:HG3    | 2.49                     | 0.47              |
| 3:H:1248:GLN:C   | 3:H:1251:SER:HG   | 2.17                     | 0.47              |
| 4:j:61:LEU:O     | 4:j:65:GLY:N      | 2.40                     | 0.47              |
| 3:N:1201:ARG:HB2 | 3:N:1202:PRO:HD2  | 1.95                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:O:698:GLU:OE1   | 3:P:621:ARG:NH2   | 2.47                     | 0.47              |
| 3:O:1058:PHE:HE2  | 3:O:1369:LEU:HD11 | 1.78                     | 0.47              |
| 3:P:403:VAL:HG22  | 3:P:1053:VAL:HG22 | 1.95                     | 0.47              |
| 3:P:752:ARG:HG3   | 3:P:913:ALA:H     | 1.79                     | 0.47              |
| 3:B:668:TYR:HD2   | 3:B:809:HIS:CE1   | 2.32                     | 0.47              |
| 3:B:718:ALA:HB1   | 3:C:982:ASP:OD2   | 2.14                     | 0.47              |
| 3:C:274:VAL:HG11  | 3:C:376:PHE:CE2   | 2.49                     | 0.47              |
| 3:D:172:VAL:O     | 3:D:175:ALA:N     | 2.43                     | 0.47              |
| 5:q:488:ARG:HG2   | 6:s:43:ILE:HB     | 1.96                     | 0.47              |
| 5:q:526:ARG:NH1   | 6:r:39:PRO:HD3    | 2.29                     | 0.47              |
| 3:E:644:LEU:HD22  | 3:E:647:LEU:HD12  | 1.96                     | 0.47              |
| 1:1:260:LEU:HD23  | 3:M:1316:GLY:HA2  | 1.95                     | 0.47              |
| 3:I:830:VAL:HG13  | 3:I:955:PHE:HE1   | 1.79                     | 0.47              |
| 3:J:439:GLN:HG2   | 3:J:453:SER:HA    | 1.96                     | 0.47              |
| 3:K:539:LEU:O     | 3:K:542:GLU:N     | 2.36                     | 0.47              |
| 3:K:610:THR:HG21  | 3:K:692:ASP:OD2   | 2.13                     | 0.47              |
| 3:K:750:ARG:O     | 3:K:753:ASP:HB3   | 2.13                     | 0.47              |
| 3:K:867:PRO:HA    | 3:K:870:LEU:HD12  | 1.96                     | 0.47              |
| 3:L:399:ASP:CG    | 3:L:1321:VAL:HG11 | 2.39                     | 0.47              |
| 3:L:440:LEU:HD13  | 3:L:1336:CYS:SG   | 2.54                     | 0.47              |
| 3:L:462:CYS:SG    | 3:L:1147:LEU:HD22 | 2.54                     | 0.47              |
| 3:L:506:LEU:O     | 3:L:510:ARG:HG3   | 2.14                     | 0.47              |
| 3:L:836:TYR:CE1   | 3:L:897:LEU:HD22  | 2.47                     | 0.47              |
| 3:M:50:TYR:OH     | 3:C:161:ALA:HA    | 2.14                     | 0.47              |
| 3:M:259:VAL:HG12  | 3:N:23:ILE:HG12   | 1.97                     | 0.47              |
| 3:M:752:ARG:NH2   | 3:M:915:ASP:HA    | 2.28                     | 0.47              |
| 3:M:827:THR:OG1   | 3:M:958:LEU:O     | 2.26                     | 0.47              |
| 3:A:887:ASP:O     | 3:A:891:MET:HG2   | 2.14                     | 0.47              |
| 3:H:873:ASN:OD1   | 4:m:92:PHE:N      | 2.47                     | 0.47              |
| 3:H:1196:ILE:O    | 3:H:1199:PHE:N    | 2.36                     | 0.47              |
| 3:N:866:HIS:HD2   | 3:N:868:ALA:HB3   | 1.79                     | 0.47              |
| 3:N:1243:ASN:HD22 | 3:N:1246:ALA:HB3  | 1.79                     | 0.47              |
| 3:O:194:PRO:HA    | 3:O:1110:ALA:O    | 2.15                     | 0.47              |
| 3:O:1227:TYR:CD1  | 3:O:1249:ARG:HB2  | 2.49                     | 0.47              |
| 3:P:1128:ASN:HD21 | 3:P:1155:ASN:CG   | 2.21                     | 0.47              |
| 3:C:691:ARG:NH1   | 3:D:620:ASP:OD1   | 2.47                     | 0.47              |
| 3:C:839:LEU:O     | 3:C:875:VAL:HG21  | 2.14                     | 0.47              |
| 3:D:454:MET:HE3   | 3:D:1045:HIS:ND1  | 2.29                     | 0.47              |
| 3:D:577:VAL:O     | 3:D:1031:MET:N    | 2.36                     | 0.47              |
| 3:D:771:VAL:HG23  | 3:D:898:ALA:O     | 2.14                     | 0.47              |
| 3:D:1000:SER:O    | 3:D:1003:ARG:NH1  | 2.47                     | 0.47              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 5:q:510:TYR:HE1  | 5:q:644:GLU:HG2   | 1.80                     | 0.47              |
| 3:E:189:LEU:HD23 | 3:E:1064:LEU:HD21 | 1.95                     | 0.47              |
| 3:E:214:VAL:O    | 3:E:217:ALA:N     | 2.47                     | 0.47              |
| 3:E:580:GLY:HA2  | 3:E:592:ARG:NH1   | 2.28                     | 0.47              |
| 3:E:1004:GLN:NE2 | 3:E:1007:VAL:HB   | 2.29                     | 0.47              |
| 3:E:1067:GLU:O   | 3:E:1068:ARG:C    | 2.57                     | 0.47              |
| 3:F:826:CYS:HB3  | 3:F:966:GLY:N     | 2.28                     | 0.47              |
| 3:F:1215:ALA:O   | 3:F:1287:ARG:NH2  | 2.39                     | 0.47              |
| 1:Q:307:ALA:HB3  | 2:S:37:ILE:HD12   | 1.96                     | 0.47              |
| 3:I:279:VAL:HG12 | 3:I:394:LEU:HD22  | 1.96                     | 0.47              |
| 3:I:873:ASN:HB3  | 4:h:89:ARG:NH1    | 2.21                     | 0.47              |
| 3:J:630:LEU:O    | 3:J:634:ILE:HD12  | 2.14                     | 0.47              |
| 3:J:1336:CYS:O   | 3:J:1362:LEU:HG   | 2.14                     | 0.47              |
| 3:K:435:PHE:O    | 3:K:1359:THR:OG1  | 2.28                     | 0.47              |
| 3:K:1051:THR:OG1 | 3:K:1188:ILE:HB   | 2.14                     | 0.47              |
| 3:L:238:GLY:CA   | 3:L:244:ILE:HD11  | 2.39                     | 0.47              |
| 3:M:576:ARG:NH1  | 3:M:582:LEU:HD23  | 2.29                     | 0.47              |
| 3:M:721:GLU:HG2  | 3:M:727:ARG:HB3   | 1.96                     | 0.47              |
| 3:M:1226:MET:HE1 | 3:M:1282:ILE:HD13 | 1.97                     | 0.47              |
| 3:A:907:ALA:HA   | 3:A:933:LEU:HD23  | 1.95                     | 0.47              |
| 3:H:490:TYR:CD1  | 3:H:564:PRO:HB3   | 2.48                     | 0.47              |
| 4:n:68:HIS:CD2   | 3:N:892:LEU:HD21  | 2.49                     | 0.47              |
| 3:N:322:MET:HE3  | 3:E:324:LYS:CD    | 2.44                     | 0.47              |
| 3:N:440:LEU:HD13 | 3:N:1336:CYS:SG   | 2.55                     | 0.47              |
| 3:N:1148:ARG:NH2 | 3:N:1163:LEU:HG   | 2.28                     | 0.47              |
| 3:O:830:VAL:HG22 | 3:O:955:PHE:HD1   | 1.78                     | 0.47              |
| 3:P:490:TYR:CG   | 3:P:564:PRO:HB3   | 2.50                     | 0.47              |
| 3:P:838:THR:O    | 3:P:875:VAL:HG22  | 2.14                     | 0.47              |
| 3:P:875:VAL:HG12 | 3:P:879:PHE:CE2   | 2.49                     | 0.47              |
| 3:P:960:VAL:HA   | 3:P:994:LEU:HD13  | 1.96                     | 0.47              |
| 3:D:1202:PRO:HB3 | 3:D:1332:TYR:HD1  | 1.79                     | 0.47              |
| 3:E:400:LEU:HD12 | 3:E:1058:PHE:CE2  | 2.50                     | 0.47              |
| 3:E:755:ARG:O    | 3:E:910:CYS:HA    | 2.15                     | 0.47              |
| 3:E:1334:ILE:HA  | 3:E:1365:ASP:HB3  | 1.96                     | 0.47              |
| 3:F:448:GLN:CB   | 3:G:1201:ARG:NH1  | 2.77                     | 0.47              |
| 3:F:469:ILE:HD11 | 3:F:547:PHE:CZ    | 2.49                     | 0.47              |
| 3:G:737:TRP:CZ2  | 3:G:937:VAL:HG22  | 2.49                     | 0.47              |
| 1:Q:85:GLN:O     | 1:Q:89:LYS:N      | 2.47                     | 0.47              |
| 2:S:39:ARG:NH1   | 3:B:1083:HIS:CD2  | 2.82                     | 0.47              |
| 1:W:191:VAL:HB   | 1:W:207:VAL:HG11  | 1.95                     | 0.47              |
| 1:I:78:ALA:HB3   | 3:M:308:GLU:OE1   | 2.14                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:I:227:PHE:O     | 3:I:231:SER:OG    | 2.25                     | 0.47              |
| 3:I:863:HIS:CD2   | 3:I:865:LEU:HB2   | 2.49                     | 0.47              |
| 3:I:1081:ALA:HB3  | 3:I:1092:THR:OG1  | 2.15                     | 0.47              |
| 3:I:1198:TYR:OH   | 3:I:1204:ASN:O    | 2.24                     | 0.47              |
| 3:J:405:PRO:O     | 3:J:440:LEU:HD11  | 2.14                     | 0.47              |
| 3:J:784:LEU:HG    | 3:J:934:HIS:NE2   | 2.29                     | 0.47              |
| 3:J:887:ASP:O     | 3:J:891:MET:HG2   | 2.14                     | 0.47              |
| 3:J:1202:PRO:HB3  | 3:J:1332:TYR:CD1  | 2.49                     | 0.47              |
| 3:L:368:VAL:HG12  | 3:L:370:ILE:HG13  | 1.96                     | 0.47              |
| 3:L:784:LEU:HD13  | 3:L:786:ASN:CG    | 2.40                     | 0.47              |
| 3:M:638:GLU:HB2   | 3:M:789:ALA:HA    | 1.96                     | 0.47              |
| 3:M:944:HIS:CE1   | 3:M:972:ASN:HD22  | 2.32                     | 0.47              |
| 3:H:318:THR:O     | 3:H:323:GLY:N     | 2.43                     | 0.47              |
| 3:N:615:ARG:NH2   | 3:N:1017:GLU:HG2  | 2.29                     | 0.47              |
| 3:N:624:PRO:HB2   | 3:N:627:PHE:CD2   | 2.50                     | 0.47              |
| 3:O:132:ALA:HB3   | 3:P:114:GLN:HG2   | 1.95                     | 0.47              |
| 3:P:512:ARG:HH12  | 3:P:564:PRO:HD2   | 1.79                     | 0.47              |
| 3:P:778:ARG:HH12  | 3:P:782:ARG:HD2   | 1.80                     | 0.47              |
| 3:B:354:LEU:HD12  | 3:G:58:LEU:HD13   | 1.97                     | 0.47              |
| 3:B:711:GLY:HA3   | 3:B:719:GLN:HE21  | 1.80                     | 0.47              |
| 3:B:861:PRO:HA    | 3:B:866:HIS:CD2   | 2.49                     | 0.47              |
| 3:B:1344:ARG:HH12 | 3:C:1356:THR:HG23 | 1.80                     | 0.47              |
| 3:C:398:MET:SD    | 3:C:1322:GLU:HG3  | 2.54                     | 0.47              |
| 3:C:512:ARG:HA    | 3:C:515:HIS:CD2   | 2.47                     | 0.47              |
| 3:D:58:LEU:HD12   | 3:E:124:ILE:HD11  | 1.96                     | 0.47              |
| 3:D:408:LEU:HD11  | 3:D:1199:PHE:HE2  | 1.79                     | 0.47              |
| 3:D:593:ASP:O     | 3:D:596:GLY:N     | 2.47                     | 0.47              |
| 3:D:958:LEU:HA    | 3:D:958:LEU:HD23  | 1.61                     | 0.47              |
| 5:q:80:TYR:CE1    | 5:q:109:GLY:HA2   | 2.49                     | 0.47              |
| 5:q:110:LEU:HD13  | 5:q:112:VAL:HG23  | 1.96                     | 0.47              |
| 3:E:310:VAL:HG12  | 3:E:312:ASN:H     | 1.79                     | 0.47              |
| 3:F:14:ALA:HB1    | 3:G:321:VAL:CG2   | 2.42                     | 0.47              |
| 3:F:52:VAL:HG22   | 3:G:320:LEU:HD22  | 1.96                     | 0.47              |
| 3:F:1176:GLY:O    | 3:G:1234:PRO:HB3  | 2.14                     | 0.47              |
| 3:G:406:LEU:HD12  | 3:G:1050:PHE:HB2  | 1.95                     | 0.47              |
| 3:G:454:MET:O     | 3:G:455:GLU:C     | 2.52                     | 0.47              |
| 3:G:666:ASN:HB3   | 3:G:938:LEU:HD21  | 1.97                     | 0.47              |
| 1:Q:317:ARG:NH1   | 1:Q:322:GLN:O     | 2.48                     | 0.47              |
| 1:T:280:GLY:O     | 3:H:51:ASP:CA     | 2.62                     | 0.47              |
| 2:V:195:LEU:O     | 2:V:199:ASN:ND2   | 2.48                     | 0.47              |
| 2:2:58:PRO:HG2    | 2:2:63:LEU:HD13   | 1.95                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:J:485:ASN:ND2  | 3:J:516:GLY:C    | 2.73                     | 0.47              |
| 3:J:601:VAL:O    | 3:J:601:VAL:HG12 | 2.15                     | 0.47              |
| 3:J:790:ARG:NH2  | 3:J:793:ASP:HB2  | 2.30                     | 0.47              |
| 3:J:950:GLN:HG3  | 4:i:80:ALA:HB3   | 1.95                     | 0.47              |
| 3:M:214:VAL:O    | 3:M:217:ALA:N    | 2.48                     | 0.47              |
| 3:M:502:GLN:O    | 3:M:505:PHE:HB3  | 2.15                     | 0.47              |
| 3:M:866:HIS:HD2  | 3:M:868:ALA:HB3  | 1.79                     | 0.47              |
| 4:p:57:GLN:NE2   | 3:P:841:ASN:OD1  | 2.47                     | 0.47              |
| 3:N:485:ASN:ND2  | 3:N:516:GLY:H    | 2.09                     | 0.47              |
| 3:N:876:ASN:HA   | 3:N:879:PHE:CD2  | 2.39                     | 0.47              |
| 3:O:309:MET:HE1  | 3:O:327:ARG:HA   | 1.96                     | 0.47              |
| 3:O:942:PRO:HA   | 3:O:969:HIS:CE1  | 2.50                     | 0.47              |
| 3:O:1044:LEU:O   | 3:O:1046:PRO:HD3 | 2.15                     | 0.47              |
| 3:B:95:VAL:O     | 3:B:121:THR:HA   | 2.14                     | 0.47              |
| 3:B:1205:PRO:HG2 | 3:B:1276:PHE:CE2 | 2.49                     | 0.47              |
| 3:C:873:ASN:HA   | 4:b:92:PHE:CB    | 2.39                     | 0.47              |
| 3:D:1155:ASN:OD1 | 3:D:1156:ARG:N   | 2.47                     | 0.47              |
| 3:E:383:ARG:HB2  | 3:E:384:ILE:HD12 | 1.96                     | 0.47              |
| 3:E:542:GLU:HG3  | 3:E:1245:TRP:HE1 | 1.79                     | 0.47              |
| 3:E:641:PHE:O    | 3:E:645:ALA:N    | 2.47                     | 0.47              |
| 3:F:368:VAL:HG12 | 3:F:370:ILE:HG13 | 1.97                     | 0.47              |
| 3:G:923:THR:HA   | 3:G:926:MET:HE3  | 1.96                     | 0.47              |
| 1:W:199:ASP:CB   | 6:r:17:ARG:C     | 2.87                     | 0.47              |
| 2:3:38:ARG:CZ    | 3:E:109:PRO:HA   | 2.44                     | 0.47              |
| 2:2:102:ASN:ND2  | 2:2:307:GLN:O    | 2.41                     | 0.47              |
| 3:I:1155:ASN:OD1 | 3:I:1156:ARG:N   | 2.47                     | 0.47              |
| 3:J:724:HIS:O    | 3:J:1030:LYS:NZ  | 2.48                     | 0.47              |
| 3:K:460:THR:HA   | 3:K:1129:PHE:HD2 | 1.80                     | 0.47              |
| 3:K:1339:ASP:OD2 | 3:K:1360:GLN:HG3 | 2.15                     | 0.47              |
| 3:L:151:THR:HG21 | 3:O:86:GLU:HB3   | 1.95                     | 0.47              |
| 3:L:227:PHE:O    | 3:L:231:SER:OG   | 2.20                     | 0.47              |
| 3:M:405:PRO:O    | 3:M:440:LEU:HD11 | 2.14                     | 0.47              |
| 3:H:383:ARG:HB2  | 3:H:384:ILE:HD12 | 1.96                     | 0.47              |
| 3:H:607:ALA:O    | 3:H:610:THR:OG1  | 2.23                     | 0.47              |
| 3:H:790:ARG:HE   | 3:H:792:ALA:HB3  | 1.80                     | 0.47              |
| 3:O:1201:ARG:HB2 | 3:O:1202:PRO:HD2 | 1.96                     | 0.47              |
| 3:P:1201:ARG:HB2 | 3:P:1202:PRO:HD2 | 1.97                     | 0.47              |
| 3:B:55:ASP:OD1   | 3:C:91:ASN:HB2   | 2.13                     | 0.47              |
| 3:B:875:VAL:HG12 | 3:B:879:PHE:CE2  | 2.50                     | 0.47              |
| 3:D:836:TYR:HE1  | 3:D:897:LEU:HD22 | 1.79                     | 0.47              |
| 3:D:840:GLN:C    | 3:D:842:MET:HG2  | 2.39                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:D:961:HIS:O    | 3:D:964:PHE:N    | 2.40                     | 0.47              |
| 3:D:1181:GLN:HB2 | 3:D:1309:VAL:O   | 2.15                     | 0.47              |
| 3:E:742:LEU:HA   | 3:E:745:HIS:HB3  | 1.96                     | 0.47              |
| 3:F:887:ASP:O    | 3:F:891:MET:HG2  | 2.14                     | 0.47              |
| 3:F:960:VAL:HA   | 3:F:994:LEU:HD13 | 1.97                     | 0.47              |
| 3:F:1160:ALA:HB2 | 3:F:1172:PRO:HG3 | 1.96                     | 0.47              |
| 3:G:496:GLY:HA3  | 3:G:504:ARG:NH2  | 2.29                     | 0.47              |
| 2:R:161:ARG:HE   | 2:S:271:LEU:HD12 | 1.80                     | 0.47              |
| 2:Y:93:THR:HB    | 2:Y:96:GLY:H     | 1.79                     | 0.47              |
| 1:1:196:ALA:HB3  | 1:1:232:ARG:HH22 | 1.78                     | 0.47              |
| 3:I:392:TYR:CE2  | 3:I:394:LEU:HB3  | 2.50                     | 0.47              |
| 3:I:756:ILE:HD12 | 3:I:763:PRO:HB3  | 1.96                     | 0.47              |
| 3:I:1245:TRP:O   | 3:I:1251:SER:HB3 | 2.14                     | 0.47              |
| 3:J:231:SER:O    | 3:J:1112:THR:OG1 | 2.29                     | 0.47              |
| 3:J:865:LEU:HD22 | 3:J:879:PHE:HB2  | 1.97                     | 0.47              |
| 3:J:1335:THR:H   | 3:J:1365:ASP:HB3 | 1.79                     | 0.47              |
| 3:K:469:ILE:HD11 | 3:K:547:PHE:CZ   | 2.50                     | 0.47              |
| 3:K:594:ALA:O    | 3:K:598:GLU:N    | 2.43                     | 0.47              |
| 3:K:966:GLY:HA3  | 3:K:969:HIS:HD2  | 1.79                     | 0.47              |
| 3:L:87:LEU:O     | 3:L:90:MET:N     | 2.44                     | 0.47              |
| 3:L:266:HIS:HE1  | 3:L:302:VAL:HG13 | 1.79                     | 0.47              |
| 3:L:441:PHE:CE2  | 3:L:1340:PRO:HD3 | 2.49                     | 0.47              |
| 3:L:778:ARG:HD3  | 3:L:782:ARG:HD2  | 1.96                     | 0.47              |
| 3:L:834:ARG:NH1  | 3:L:953:GLU:HA   | 2.27                     | 0.47              |
| 3:L:843:VAL:HB   | 3:L:876:ASN:HD22 | 1.80                     | 0.47              |
| 3:L:881:ASN:HD21 | 3:L:948:THR:HG21 | 1.80                     | 0.47              |
| 3:M:264:LEU:O    | 3:M:265:THR:OG1  | 2.28                     | 0.47              |
| 3:M:467:MET:SD   | 3:M:918:ALA:HA   | 2.55                     | 0.47              |
| 3:M:790:ARG:HG3  | 3:M:792:ALA:H    | 1.80                     | 0.47              |
| 3:A:405:PRO:O    | 3:A:440:LEU:HD11 | 2.15                     | 0.47              |
| 3:A:453:SER:H    | 3:A:456:ASN:HD22 | 1.61                     | 0.47              |
| 3:A:536:ASN:HD22 | 3:A:538:ASN:HB2  | 1.78                     | 0.47              |
| 3:A:576:ARG:NH1  | 3:A:582:LEU:HD23 | 2.29                     | 0.47              |
| 3:H:204:TYR:HB2  | 3:H:219:LEU:HD21 | 1.96                     | 0.47              |
| 3:H:744:ARG:HH12 | 3:H:799:PRO:HG3  | 1.80                     | 0.47              |
| 3:H:749:ASP:N    | 3:H:749:ASP:OD1  | 2.46                     | 0.47              |
| 3:H:1004:GLN:NE2 | 3:H:1007:VAL:HB  | 2.30                     | 0.47              |
| 3:N:58:LEU:HD12  | 3:O:124:ILE:CD1  | 2.44                     | 0.47              |
| 3:N:119:TYR:CE2  | 3:D:42:VAL:HG21  | 2.48                     | 0.47              |
| 3:N:745:HIS:C    | 3:N:745:HIS:ND1  | 2.73                     | 0.47              |
| 3:N:748:LEU:HD13 | 3:N:752:ARG:HD2  | 1.96                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:N:867:PRO:HA    | 3:N:870:LEU:HG    | 1.97                     | 0.47              |
| 3:P:264:LEU:O     | 3:P:265:THR:OG1   | 2.30                     | 0.47              |
| 3:P:512:ARG:HA    | 3:P:515:HIS:HD2   | 1.76                     | 0.47              |
| 3:P:630:LEU:O     | 3:P:634:ILE:HD12  | 2.14                     | 0.47              |
| 3:B:311:LEU:HD23  | 3:G:55:ASP:CG     | 2.36                     | 0.47              |
| 3:B:446:ASP:HB3   | 3:C:1201:ARG:HH12 | 1.79                     | 0.47              |
| 3:B:524:CYS:HA    | 3:B:1008:GLN:NE2  | 2.28                     | 0.47              |
| 3:B:756:ILE:HG12  | 3:B:910:CYS:HB3   | 1.96                     | 0.47              |
| 3:B:781:GLY:O     | 3:B:783:LEU:HG    | 2.15                     | 0.47              |
| 3:B:846:GLU:OE2   | 4:b:67:THR:O      | 2.31                     | 0.47              |
| 3:B:1334:ILE:HG22 | 3:B:1335:THR:H    | 1.78                     | 0.47              |
| 3:C:463:HIS:CD2   | 3:C:465:SER:H     | 2.33                     | 0.47              |
| 3:C:703:LEU:HA    | 3:C:703:LEU:HD23  | 1.68                     | 0.47              |
| 3:C:739:CYS:HG    | 3:C:765:TYR:HD1   | 1.61                     | 0.47              |
| 3:C:776:PHE:HD2   | 3:C:833:ASP:OD1   | 1.97                     | 0.47              |
| 3:D:71:LEU:HD13   | 3:D:304:VAL:O     | 2.14                     | 0.47              |
| 3:D:274:VAL:HG11  | 3:D:376:PHE:CD2   | 2.50                     | 0.47              |
| 3:D:638:GLU:C     | 4:d:79:PHE:HZ     | 2.23                     | 0.47              |
| 3:D:1156:ARG:NH2  | 3:E:1237:PRO:HB2  | 2.30                     | 0.47              |
| 3:D:1354:ARG:HG3  | 3:D:1354:ARG:O    | 2.14                     | 0.47              |
| 5:q:65:HIS:HB2    | 5:q:128:THR:CG2   | 2.45                     | 0.47              |
| 5:q:138:PRO:HG2   | 5:q:139:TRP:CD1   | 2.50                     | 0.47              |
| 5:q:435:VAL:HG12  | 5:q:437:ARG:H     | 1.80                     | 0.47              |
| 5:q:477:ALA:HB2   | 6:s:54:VAL:HG21   | 1.95                     | 0.47              |
| 3:E:194:PRO:HA    | 3:E:1110:ALA:O    | 2.14                     | 0.47              |
| 3:E:718:ALA:HB1   | 3:F:982:ASP:OD2   | 2.14                     | 0.47              |
| 3:E:781:GLY:O     | 3:E:782:ARG:HG3   | 2.14                     | 0.47              |
| 3:E:983:LEU:CD2   | 3:E:987:VAL:HG21  | 2.41                     | 0.47              |
| 3:E:1174:ARG:HH12 | 3:F:1232:SER:HG   | 1.59                     | 0.47              |
| 3:E:1174:ARG:NH1  | 3:F:1232:SER:OG   | 2.45                     | 0.47              |
| 3:F:86:GLU:O      | 3:F:86:GLU:HG2    | 2.13                     | 0.47              |
| 3:F:98:GLU:HG2    | 3:F:119:TYR:HD1   | 1.79                     | 0.47              |
| 3:F:259:VAL:HG22  | 3:F:1102:LEU:HD13 | 1.95                     | 0.47              |
| 3:F:384:ILE:HG22  | 3:F:385:TYR:N     | 2.30                     | 0.47              |
| 3:F:578:VAL:HB    | 3:F:1027:GLY:O    | 2.15                     | 0.47              |
| 3:G:101:GLN:NE2   | 3:G:118:ASN:HD21  | 2.12                     | 0.47              |
| 2:R:60:THR:HG23   | 2:R:201:GLU:HG3   | 1.97                     | 0.47              |
| 2:X:80:PRO:HG2    | 3:M:53:GLU:OE2    | 2.14                     | 0.47              |
| 2:3:38:ARG:HH12   | 3:E:109:PRO:C     | 2.23                     | 0.47              |
| 2:y:56:VAL:N      | 3:L:1262:HIS:NE2  | 2.58                     | 0.47              |
| 3:I:435:PHE:HB3   | 3:I:436:PRO:HD2   | 1.97                     | 0.47              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:I:840:GLN:O    | 3:I:842:MET:HG2   | 2.14                     | 0.47              |
| 3:J:148:LEU:HD11 | 3:J:158:GLN:NE2   | 2.30                     | 0.47              |
| 3:J:293:LEU:HD13 | 3:J:368:VAL:HG11  | 1.96                     | 0.47              |
| 3:J:718:ALA:HB1  | 3:K:982:ASP:OD2   | 2.15                     | 0.47              |
| 3:J:888:GLY:O    | 3:J:891:MET:HB2   | 2.14                     | 0.47              |
| 3:K:828:ALA:HA   | 3:K:958:LEU:H     | 1.78                     | 0.47              |
| 3:K:863:HIS:CD2  | 3:K:865:LEU:HB2   | 2.50                     | 0.47              |
| 3:L:641:PHE:CE2  | 3:L:677:TYR:HD2   | 2.33                     | 0.47              |
| 3:L:647:LEU:O    | 3:L:651:CYS:N     | 2.46                     | 0.47              |
| 3:L:740:ASP:HB2  | 3:L:799:PRO:HB3   | 1.97                     | 0.47              |
| 3:M:462:CYS:SG   | 3:M:1147:LEU:HD22 | 2.55                     | 0.47              |
| 3:M:620:ASP:HB2  | 3:M:623:TYR:HB2   | 1.96                     | 0.47              |
| 3:A:1254:ASP:HB3 | 3:A:1258:ASN:HD21 | 1.80                     | 0.47              |
| 3:N:542:GLU:CD   | 3:N:576:ARG:HH22  | 2.22                     | 0.47              |
| 3:O:410:ASN:ND2  | 3:O:1359:THR:O    | 2.46                     | 0.47              |
| 3:O:863:HIS:ND1  | 3:O:864:PRO:HD2   | 2.30                     | 0.47              |
| 3:P:830:VAL:HG22 | 3:P:955:PHE:HD1   | 1.80                     | 0.47              |
| 3:B:481:VAL:HG21 | 3:B:571:ILE:HD11  | 1.97                     | 0.47              |
| 3:B:505:PHE:CD1  | 3:B:509:TRP:CD1   | 3.03                     | 0.47              |
| 3:C:187:VAL:HG11 | 3:C:1071:GLU:OE2  | 2.14                     | 0.47              |
| 3:C:745:HIS:CE1  | 3:C:910:CYS:HB2   | 2.50                     | 0.47              |
| 3:D:103:LEU:HD11 | 3:D:115:PRO:CA    | 2.42                     | 0.47              |
| 3:D:451:ARG:NH1  | 3:E:529:GLU:OE1   | 2.48                     | 0.47              |
| 3:D:512:ARG:HA   | 3:D:515:HIS:NE2   | 2.30                     | 0.47              |
| 3:D:604:HIS:HD2  | 3:D:696:HIS:CD2   | 2.33                     | 0.47              |
| 3:D:684:GLU:HG2  | 3:E:658:ASN:O     | 2.14                     | 0.47              |
| 3:E:154:SER:O    | 3:E:157:ARG:N     | 2.48                     | 0.47              |
| 3:E:880:HIS:CE1  | 3:E:883:ARG:HH11  | 2.32                     | 0.47              |
| 3:F:518:VAL:HB   | 3:F:521:VAL:HB    | 1.96                     | 0.47              |
| 3:F:784:LEU:HD13 | 3:F:786:ASN:CG    | 2.39                     | 0.47              |
| 3:F:790:ARG:NH2  | 4:f:81:GLY:HA3    | 2.30                     | 0.47              |
| 2:S:300:PHE:CD2  | 3:A:111:PRO:CA    | 2.55                     | 0.47              |
| 1:T:125:GLU:OE2  | 1:T:215:TYR:OH    | 2.30                     | 0.47              |
| 2:2:241:LEU:HD12 | 2:2:248:ARG:HH21  | 1.79                     | 0.47              |
| 3:I:543:LEU:HD23 | 3:I:1248:GLN:OE1  | 2.14                     | 0.47              |
| 3:I:545:PRO:O    | 3:I:576:ARG:NH1   | 2.48                     | 0.47              |
| 3:I:866:HIS:HD2  | 3:I:868:ALA:HB3   | 1.80                     | 0.47              |
| 3:I:895:GLN:HG2  | 4:i:61:LEU:HB3    | 1.97                     | 0.47              |
| 3:J:56:ALA:HA    | 3:K:325:ALA:O     | 2.15                     | 0.47              |
| 3:J:185:LEU:HD11 | 3:J:380:LEU:HD12  | 1.96                     | 0.47              |
| 3:J:402:PHE:HA   | 3:J:1332:TYR:O    | 2.14                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:K:300:ALA:HB2   | 3:K:367:LEU:HD11  | 1.97                     | 0.47              |
| 3:K:724:HIS:CE1   | 3:K:1028:TYR:HB2  | 2.50                     | 0.47              |
| 3:K:801:ARG:HB3   | 3:K:802:PRO:HD2   | 1.96                     | 0.47              |
| 3:L:880:HIS:HD2   | 4:k:94:LEU:HD22   | 1.80                     | 0.47              |
| 3:M:86:GLU:HG2    | 3:M:86:GLU:O      | 2.15                     | 0.47              |
| 3:M:895:GLN:NE2   | 4:m:65:GLY:HA3    | 2.30                     | 0.47              |
| 3:M:948:THR:HA    | 4:l:80:ALA:N      | 2.30                     | 0.47              |
| 3:M:1178:ASP:O    | 3:H:217:ALA:HB1   | 2.15                     | 0.47              |
| 3:A:509:TRP:CZ3   | 3:A:512:ARG:HG2   | 2.50                     | 0.47              |
| 3:A:543:LEU:HB2   | 3:A:549:PHE:CE2   | 2.49                     | 0.47              |
| 3:H:709:LEU:CB    | 3:H:1038:HIS:ND1  | 2.78                     | 0.47              |
| 3:H:1271:SER:OG   | 3:H:1274:PHE:HB2  | 2.15                     | 0.47              |
| 4:l:42:HIS:HE1    | 4:l:44:HIS:HB2    | 1.80                     | 0.47              |
| 4:p:71:ASN:HA     | 4:p:102:VAL:HB    | 1.97                     | 0.47              |
| 3:N:352:ASP:OD2   | 3:D:21:GLY:HA3    | 2.15                     | 0.47              |
| 3:O:57:LEU:O      | 3:O:58:LEU:HD23   | 2.15                     | 0.47              |
| 3:O:178:ARG:HB3   | 3:P:104:ILE:HG22  | 1.97                     | 0.47              |
| 3:O:244:ILE:HD13  | 3:O:292:PHE:CE2   | 2.50                     | 0.47              |
| 3:O:460:THR:HA    | 3:O:1129:PHE:CD2  | 2.50                     | 0.47              |
| 3:O:752:ARG:HH22  | 3:O:915:ASP:HA    | 1.79                     | 0.47              |
| 3:P:1103:GLY:HA3  | 3:P:1107:THR:HG21 | 1.96                     | 0.47              |
| 3:B:205:LEU:HD21  | 3:B:1290:GLU:OE2  | 2.15                     | 0.47              |
| 3:B:512:ARG:HH12  | 3:B:564:PRO:HG2   | 1.80                     | 0.47              |
| 3:B:880:HIS:NE2   | 4:g:98:TYR:HB3    | 2.30                     | 0.47              |
| 3:B:1206:ARG:NH2  | 3:B:1208:ARG:O    | 2.47                     | 0.47              |
| 3:D:399:ASP:OD1   | 3:D:1057:ARG:HG2  | 2.15                     | 0.47              |
| 3:D:610:THR:HG21  | 3:D:692:ASP:OD2   | 2.15                     | 0.47              |
| 3:D:866:HIS:CD2   | 3:D:868:ALA:HB3   | 2.50                     | 0.47              |
| 3:D:1328:PHE:O    | 3:D:1330:GLU:HG3  | 2.15                     | 0.47              |
| 5:q:495:ARG:HH22  | 6:s:42:ASN:CG     | 2.23                     | 0.47              |
| 3:E:213:ARG:HH12  | 3:E:1216:GLY:HA3  | 1.80                     | 0.47              |
| 3:E:524:CYS:CB    | 3:E:1008:GLN:HE22 | 2.27                     | 0.47              |
| 3:E:1051:THR:HG23 | 3:E:1190:THR:HG21 | 1.97                     | 0.47              |
| 3:E:1222:VAL:HG11 | 3:E:1283:THR:HA   | 1.97                     | 0.47              |
| 3:F:280:THR:HG22  | 3:F:1063:VAL:HG13 | 1.96                     | 0.47              |
| 3:F:1131:LEU:HB3  | 3:F:1267:SER:HB2  | 1.97                     | 0.47              |
| 3:G:469:ILE:O     | 3:G:469:ILE:CG2   | 2.60                     | 0.47              |
| 2:2:224:ILE:HG22  | 2:2:251:ALA:HB2   | 1.97                     | 0.47              |
| 3:I:1208:ARG:NH2  | 3:I:1228:ASP:O    | 2.48                     | 0.47              |
| 3:K:446:ASP:OD2   | 3:L:1201:ARG:NH2  | 2.44                     | 0.47              |
| 3:M:460:THR:HA    | 3:M:1129:PHE:HD2  | 1.78                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:M:919:ASN:ND2   | 3:M:1139:LEU:HD12 | 2.30                     | 0.47              |
| 3:A:593:ASP:O     | 3:A:597:LEU:N     | 2.35                     | 0.47              |
| 3:A:1128:ASN:HB2  | 3:A:1131:LEU:HD12 | 1.97                     | 0.47              |
| 3:A:1229:HIS:CE1  | 3:A:1248:GLN:HA   | 2.50                     | 0.47              |
| 3:H:1342:LEU:CD2  | 3:H:1362:LEU:HB2  | 2.45                     | 0.47              |
| 4:o:57:GLN:HB3    | 3:O:840:GLN:CB    | 2.44                     | 0.47              |
| 3:N:227:PHE:CE2   | 3:N:1324:PRO:HB3  | 2.49                     | 0.47              |
| 3:O:802:PRO:HG2   | 3:O:805:TRP:HB2   | 1.96                     | 0.47              |
| 3:O:861:PRO:HA    | 3:O:866:HIS:CD2   | 2.50                     | 0.47              |
| 3:B:58:LEU:HD12   | 3:C:124:ILE:CD1   | 2.46                     | 0.47              |
| 3:C:201:MET:O     | 3:C:204:TYR:N     | 2.48                     | 0.47              |
| 3:C:397:ALA:HB3   | 3:C:1321:VAL:HG22 | 1.97                     | 0.47              |
| 3:C:1357:HIS:O    | 3:C:1358:PHE:C    | 2.58                     | 0.47              |
| 5:q:532:GLU:O     | 5:q:536:ARG:HG2   | 2.15                     | 0.47              |
| 5:q:586:HIS:HA    | 5:q:609:VAL:HG22  | 1.96                     | 0.47              |
| 3:E:267:ALA:HA    | 3:E:273:PRO:HA    | 1.97                     | 0.47              |
| 3:E:865:LEU:CD1   | 3:E:886:VAL:H     | 2.27                     | 0.47              |
| 3:E:1013:SER:OG   | 3:E:1020:LEU:HD21 | 2.14                     | 0.47              |
| 3:F:262:PRO:HD2   | 3:F:352:ASP:HB3   | 1.97                     | 0.47              |
| 3:F:523:GLU:HA    | 3:F:526:MET:HG2   | 1.96                     | 0.47              |
| 3:F:873:ASN:HA    | 4:e:92:PHE:CG     | 2.50                     | 0.47              |
| 3:F:1075:LEU:HD12 | 3:F:1075:LEU:O    | 2.15                     | 0.47              |
| 2:S:77:ARG:NH2    | 3:G:40:ALA:C      | 2.73                     | 0.46              |
| 2:U:89:ASP:HB3    | 2:V:315:ILE:HG21  | 1.97                     | 0.46              |
| 3:I:607:ALA:O     | 3:I:610:THR:OG1   | 2.28                     | 0.46              |
| 3:I:718:ALA:HB3   | 3:I:721:GLU:HG3   | 1.97                     | 0.46              |
| 3:I:1344:ARG:HH12 | 3:J:1356:THR:HG23 | 1.81                     | 0.46              |
| 3:K:438:ARG:HB2   | 3:K:454:MET:CG    | 2.45                     | 0.46              |
| 3:K:1004:GLN:HE22 | 3:K:1007:VAL:HB   | 1.77                     | 0.46              |
| 3:L:213:ARG:HH12  | 3:L:1216:GLY:HA3  | 1.80                     | 0.46              |
| 3:L:426:ALA:HB3   | 3:L:429:HIS:CD2   | 2.50                     | 0.46              |
| 3:L:634:ILE:HG22  | 3:L:636:GLY:N     | 2.30                     | 0.46              |
| 3:M:158:GLN:O     | 3:M:161:ALA:N     | 2.47                     | 0.46              |
| 3:M:460:THR:HA    | 3:M:1129:PHE:CD2  | 2.50                     | 0.46              |
| 3:M:1105:GLY:HA2  | 3:N:32:HIS:NE2    | 2.29                     | 0.46              |
| 3:A:605:ALA:HA    | 3:A:1018:ASN:HD21 | 1.79                     | 0.46              |
| 3:A:786:ASN:ND2   | 3:A:901:MET:O     | 2.48                     | 0.46              |
| 3:A:1318:ARG:HG2  | 3:A:1322:GLU:HG2  | 1.97                     | 0.46              |
| 3:H:669:SER:O     | 3:H:672:SER:OG    | 2.29                     | 0.46              |
| 3:H:864:PRO:HB2   | 3:H:876:ASN:OD1   | 2.15                     | 0.46              |
| 3:H:1209:ALA:HB3  | 3:H:1234:PRO:HG2  | 1.98                     | 0.46              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 4:j:62:THR:O     | 4:j:66:VAL:HG23   | 2.15                     | 0.46              |
| 3:N:433:ARG:NH2  | 3:O:413:MET:O     | 2.47                     | 0.46              |
| 3:O:124:ILE:HG12 | 3:O:1100:VAL:CG2  | 2.45                     | 0.46              |
| 3:P:198:LEU:O    | 3:P:201:MET:N     | 2.47                     | 0.46              |
| 3:B:200:PRO:HA   | 3:B:203:ARG:HH21  | 1.81                     | 0.46              |
| 3:B:533:GLN:C    | 3:B:535:ASP:H     | 2.23                     | 0.46              |
| 3:B:925:ASN:O    | 3:B:927:ARG:NH1   | 2.48                     | 0.46              |
| 3:C:730:ALA:HB2  | 3:C:752:ARG:HH11  | 1.80                     | 0.46              |
| 3:D:38:PHE:O     | 3:D:39:PHE:C      | 2.58                     | 0.46              |
| 3:D:1191:PRO:HG2 | 3:D:1194:THR:CG2  | 2.43                     | 0.46              |
| 3:E:496:GLY:HA3  | 3:E:504:ARG:NH2   | 2.31                     | 0.46              |
| 3:F:1072:ALA:HB2 | 3:F:1102:LEU:HD23 | 1.96                     | 0.46              |
| 3:G:469:ILE:CD1  | 3:G:547:PHE:CD1   | 2.98                     | 0.46              |
| 3:G:550:PHE:HD1  | 3:G:998:TYR:CZ    | 2.33                     | 0.46              |
| 3:G:863:HIS:CD2  | 3:G:865:LEU:H     | 2.34                     | 0.46              |
| 2:R:24:LEU:HD21  | 2:R:130:LEU:HD11  | 1.98                     | 0.46              |
| 3:I:238:GLY:HA2  | 3:I:244:ILE:HD11  | 1.97                     | 0.46              |
| 3:I:259:VAL:HG22 | 3:I:1102:LEU:HD13 | 1.97                     | 0.46              |
| 3:I:1082:ARG:HG3 | 3:I:1091:PHE:HE1  | 1.80                     | 0.46              |
| 3:J:99:VAL:HB    | 3:J:118:ASN:HB2   | 1.97                     | 0.46              |
| 3:J:1004:GLN:NE2 | 3:J:1007:VAL:HB   | 2.31                     | 0.46              |
| 3:K:646:ARG:HH11 | 3:K:890:ALA:CB    | 2.23                     | 0.46              |
| 3:K:668:TYR:HB2  | 3:K:812:TYR:CD2   | 2.50                     | 0.46              |
| 3:K:841:ASN:O    | 3:K:875:VAL:HG23  | 2.16                     | 0.46              |
| 3:M:119:TYR:HD1  | 3:N:11:TYR:OH     | 1.98                     | 0.46              |
| 3:M:241:ARG:O    | 3:M:244:ILE:N     | 2.48                     | 0.46              |
| 3:M:684:GLU:HA   | 3:H:658:ASN:O     | 2.14                     | 0.46              |
| 3:M:845:PRO:HG3  | 3:M:869:ASN:ND2   | 2.31                     | 0.46              |
| 3:A:1292:LEU:HA  | 3:A:1295:GLU:HB2  | 1.97                     | 0.46              |
| 4:i:88:LEU:HD12  | 4:i:89:ARG:N      | 2.30                     | 0.46              |
| 4:l:57:GLN:O     | 4:l:61:LEU:N      | 2.38                     | 0.46              |
| 3:N:915:ASP:O    | 3:N:919:ASN:HB2   | 2.15                     | 0.46              |
| 3:O:578:VAL:HB   | 3:O:1028:TYR:HA   | 1.96                     | 0.46              |
| 3:O:700:LEU:HB3  | 3:O:1025:MET:HG3  | 1.97                     | 0.46              |
| 3:O:802:PRO:HG3  | 3:P:944:HIS:NE2   | 2.30                     | 0.46              |
| 3:B:58:LEU:HA    | 3:B:58:LEU:HD23   | 1.58                     | 0.46              |
| 3:C:652:ILE:O    | 3:C:655:TYR:N     | 2.48                     | 0.46              |
| 3:C:707:PHE:N    | 3:C:707:PHE:CD1   | 2.82                     | 0.46              |
| 3:D:781:GLY:O    | 3:D:783:LEU:HG    | 2.16                     | 0.46              |
| 3:D:843:VAL:O    | 3:D:876:ASN:ND2   | 2.48                     | 0.46              |
| 3:E:163:GLN:O    | 3:E:167:ARG:HG2   | 2.15                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:E:440:LEU:HD13  | 3:E:1336:CYS:SG   | 2.54                     | 0.46              |
| 3:E:606:MET:HE3   | 3:E:611:ILE:HG12  | 1.97                     | 0.46              |
| 3:E:756:ILE:HA    | 3:E:909:LEU:O     | 2.14                     | 0.46              |
| 3:F:843:VAL:HB    | 3:F:876:ASN:ND2   | 2.30                     | 0.46              |
| 3:G:547:PHE:HB3   | 3:G:549:PHE:CE2   | 2.50                     | 0.46              |
| 1:T:335:PRO:HB2   | 1:T:337:ARG:HG2   | 1.96                     | 0.46              |
| 2:U:272:TYR:OH    | 2:V:164:ASN:ND2   | 2.48                     | 0.46              |
| 1:W:28:ALA:HB1    | 3:H:148:LEU:HD11  | 1.90                     | 0.46              |
| 2:X:189:VAL:HA    | 2:X:195:LEU:HD12  | 1.97                     | 0.46              |
| 2:Y:197:SER:O     | 2:Y:200:THR:OG1   | 2.29                     | 0.46              |
| 2:3:38:ARG:NH1    | 3:E:109:PRO:CA    | 2.79                     | 0.46              |
| 2:3:38:ARG:HH12   | 3:E:109:PRO:CA    | 2.28                     | 0.46              |
| 3:I:148:LEU:HD21  | 3:I:158:GLN:CD    | 2.40                     | 0.46              |
| 3:I:448:GLN:HG2   | 3:J:1201:ARG:NE   | 2.30                     | 0.46              |
| 3:I:889:PRO:HA    | 3:I:892:LEU:HD12  | 1.97                     | 0.46              |
| 3:J:103:LEU:HD11  | 3:J:115:PRO:CA    | 2.45                     | 0.46              |
| 3:K:1201:ARG:HB2  | 3:K:1202:PRO:HD2  | 1.96                     | 0.46              |
| 3:L:757:ASP:N     | 3:L:909:LEU:O     | 2.35                     | 0.46              |
| 3:L:1218:LYS:HB3  | 3:L:1221:ASP:CG   | 2.40                     | 0.46              |
| 3:M:103:LEU:HD11  | 3:M:115:PRO:HA    | 1.96                     | 0.46              |
| 3:A:124:ILE:HA    | 3:A:1100:VAL:HG22 | 1.98                     | 0.46              |
| 3:A:266:HIS:CE1   | 3:A:302:VAL:HG13  | 2.50                     | 0.46              |
| 3:A:853:CYS:SG    | 3:A:889:PRO:HD3   | 2.56                     | 0.46              |
| 3:A:1054:ARG:HH12 | 3:A:1123:GLY:H    | 1.63                     | 0.46              |
| 3:H:116:VAL:HG12  | 3:H:117:HIS:N     | 2.30                     | 0.46              |
| 3:H:231:SER:O     | 3:H:1112:THR:OG1  | 2.33                     | 0.46              |
| 3:O:103:LEU:HD11  | 3:O:115:PRO:CA    | 2.43                     | 0.46              |
| 3:O:1229:HIS:CE1  | 3:O:1248:GLN:HA   | 2.51                     | 0.46              |
| 3:P:766:ALA:N     | 3:P:783:LEU:O     | 2.36                     | 0.46              |
| 3:B:107:ASP:HB2   | 3:G:183:GLN:HE22  | 1.80                     | 0.46              |
| 3:B:351:LEU:CD2   | 3:G:58:LEU:HD13   | 2.41                     | 0.46              |
| 3:B:765:TYR:HA    | 3:B:783:LEU:HB2   | 1.97                     | 0.46              |
| 3:C:749:ASP:OD2   | 3:C:751:HIS:HB2   | 2.15                     | 0.46              |
| 3:C:828:ALA:HA    | 3:C:958:LEU:H     | 1.80                     | 0.46              |
| 3:C:1124:ASN:O    | 3:C:1156:ARG:NH1  | 2.48                     | 0.46              |
| 3:D:390:VAL:HG21  | 3:E:104:ILE:HD11  | 1.98                     | 0.46              |
| 3:D:1292:LEU:HB3  | 3:D:1327:LEU:HD21 | 1.98                     | 0.46              |
| 3:E:195:LEU:O     | 3:E:196:ALA:C     | 2.58                     | 0.46              |
| 3:E:302:VAL:HG12  | 3:E:303:PRO:O     | 2.15                     | 0.46              |
| 3:E:684:GLU:HG2   | 3:F:658:ASN:O     | 2.15                     | 0.46              |
| 3:F:158:GLN:O     | 3:F:162:ILE:N     | 2.48                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:G:1197:ASN:OD1  | 3:G:1197:ASN:N    | 2.48                     | 0.46              |
| 1:W:118:ASP:O     | 1:W:223:ARG:NH1   | 2.48                     | 0.46              |
| 2:X:162:ASP:OD2   | 2:X:199:ASN:ND2   | 2.48                     | 0.46              |
| 2:Y:248:ARG:CZ    | 3:H:1141:ASN:HD21 | 2.29                     | 0.46              |
| 2:3:295:VAL:HG13  | 2:3:314:VAL:HG13  | 1.98                     | 0.46              |
| 2:2:31:VAL:HG11   | 2:2:116:LEU:HD22  | 1.97                     | 0.46              |
| 2:2:92:LEU:HD12   | 2:2:98:VAL:HG21   | 1.97                     | 0.46              |
| 2:x:208:ASN:HB3   | 2:x:285:LEU:HD11  | 1.97                     | 0.46              |
| 2:y:222:THR:HG21  | 2:y:258:ALA:HB2   | 1.97                     | 0.46              |
| 3:I:701:ALA:O     | 3:I:727:ARG:NH2   | 2.49                     | 0.46              |
| 3:J:469:ILE:CD1   | 3:J:547:PHE:CG    | 2.80                     | 0.46              |
| 3:J:482:GLU:O     | 3:J:569:GLY:HA3   | 2.15                     | 0.46              |
| 3:J:543:LEU:HD23  | 3:J:1248:GLN:OE1  | 2.15                     | 0.46              |
| 3:J:679:GLY:HA2   | 3:K:622:SER:HB2   | 1.98                     | 0.46              |
| 3:K:397:ALA:HB3   | 3:K:1321:VAL:HG22 | 1.97                     | 0.46              |
| 3:K:502:GLN:HE22  | 3:K:970:VAL:HG13  | 1.79                     | 0.46              |
| 3:K:861:PRO:HA    | 3:K:866:HIS:CG    | 2.50                     | 0.46              |
| 3:L:85:PRO:HG2    | 3:L:86:GLU:OE1    | 2.15                     | 0.46              |
| 3:L:639:HIS:HA    | 4:l:79:PHE:CZ     | 2.50                     | 0.46              |
| 3:L:755:ARG:O     | 3:L:756:ILE:HG13  | 2.16                     | 0.46              |
| 3:L:837:ALA:HA    | 4:l:57:GLN:HE22   | 1.81                     | 0.46              |
| 3:L:841:ASN:O     | 3:L:875:VAL:HG23  | 2.16                     | 0.46              |
| 3:L:875:VAL:HG12  | 3:L:879:PHE:CE2   | 2.50                     | 0.46              |
| 3:M:547:PHE:CD1   | 3:M:575:TRP:HA    | 2.50                     | 0.46              |
| 3:M:828:ALA:HA    | 3:M:958:LEU:H     | 1.81                     | 0.46              |
| 3:H:545:PRO:HB2   | 3:H:1048:PHE:HE1  | 1.80                     | 0.46              |
| 4:l:88:LEU:HD12   | 4:l:89:ARG:N      | 2.30                     | 0.46              |
| 4:n:61:LEU:HD13   | 3:N:895:GLN:HA    | 1.96                     | 0.46              |
| 3:O:108:GLY:HA2   | 3:O:110:HIS:N     | 2.30                     | 0.46              |
| 3:O:488:GLY:N     | 3:O:520:TRP:HH2   | 2.10                     | 0.46              |
| 3:O:1029:PHE:HB3  | 3:O:1039:GLN:HE22 | 1.77                     | 0.46              |
| 3:P:385:TYR:CE1   | 3:P:393:PRO:HD3   | 2.50                     | 0.46              |
| 3:P:600:GLY:O     | 3:P:602:GLY:N     | 2.48                     | 0.46              |
| 3:P:1186:GLU:CD   | 3:P:1272:PRO:HD2  | 2.40                     | 0.46              |
| 3:B:96:GLN:HA     | 3:B:120:MET:O     | 2.15                     | 0.46              |
| 3:C:315:ASN:O     | 3:C:318:THR:OG1   | 2.31                     | 0.46              |
| 3:C:756:ILE:HA    | 3:C:909:LEU:O     | 2.14                     | 0.46              |
| 3:D:762:GLU:HB3   | 3:D:763:PRO:HD2   | 1.97                     | 0.46              |
| 3:D:1004:GLN:HE22 | 3:D:1007:VAL:HB   | 1.79                     | 0.46              |
| 3:D:1051:THR:OG1  | 3:D:1188:ILE:HB   | 2.15                     | 0.46              |
| 3:E:124:ILE:HG12  | 3:E:1100:VAL:CG2  | 2.46                     | 0.46              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:E:662:ALA:HB1  | 3:E:690:TYR:CZ    | 2.50                     | 0.46              |
| 3:F:222:GLU:O    | 3:F:225:ARG:N     | 2.47                     | 0.46              |
| 3:F:639:HIS:CD2  | 4:f:78:MET:SD     | 3.08                     | 0.46              |
| 3:F:873:ASN:OD1  | 4:e:92:PHE:HB2    | 2.13                     | 0.46              |
| 3:F:1117:ASN:ND2 | 3:G:222:GLU:HG3   | 2.30                     | 0.46              |
| 3:F:1357:HIS:O   | 3:F:1360:GLN:N    | 2.46                     | 0.46              |
| 3:G:453:SER:OG   | 3:G:455:GLU:HG2   | 2.16                     | 0.46              |
| 3:G:697:VAL:CG2  | 3:G:816:LEU:CD1   | 2.90                     | 0.46              |
| 3:G:1236:ARG:O   | 3:G:1236:ARG:HG3  | 2.15                     | 0.46              |
| 1:W:139:ASP:OD2  | 2:X:182:ASN:N     | 2.49                     | 0.46              |
| 3:I:762:GLU:HB3  | 3:I:763:PRO:HD2   | 1.96                     | 0.46              |
| 3:J:616:GLY:HA3  | 3:J:661:CYS:SG    | 2.55                     | 0.46              |
| 3:J:802:PRO:HD3  | 3:K:945:LEU:HD21  | 1.98                     | 0.46              |
| 3:J:1081:ALA:HB3 | 3:J:1092:THR:OG1  | 2.16                     | 0.46              |
| 3:K:1058:PHE:CE2 | 3:K:1369:LEU:HD11 | 2.50                     | 0.46              |
| 3:L:863:HIS:O    | 3:L:869:ASN:ND2   | 2.29                     | 0.46              |
| 3:M:102:PRO:O    | 3:M:103:LEU:HD12  | 2.15                     | 0.46              |
| 3:M:634:ILE:HA   | 3:M:640:VAL:HG11  | 1.96                     | 0.46              |
| 3:M:775:ASP:HB2  | 3:M:778:ARG:HH21  | 1.79                     | 0.46              |
| 3:M:1217:ASP:OD1 | 3:M:1287:ARG:NH1  | 2.47                     | 0.46              |
| 3:A:258:SER:OG   | 3:A:259:VAL:N     | 2.49                     | 0.46              |
| 3:H:414:GLU:HG2  | 3:H:1356:THR:HG21 | 1.97                     | 0.46              |
| 3:H:978:PRO:HA   | 3:H:981:ARG:HG3   | 1.96                     | 0.46              |
| 3:H:1188:ILE:O   | 3:H:1190:THR:HG23 | 2.14                     | 0.46              |
| 4:h:88:LEU:HD12  | 4:h:89:ARG:N      | 2.30                     | 0.46              |
| 4:n:22:MET:O     | 4:n:26:VAL:HG23   | 2.15                     | 0.46              |
| 3:N:185:LEU:HD11 | 3:N:380:LEU:HD12  | 1.97                     | 0.46              |
| 3:N:272:ARG:CZ   | 3:N:374:LEU:HD11  | 2.46                     | 0.46              |
| 3:N:296:GLU:CD   | 3:N:369:ALA:HB2   | 2.40                     | 0.46              |
| 3:N:887:ASP:O    | 3:N:891:MET:HG2   | 2.15                     | 0.46              |
| 3:N:1260:ALA:O   | 3:N:1262:HIS:NE2  | 2.42                     | 0.46              |
| 3:O:238:GLY:HA2  | 3:O:244:ILE:HD11  | 1.97                     | 0.46              |
| 3:O:279:VAL:HG12 | 3:O:394:LEU:HD22  | 1.97                     | 0.46              |
| 3:O:1181:GLN:HB2 | 3:O:1309:VAL:O    | 2.15                     | 0.46              |
| 3:B:227:PHE:O    | 3:B:231:SER:OG    | 2.25                     | 0.46              |
| 3:B:309:MET:HB3  | 3:G:55:ASP:HB3    | 1.98                     | 0.46              |
| 3:C:505:PHE:CD1  | 3:C:509:TRP:CD1   | 3.03                     | 0.46              |
| 3:C:625:ALA:HB3  | 3:C:878:MET:HE1   | 1.98                     | 0.46              |
| 3:D:776:PHE:HD2  | 3:D:833:ASP:OD1   | 1.98                     | 0.46              |
| 5:q:114:LEU:HD21 | 5:q:132:LEU:HD21  | 1.97                     | 0.46              |
| 3:E:263:ARG:NH2  | 3:E:306:TYR:O     | 2.47                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:F:399:ASP:HB2   | 3:F:1323:ASP:OD1  | 2.16                     | 0.46              |
| 3:F:577:VAL:HG12  | 3:F:578:VAL:HG13  | 1.97                     | 0.46              |
| 3:F:766:ALA:HB2   | 3:F:782:ARG:HB3   | 1.97                     | 0.46              |
| 3:F:888:GLY:O     | 3:F:892:LEU:HG    | 2.16                     | 0.46              |
| 3:G:433:ARG:O     | 3:G:1359:THR:OG1  | 2.32                     | 0.46              |
| 3:G:554:ALA:CA    | 3:G:569:GLY:HA2   | 2.45                     | 0.46              |
| 3:G:745:HIS:ND1   | 3:G:745:HIS:C     | 2.73                     | 0.46              |
| 2:x:145:THR:HA    | 2:x:148:ALA:HB3   | 1.98                     | 0.46              |
| 3:I:621:ARG:HB2   | 3:H:675:VAL:HG12  | 1.98                     | 0.46              |
| 3:I:634:ILE:HA    | 3:I:640:VAL:HG11  | 1.97                     | 0.46              |
| 3:I:834:ARG:HG2   | 4:h:88:LEU:O      | 2.15                     | 0.46              |
| 3:J:124:ILE:HG12  | 3:J:1100:VAL:CG2  | 2.46                     | 0.46              |
| 3:K:443:TRP:NE1   | 3:K:1343:LEU:HD21 | 2.31                     | 0.46              |
| 3:K:895:GLN:NE2   | 4:k:65:GLY:HA3    | 2.31                     | 0.46              |
| 3:L:44:SER:O      | 3:N:168:ASN:ND2   | 2.34                     | 0.46              |
| 3:L:1222:VAL:HG11 | 3:L:1283:THR:HA   | 1.97                     | 0.46              |
| 3:M:195:LEU:O     | 3:M:198:LEU:N     | 2.32                     | 0.46              |
| 3:M:740:ASP:CG    | 3:M:799:PRO:HB3   | 2.41                     | 0.46              |
| 3:M:765:TYR:CE1   | 3:M:783:LEU:HD12  | 2.50                     | 0.46              |
| 3:M:866:HIS:O     | 3:M:870:LEU:HG    | 2.16                     | 0.46              |
| 3:M:920:THR:HG22  | 3:M:921:ALA:N     | 2.30                     | 0.46              |
| 3:A:439:GLN:NE2   | 3:A:451:ARG:HH21  | 2.10                     | 0.46              |
| 3:A:582:LEU:HB2   | 3:A:587:CYS:SG    | 2.56                     | 0.46              |
| 3:A:626:VAL:HG11  | 3:A:879:PHE:CE1   | 2.50                     | 0.46              |
| 3:H:309:MET:SD    | 3:H:327:ARG:HG3   | 2.56                     | 0.46              |
| 3:H:405:PRO:HB3   | 3:H:1199:PHE:CE2  | 2.50                     | 0.46              |
| 3:H:604:HIS:NE2   | 3:H:605:ALA:O     | 2.49                     | 0.46              |
| 3:H:866:HIS:HD2   | 3:H:868:ALA:HB3   | 1.80                     | 0.46              |
| 4:j:56:GLY:O      | 4:j:60:ALA:N      | 2.39                     | 0.46              |
| 4:m:52:GLU:HA     | 4:m:55:ARG:HH11   | 1.81                     | 0.46              |
| 3:N:1155:ASN:OD1  | 3:N:1156:ARG:N    | 2.49                     | 0.46              |
| 3:P:879:PHE:CD1   | 3:P:884:VAL:HB    | 2.50                     | 0.46              |
| 3:B:132:ALA:HB3   | 3:C:114:GLN:HG2   | 1.96                     | 0.46              |
| 3:B:224:LYS:NZ    | 3:B:1330:GLU:OE2  | 2.42                     | 0.46              |
| 3:B:970:VAL:HG11  | 3:B:989:LEU:HD12  | 1.98                     | 0.46              |
| 3:E:33:ARG:O      | 3:E:35:LEU:N      | 2.48                     | 0.46              |
| 3:E:264:LEU:HB2   | 3:E:1068:ARG:NH2  | 2.30                     | 0.46              |
| 3:E:681:ASP:N     | 3:E:681:ASP:OD1   | 2.46                     | 0.46              |
| 3:E:853:CYS:SG    | 3:E:889:PRO:HD3   | 2.56                     | 0.46              |
| 3:E:1321:VAL:HG12 | 3:E:1322:GLU:N    | 2.30                     | 0.46              |
| 3:F:96:GLN:HG2    | 3:F:121:THR:HG22  | 1.98                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:F:895:GLN:HE22  | 4:f:65:GLY:HA3    | 1.80                     | 0.46              |
| 3:G:1233:ASP:OD2  | 3:G:1236:ARG:CG   | 2.64                     | 0.46              |
| 2:S:77:ARG:NH2    | 3:G:37:ASP:O      | 2.49                     | 0.46              |
| 1:T:281:ARG:HA    | 3:H:51:ASP:CG     | 2.41                     | 0.46              |
| 1:W:349:ARG:CA    | 6:r:14:GLU:CG     | 2.91                     | 0.46              |
| 2:y:152:VAL:HG21  | 2:y:290:ALA:HB2   | 1.97                     | 0.46              |
| 3:K:108:GLY:HA2   | 3:K:110:HIS:H     | 1.81                     | 0.46              |
| 3:K:1155:ASN:OD1  | 3:K:1156:ARG:N    | 2.49                     | 0.46              |
| 3:L:280:THR:HG22  | 3:L:1063:VAL:HG22 | 1.98                     | 0.46              |
| 3:L:802:PRO:HB3   | 3:M:945:LEU:HD21  | 1.97                     | 0.46              |
| 3:L:863:HIS:CD2   | 3:L:865:LEU:HB2   | 2.51                     | 0.46              |
| 3:M:463:HIS:HD2   | 3:M:465:SER:CB    | 2.28                     | 0.46              |
| 3:M:865:LEU:HD22  | 3:M:879:PHE:HB2   | 1.98                     | 0.46              |
| 3:A:1209:ALA:HB3  | 3:A:1234:PRO:HG2  | 1.98                     | 0.46              |
| 3:H:638:GLU:OE1   | 3:H:677:TYR:OH    | 2.30                     | 0.46              |
| 3:H:653:THR:HG22  | 3:H:683:PRO:HD3   | 1.98                     | 0.46              |
| 3:H:709:LEU:HB3   | 3:H:1038:HIS:ND1  | 2.31                     | 0.46              |
| 3:H:1215:ALA:O    | 3:H:1287:ARG:NH2  | 2.48                     | 0.46              |
| 3:N:86:GLU:HB3    | 3:D:151:THR:HG21  | 1.97                     | 0.46              |
| 3:N:1115:VAL:HG12 | 3:N:1116:ARG:O    | 2.16                     | 0.46              |
| 3:N:1321:VAL:HG12 | 3:N:1322:GLU:N    | 2.31                     | 0.46              |
| 3:C:162:ILE:HG22  | 3:D:344:LEU:HD13  | 1.98                     | 0.46              |
| 3:C:811:ILE:O     | 3:C:815:VAL:HB    | 2.15                     | 0.46              |
| 5:q:93:VAL:CG1    | 5:q:98:PRO:HA     | 2.46                     | 0.46              |
| 5:q:610:ILE:HG22  | 5:q:611:ASP:N     | 2.31                     | 0.46              |
| 3:E:398:MET:SD    | 3:E:1322:GLU:HG3  | 2.55                     | 0.46              |
| 3:F:12:ARG:NE     | 3:G:321:VAL:O     | 2.49                     | 0.46              |
| 3:F:558:LEU:HD13  | 3:F:929:PHE:HE2   | 1.80                     | 0.46              |
| 3:F:776:PHE:O     | 3:F:904:ARG:HB3   | 2.16                     | 0.46              |
| 2:U:162:ASP:OD2   | 2:U:199:ASN:ND2   | 2.49                     | 0.46              |
| 1:W:328:TYR:CD1   | 6:r:18:PHE:CZ     | 2.88                     | 0.46              |
| 2:X:80:PRO:HG2    | 3:M:53:GLU:CD     | 2.41                     | 0.46              |
| 2:Y:92:LEU:HD12   | 2:Y:98:VAL:HG21   | 1.98                     | 0.46              |
| 1:w:283:ARG:NH1   | 3:N:47:ASN:ND2    | 2.64                     | 0.46              |
| 2:x:295:VAL:HG13  | 2:x:314:VAL:HG13  | 1.97                     | 0.46              |
| 3:I:159:LEU:HD23  | 3:I:159:LEU:HA    | 1.76                     | 0.46              |
| 3:I:456:ASN:HB3   | 3:I:1126:PRO:HG3  | 1.96                     | 0.46              |
| 3:J:604:HIS:NE2   | 3:J:605:ALA:O     | 2.48                     | 0.46              |
| 3:J:1271:SER:OG   | 3:J:1274:PHE:HB2  | 2.16                     | 0.46              |
| 3:K:278:LEU:HG    | 3:K:375:VAL:HG11  | 1.97                     | 0.46              |
| 3:K:421:GLY:HA3   | 3:L:420:ALA:HB2   | 1.97                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:K:467:MET:O     | 3:K:922:SER:OG    | 2.32                     | 0.46              |
| 3:K:521:VAL:HG21  | 3:K:987:VAL:HG12  | 1.97                     | 0.46              |
| 3:K:1008:GLN:O    | 3:K:1012:GLU:HB2  | 2.16                     | 0.46              |
| 3:M:802:PRO:HG2   | 3:M:805:TRP:HB2   | 1.98                     | 0.46              |
| 3:A:129:LEU:HD12  | 3:A:1097:ARG:NH1  | 2.30                     | 0.46              |
| 3:A:668:TYR:CE1   | 3:A:694:VAL:HG22  | 2.51                     | 0.46              |
| 3:H:94:ARG:HH12   | 3:C:9:PRO:CB      | 1.99                     | 0.46              |
| 3:H:462:CYS:SG    | 3:H:1147:LEU:HD22 | 2.56                     | 0.46              |
| 3:H:666:ASN:HB3   | 3:H:940:MET:SD    | 2.56                     | 0.46              |
| 3:H:668:TYR:HD2   | 3:H:809:HIS:CE1   | 2.33                     | 0.46              |
| 3:N:187:VAL:HG11  | 3:N:1071:GLU:OE2  | 2.15                     | 0.46              |
| 3:O:93:GLY:HA3    | 3:O:124:ILE:HD12  | 1.98                     | 0.46              |
| 3:O:736:VAL:HG12  | 3:O:738:ASP:H     | 1.81                     | 0.46              |
| 3:B:691:ARG:NH1   | 3:C:620:ASP:OD1   | 2.49                     | 0.46              |
| 3:B:1036:LEU:O    | 3:B:1039:GLN:N    | 2.49                     | 0.46              |
| 3:B:1186:GLU:CD   | 3:B:1272:PRO:HD2  | 2.41                     | 0.46              |
| 3:B:1218:LYS:HB2  | 3:B:1221:ASP:CG   | 2.40                     | 0.46              |
| 3:C:86:GLU:O      | 3:C:86:GLU:HG2    | 2.15                     | 0.46              |
| 3:C:263:ARG:HH12  | 3:C:307:GLY:HA2   | 1.79                     | 0.46              |
| 3:D:417:ALA:HB2   | 3:D:1358:PHE:CZ   | 2.51                     | 0.46              |
| 3:D:1335:THR:HA   | 3:D:1363:ILE:O    | 2.14                     | 0.46              |
| 3:F:198:LEU:O     | 3:F:201:MET:N     | 2.49                     | 0.46              |
| 3:F:829:GLY:HA3   | 3:F:956:TYR:CZ    | 2.50                     | 0.46              |
| 3:F:1054:ARG:NH1  | 3:F:1123:GLY:O    | 2.48                     | 0.46              |
| 3:G:106:ARG:NH1   | 3:G:113:GLU:OE2   | 2.48                     | 0.46              |
| 3:G:119:TYR:C     | 3:G:120:MET:HG3   | 2.37                     | 0.46              |
| 2:R:272:TYR:OH    | 2:S:164:ASN:ND2   | 2.47                     | 0.46              |
| 1:1:150:PRO:HA    | 2:2:267:ARG:HH21  | 1.80                     | 0.46              |
| 2:2:285:LEU:HA    | 2:2:288:ILE:HD12  | 1.96                     | 0.46              |
| 3:I:438:ARG:HG3   | 3:I:439:GLN:HG3   | 1.97                     | 0.46              |
| 3:I:579:ASN:ND2   | 3:I:595:ARG:HH12  | 2.13                     | 0.46              |
| 3:I:752:ARG:HG3   | 3:I:912:ALA:HB1   | 1.98                     | 0.46              |
| 3:J:381:GLU:HB3   | 3:J:392:TYR:CD1   | 2.51                     | 0.46              |
| 3:J:490:TYR:CD1   | 3:J:564:PRO:HB3   | 2.50                     | 0.46              |
| 3:J:837:ALA:O     | 3:J:841:ASN:N     | 2.49                     | 0.46              |
| 3:K:1184:VAL:HG21 | 3:K:1269:VAL:HG13 | 1.97                     | 0.46              |
| 3:L:86:GLU:O      | 3:L:86:GLU:HG2    | 2.15                     | 0.46              |
| 3:L:989:LEU:HD23  | 3:L:989:LEU:HA    | 1.74                     | 0.46              |
| 3:L:1115:VAL:HG11 | 3:L:1374:LEU:HD11 | 1.98                     | 0.46              |
| 3:M:86:GLU:OE1    | 3:M:86:GLU:N      | 2.49                     | 0.46              |
| 3:M:204:TYR:CD2   | 3:M:219:LEU:HD11  | 2.50                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:M:279:VAL:HG12  | 3:M:394:LEU:HD22  | 1.98                     | 0.46              |
| 3:M:1215:ALA:HB3  | 3:M:1287:ARG:HE   | 1.81                     | 0.46              |
| 3:A:610:THR:HG22  | 3:A:689:VAL:HA    | 1.97                     | 0.46              |
| 3:H:182:ASP:OD1   | 3:H:385:TYR:OH    | 2.24                     | 0.46              |
| 3:H:1182:ASP:HB2  | 3:H:1309:VAL:HG13 | 1.97                     | 0.46              |
| 4:n:42:HIS:CE1    | 4:n:44:HIS:HB2    | 2.51                     | 0.46              |
| 3:N:120:MET:HE2   | 3:D:39:PHE:CE1    | 2.51                     | 0.46              |
| 3:N:521:VAL:HG11  | 3:N:987:VAL:HG12  | 1.97                     | 0.46              |
| 3:N:578:VAL:HA    | 3:N:1029:PHE:O    | 2.16                     | 0.46              |
| 3:N:704:VAL:O     | 3:N:708:THR:HG23  | 2.15                     | 0.46              |
| 3:P:241:ARG:NE    | 3:P:245:GLU:OE2   | 2.38                     | 0.46              |
| 3:P:1354:ARG:HG3  | 3:P:1354:ARG:O    | 2.15                     | 0.46              |
| 3:B:1201:ARG:CG   | 3:B:1202:PRO:HD2  | 2.46                     | 0.46              |
| 3:C:31:SER:HG     | 3:C:32:HIS:CE1    | 2.33                     | 0.46              |
| 3:C:906:THR:OG1   | 3:C:934:HIS:HB3   | 2.15                     | 0.46              |
| 3:C:913:ALA:HB1   | 3:C:914:PRO:HD2   | 1.98                     | 0.46              |
| 3:D:945:LEU:HA    | 3:D:945:LEU:HD23  | 1.57                     | 0.46              |
| 5:q:260:ILE:HB    | 5:q:261:LEU:HD13  | 1.98                     | 0.46              |
| 5:q:592:TYR:HB2   | 5:q:649:LEU:HB3   | 1.97                     | 0.46              |
| 3:E:186:HIS:CE1   | 3:E:393:PRO:HB3   | 2.51                     | 0.46              |
| 3:E:234:LEU:HD23  | 3:E:234:LEU:HA    | 1.76                     | 0.46              |
| 3:E:266:HIS:CE1   | 3:E:303:PRO:HD2   | 2.51                     | 0.46              |
| 3:E:430:PRO:O     | 3:E:432:PRO:HD3   | 2.15                     | 0.46              |
| 3:E:463:HIS:CD2   | 3:E:465:SER:HB3   | 2.49                     | 0.46              |
| 3:E:499:ALA:HA    | 3:E:956:TYR:CD1   | 2.50                     | 0.46              |
| 3:E:1166:PHE:CD1  | 3:E:1167:GLY:N    | 2.84                     | 0.46              |
| 3:F:593:ASP:O     | 3:F:597:LEU:N     | 2.38                     | 0.46              |
| 3:G:1075:LEU:HA   | 3:G:1097:ARG:HG2  | 1.97                     | 0.46              |
| 2:3:300:PHE:CG    | 3:M:1083:HIS:CD2  | 2.88                     | 0.46              |
| 2:x:306:VAL:HG11  | 2:x:312:ALA:HB2   | 1.96                     | 0.46              |
| 3:I:948:THR:HA    | 4:h:80:ALA:H      | 1.81                     | 0.46              |
| 3:J:264:LEU:O     | 3:J:265:THR:OG1   | 2.28                     | 0.46              |
| 3:J:875:VAL:HG11  | 3:J:891:MET:HE1   | 1.97                     | 0.46              |
| 3:J:878:MET:HE2   | 4:i:92:PHE:CZ     | 2.51                     | 0.46              |
| 3:J:1004:GLN:HE21 | 3:J:1007:VAL:HB   | 1.81                     | 0.46              |
| 3:K:263:ARG:HH12  | 3:K:307:GLY:HA2   | 1.81                     | 0.46              |
| 3:K:834:ARG:HB3   | 4:j:90:PRO:HD3    | 1.98                     | 0.46              |
| 3:L:59:GLY:HA2    | 3:N:20:THR:HG21   | 1.98                     | 0.46              |
| 3:L:1148:ARG:NH2  | 3:L:1163:LEU:HG   | 2.30                     | 0.46              |
| 3:M:23:ILE:HG22   | 3:M:24:LEU:N      | 2.30                     | 0.46              |
| 3:M:27:ILE:CD1    | 3:D:256:GLN:CD    | 2.88                     | 0.46              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:M:1029:PHE:HB3 | 3:M:1039:GLN:HE21 | 1.80                     | 0.46              |
| 3:M:1227:TYR:O   | 3:M:1229:HIS:ND1  | 2.48                     | 0.46              |
| 3:A:728:ASP:CG   | 3:A:1030:LYS:HZ1  | 2.24                     | 0.46              |
| 4:p:71:ASN:ND2   | 3:P:847:ILE:HD13  | 2.31                     | 0.46              |
| 3:N:79:CYS:HB3   | 3:N:81:CYS:SG     | 2.55                     | 0.46              |
| 3:N:130:ASN:OD1  | 3:N:1094:THR:HG22 | 2.16                     | 0.46              |
| 3:N:749:ASP:O    | 3:N:752:ARG:N     | 2.48                     | 0.46              |
| 3:O:99:VAL:HB    | 3:O:118:ASN:HB2   | 1.98                     | 0.46              |
| 3:O:748:LEU:HD13 | 3:O:752:ARG:HD2   | 1.98                     | 0.46              |
| 3:P:830:VAL:HG22 | 3:P:955:PHE:CD1   | 2.51                     | 0.46              |
| 3:B:399:ASP:OD1  | 3:B:1057:ARG:HG2  | 2.16                     | 0.46              |
| 3:B:460:THR:HA   | 3:B:1129:PHE:CD2  | 2.50                     | 0.46              |
| 3:B:543:LEU:HD23 | 3:B:1248:GLN:OE1  | 2.16                     | 0.46              |
| 3:B:615:ARG:NH2  | 3:B:1017:GLU:HG2  | 2.31                     | 0.46              |
| 3:B:827:THR:OG1  | 3:B:960:VAL:HG23  | 2.16                     | 0.46              |
| 3:C:130:ASN:OD1  | 3:C:1094:THR:HG22 | 2.15                     | 0.46              |
| 3:C:542:GLU:CD   | 3:C:576:ARG:HH22  | 2.23                     | 0.46              |
| 3:C:778:ARG:HH11 | 3:C:782:ARG:HD2   | 1.81                     | 0.46              |
| 3:C:1241:THR:OG1 | 3:C:1247:SER:OG   | 2.25                     | 0.46              |
| 3:D:108:GLY:HA2  | 3:D:110:HIS:N     | 2.30                     | 0.46              |
| 3:D:730:ALA:HB2  | 3:D:752:ARG:NH1   | 2.29                     | 0.46              |
| 3:D:842:MET:HG3  | 4:d:61:LEU:HD21   | 1.98                     | 0.46              |
| 3:D:948:THR:HG21 | 4:c:95:LYS:HE3    | 1.98                     | 0.46              |
| 5:q:493:SER:OG   | 5:q:673:THR:HG22  | 2.15                     | 0.46              |
| 5:q:591:TYR:HD2  | 5:q:602:THR:HG21  | 1.79                     | 0.46              |
| 3:E:826:CYS:SG   | 3:E:939:LEU:HB2   | 2.56                     | 0.46              |
| 3:F:124:ILE:HA   | 3:F:1100:VAL:HG22 | 1.98                     | 0.46              |
| 3:F:505:PHE:CD1  | 3:F:992:PRO:HD3   | 2.50                     | 0.46              |
| 1:Q:118:ASP:O    | 1:Q:223:ARG:NH1   | 2.49                     | 0.45              |
| 2:R:110:ASN:N    | 2:R:304:ALA:O     | 2.49                     | 0.45              |
| 2:U:253:LEU:O    | 2:U:257:GLU:N     | 2.47                     | 0.45              |
| 2:X:90:LEU:O     | 2:X:93:THR:OG1    | 2.31                     | 0.45              |
| 2:3:78:VAL:HG13  | 2:3:83:ILE:HG12   | 1.98                     | 0.45              |
| 2:2:53:SER:OG    | 2:2:54:GLY:N      | 2.49                     | 0.45              |
| 2:2:245:SER:OG   | 2:2:246:VAL:N     | 2.49                     | 0.45              |
| 3:I:104:ILE:HD11 | 3:H:390:VAL:HG21  | 1.98                     | 0.45              |
| 3:I:180:THR:HG22 | 3:I:1097:ARG:NH1  | 2.31                     | 0.45              |
| 3:J:85:PRO:HG2   | 3:J:86:GLU:OE1    | 2.16                     | 0.45              |
| 3:J:505:PHE:CE1  | 3:J:992:PRO:HD3   | 2.51                     | 0.45              |
| 3:J:728:ASP:HB3  | 3:J:730:ALA:H     | 1.81                     | 0.45              |
| 3:K:698:GLU:OE1  | 3:L:621:ARG:NH2   | 2.49                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:L:77:VAL:HG12   | 3:L:1068:ARG:O    | 2.17                     | 0.45              |
| 3:L:748:LEU:HB2   | 3:L:754:CYS:SG    | 2.56                     | 0.45              |
| 3:M:43:ARG:C      | 3:M:45:ASP:H      | 2.23                     | 0.45              |
| 3:M:414:GLU:HG2   | 3:M:1356:THR:HG21 | 1.98                     | 0.45              |
| 3:M:879:PHE:O     | 3:M:883:ARG:N     | 2.50                     | 0.45              |
| 3:A:577:VAL:H     | 3:A:581:ASN:ND2   | 2.14                     | 0.45              |
| 3:A:1291:ARG:O    | 3:A:1295:GLU:HG2  | 2.16                     | 0.45              |
| 3:H:172:VAL:HG11  | 3:H:1093:LEU:HD12 | 1.97                     | 0.45              |
| 3:H:440:LEU:HD22  | 3:H:1336:CYS:SG   | 2.56                     | 0.45              |
| 3:H:727:ARG:O     | 3:H:729:PRO:HD3   | 2.17                     | 0.45              |
| 3:H:763:PRO:HB2   | 3:H:765:TYR:CE1   | 2.50                     | 0.45              |
| 3:O:129:LEU:O     | 3:O:1094:THR:HA   | 2.15                     | 0.45              |
| 3:O:1170:GLN:OE1  | 3:O:1170:GLN:N    | 2.48                     | 0.45              |
| 3:P:29:VAL:O      | 3:P:32:HIS:N      | 2.47                     | 0.45              |
| 3:P:205:LEU:HD21  | 3:P:1290:GLU:OE2  | 2.16                     | 0.45              |
| 3:P:558:LEU:HA    | 3:P:559:PRO:C     | 2.41                     | 0.45              |
| 3:B:277:VAL:HG22  | 3:B:376:PHE:HB2   | 1.98                     | 0.45              |
| 3:B:411:PRO:O     | 3:B:415:ARG:NH1   | 2.49                     | 0.45              |
| 3:B:460:THR:HA    | 3:B:1129:PHE:CE2  | 2.51                     | 0.45              |
| 3:B:1256:LEU:HD23 | 3:B:1256:LEU:HA   | 1.72                     | 0.45              |
| 3:B:1370:LYS:HE2  | 3:B:1370:LYS:HB2  | 1.74                     | 0.45              |
| 3:C:425:PRO:HG3   | 3:C:431:GLU:HG2   | 1.98                     | 0.45              |
| 3:C:452:LEU:HD12  | 3:C:456:ASN:HD22  | 1.81                     | 0.45              |
| 3:D:213:ARG:NH1   | 3:D:1216:GLY:HA3  | 2.29                     | 0.45              |
| 3:D:286:GLN:O     | 3:D:289:LEU:N     | 2.48                     | 0.45              |
| 3:F:888:GLY:O     | 3:F:891:MET:HB2   | 2.15                     | 0.45              |
| 3:F:1232:SER:HB2  | 3:F:1237:PRO:O    | 2.16                     | 0.45              |
| 3:G:37:ASP:O      | 3:G:40:ALA:O      | 2.34                     | 0.45              |
| 2:S:130:LEU:HD12  | 2:S:135:LEU:HB2   | 1.97                     | 0.45              |
| 1:W:28:ALA:C      | 3:H:145:GLY:HA3   | 2.41                     | 0.45              |
| 3:I:411:PRO:HD2   | 3:I:414:GLU:OE1   | 2.17                     | 0.45              |
| 3:I:801:ARG:HD3   | 3:I:805:TRP:CD1   | 2.51                     | 0.45              |
| 3:J:130:ASN:HA    | 3:J:1093:LEU:O    | 2.16                     | 0.45              |
| 3:J:620:ASP:OD2   | 3:J:655:TYR:OH    | 2.33                     | 0.45              |
| 3:J:845:PRO:HG2   | 3:J:862:ALA:HA    | 1.98                     | 0.45              |
| 3:L:187:VAL:HG11  | 3:L:1071:GLU:OE2  | 2.16                     | 0.45              |
| 3:L:469:ILE:HD11  | 3:L:547:PHE:CD2   | 2.52                     | 0.45              |
| 3:L:682:LEU:HB2   | 3:L:687:MET:HG2   | 1.97                     | 0.45              |
| 3:M:983:LEU:O     | 3:M:987:VAL:HG22  | 2.15                     | 0.45              |
| 3:A:70:PHE:CZ     | 3:A:184:MET:HG3   | 2.51                     | 0.45              |
| 3:H:1186:GLU:CD   | 3:H:1272:PRO:HD2  | 2.41                     | 0.45              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:N:600:GLY:C    | 3:N:602:GLY:N     | 2.74                     | 0.45              |
| 3:N:718:ALA:HB3  | 3:N:721:GLU:HG3   | 1.98                     | 0.45              |
| 3:N:1008:GLN:HB3 | 3:N:1012:GLU:CD   | 2.41                     | 0.45              |
| 3:O:1215:ALA:HB1 | 3:O:1221:ASP:HB3  | 1.97                     | 0.45              |
| 3:P:311:LEU:O    | 3:P:316:LEU:HB2   | 2.15                     | 0.45              |
| 3:B:189:LEU:HD23 | 3:B:1064:LEU:HD21 | 1.97                     | 0.45              |
| 3:B:621:ARG:C    | 3:B:943:GLN:HE21  | 2.23                     | 0.45              |
| 3:B:870:LEU:HD23 | 3:B:876:ASN:HB3   | 1.97                     | 0.45              |
| 3:B:978:PRO:O    | 3:B:981:ARG:NH1   | 2.50                     | 0.45              |
| 3:B:1202:PRO:HB3 | 3:B:1332:TYR:HD1  | 1.81                     | 0.45              |
| 3:D:845:PRO:HG3  | 3:D:869:ASN:HD21  | 1.80                     | 0.45              |
| 3:E:543:LEU:HD23 | 3:E:1248:GLN:OE1  | 2.16                     | 0.45              |
| 3:E:600:GLY:C    | 3:E:602:GLY:N     | 2.72                     | 0.45              |
| 3:E:983:LEU:HD23 | 3:E:987:VAL:HG22  | 1.99                     | 0.45              |
| 3:F:380:LEU:O    | 3:F:382:LYS:N     | 2.49                     | 0.45              |
| 3:F:700:LEU:O    | 3:F:1025:MET:HE2  | 2.16                     | 0.45              |
| 3:G:709:LEU:HD12 | 3:G:1037:TYR:HE1  | 1.81                     | 0.45              |
| 2:R:174:PRO:CB   | 5:q:371:GLY:HA3   | 2.43                     | 0.45              |
| 1:1:117:THR:O    | 1:1:121:GLN:NE2   | 2.49                     | 0.45              |
| 2:3:91:GLY:O     | 2:3:95:ALA:N      | 2.42                     | 0.45              |
| 2:2:248:ARG:HD3  | 3:D:1141:ASN:ND2  | 2.31                     | 0.45              |
| 1:w:166:GLU:HG2  | 3:O:1262:HIS:NE2  | 2.30                     | 0.45              |
| 3:I:171:ALA:O    | 3:J:103:LEU:HD13  | 2.15                     | 0.45              |
| 3:J:836:TYR:O    | 3:J:840:GLN:N     | 2.44                     | 0.45              |
| 3:K:1004:GLN:NE2 | 3:K:1008:GLN:HG3  | 2.31                     | 0.45              |
| 3:K:1196:ILE:O   | 3:K:1199:PHE:N    | 2.43                     | 0.45              |
| 3:L:1020:LEU:HA  | 3:L:1023:ALA:HB3  | 1.97                     | 0.45              |
| 4:n:88:LEU:HD12  | 4:n:89:ARG:N      | 2.31                     | 0.45              |
| 3:N:961:HIS:O    | 3:N:964:PHE:N     | 2.41                     | 0.45              |
| 3:N:1241:THR:OG1 | 3:N:1247:SER:OG   | 2.19                     | 0.45              |
| 3:P:130:ASN:OD1  | 3:P:1094:THR:HG22 | 2.16                     | 0.45              |
| 3:B:523:GLU:OE2  | 3:B:538:ASN:ND2   | 2.45                     | 0.45              |
| 3:B:578:VAL:H    | 3:B:581:ASN:HD22  | 1.63                     | 0.45              |
| 3:B:606:MET:H    | 3:B:1018:ASN:HD21 | 1.64                     | 0.45              |
| 3:B:857:PRO:O    | 3:B:866:HIS:HA    | 2.16                     | 0.45              |
| 5:q:38:VAL:HG13  | 5:q:136:TRP:CZ2   | 2.36                     | 0.45              |
| 5:q:257:ASN:HA   | 6:s:90:GLN:NE2    | 2.15                     | 0.45              |
| 5:q:512:PHE:CD1  | 5:q:520:LEU:HD11  | 2.51                     | 0.45              |
| 3:E:748:LEU:HD13 | 3:E:752:ARG:HD2   | 1.97                     | 0.45              |
| 3:E:1245:TRP:N   | 3:E:1245:TRP:CD1  | 2.81                     | 0.45              |
| 3:E:1256:LEU:HB2 | 3:E:1257:TYR:CD2  | 2.52                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:F:1195:ASP:OD1  | 3:F:1195:ASP:N    | 2.49                     | 0.45              |
| 3:G:106:ARG:HB3   | 3:G:110:HIS:CG    | 2.52                     | 0.45              |
| 3:G:505:PHE:HE1   | 3:G:992:PRO:CD    | 2.30                     | 0.45              |
| 2:S:246:VAL:O     | 2:S:250:ALA:N     | 2.48                     | 0.45              |
| 2:3:306:VAL:HG11  | 2:3:312:ALA:HB2   | 1.99                     | 0.45              |
| 2:x:47:ALA:HA     | 2:x:137:LEU:HD23  | 1.98                     | 0.45              |
| 3:I:175:ALA:HB2   | 3:J:103:LEU:HB2   | 1.98                     | 0.45              |
| 3:J:1202:PRO:HB3  | 3:J:1332:TYR:HD1  | 1.82                     | 0.45              |
| 3:L:584:LEU:HA    | 3:L:584:LEU:HD23  | 1.73                     | 0.45              |
| 3:L:1051:THR:OG1  | 3:L:1188:ILE:HB   | 2.17                     | 0.45              |
| 3:M:44:SER:N      | 3:D:115:PRO:O     | 2.49                     | 0.45              |
| 3:M:1197:ASN:OD1  | 3:M:1200:ARG:NH1  | 2.49                     | 0.45              |
| 3:M:1357:HIS:O    | 3:M:1358:PHE:C    | 2.59                     | 0.45              |
| 3:A:639:HIS:HB2   | 3:A:789:ALA:C     | 2.42                     | 0.45              |
| 3:A:707:PHE:HA    | 3:A:1042:THR:HG21 | 1.99                     | 0.45              |
| 3:H:639:HIS:CD2   | 4:h:78:MET:HE3    | 2.51                     | 0.45              |
| 3:H:1218:LYS:N    | 3:H:1221:ASP:OD2  | 2.49                     | 0.45              |
| 3:N:521:VAL:HG21  | 3:N:987:VAL:HG12  | 1.97                     | 0.45              |
| 3:N:721:GLU:HG2   | 3:N:727:ARG:O     | 2.15                     | 0.45              |
| 3:N:1024:LEU:O    | 3:N:1027:GLY:N    | 2.49                     | 0.45              |
| 3:O:783:LEU:HD22  | 3:O:934:HIS:CD2   | 2.52                     | 0.45              |
| 3:B:543:LEU:HB3   | 3:B:1251:SER:HA   | 1.99                     | 0.45              |
| 3:B:739:CYS:O     | 3:B:743:MET:HG2   | 2.17                     | 0.45              |
| 3:C:108:GLY:HA2   | 3:C:110:HIS:N     | 2.32                     | 0.45              |
| 3:C:873:ASN:HA    | 4:b:92:PHE:CG     | 2.51                     | 0.45              |
| 3:D:398:MET:SD    | 3:D:1322:GLU:HG3  | 2.56                     | 0.45              |
| 3:D:405:PRO:O     | 3:D:440:LEU:HD11  | 2.17                     | 0.45              |
| 3:D:863:HIS:HD2   | 3:D:865:LEU:HB2   | 1.82                     | 0.45              |
| 3:D:1233:ASP:HB3  | 3:D:1236:ARG:O    | 2.17                     | 0.45              |
| 3:D:1335:THR:HG22 | 3:D:1365:ASP:H    | 1.82                     | 0.45              |
| 5:q:495:ARG:HA    | 6:s:36:TRP:CZ3    | 2.46                     | 0.45              |
| 3:E:867:PRO:HA    | 3:E:870:LEU:HB2   | 1.99                     | 0.45              |
| 3:E:1124:ASN:OD1  | 3:E:1124:ASN:N    | 2.48                     | 0.45              |
| 3:F:367:LEU:HD21  | 3:F:376:PHE:CE1   | 2.52                     | 0.45              |
| 3:F:879:PHE:CE2   | 3:F:891:MET:HE1   | 2.51                     | 0.45              |
| 3:G:31:SER:O      | 3:G:53:GLU:CB     | 2.64                     | 0.45              |
| 3:G:1282:ILE:HD12 | 3:G:1282:ILE:H    | 1.77                     | 0.45              |
| 1:W:344:GLU:O     | 6:r:13:TRP:HE3    | 1.29                     | 0.45              |
| 1:1:259:GLU:OE1   | 3:M:1315:PRO:HB3  | 2.16                     | 0.45              |
| 2:x:63:LEU:HD11   | 2:x:138:ARG:HH21  | 1.81                     | 0.45              |
| 3:I:198:LEU:HD23  | 3:I:198:LEU:HA    | 1.68                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:I:634:ILE:HG22  | 3:I:636:GLY:N     | 2.31                     | 0.45              |
| 3:I:658:ASN:O     | 3:H:684:GLU:HG2   | 2.17                     | 0.45              |
| 3:I:829:GLY:HA3   | 3:I:956:TYR:CZ    | 2.52                     | 0.45              |
| 3:J:313:GLY:O     | 3:J:316:LEU:N     | 2.39                     | 0.45              |
| 3:J:983:LEU:O     | 3:J:987:VAL:HG22  | 2.17                     | 0.45              |
| 3:J:1125:LEU:HD12 | 3:J:1156:ARG:NH2  | 2.31                     | 0.45              |
| 3:K:311:LEU:O     | 3:K:316:LEU:HB2   | 2.17                     | 0.45              |
| 3:K:1245:TRP:O    | 3:K:1251:SER:HB3  | 2.17                     | 0.45              |
| 3:L:712:PRO:HD2   | 3:L:1146:TYR:CE1  | 2.51                     | 0.45              |
| 3:L:863:HIS:HD2   | 3:L:865:LEU:HB2   | 1.80                     | 0.45              |
| 3:M:1190:THR:HG22 | 3:M:1243:ASN:ND2  | 2.31                     | 0.45              |
| 3:A:266:HIS:HE1   | 3:A:302:VAL:HG13  | 1.82                     | 0.45              |
| 3:H:279:VAL:HG12  | 3:H:394:LEU:HD22  | 1.98                     | 0.45              |
| 4:o:5:GLN:H       | 4:o:11:THR:HG21   | 1.80                     | 0.45              |
| 3:N:496:GLY:HA3   | 3:N:504:ARG:NH2   | 2.32                     | 0.45              |
| 3:O:463:HIS:HD2   | 3:O:465:SER:OG    | 1.99                     | 0.45              |
| 3:O:580:GLY:HA2   | 3:O:592:ARG:NH1   | 2.25                     | 0.45              |
| 3:O:1032:SER:H    | 3:O:1035:ALA:HB3  | 1.81                     | 0.45              |
| 3:P:116:VAL:HG12  | 3:P:117:HIS:N     | 2.31                     | 0.45              |
| 3:P:1304:THR:HG23 | 3:P:1313:ARG:HA   | 1.99                     | 0.45              |
| 3:B:846:GLU:HA    | 4:b:68:HIS:CE1    | 2.37                     | 0.45              |
| 3:B:1004:GLN:O    | 3:B:1007:VAL:N    | 2.49                     | 0.45              |
| 3:B:1138:LEU:HD11 | 3:B:1144:ALA:N    | 2.32                     | 0.45              |
| 3:C:383:ARG:HB2   | 3:C:384:ILE:HD12  | 1.98                     | 0.45              |
| 3:C:481:VAL:HG11  | 3:C:571:ILE:HD12  | 1.98                     | 0.45              |
| 3:D:367:LEU:HD23  | 3:D:367:LEU:HA    | 1.69                     | 0.45              |
| 3:D:627:PHE:HD1   | 3:D:664:PHE:CZ    | 2.34                     | 0.45              |
| 3:D:696:HIS:HE1   | 3:D:1021:THR:HG21 | 1.82                     | 0.45              |
| 3:D:880:HIS:NE2   | 4:c:98:TYR:CD2    | 2.79                     | 0.45              |
| 5:q:25:HIS:ND1    | 5:q:113:SER:HB3   | 2.32                     | 0.45              |
| 3:E:485:ASN:ND2   | 3:E:516:GLY:O     | 2.49                     | 0.45              |
| 3:E:491:VAL:HG21  | 3:E:929:PHE:HD2   | 1.81                     | 0.45              |
| 3:E:606:MET:HB3   | 3:E:606:MET:HE2   | 1.71                     | 0.45              |
| 3:F:761:HIS:CD2   | 3:F:780:ASP:HA    | 2.51                     | 0.45              |
| 3:F:765:TYR:HE1   | 3:F:783:LEU:HD12  | 1.81                     | 0.45              |
| 3:F:834:ARG:HD3   | 4:e:90:PRO:HD3    | 1.99                     | 0.45              |
| 3:G:231:SER:O     | 3:G:1112:THR:OG1  | 2.35                     | 0.45              |
| 3:G:293:LEU:HD13  | 3:G:368:VAL:HG11  | 1.97                     | 0.45              |
| 3:G:503:GLN:OE1   | 3:G:503:GLN:HA    | 2.17                     | 0.45              |
| 2:S:2:ILE:HD12    | 3:B:1084:GLU:C    | 2.38                     | 0.45              |
| 2:U:276:VAL:HG21  | 2:V:176:LEU:HD11  | 1.99                     | 0.45              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:W:45:ASP:C     | 3:I:345:GLU:HG2   | 2.41                     | 0.45              |
| 2:X:10:ILE:HD13  | 2:X:46:VAL:HG21   | 1.99                     | 0.45              |
| 3:I:475:GLY:O    | 3:I:478:HIS:HD2   | 2.00                     | 0.45              |
| 3:I:784:LEU:HG   | 3:I:934:HIS:NE2   | 2.32                     | 0.45              |
| 3:I:845:PRO:HG2  | 3:I:862:ALA:O     | 2.17                     | 0.45              |
| 3:J:204:TYR:CD2  | 3:J:219:LEU:HD11  | 2.51                     | 0.45              |
| 3:J:905:THR:HB   | 3:J:956:TYR:OH    | 2.17                     | 0.45              |
| 3:M:129:LEU:O    | 3:M:1094:THR:HA   | 2.16                     | 0.45              |
| 3:M:527:THR:HG22 | 3:M:528:ALA:N     | 2.32                     | 0.45              |
| 3:M:714:LEU:HD22 | 3:M:1143:ALA:HA   | 1.99                     | 0.45              |
| 3:M:771:VAL:HG23 | 3:M:898:ALA:O     | 2.17                     | 0.45              |
| 3:M:840:GLN:C    | 3:M:842:MET:HG2   | 2.41                     | 0.45              |
| 4:j:79:PHE:CA    | 4:j:93:GLY:HA3    | 2.47                     | 0.45              |
| 4:n:79:PHE:HA    | 3:O:948:THR:HA    | 1.99                     | 0.45              |
| 3:N:339:MET:SD   | 3:N:339:MET:C     | 3.00                     | 0.45              |
| 3:N:746:ALA:HA   | 3:N:754:CYS:CB    | 2.47                     | 0.45              |
| 3:O:1155:ASN:OD1 | 3:O:1156:ARG:N    | 2.50                     | 0.45              |
| 3:P:193:PRO:HB2  | 3:P:1293:ILE:HG22 | 1.98                     | 0.45              |
| 3:P:1034:VAL:HA  | 3:P:1147:LEU:HD21 | 1.98                     | 0.45              |
| 3:P:1205:PRO:HG2 | 3:P:1276:PHE:CE2  | 2.51                     | 0.45              |
| 3:P:1281:ASP:O   | 3:P:1284:ALA:N    | 2.44                     | 0.45              |
| 3:B:1342:LEU:CD2 | 3:B:1362:LEU:HB2  | 2.43                     | 0.45              |
| 3:C:703:LEU:O    | 3:C:706:ASP:N     | 2.46                     | 0.45              |
| 3:C:714:LEU:HD23 | 3:C:714:LEU:HA    | 1.73                     | 0.45              |
| 3:D:199:LEU:HA   | 3:D:199:LEU:HD23  | 1.63                     | 0.45              |
| 3:D:280:THR:HG22 | 3:D:1063:VAL:HG22 | 1.98                     | 0.45              |
| 3:D:499:ALA:HA   | 3:D:956:TYR:CD1   | 2.52                     | 0.45              |
| 3:E:96:GLN:HG2   | 3:E:121:THR:HG22  | 1.98                     | 0.45              |
| 3:E:578:VAL:HB   | 3:E:1027:GLY:O    | 2.17                     | 0.45              |
| 3:E:724:HIS:HE1  | 3:E:1025:MET:O    | 1.99                     | 0.45              |
| 3:E:775:ASP:CG   | 3:E:778:ARG:HH21  | 2.25                     | 0.45              |
| 3:F:524:CYS:CB   | 3:F:1008:GLN:HE22 | 2.28                     | 0.45              |
| 3:F:543:LEU:HD23 | 3:F:1248:GLN:OE1  | 2.16                     | 0.45              |
| 3:F:879:PHE:CE1  | 3:F:886:VAL:HG21  | 2.52                     | 0.45              |
| 2:S:268:ARG:NH2  | 2:S:273:GLU:OE1   | 2.50                     | 0.45              |
| 2:X:50:SER:OG    | 2:X:70:ARG:NH2    | 2.43                     | 0.45              |
| 3:I:496:GLY:HA3  | 3:I:504:ARG:HH12  | 1.82                     | 0.45              |
| 3:I:866:HIS:CG   | 3:I:867:PRO:HD2   | 2.52                     | 0.45              |
| 3:I:873:ASN:HA   | 4:h:92:PHE:CD2    | 2.52                     | 0.45              |
| 3:J:492:ALA:H    | 3:J:992:PRO:HB2   | 1.81                     | 0.45              |
| 3:J:1198:TYR:HD1 | 3:J:1236:ARG:HH11 | 1.65                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:K:473:VAL:O     | 3:K:477:ASN:ND2   | 2.36                     | 0.45              |
| 3:L:778:ARG:HG2   | 3:L:904:ARG:HH12  | 1.82                     | 0.45              |
| 3:L:863:HIS:CD2   | 3:L:865:LEU:H     | 2.35                     | 0.45              |
| 3:L:1178:ASP:O    | 3:M:217:ALA:HB1   | 2.17                     | 0.45              |
| 3:M:412:ALA:HA    | 3:M:415:ARG:NH2   | 2.32                     | 0.45              |
| 3:H:895:GLN:NE2   | 4:h:65:GLY:HA3    | 2.32                     | 0.45              |
| 4:n:100:PRO:HD2   | 3:N:646:ARG:NH1   | 2.31                     | 0.45              |
| 3:N:58:LEU:HD12   | 3:O:124:ILE:HD11  | 1.99                     | 0.45              |
| 3:N:765:TYR:HE1   | 3:N:783:LEU:HD12  | 1.82                     | 0.45              |
| 3:N:1355:GLU:OE1  | 3:N:1355:GLU:N    | 2.47                     | 0.45              |
| 3:O:577:VAL:HG12  | 3:O:578:VAL:HG13  | 1.99                     | 0.45              |
| 3:O:756:ILE:HA    | 3:O:909:LEU:O     | 2.16                     | 0.45              |
| 3:O:866:HIS:CD2   | 3:O:868:ALA:HB3   | 2.51                     | 0.45              |
| 3:P:122:LYS:NZ    | 3:P:1103:GLY:O    | 2.50                     | 0.45              |
| 3:P:213:ARG:NH1   | 3:P:1216:GLY:HA3  | 2.24                     | 0.45              |
| 3:P:476:VAL:HG12  | 3:P:571:ILE:HD13  | 1.99                     | 0.45              |
| 3:B:213:ARG:HH21  | 3:G:1176:GLY:HA2  | 1.81                     | 0.45              |
| 3:B:405:PRO:HB3   | 3:B:1199:PHE:CE2  | 2.51                     | 0.45              |
| 3:B:1215:ALA:O    | 3:B:1287:ARG:NH2  | 2.47                     | 0.45              |
| 3:C:469:ILE:O     | 3:C:471:ALA:N     | 2.50                     | 0.45              |
| 3:C:490:TYR:OH    | 3:C:561:GLY:N     | 2.50                     | 0.45              |
| 3:C:528:ALA:O     | 3:C:531:PHE:N     | 2.49                     | 0.45              |
| 3:C:732:LEU:HD21  | 3:C:745:HIS:HB2   | 1.98                     | 0.45              |
| 3:C:784:LEU:HD23  | 3:C:903:GLU:HG2   | 1.99                     | 0.45              |
| 3:C:1034:VAL:HG22 | 3:C:1147:LEU:HD21 | 1.98                     | 0.45              |
| 3:C:1202:PRO:HB3  | 3:C:1332:TYR:CD1  | 2.49                     | 0.45              |
| 3:D:675:VAL:HG21  | 3:D:694:VAL:HG21  | 1.99                     | 0.45              |
| 3:D:954:TYR:OH    | 4:c:92:PHE:CZ     | 2.69                     | 0.45              |
| 5:q:93:VAL:CG2    | 5:q:103:ARG:HH12  | 2.30                     | 0.45              |
| 5:q:119:ASP:H     | 5:q:122:GLY:HA2   | 1.81                     | 0.45              |
| 5:q:393:THR:C     | 5:q:395:GLN:H     | 2.25                     | 0.45              |
| 5:q:422:LEU:HD23  | 5:q:453:PHE:CD2   | 2.52                     | 0.45              |
| 3:F:134:SER:CB    | 3:G:114:GLN:HE22  | 2.18                     | 0.45              |
| 3:F:828:ALA:HA    | 3:F:958:LEU:H     | 1.82                     | 0.45              |
| 3:F:867:PRO:HA    | 3:F:870:LEU:HD12  | 1.98                     | 0.45              |
| 1:Q:317:ARG:HB2   | 1:Q:350:LEU:HD22  | 1.98                     | 0.45              |
| 1:W:25:ARG:O      | 1:W:29:GLY:N      | 2.49                     | 0.45              |
| 2:2:100:LEU:HD13  | 2:2:314:VAL:HG21  | 1.99                     | 0.45              |
| 3:I:10:GLY:HA2    | 3:I:38:PHE:CE2    | 2.52                     | 0.45              |
| 3:I:432:PRO:HA    | 3:I:435:PHE:CD2   | 2.52                     | 0.45              |
| 3:I:496:GLY:HA3   | 3:I:504:ARG:HH22  | 1.82                     | 0.45              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:J:163:GLN:NE2  | 3:K:348:ARG:HH22  | 2.11                     | 0.45              |
| 3:J:280:THR:HG22 | 3:J:1063:VAL:HG22 | 1.98                     | 0.45              |
| 3:J:829:GLY:N    | 3:J:956:TYR:O     | 2.50                     | 0.45              |
| 3:J:1148:ARG:NH2 | 3:J:1162:PRO:HA   | 2.32                     | 0.45              |
| 3:K:255:THR:CG2  | 3:K:1109:VAL:HG23 | 2.47                     | 0.45              |
| 3:K:879:PHE:O    | 3:K:883:ARG:N     | 2.49                     | 0.45              |
| 3:L:23:ILE:HB    | 3:N:63:ASN:OD1    | 2.17                     | 0.45              |
| 3:L:63:ASN:HD21  | 3:M:99:VAL:HG13   | 1.80                     | 0.45              |
| 3:L:477:ASN:OD1  | 3:L:571:ILE:HB    | 2.17                     | 0.45              |
| 3:L:784:LEU:HD22 | 3:L:786:ASN:ND2   | 2.32                     | 0.45              |
| 3:M:989:LEU:HD23 | 3:M:989:LEU:HA    | 1.74                     | 0.45              |
| 3:A:406:LEU:HD23 | 3:A:440:LEU:HG    | 1.99                     | 0.45              |
| 3:A:645:ALA:HB1  | 3:A:678:LEU:HD21  | 1.99                     | 0.45              |
| 3:A:733:PRO:HG3  | 3:A:810:LYS:HG3   | 1.97                     | 0.45              |
| 3:H:98:GLU:OE2   | 3:C:16:ALA:HB1    | 2.17                     | 0.45              |
| 3:H:752:ARG:NH2  | 3:H:915:ASP:OD1   | 2.50                     | 0.45              |
| 3:H:784:LEU:HB2  | 3:H:786:ASN:OD1   | 2.17                     | 0.45              |
| 3:H:1105:GLY:CA  | 3:C:32:HIS:NE2    | 2.74                     | 0.45              |
| 3:N:258:SER:O    | 3:D:24:LEU:CD1    | 2.62                     | 0.45              |
| 3:N:399:ASP:OD1  | 3:N:1057:ARG:HG2  | 2.17                     | 0.45              |
| 3:N:1202:PRO:HB3 | 3:N:1332:TYR:HD1  | 1.82                     | 0.45              |
| 3:O:630:LEU:O    | 3:O:634:ILE:HD12  | 2.17                     | 0.45              |
| 3:O:652:ILE:O    | 3:O:655:TYR:N     | 2.50                     | 0.45              |
| 3:O:842:MET:HE1  | 3:O:891:MET:HB3   | 1.97                     | 0.45              |
| 3:O:1233:ASP:HB3 | 3:O:1236:ARG:O    | 2.17                     | 0.45              |
| 3:P:763:PRO:HB2  | 3:P:765:TYR:CZ    | 2.52                     | 0.45              |
| 3:P:864:PRO:O    | 3:P:876:ASN:HB3   | 2.17                     | 0.45              |
| 3:B:33:ARG:HD3   | 3:B:39:PHE:CD2    | 2.52                     | 0.45              |
| 3:B:262:PRO:HA   | 3:G:60:SER:OG     | 2.17                     | 0.45              |
| 3:B:438:ARG:HB2  | 3:B:454:MET:HG2   | 1.98                     | 0.45              |
| 3:B:630:LEU:O    | 3:B:634:ILE:HD12  | 2.17                     | 0.45              |
| 3:B:708:THR:HG22 | 3:B:723:ASN:HD22  | 1.82                     | 0.45              |
| 3:B:724:HIS:HE1  | 3:B:1028:TYR:HB2  | 1.78                     | 0.45              |
| 3:B:834:ARG:HD2  | 3:B:953:GLU:O     | 2.16                     | 0.45              |
| 3:E:634:ILE:HG22 | 3:E:636:GLY:H     | 1.80                     | 0.45              |
| 3:F:958:LEU:HD23 | 3:F:958:LEU:HA    | 1.83                     | 0.45              |
| 3:F:1170:GLN:OE1 | 3:F:1170:GLN:N    | 2.41                     | 0.45              |
| 3:G:392:TYR:HD2  | 3:G:395:VAL:HG23  | 1.82                     | 0.45              |
| 3:G:577:VAL:HG12 | 3:G:578:VAL:HG13  | 1.99                     | 0.45              |
| 1:T:228:SER:O    | 1:T:232:ARG:N     | 2.46                     | 0.45              |
| 2:X:300:PHE:CE2  | 3:C:1083:HIS:CB   | 3.00                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:y:18:ARG:HA     | 2:y:21:ALA:HB3    | 1.98                     | 0.45              |
| 3:I:279:VAL:O     | 3:I:394:LEU:HD21  | 2.17                     | 0.45              |
| 3:K:745:HIS:HE1   | 3:K:754:CYS:HA    | 1.82                     | 0.45              |
| 3:K:1229:HIS:CE1  | 3:K:1248:GLN:HA   | 2.52                     | 0.45              |
| 3:K:1269:VAL:HG12 | 3:K:1270:LEU:O    | 2.17                     | 0.45              |
| 3:L:485:ASN:HD21  | 3:L:516:GLY:H     | 1.65                     | 0.45              |
| 3:L:906:THR:OG1   | 3:L:934:HIS:HB3   | 2.17                     | 0.45              |
| 3:A:335:HIS:O     | 3:A:338:GLU:HB3   | 2.17                     | 0.45              |
| 3:H:129:LEU:O     | 3:H:1094:THR:HA   | 2.17                     | 0.45              |
| 3:H:638:GLU:HB2   | 3:H:789:ALA:HA    | 1.97                     | 0.45              |
| 3:O:487:TYR:OH    | 3:O:989:LEU:HA    | 2.17                     | 0.45              |
| 3:O:618:PHE:O     | 3:O:941:ALA:HB2   | 2.16                     | 0.45              |
| 3:O:841:ASN:O     | 3:O:875:VAL:HG23  | 2.17                     | 0.45              |
| 3:P:1181:GLN:HB2  | 3:P:1309:VAL:O    | 2.17                     | 0.45              |
| 3:B:315:ASN:HD21  | 3:B:339:MET:HB3   | 1.82                     | 0.45              |
| 3:B:804:ASP:HB3   | 3:B:808:HIS:NE2   | 2.31                     | 0.45              |
| 3:B:1365:ASP:OD1  | 3:B:1365:ASP:N    | 2.49                     | 0.45              |
| 3:C:137:THR:HG22  | 3:C:1087:GLY:O    | 2.16                     | 0.45              |
| 3:C:158:GLN:O     | 3:C:162:ILE:N     | 2.40                     | 0.45              |
| 3:C:841:ASN:O     | 3:C:875:VAL:HG23  | 2.17                     | 0.45              |
| 3:C:1222:VAL:HG11 | 3:C:1283:THR:HA   | 1.99                     | 0.45              |
| 3:D:1072:ALA:HB3  | 3:D:1100:VAL:HB   | 1.99                     | 0.45              |
| 3:E:11:TYR:HB2    | 3:E:38:PHE:CE2    | 2.52                     | 0.45              |
| 3:E:983:LEU:HD21  | 3:E:987:VAL:CG2   | 2.44                     | 0.45              |
| 3:F:1059:VAL:HG23 | 3:F:1119:VAL:HG23 | 1.99                     | 0.45              |
| 6:s:91:VAL:HG12   | 7:t:3089:CYS:O    | 2.17                     | 0.45              |
| 3:G:554:ALA:N     | 3:G:569:GLY:HA2   | 2.31                     | 0.45              |
| 3:G:1346:ALA:HB2  | 3:G:1362:LEU:HD11 | 1.97                     | 0.45              |
| 2:V:68:ARG:NH1    | 2:V:288:ILE:O     | 2.50                     | 0.45              |
| 3:I:178:ARG:HB3   | 3:J:104:ILE:HG22  | 2.00                     | 0.45              |
| 3:I:193:PRO:HG2   | 3:I:198:LEU:HD11  | 1.98                     | 0.45              |
| 3:I:309:MET:HE1   | 3:I:327:ARG:HA    | 1.99                     | 0.45              |
| 3:J:462:CYS:SG    | 3:J:1147:LEU:HD22 | 2.57                     | 0.45              |
| 3:J:765:TYR:CE1   | 3:J:783:LEU:HD12  | 2.52                     | 0.45              |
| 3:K:484:ALA:O     | 3:K:486:PRO:CD    | 2.63                     | 0.45              |
| 3:K:668:TYR:HD2   | 3:K:809:HIS:CE1   | 2.35                     | 0.45              |
| 3:L:23:ILE:HG22   | 3:L:24:LEU:N      | 2.32                     | 0.45              |
| 3:L:32:HIS:HE2    | 3:O:1105:GLY:HA2  | 1.81                     | 0.45              |
| 3:M:268:ASP:OD1   | 3:M:367:LEU:HD13  | 2.17                     | 0.45              |
| 3:M:802:PRO:HG3   | 3:H:945:LEU:HD21  | 1.99                     | 0.45              |
| 3:H:176:PHE:O     | 3:H:180:THR:HG23  | 2.17                     | 0.45              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:H:424:VAL:HG12 | 3:H:425:PRO:O     | 2.17                     | 0.45              |
| 4:k:88:LEU:HD12  | 4:k:89:ARG:N      | 2.32                     | 0.45              |
| 3:N:526:MET:HE1  | 3:N:536:ASN:HB3   | 1.98                     | 0.45              |
| 3:N:651:CYS:O    | 3:N:654:SER:OG    | 2.29                     | 0.45              |
| 3:N:825:CYS:HB2  | 3:N:939:LEU:O     | 2.16                     | 0.45              |
| 3:N:1249:ARG:HA  | 3:N:1254:ASP:OD2  | 2.17                     | 0.45              |
| 3:O:198:LEU:HD21 | 3:O:1106:TYR:CD2  | 2.51                     | 0.45              |
| 3:O:662:ALA:HB2  | 3:O:689:VAL:HG11  | 1.99                     | 0.45              |
| 3:P:460:THR:HA   | 3:P:1129:PHE:CD2  | 2.52                     | 0.45              |
| 3:P:845:PRO:HG3  | 3:P:869:ASN:HD21  | 1.82                     | 0.45              |
| 3:P:914:PRO:HD3  | 3:P:926:MET:O     | 2.17                     | 0.45              |
| 3:B:423:LEU:HA   | 3:B:423:LEU:HD23  | 1.69                     | 0.45              |
| 3:B:469:ILE:HG22 | 3:B:473:VAL:HG23  | 1.99                     | 0.45              |
| 3:D:631:GLN:HG2  | 3:D:670:LEU:HD11  | 1.99                     | 0.45              |
| 5:q:134:LEU:O    | 5:q:143:ALA:HA    | 2.17                     | 0.45              |
| 5:q:438:PRO:O    | 5:q:441:LEU:HB3   | 2.16                     | 0.45              |
| 5:q:586:HIS:CD2  | 5:q:625:MET:HE2   | 2.51                     | 0.45              |
| 3:E:172:VAL:HG11 | 3:E:1093:LEU:HD12 | 1.99                     | 0.45              |
| 3:E:589:VAL:O    | 3:E:592:ARG:N     | 2.49                     | 0.45              |
| 3:E:1241:THR:OG1 | 3:E:1243:ASN:O    | 2.27                     | 0.45              |
| 3:F:12:ARG:CD    | 3:G:321:VAL:O     | 2.65                     | 0.45              |
| 3:F:124:ILE:HG12 | 3:F:1100:VAL:CG2  | 2.47                     | 0.45              |
| 3:F:302:VAL:HG12 | 3:F:303:PRO:O     | 2.17                     | 0.45              |
| 3:F:714:LEU:HA   | 3:F:714:LEU:HD23  | 1.75                     | 0.45              |
| 3:F:714:LEU:HD12 | 3:F:722:LEU:HD22  | 1.99                     | 0.45              |
| 3:F:755:ARG:HG3  | 3:F:755:ARG:O     | 2.17                     | 0.45              |
| 3:G:104:ILE:O    | 3:G:113:GLU:OE2   | 2.35                     | 0.45              |
| 3:G:133:PHE:HB3  | 3:G:1091:PHE:HB2  | 1.98                     | 0.45              |
| 2:X:300:PHE:CE2  | 3:C:1083:HIS:HB3  | 2.53                     | 0.44              |
| 1:w:427:VAL:HG21 | 1:w:458:ARG:HH21  | 1.83                     | 0.44              |
| 3:I:86:GLU:OE1   | 3:I:86:GLU:N      | 2.50                     | 0.44              |
| 3:I:94:ARG:HB2   | 3:H:57:LEU:HD23   | 1.99                     | 0.44              |
| 3:I:136:ALA:O    | 3:I:140:ILE:HG13  | 2.17                     | 0.44              |
| 3:I:749:ASP:OD1  | 3:I:752:ARG:HB3   | 2.17                     | 0.44              |
| 3:I:846:GLU:HA   | 4:i:68:HIS:HE1    | 1.81                     | 0.44              |
| 3:J:373:ARG:NH1  | 3:J:1067:GLU:OE2  | 2.45                     | 0.44              |
| 3:J:463:HIS:CD2  | 3:J:465:SER:HB3   | 2.52                     | 0.44              |
| 3:K:132:ALA:HB3  | 3:L:114:GLN:HG2   | 1.99                     | 0.44              |
| 3:K:326:VAL:HB   | 3:K:329:LEU:HD12  | 1.99                     | 0.44              |
| 3:K:1178:ASP:O   | 3:L:217:ALA:HB1   | 2.16                     | 0.44              |
| 3:L:296:GLU:OE1  | 3:L:374:LEU:HD21  | 2.17                     | 0.44              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:M:69:ARG:HA    | 3:M:177:GLU:HG2   | 1.99                     | 0.44              |
| 3:A:94:ARG:HH12  | 3:G:47:ASN:C      | 2.25                     | 0.44              |
| 3:A:129:LEU:HD12 | 3:A:1097:ARG:HH11 | 1.82                     | 0.44              |
| 3:A:578:VAL:HB   | 3:A:1027:GLY:O    | 2.18                     | 0.44              |
| 3:A:727:ARG:NH1  | 3:A:807:VAL:HG11  | 2.32                     | 0.44              |
| 3:A:1054:ARG:NH1 | 3:A:1123:GLY:H    | 2.15                     | 0.44              |
| 3:H:502:GLN:O    | 3:H:505:PHE:HB3   | 2.17                     | 0.44              |
| 3:H:755:ARG:HG2  | 3:H:911:SER:OG    | 2.17                     | 0.44              |
| 3:N:126:ARG:HG3  | 3:N:1097:ARG:O    | 2.17                     | 0.44              |
| 3:N:266:HIS:HE1  | 3:N:302:VAL:HG13  | 1.83                     | 0.44              |
| 3:N:745:HIS:HE2  | 3:N:910:CYS:HB2   | 1.82                     | 0.44              |
| 3:N:1034:VAL:HA  | 3:N:1147:LEU:HD21 | 1.98                     | 0.44              |
| 3:O:834:ARG:HA   | 3:O:837:ALA:HB3   | 1.99                     | 0.44              |
| 3:B:331:ASP:HA   | 3:B:334:ARG:HB2   | 1.98                     | 0.44              |
| 3:C:36:PHE:HD2   | 3:C:39:PHE:HD1    | 1.64                     | 0.44              |
| 3:C:195:LEU:O    | 3:C:198:LEU:N     | 2.43                     | 0.44              |
| 3:C:802:PRO:HG3  | 3:D:945:LEU:HD11  | 1.99                     | 0.44              |
| 3:C:866:HIS:O    | 3:C:870:LEU:N     | 2.50                     | 0.44              |
| 3:D:58:LEU:HA    | 3:E:327:ARG:HB2   | 1.98                     | 0.44              |
| 3:D:714:LEU:HD23 | 3:D:714:LEU:HA    | 1.80                     | 0.44              |
| 3:D:1195:ASP:OD1 | 3:D:1195:ASP:N    | 2.49                     | 0.44              |
| 3:D:1218:LYS:HB3 | 3:D:1221:ASP:CG   | 2.43                     | 0.44              |
| 3:E:443:TRP:NE1  | 3:E:1343:LEU:HD21 | 2.32                     | 0.44              |
| 3:E:475:GLY:HA3  | 3:E:1250:PHE:CE2  | 2.52                     | 0.44              |
| 3:E:512:ARG:HD3  | 3:E:515:HIS:CD2   | 2.52                     | 0.44              |
| 3:E:1251:SER:O   | 3:E:1255:LEU:HG   | 2.18                     | 0.44              |
| 3:F:402:PHE:CG   | 3:F:1334:ILE:HD11 | 2.52                     | 0.44              |
| 3:F:424:VAL:HG12 | 3:F:425:PRO:O     | 2.17                     | 0.44              |
| 3:F:544:HIS:CG   | 3:F:545:PRO:HD2   | 2.52                     | 0.44              |
| 3:F:906:THR:OG1  | 3:F:934:HIS:HB3   | 2.17                     | 0.44              |
| 3:G:1156:ARG:NH2 | 3:G:1182:ASP:OD2  | 2.50                     | 0.44              |
| 2:S:130:LEU:HD13 | 2:S:133:LEU:HD12  | 1.99                     | 0.44              |
| 3:I:43:ARG:C     | 3:I:45:ASP:H      | 2.25                     | 0.44              |
| 3:I:836:TYR:CE1  | 3:I:897:LEU:HD22  | 2.51                     | 0.44              |
| 3:I:1036:LEU:HA  | 3:I:1036:LEU:HD23 | 1.72                     | 0.44              |
| 3:J:125:ASP:O    | 3:J:1098:GLY:HA2  | 2.16                     | 0.44              |
| 3:J:491:VAL:O    | 3:J:559:PRO:HA    | 2.17                     | 0.44              |
| 3:K:599:LEU:C    | 3:K:601:VAL:H     | 2.24                     | 0.44              |
| 3:K:647:LEU:HG   | 3:K:890:ALA:HB1   | 1.98                     | 0.44              |
| 3:K:840:GLN:NE2  | 4:k:58:ALA:HB2    | 2.32                     | 0.44              |
| 3:L:948:THR:HB   | 4:k:95:LYS:HE3    | 2.00                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:L:1245:TRP:O    | 3:L:1251:SER:HB3  | 2.17                     | 0.44              |
| 3:L:1304:THR:HG21 | 3:L:1314:PRO:HD2  | 1.97                     | 0.44              |
| 3:M:96:GLN:NE2    | 3:N:11:TYR:HD1    | 2.16                     | 0.44              |
| 3:M:520:TRP:CD1   | 3:M:997:ASN:HD22  | 2.36                     | 0.44              |
| 3:M:647:LEU:O     | 3:M:651:CYS:N     | 2.45                     | 0.44              |
| 3:M:1209:ALA:HB2  | 3:M:1235:ALA:HB2  | 1.99                     | 0.44              |
| 3:A:184:MET:HE3   | 3:A:184:MET:HB3   | 1.77                     | 0.44              |
| 3:H:43:ARG:O      | 3:H:45:ASP:N      | 2.49                     | 0.44              |
| 4:k:68:HIS:HB3    | 4:k:71:ASN:HB3    | 2.00                     | 0.44              |
| 4:n:95:LYS:HG2    | 3:N:642:CYS:SG    | 2.57                     | 0.44              |
| 4:p:79:PHE:CZ     | 3:P:639:HIS:HA    | 2.52                     | 0.44              |
| 3:N:251:LEU:HD21  | 3:N:1111:ALA:HB2  | 1.99                     | 0.44              |
| 3:O:264:LEU:O     | 3:O:265:THR:OG1   | 2.29                     | 0.44              |
| 3:O:363:VAL:HG12  | 3:O:364:ARG:H     | 1.81                     | 0.44              |
| 3:O:755:ARG:HG2   | 3:O:911:SER:OG    | 2.16                     | 0.44              |
| 3:O:1058:PHE:CE2  | 3:O:1369:LEU:HD11 | 2.52                     | 0.44              |
| 3:O:1241:THR:OG1  | 3:O:1247:SER:OG   | 2.30                     | 0.44              |
| 3:B:103:LEU:O     | 3:G:175:ALA:HB1   | 2.14                     | 0.44              |
| 3:B:383:ARG:HB2   | 3:B:384:ILE:HD12  | 1.99                     | 0.44              |
| 3:B:433:ARG:O     | 3:B:1360:GLN:NE2  | 2.38                     | 0.44              |
| 3:B:778:ARG:HH12  | 3:B:782:ARG:NH1   | 2.15                     | 0.44              |
| 3:C:475:GLY:HA2   | 3:C:478:HIS:CD2   | 2.52                     | 0.44              |
| 3:D:238:GLY:HA2   | 3:D:244:ILE:HD11  | 1.99                     | 0.44              |
| 3:D:734:PRO:O     | 3:D:735:LEU:HD23  | 2.18                     | 0.44              |
| 5:q:85:ALA:HB1    | 5:q:111:PHE:CE1   | 2.52                     | 0.44              |
| 5:q:431:ALA:HA    | 7:u:3115:HIS:HD2  | 1.82                     | 0.44              |
| 5:q:465:PRO:HB2   | 5:q:467:LEU:O     | 2.17                     | 0.44              |
| 3:F:130:ASN:OD1   | 3:F:1094:THR:HG22 | 2.17                     | 0.44              |
| 3:F:397:ALA:HB3   | 3:F:1321:VAL:HG22 | 2.00                     | 0.44              |
| 3:G:258:SER:OG    | 3:G:259:VAL:N     | 2.49                     | 0.44              |
| 1:W:197:ALA:HB2   | 1:W:324:LEU:HD22  | 1.99                     | 0.44              |
| 1:W:271:GLN:OE1   | 1:W:457:TRP:NE1   | 2.46                     | 0.44              |
| 2:x:219:LEU:HD13  | 2:x:275:LEU:HD23  | 1.99                     | 0.44              |
| 3:I:1227:TYR:O    | 3:I:1229:HIS:ND1  | 2.50                     | 0.44              |
| 3:I:1241:THR:OG1  | 3:I:1247:SER:OG   | 2.32                     | 0.44              |
| 3:I:1344:ARG:NH1  | 3:J:1355:GLU:HB2  | 2.32                     | 0.44              |
| 3:J:663:ALA:O     | 3:J:690:TYR:OH    | 2.20                     | 0.44              |
| 3:K:1237:PRO:HD2  | 3:K:1238:PHE:CD2  | 2.51                     | 0.44              |
| 3:L:406:LEU:HD23  | 3:L:440:LEU:HG    | 1.99                     | 0.44              |
| 3:L:829:GLY:HA3   | 3:L:956:TYR:CZ    | 2.52                     | 0.44              |
| 3:M:178:ARG:HB3   | 3:H:104:ILE:HG22  | 1.98                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:M:402:PHE:HA    | 3:M:1332:TYR:O    | 2.17                     | 0.44              |
| 3:M:511:GLN:HB3   | 3:M:515:HIS:CE1   | 2.53                     | 0.44              |
| 3:M:767:ALA:HA    | 3:M:785:HIS:HB3   | 1.98                     | 0.44              |
| 3:M:950:GLN:HB2   | 3:M:953:GLU:HG3   | 1.98                     | 0.44              |
| 3:A:406:LEU:HD11  | 3:A:1187:PHE:HE1  | 1.82                     | 0.44              |
| 3:A:764:VAL:HB    | 3:A:782:ARG:HA    | 1.99                     | 0.44              |
| 3:H:634:ILE:HG22  | 3:H:636:GLY:N     | 2.33                     | 0.44              |
| 3:H:765:TYR:CE1   | 3:H:783:LEU:HD12  | 2.52                     | 0.44              |
| 3:H:793:ASP:OD2   | 3:H:800:HIS:NE2   | 2.50                     | 0.44              |
| 3:H:1365:ASP:O    | 3:H:1370:LYS:NZ   | 2.50                     | 0.44              |
| 4:n:23:ARG:HH12   | 4:n:27:LEU:HG     | 1.82                     | 0.44              |
| 4:o:79:PHE:HE2    | 3:O:639:HIS:CD2   | 2.35                     | 0.44              |
| 4:o:97:THR:HA     | 3:O:646:ARG:HB3   | 1.99                     | 0.44              |
| 3:N:58:LEU:HD23   | 3:N:58:LEU:HA     | 1.60                     | 0.44              |
| 3:O:638:GLU:HB2   | 3:O:789:ALA:HA    | 1.99                     | 0.44              |
| 3:O:866:HIS:O     | 3:O:870:LEU:HG    | 2.18                     | 0.44              |
| 3:P:490:TYR:HH    | 3:P:561:GLY:N     | 2.15                     | 0.44              |
| 3:P:725:LEU:HB3   | 3:P:1028:TYR:HB3  | 1.99                     | 0.44              |
| 3:P:876:ASN:O     | 3:P:879:PHE:HB2   | 2.17                     | 0.44              |
| 3:B:1201:ARG:HG2  | 3:B:1202:PRO:HD2  | 1.99                     | 0.44              |
| 3:C:198:LEU:O     | 3:C:199:LEU:C     | 2.59                     | 0.44              |
| 3:C:446:ASP:HB3   | 3:D:1201:ARG:HH12 | 1.82                     | 0.44              |
| 3:C:631:GLN:HE22  | 3:C:666:ASN:CG    | 2.23                     | 0.44              |
| 3:C:706:ASP:O     | 3:D:525:GLN:NE2   | 2.50                     | 0.44              |
| 3:D:198:LEU:HD23  | 3:D:198:LEU:HA    | 1.68                     | 0.44              |
| 3:D:331:ASP:O     | 3:D:334:ARG:N     | 2.51                     | 0.44              |
| 3:D:541:LEU:HA    | 3:D:541:LEU:HD23  | 1.82                     | 0.44              |
| 3:D:1229:HIS:CE1  | 3:D:1248:GLN:HA   | 2.52                     | 0.44              |
| 5:q:384:SER:OG    | 5:q:401:SER:OG    | 2.19                     | 0.44              |
| 5:q:597:ASP:HA    | 6:r:40:VAL:O      | 2.17                     | 0.44              |
| 3:E:863:HIS:CD2   | 3:E:865:LEU:HB2   | 2.52                     | 0.44              |
| 3:F:251:LEU:HD23  | 3:F:251:LEU:HA    | 1.65                     | 0.44              |
| 3:F:279:VAL:HG12  | 3:F:394:LEU:HD22  | 1.98                     | 0.44              |
| 3:F:452:LEU:HD12  | 3:F:456:ASN:HD22  | 1.83                     | 0.44              |
| 3:F:469:ILE:O     | 3:F:472:ALA:N     | 2.51                     | 0.44              |
| 3:F:490:TYR:OH    | 3:F:561:GLY:N     | 2.51                     | 0.44              |
| 3:F:1152:VAL:HG13 | 3:F:1159:PRO:HD2  | 1.99                     | 0.44              |
| 3:F:1354:ARG:HG3  | 3:F:1354:ARG:O    | 2.16                     | 0.44              |
| 3:G:266:HIS:CE1   | 3:G:302:VAL:HG13  | 2.52                     | 0.44              |
| 3:G:1034:VAL:HG22 | 3:G:1147:LEU:HD21 | 1.99                     | 0.44              |
| 2:R:172:GLU:O     | 5:q:372:ASP:N     | 2.50                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:I:185:LEU:HD11  | 3:I:380:LEU:HD12  | 1.98                     | 0.44              |
| 3:I:264:LEU:O     | 3:I:265:THR:OG1   | 2.31                     | 0.44              |
| 3:I:399:ASP:OD1   | 3:I:1057:ARG:HG2  | 2.16                     | 0.44              |
| 3:J:592:ARG:O     | 3:J:595:ARG:HB3   | 2.17                     | 0.44              |
| 3:L:205:LEU:HD21  | 3:L:1290:GLU:OE2  | 2.17                     | 0.44              |
| 3:L:961:HIS:O     | 3:L:964:PHE:N     | 2.47                     | 0.44              |
| 3:A:137:THR:HA    | 3:A:140:ILE:HD12  | 2.00                     | 0.44              |
| 3:A:592:ARG:O     | 3:A:595:ARG:HB3   | 2.17                     | 0.44              |
| 3:A:914:PRO:HG3   | 3:A:923:THR:HG22  | 1.99                     | 0.44              |
| 3:A:1292:LEU:HD21 | 3:A:1320:LEU:HD21 | 1.99                     | 0.44              |
| 3:H:740:ASP:CG    | 3:H:799:PRO:HB3   | 2.43                     | 0.44              |
| 3:H:1081:ALA:HB3  | 3:H:1092:THR:OG1  | 2.17                     | 0.44              |
| 3:H:1256:LEU:HA   | 3:H:1256:LEU:HD23 | 1.79                     | 0.44              |
| 3:N:274:VAL:HG11  | 3:N:376:PHE:CE2   | 2.52                     | 0.44              |
| 3:N:399:ASP:CG    | 3:N:1321:VAL:HG11 | 2.42                     | 0.44              |
| 3:N:838:THR:HG21  | 3:N:954:TYR:OH    | 2.17                     | 0.44              |
| 3:N:1206:ARG:NH1  | 3:N:1208:ARG:O    | 2.50                     | 0.44              |
| 3:N:1254:ASP:HB3  | 3:N:1258:ASN:ND2  | 2.33                     | 0.44              |
| 3:O:842:MET:CE    | 3:O:891:MET:HE3   | 2.45                     | 0.44              |
| 3:O:1036:LEU:HD23 | 3:O:1036:LEU:HA   | 1.80                     | 0.44              |
| 3:P:700:LEU:HD22  | 3:P:1025:MET:HG3  | 1.99                     | 0.44              |
| 3:P:753:ASP:OD2   | 3:P:927:ARG:NH2   | 2.50                     | 0.44              |
| 3:P:1082:ARG:HG2  | 3:P:1091:PHE:CE1  | 2.52                     | 0.44              |
| 3:B:263:ARG:HB2   | 3:G:59:GLY:CA     | 2.40                     | 0.44              |
| 3:B:682:LEU:HB2   | 3:B:687:MET:HG2   | 2.00                     | 0.44              |
| 3:B:863:HIS:ND1   | 3:B:864:PRO:HD2   | 2.33                     | 0.44              |
| 3:C:624:PRO:HB2   | 3:C:627:PHE:CE2   | 2.52                     | 0.44              |
| 3:D:1227:TYR:CD1  | 3:D:1249:ARG:HB2  | 2.52                     | 0.44              |
| 3:E:133:PHE:HZ    | 3:E:165:LEU:HD22  | 1.83                     | 0.44              |
| 3:E:591:PHE:HZ    | 3:E:1045:HIS:CD2  | 2.34                     | 0.44              |
| 3:E:638:GLU:HG3   | 3:F:947:HIS:CD2   | 2.52                     | 0.44              |
| 3:E:879:PHE:HE2   | 3:E:891:MET:HE1   | 1.81                     | 0.44              |
| 3:E:1050:PHE:HD1  | 3:E:1187:PHE:HB3  | 1.82                     | 0.44              |
| 3:F:460:THR:HA    | 3:F:1129:PHE:CD2  | 2.52                     | 0.44              |
| 3:F:487:TYR:CD1   | 3:F:513:LEU:HD21  | 2.53                     | 0.44              |
| 3:F:842:MET:CE    | 3:F:891:MET:HB3   | 2.37                     | 0.44              |
| 2:S:6:PHE:HB3     | 2:S:87:PRO:HD2    | 1.99                     | 0.44              |
| 1:T:256:THR:HA    | 1:T:261:ALA:HA    | 1.99                     | 0.44              |
| 1:W:349:ARG:HA    | 6:r:14:GLU:CG     | 2.48                     | 0.44              |
| 3:I:331:ASP:HB2   | 3:I:351:LEU:HD11  | 1.98                     | 0.44              |
| 3:I:892:LEU:O     | 3:I:895:GLN:HG3   | 2.18                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:I:968:ASP:O     | 3:I:971:ALA:N     | 2.50                     | 0.44              |
| 3:I:1256:LEU:HD23 | 3:I:1256:LEU:HA   | 1.70                     | 0.44              |
| 3:J:724:HIS:HD2   | 3:J:726:MET:HB2   | 1.83                     | 0.44              |
| 3:J:804:ASP:HB3   | 3:J:808:HIS:CD2   | 2.53                     | 0.44              |
| 3:J:1208:ARG:HH12 | 3:J:1229:HIS:HA   | 1.83                     | 0.44              |
| 3:K:180:THR:HG22  | 3:K:1097:ARG:NH1  | 2.32                     | 0.44              |
| 3:K:778:ARG:HH11  | 3:K:782:ARG:CD    | 2.30                     | 0.44              |
| 3:L:263:ARG:HH12  | 3:L:307:GLY:CA    | 2.30                     | 0.44              |
| 3:M:159:LEU:HD11  | 3:H:340:GLN:HA    | 1.98                     | 0.44              |
| 3:M:266:HIS:HE1   | 3:M:302:VAL:HG13  | 1.81                     | 0.44              |
| 3:M:490:TYR:CD1   | 3:M:564:PRO:HB3   | 2.53                     | 0.44              |
| 3:M:1004:GLN:O    | 3:M:1007:VAL:N    | 2.45                     | 0.44              |
| 3:A:763:PRO:HB2   | 3:A:765:TYR:CZ    | 2.52                     | 0.44              |
| 3:H:487:TYR:HD2   | 3:H:520:TRP:CH2   | 2.36                     | 0.44              |
| 3:H:634:ILE:HG22  | 3:H:636:GLY:H     | 1.83                     | 0.44              |
| 3:H:837:ALA:HA    | 4:h:57:GLN:OE1    | 2.18                     | 0.44              |
| 3:H:1208:ARG:NH2  | 3:H:1228:ASP:O    | 2.51                     | 0.44              |
| 4:l:51:ARG:O      | 4:l:55:ARG:NH1    | 2.50                     | 0.44              |
| 3:N:634:ILE:HA    | 3:N:640:VAL:CG1   | 2.47                     | 0.44              |
| 3:N:778:ARG:O     | 3:N:904:ARG:NE    | 2.50                     | 0.44              |
| 3:O:533:GLN:HB3   | 3:O:534:PRO:HD2   | 1.98                     | 0.44              |
| 3:O:880:HIS:CE1   | 3:O:883:ARG:HH11  | 2.35                     | 0.44              |
| 3:P:218:THR:O     | 3:P:222:GLU:HG2   | 2.18                     | 0.44              |
| 3:P:239:HIS:CD2   | 3:P:240:ARG:HG3   | 2.52                     | 0.44              |
| 3:P:769:CYS:HB2   | 3:P:901:MET:O     | 2.18                     | 0.44              |
| 3:P:866:HIS:O     | 3:P:870:LEU:N     | 2.50                     | 0.44              |
| 3:P:1251:SER:O    | 3:P:1255:LEU:HG   | 2.18                     | 0.44              |
| 3:B:351:LEU:CD2   | 3:G:58:LEU:HD11   | 2.48                     | 0.44              |
| 3:B:488:GLY:HA3   | 3:B:520:TRP:CZ3   | 2.53                     | 0.44              |
| 3:B:989:LEU:HA    | 3:B:989:LEU:HD23  | 1.61                     | 0.44              |
| 3:B:1334:ILE:CA   | 3:B:1365:ASP:HB3  | 2.46                     | 0.44              |
| 3:C:381:GLU:HB3   | 3:C:392:TYR:CD1   | 2.52                     | 0.44              |
| 3:C:406:LEU:HD23  | 3:C:440:LEU:HG    | 1.98                     | 0.44              |
| 3:C:411:PRO:O     | 3:C:415:ARG:NH1   | 2.50                     | 0.44              |
| 3:C:639:HIS:HA    | 4:c:79:PHE:CE2    | 2.53                     | 0.44              |
| 3:C:807:VAL:O     | 3:C:810:LYS:N     | 2.50                     | 0.44              |
| 3:D:204:TYR:CG    | 3:D:219:LEU:HD11  | 2.53                     | 0.44              |
| 3:D:399:ASP:CG    | 3:D:1321:VAL:HG11 | 2.43                     | 0.44              |
| 3:D:544:HIS:ND1   | 3:D:545:PRO:HD2   | 2.33                     | 0.44              |
| 3:D:717:GLN:HE22  | 3:D:752:ARG:HH12  | 1.66                     | 0.44              |
| 3:D:749:ASP:OD2   | 3:D:751:HIS:HB2   | 2.18                     | 0.44              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 5:q:537:ALA:O    | 5:q:541:THR:HG23  | 2.17                     | 0.44              |
| 3:F:755:ARG:HG2  | 3:F:911:SER:OG    | 2.18                     | 0.44              |
| 6:s:62:ALA:HA    | 7:u:3120:LEU:HD22 | 2.00                     | 0.44              |
| 6:s:92:HIS:HA    | 7:t:3093:GLN:HE21 | 1.83                     | 0.44              |
| 3:G:469:ILE:HG23 | 3:G:472:ALA:HB3   | 2.00                     | 0.44              |
| 2:U:52:VAL:HG12  | 2:U:57:SER:HA     | 1.99                     | 0.44              |
| 2:3:80:PRO:HG2   | 3:C:53:GLU:CD     | 2.39                     | 0.44              |
| 3:I:802:PRO:HG3  | 3:J:945:LEU:HD11  | 1.99                     | 0.44              |
| 3:I:845:PRO:HG3  | 3:I:869:ASN:ND2   | 2.32                     | 0.44              |
| 3:I:895:GLN:NE2  | 4:i:65:GLY:HA3    | 2.32                     | 0.44              |
| 3:J:238:GLY:HA2  | 3:J:244:ILE:HD11  | 2.00                     | 0.44              |
| 3:J:258:SER:OG   | 3:J:259:VAL:N     | 2.48                     | 0.44              |
| 3:J:904:ARG:NE   | 3:J:906:THR:HG22  | 2.32                     | 0.44              |
| 3:K:426:ALA:HA   | 3:L:1358:PHE:CE1  | 2.52                     | 0.44              |
| 3:L:63:ASN:ND2   | 3:M:99:VAL:HG13   | 2.32                     | 0.44              |
| 3:L:879:PHE:HB3  | 3:L:884:VAL:O     | 2.17                     | 0.44              |
| 3:M:23:ILE:HB    | 3:C:63:ASN:OD1    | 2.18                     | 0.44              |
| 3:M:870:LEU:HD22 | 3:M:876:ASN:C     | 2.42                     | 0.44              |
| 3:A:1032:SER:HB3 | 3:A:1035:ALA:CB   | 2.47                     | 0.44              |
| 3:H:1339:ASP:OD2 | 3:H:1360:GLN:HG3  | 2.17                     | 0.44              |
| 4:h:65:GLY:O     | 4:h:69:ALA:N      | 2.51                     | 0.44              |
| 3:N:558:LEU:HD13 | 3:N:929:PHE:HE2   | 1.82                     | 0.44              |
| 3:O:684:GLU:HG2  | 3:P:658:ASN:O     | 2.16                     | 0.44              |
| 3:O:830:VAL:HG22 | 3:O:955:PHE:CD1   | 2.53                     | 0.44              |
| 3:P:452:LEU:HD21 | 3:P:1052:VAL:HG21 | 2.00                     | 0.44              |
| 3:B:887:ASP:O    | 3:B:891:MET:HG2   | 2.17                     | 0.44              |
| 3:B:920:THR:HA   | 3:B:1139:LEU:HG   | 1.99                     | 0.44              |
| 3:C:615:ARG:O    | 3:C:619:GLU:N     | 2.48                     | 0.44              |
| 3:D:789:ALA:O    | 4:d:79:PHE:CE2    | 2.70                     | 0.44              |
| 3:E:85:PRO:HG3   | 3:E:310:VAL:HG22  | 1.99                     | 0.44              |
| 3:E:448:GLN:HG2  | 3:F:1201:ARG:NH1  | 2.32                     | 0.44              |
| 3:E:519:ARG:O    | 3:E:522:ALA:N     | 2.51                     | 0.44              |
| 3:F:194:PRO:HG2  | 3:F:197:LEU:HD12  | 2.00                     | 0.44              |
| 3:F:1201:ARG:HB2 | 3:F:1202:PRO:HD2  | 2.00                     | 0.44              |
| 3:G:405:PRO:O    | 3:G:1361:TYR:OH   | 2.36                     | 0.44              |
| 4:f:21:GLY:O     | 4:f:25:LEU:N      | 2.50                     | 0.44              |
| 7:u:3090:ARG:O   | 7:u:3094:GLN:HG3  | 2.18                     | 0.44              |
| 1:w:283:ARG:HH11 | 3:N:47:ASN:ND2    | 2.16                     | 0.44              |
| 3:J:159:LEU:HD23 | 3:J:159:LEU:HA    | 1.73                     | 0.44              |
| 3:J:194:PRO:HG2  | 3:J:197:LEU:HD12  | 2.00                     | 0.44              |
| 3:J:485:ASN:ND2  | 3:J:516:GLY:H     | 2.13                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:J:642:CYS:CB    | 4:j:78:MET:HB3    | 2.48                     | 0.44              |
| 3:J:863:HIS:ND1   | 3:J:864:PRO:HD2   | 2.32                     | 0.44              |
| 3:J:1143:ALA:O    | 3:J:1146:TYR:HB3  | 2.18                     | 0.44              |
| 3:K:1079:GLN:OE1  | 3:K:1094:THR:OG1  | 2.32                     | 0.44              |
| 3:K:1229:HIS:HE1  | 3:K:1248:GLN:HA   | 1.82                     | 0.44              |
| 3:L:198:LEU:HD21  | 3:L:1106:TYR:CD2  | 2.53                     | 0.44              |
| 3:L:244:ILE:O     | 3:L:247:TRP:HB3   | 2.18                     | 0.44              |
| 3:M:20:THR:O      | 3:D:352:ASP:CA    | 2.65                     | 0.44              |
| 3:M:97:PHE:N      | 3:M:120:MET:O     | 2.47                     | 0.44              |
| 3:M:639:HIS:CD2   | 4:m:78:MET:HE3    | 2.51                     | 0.44              |
| 3:M:764:VAL:HB    | 3:M:782:ARG:HG2   | 2.00                     | 0.44              |
| 3:A:96:GLN:HG2    | 3:A:121:THR:CG2   | 2.46                     | 0.44              |
| 3:A:463:HIS:CG    | 3:A:464:PRO:HD2   | 2.53                     | 0.44              |
| 3:A:550:PHE:O     | 3:A:571:ILE:HA    | 2.18                     | 0.44              |
| 3:A:629:LEU:HD12  | 3:A:878:MET:HE2   | 1.98                     | 0.44              |
| 3:A:783:LEU:HD22  | 3:A:934:HIS:CG    | 2.53                     | 0.44              |
| 3:H:116:VAL:HG12  | 3:H:117:HIS:H     | 1.82                     | 0.44              |
| 4:l:9:PRO:HG2     | 4:l:36:MET:HE3    | 1.98                     | 0.44              |
| 3:N:99:VAL:HB     | 3:N:118:ASN:HB2   | 2.00                     | 0.44              |
| 3:N:301:ASP:HA    | 3:N:361:THR:O     | 2.18                     | 0.44              |
| 3:N:462:CYS:SG    | 3:N:1147:LEU:HD22 | 2.57                     | 0.44              |
| 3:N:631:GLN:HG2   | 3:N:670:LEU:HD11  | 2.00                     | 0.44              |
| 3:N:765:TYR:CE1   | 3:N:783:LEU:HD12  | 2.53                     | 0.44              |
| 3:N:830:VAL:HG22  | 3:N:955:PHE:CD1   | 2.53                     | 0.44              |
| 3:P:920:THR:O     | 3:P:923:THR:N     | 2.48                     | 0.44              |
| 3:P:1051:THR:HG23 | 3:P:1190:THR:HG21 | 2.00                     | 0.44              |
| 3:P:1081:ALA:HB3  | 3:P:1092:THR:OG1  | 2.18                     | 0.44              |
| 3:B:599:LEU:HA    | 3:B:599:LEU:HD23  | 1.76                     | 0.44              |
| 3:C:700:LEU:HD23  | 3:C:700:LEU:HA    | 1.77                     | 0.44              |
| 3:C:989:LEU:HD23  | 3:C:989:LEU:HA    | 1.59                     | 0.44              |
| 3:D:130:ASN:OD1   | 3:D:1094:THR:HG22 | 2.18                     | 0.44              |
| 3:D:175:ALA:HB2   | 3:E:103:LEU:HB2   | 1.99                     | 0.44              |
| 3:D:740:ASP:CG    | 3:D:799:PRO:HB3   | 2.43                     | 0.44              |
| 5:q:571:PRO:HA    | 5:q:692:CYS:HA    | 1.99                     | 0.44              |
| 5:q:681:ASP:N     | 5:q:682:PRO:HD2   | 2.33                     | 0.44              |
| 3:E:201:MET:O     | 3:E:204:TYR:N     | 2.51                     | 0.44              |
| 3:E:580:GLY:HA3   | 3:E:1006:VAL:HG22 | 2.00                     | 0.44              |
| 3:E:989:LEU:HD23  | 3:E:989:LEU:HA    | 1.79                     | 0.44              |
| 3:F:724:HIS:HE1   | 3:F:1028:TYR:HB2  | 1.82                     | 0.44              |
| 3:F:1020:LEU:HA   | 3:F:1020:LEU:HD23 | 1.57                     | 0.44              |
| 3:F:1072:ALA:HB2  | 3:F:1102:LEU:CD2  | 2.48                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:Q:89:LYS:HA     | 1:Q:92:ARG:HB2    | 2.00                     | 0.44              |
| 2:X:161:ARG:NH1   | 2:X:172:GLU:O     | 2.51                     | 0.44              |
| 1:1:141:PRO:HD3   | 3:M:1166:PHE:HB3  | 2.00                     | 0.44              |
| 2:2:183:GLY:N     | 3:D:1170:GLN:HG3  | 2.29                     | 0.44              |
| 3:I:743:MET:HE2   | 3:I:797:ASP:O     | 2.17                     | 0.44              |
| 3:I:906:THR:OG1   | 3:I:934:HIS:HB3   | 2.18                     | 0.44              |
| 3:I:1128:ASN:HD21 | 3:I:1155:ASN:ND2  | 2.15                     | 0.44              |
| 3:J:714:LEU:HD23  | 3:J:714:LEU:HA    | 1.81                     | 0.44              |
| 3:J:861:PRO:HA    | 3:J:866:HIS:CG    | 2.53                     | 0.44              |
| 3:K:309:MET:HE1   | 3:K:327:ARG:HA    | 1.99                     | 0.44              |
| 3:L:198:LEU:HA    | 3:L:198:LEU:HD23  | 1.78                     | 0.44              |
| 3:L:578:VAL:HB    | 3:L:1027:GLY:O    | 2.17                     | 0.44              |
| 3:L:740:ASP:CB    | 3:L:799:PRO:HB3   | 2.48                     | 0.44              |
| 3:L:958:LEU:HD23  | 3:L:958:LEU:HA    | 1.73                     | 0.44              |
| 3:M:392:TYR:CE2   | 3:M:394:LEU:HB3   | 2.52                     | 0.44              |
| 3:M:492:ALA:H     | 3:M:992:PRO:HB2   | 1.83                     | 0.44              |
| 3:M:1127:GLN:NE2  | 3:M:1264:ASN:HD21 | 2.15                     | 0.44              |
| 3:A:274:VAL:HG11  | 3:A:376:PHE:CD2   | 2.53                     | 0.44              |
| 3:A:1184:VAL:HG21 | 3:A:1269:VAL:HG13 | 2.00                     | 0.44              |
| 4:h:9:PRO:HG3     | 4:h:36:MET:HE3    | 2.00                     | 0.44              |
| 4:n:70:ASN:O      | 4:n:102:VAL:HB    | 2.18                     | 0.44              |
| 4:n:101:PHE:CD1   | 3:N:853:CYS:HB2   | 2.53                     | 0.44              |
| 4:o:79:PHE:CZ     | 3:O:639:HIS:HA    | 2.53                     | 0.44              |
| 3:N:518:VAL:HG13  | 3:N:520:TRP:CZ3   | 2.53                     | 0.44              |
| 3:O:776:PHE:O     | 3:O:904:ARG:HB3   | 2.18                     | 0.44              |
| 3:P:384:ILE:HG22  | 3:P:385:TYR:N     | 2.33                     | 0.44              |
| 3:P:520:TRP:CD1   | 3:P:1004:GLN:HB2  | 2.52                     | 0.44              |
| 3:P:1058:PHE:CD1  | 3:P:1118:PRO:HB3  | 2.53                     | 0.44              |
| 3:C:61:TYR:CD2    | 3:D:259:VAL:HG11  | 2.53                     | 0.44              |
| 3:C:485:ASN:HD21  | 3:C:516:GLY:N     | 2.16                     | 0.44              |
| 3:C:491:VAL:HG12  | 3:C:559:PRO:HB3   | 1.99                     | 0.44              |
| 3:C:867:PRO:HA    | 3:C:870:LEU:HD12  | 2.00                     | 0.44              |
| 3:C:1178:ASP:OD2  | 3:C:1179:HIS:ND1  | 2.51                     | 0.44              |
| 3:D:159:LEU:CD1   | 3:E:340:GLN:HA    | 2.47                     | 0.44              |
| 3:D:185:LEU:HD23  | 3:D:185:LEU:HA    | 1.78                     | 0.44              |
| 3:D:577:VAL:H     | 3:D:581:ASN:ND2   | 2.15                     | 0.44              |
| 3:D:755:ARG:HG3   | 3:D:755:ARG:O     | 2.18                     | 0.44              |
| 3:D:1198:TYR:HD2  | 3:D:1199:PHE:CE1  | 2.36                     | 0.44              |
| 5:q:27:ILE:HG12   | 5:q:111:PHE:CD1   | 2.53                     | 0.44              |
| 3:E:133:PHE:O     | 3:E:133:PHE:CG    | 2.70                     | 0.44              |
| 3:E:675:VAL:HG21  | 3:E:694:VAL:HG21  | 2.00                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:E:778:ARG:O     | 3:E:904:ARG:NE    | 2.50                     | 0.44              |
| 3:E:945:LEU:HD23  | 3:E:945:LEU:HA    | 1.82                     | 0.44              |
| 3:F:544:HIS:ND1   | 3:F:545:PRO:HD2   | 2.32                     | 0.44              |
| 2:X:38:ARG:NH2    | 3:I:110:HIS:O     | 2.51                     | 0.44              |
| 2:X:249:GLU:O     | 2:X:253:LEU:N     | 2.48                     | 0.44              |
| 1:I:141:PRO:HB2   | 3:M:1165:VAL:HG12 | 1.89                     | 0.44              |
| 1:I:350:LEU:O     | 1:I:354:ASN:ND2   | 2.50                     | 0.44              |
| 3:I:834:ARG:HH11  | 3:I:953:GLU:HA    | 1.82                     | 0.44              |
| 3:I:1035:ALA:O    | 3:I:1039:GLN:HG3  | 2.17                     | 0.44              |
| 3:J:302:VAL:HG12  | 3:J:303:PRO:O     | 2.18                     | 0.44              |
| 3:J:584:LEU:HA    | 3:J:584:LEU:HD23  | 1.82                     | 0.44              |
| 3:J:745:HIS:O     | 3:J:748:LEU:N     | 2.50                     | 0.44              |
| 3:J:1218:LYS:HB3  | 3:J:1221:ASP:CG   | 2.43                     | 0.44              |
| 3:K:769:CYS:HB2   | 3:K:786:ASN:ND2   | 2.32                     | 0.44              |
| 3:K:1215:ALA:HB1  | 3:K:1221:ASP:HB3  | 2.00                     | 0.44              |
| 3:L:1334:ILE:HG22 | 3:L:1335:THR:H    | 1.81                     | 0.44              |
| 3:M:463:HIS:HD2   | 3:M:465:SER:HB3   | 1.82                     | 0.44              |
| 3:M:475:GLY:HA2   | 3:M:478:HIS:CD2   | 2.53                     | 0.44              |
| 3:M:888:GLY:O     | 3:M:892:LEU:HG    | 2.17                     | 0.44              |
| 3:A:724:HIS:CE1   | 3:A:1028:TYR:HB2  | 2.53                     | 0.44              |
| 3:A:1366:ALA:HA   | 3:A:1370:LYS:NZ   | 2.33                     | 0.44              |
| 3:H:82:THR:O      | 3:H:1074:PHE:HA   | 2.18                     | 0.44              |
| 3:H:827:THR:HA    | 3:H:938:LEU:HA    | 2.00                     | 0.44              |
| 4:o:73:PHE:CE2    | 4:o:100:PRO:HA    | 2.53                     | 0.44              |
| 3:N:463:HIS:CD2   | 3:N:465:SER:HB3   | 2.42                     | 0.44              |
| 3:N:753:ASP:OD2   | 3:N:927:ARG:NH2   | 2.51                     | 0.44              |
| 3:N:770:ASN:OD1   | 3:N:900:ASN:HA    | 2.18                     | 0.44              |
| 3:N:1166:PHE:CD1  | 3:N:1167:GLY:N    | 2.85                     | 0.44              |
| 3:O:335:HIS:O     | 3:O:339:MET:HB2   | 2.18                     | 0.44              |
| 3:O:544:HIS:CG    | 3:O:545:PRO:HD2   | 2.53                     | 0.44              |
| 3:O:625:ALA:HB3   | 3:O:878:MET:HE1   | 1.98                     | 0.44              |
| 3:P:469:ILE:O     | 3:P:471:ALA:N     | 2.51                     | 0.44              |
| 3:P:481:VAL:HG11  | 3:P:571:ILE:HD12  | 2.00                     | 0.44              |
| 3:P:784:LEU:HG    | 3:P:934:HIS:HE2   | 1.81                     | 0.44              |
| 3:B:1186:GLU:OE2  | 3:B:1271:SER:HB2  | 2.18                     | 0.44              |
| 3:C:103:LEU:HD13  | 3:C:115:PRO:HA    | 1.99                     | 0.44              |
| 3:C:198:LEU:HA    | 3:C:198:LEU:HD23  | 1.71                     | 0.44              |
| 3:C:448:GLN:HG3   | 3:D:1201:ARG:HH11 | 1.83                     | 0.44              |
| 3:C:448:GLN:HG3   | 3:D:1201:ARG:NH1  | 2.33                     | 0.44              |
| 3:D:168:ASN:O     | 3:D:171:ALA:N     | 2.51                     | 0.44              |
| 3:D:494:PRO:HD3   | 3:D:909:LEU:HD12  | 1.99                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:635:HIS:CE1   | 3:D:640:VAL:HG21  | 2.52                     | 0.44              |
| 3:D:1022:TYR:O    | 3:D:1025:MET:N    | 2.51                     | 0.44              |
| 3:D:1165:VAL:HG13 | 3:D:1166:PHE:N    | 2.30                     | 0.44              |
| 5:q:23:LEU:O      | 5:q:407:ALA:HB1   | 2.17                     | 0.44              |
| 6:r:47:THR:HG22   | 6:r:49:ALA:H      | 1.82                     | 0.44              |
| 3:F:769:CYS:HB2   | 3:F:902:ALA:HA    | 1.99                     | 0.44              |
| 7:t:3103:LEU:O    | 7:t:3107:SER:N    | 2.33                     | 0.44              |
| 2:S:260:MET:HG2   | 5:q:412:ARG:NH1   | 2.33                     | 0.43              |
| 1:l:281:ARG:NH1   | 3:L:51:ASP:CG     | 2.71                     | 0.43              |
| 2:3:33:PHE:HZ     | 2:3:116:LEU:HD13  | 1.83                     | 0.43              |
| 3:I:106:ARG:HH11  | 3:H:390:VAL:HG22  | 1.83                     | 0.43              |
| 3:I:469:ILE:HD11  | 3:I:547:PHE:CG    | 2.53                     | 0.43              |
| 3:I:491:VAL:HG11  | 3:I:929:PHE:CD2   | 2.53                     | 0.43              |
| 3:I:1020:LEU:O    | 3:I:1021:THR:C    | 2.60                     | 0.43              |
| 3:J:228:CYS:HB3   | 3:J:1370:LYS:NZ   | 2.33                     | 0.43              |
| 3:J:1182:ASP:HB2  | 3:J:1309:VAL:HG13 | 1.99                     | 0.43              |
| 3:K:948:THR:HA    | 4:j:80:ALA:H      | 1.83                     | 0.43              |
| 3:K:1346:ALA:HB2  | 3:K:1362:LEU:HD11 | 2.00                     | 0.43              |
| 3:L:12:ARG:HB2    | 3:O:96:GLN:HE22   | 1.83                     | 0.43              |
| 3:L:32:HIS:HB3    | 3:O:1290:GLU:HG3  | 1.99                     | 0.43              |
| 3:L:176:PHE:O     | 3:L:180:THR:HG23  | 2.18                     | 0.43              |
| 3:L:746:ALA:HA    | 3:L:754:CYS:HB3   | 1.99                     | 0.43              |
| 3:L:983:LEU:O     | 3:L:987:VAL:HG22  | 2.18                     | 0.43              |
| 3:M:27:ILE:HD11   | 3:D:256:GLN:CD    | 2.43                     | 0.43              |
| 3:M:204:TYR:CG    | 3:M:219:LEU:HD11  | 2.53                     | 0.43              |
| 3:M:765:TYR:HD1   | 3:M:783:LEU:HB2   | 1.83                     | 0.43              |
| 3:A:86:GLU:N      | 3:A:86:GLU:OE1    | 2.51                     | 0.43              |
| 3:A:410:ASN:HD21  | 3:A:1196:ILE:H    | 1.66                     | 0.43              |
| 3:H:300:ALA:O     | 3:H:362:ARG:HD3   | 2.18                     | 0.43              |
| 3:H:322:MET:CE    | 3:D:324:LYS:C     | 2.91                     | 0.43              |
| 3:N:1198:TYR:HD1  | 3:N:1236:ARG:HH11 | 1.66                     | 0.43              |
| 3:O:99:VAL:HG23   | 3:O:120:MET:HE1   | 2.00                     | 0.43              |
| 3:O:487:TYR:CD1   | 3:O:513:LEU:HD21  | 2.53                     | 0.43              |
| 3:O:1024:LEU:HA   | 3:O:1024:LEU:HD23 | 1.76                     | 0.43              |
| 3:O:1024:LEU:O    | 3:O:1027:GLY:N    | 2.37                     | 0.43              |
| 3:P:258:SER:OG    | 3:P:259:VAL:N     | 2.48                     | 0.43              |
| 3:P:280:THR:HG22  | 3:P:1063:VAL:HG13 | 2.00                     | 0.43              |
| 3:P:399:ASP:OD1   | 3:P:1057:ARG:HG2  | 2.17                     | 0.43              |
| 3:P:914:PRO:HG3   | 3:P:923:THR:HG22  | 1.98                     | 0.43              |
| 3:B:86:GLU:HB2    | 3:B:89:TYR:CD2    | 2.53                     | 0.43              |
| 3:B:201:MET:HG3   | 3:B:1293:ILE:CD1  | 2.48                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:B:258:SER:OG    | 3:B:259:VAL:N     | 2.51                     | 0.43              |
| 3:B:1221:ASP:O    | 3:B:1224:ALA:N    | 2.51                     | 0.43              |
| 3:D:669:SER:O     | 3:D:672:SER:OG    | 2.33                     | 0.43              |
| 5:q:572:LEU:O     | 5:q:573:SER:OG    | 2.29                     | 0.43              |
| 3:E:745:HIS:NE2   | 3:E:910:CYS:HB2   | 2.33                     | 0.43              |
| 3:F:52:VAL:HG21   | 3:G:320:LEU:CD2   | 2.47                     | 0.43              |
| 3:F:367:LEU:HA    | 3:F:367:LEU:HD23  | 1.80                     | 0.43              |
| 3:G:99:VAL:HG12   | 3:G:118:ASN:ND2   | 2.24                     | 0.43              |
| 3:G:434:ALA:O     | 3:G:1359:THR:OG1  | 2.35                     | 0.43              |
| 2:R:145:THR:HG21  | 2:R:293:PRO:HB3   | 2.01                     | 0.43              |
| 1:W:166:GLU:CG    | 3:C:1262:HIS:CD2  | 2.96                     | 0.43              |
| 2:X:295:VAL:HG13  | 2:X:314:VAL:HG13  | 2.00                     | 0.43              |
| 2:2:68:ARG:NH1    | 2:2:290:ALA:O     | 2.51                     | 0.43              |
| 2:y:108:LEU:HD13  | 2:y:297:VAL:HG21  | 2.00                     | 0.43              |
| 3:I:126:ARG:HG3   | 3:I:1097:ARG:O    | 2.19                     | 0.43              |
| 3:I:496:GLY:HA3   | 3:I:504:ARG:NH2   | 2.34                     | 0.43              |
| 3:K:543:LEU:HD23  | 3:K:1248:GLN:OE1  | 2.16                     | 0.43              |
| 3:K:842:MET:CE    | 3:K:891:MET:HB3   | 2.48                     | 0.43              |
| 3:L:374:LEU:HD23  | 3:L:374:LEU:HA    | 1.57                     | 0.43              |
| 3:L:865:LEU:CD2   | 3:L:879:PHE:HB2   | 2.48                     | 0.43              |
| 3:L:1227:TYR:OH   | 3:L:1279:ALA:HB2  | 2.18                     | 0.43              |
| 3:M:528:ALA:O     | 3:M:531:PHE:N     | 2.51                     | 0.43              |
| 3:M:1013:SER:OG   | 3:M:1020:LEU:HD21 | 2.17                     | 0.43              |
| 3:M:1080:VAL:HG22 | 3:M:1093:LEU:HD22 | 2.00                     | 0.43              |
| 3:A:344:LEU:HD23  | 3:A:344:LEU:HA    | 1.61                     | 0.43              |
| 3:A:730:ALA:HB2   | 3:A:752:ARG:HH11  | 1.82                     | 0.43              |
| 3:A:950:GLN:H     | 3:A:953:GLU:CD    | 2.27                     | 0.43              |
| 3:A:1051:THR:OG1  | 3:A:1188:ILE:HB   | 2.18                     | 0.43              |
| 3:A:1357:HIS:CE1  | 3:A:1358:PHE:CD2  | 3.04                     | 0.43              |
| 3:H:85:PRO:HG2    | 3:H:86:GLU:OE1    | 2.18                     | 0.43              |
| 3:H:185:LEU:HD11  | 3:H:380:LEU:HD12  | 2.00                     | 0.43              |
| 3:H:219:LEU:HD23  | 3:H:219:LEU:HA    | 1.85                     | 0.43              |
| 3:H:255:THR:OG1   | 3:H:1067:GLU:OE2  | 2.32                     | 0.43              |
| 3:H:506:LEU:HD23  | 3:H:506:LEU:HA    | 1.87                     | 0.43              |
| 3:H:845:PRO:HG3   | 3:H:869:ASN:ND2   | 2.33                     | 0.43              |
| 4:h:57:GLN:HA     | 4:h:60:ALA:HB3    | 1.99                     | 0.43              |
| 3:N:183:GLN:O     | 3:N:187:VAL:N     | 2.50                     | 0.43              |
| 3:N:438:ARG:HG3   | 3:N:439:GLN:HG3   | 2.00                     | 0.43              |
| 3:N:687:MET:O     | 3:N:690:TYR:N     | 2.48                     | 0.43              |
| 3:N:1020:LEU:HA   | 3:N:1020:LEU:HD23 | 1.65                     | 0.43              |
| 3:N:1357:HIS:O    | 3:N:1358:PHE:C    | 2.58                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:O:1054:ARG:NH2  | 3:O:1122:MET:HB3  | 2.32                     | 0.43              |
| 3:O:1173:ARG:NH1  | 3:P:1218:LYS:HB2  | 2.33                     | 0.43              |
| 3:P:402:PHE:HA    | 3:P:1332:TYR:O    | 2.19                     | 0.43              |
| 3:P:753:ASP:HB3   | 3:P:755:ARG:HH22  | 1.83                     | 0.43              |
| 3:P:875:VAL:CG1   | 3:P:891:MET:HE1   | 2.48                     | 0.43              |
| 3:B:191:LYS:HD2   | 3:B:1101:ASP:CG   | 2.43                     | 0.43              |
| 3:B:693:LEU:HD23  | 3:B:693:LEU:HA    | 1.77                     | 0.43              |
| 3:B:1004:GLN:HE21 | 3:B:1008:GLN:HG3  | 1.83                     | 0.43              |
| 3:C:853:CYS:HB2   | 4:c:101:PHE:CD1   | 2.54                     | 0.43              |
| 3:D:176:PHE:HE2   | 3:D:1078:LEU:HD22 | 1.83                     | 0.43              |
| 3:D:826:CYS:HB3   | 3:D:966:GLY:N     | 2.33                     | 0.43              |
| 3:F:182:ASP:OD1   | 3:F:385:TYR:OH    | 2.33                     | 0.43              |
| 3:F:752:ARG:HG3   | 3:F:912:ALA:HB1   | 2.00                     | 0.43              |
| 3:F:875:VAL:HG12  | 3:F:879:PHE:CE2   | 2.50                     | 0.43              |
| 3:F:880:HIS:CE1   | 4:e:98:TYR:HB3    | 2.53                     | 0.43              |
| 3:G:34:ARG:CB     | 3:G:37:ASP:CG     | 2.92                     | 0.43              |
| 3:G:1223:ILE:O    | 3:G:1223:ILE:CG2  | 2.67                     | 0.43              |
| 2:S:261:LEU:HD21  | 5:q:378:TRP:CZ2   | 2.54                     | 0.43              |
| 2:U:33:PHE:HZ     | 2:U:116:LEU:HD13  | 1.83                     | 0.43              |
| 3:I:162:ILE:HG22  | 3:J:344:LEU:HD13  | 2.00                     | 0.43              |
| 3:J:36:PHE:HD2    | 3:J:39:PHE:HD1    | 1.65                     | 0.43              |
| 3:J:756:ILE:HA    | 3:J:909:LEU:O     | 2.18                     | 0.43              |
| 3:K:12:ARG:HD3    | 3:K:12:ARG:HA     | 1.77                     | 0.43              |
| 3:K:238:GLY:HA2   | 3:K:244:ILE:HD11  | 2.00                     | 0.43              |
| 3:K:753:ASP:OD1   | 3:K:911:SER:OG    | 2.36                     | 0.43              |
| 3:L:198:LEU:O     | 3:L:199:LEU:C     | 2.62                     | 0.43              |
| 3:L:403:VAL:HG21  | 3:L:1205:PRO:HG3  | 2.00                     | 0.43              |
| 3:L:819:ALA:O     | 3:L:822:ARG:NH1   | 2.51                     | 0.43              |
| 3:L:920:THR:O     | 3:L:923:THR:N     | 2.49                     | 0.43              |
| 3:L:1339:ASP:OD2  | 3:L:1360:GLN:HG3  | 2.18                     | 0.43              |
| 3:M:435:PHE:O     | 3:M:1359:THR:OG1  | 2.29                     | 0.43              |
| 3:M:1131:LEU:HD11 | 3:M:1157:LEU:HG   | 2.00                     | 0.43              |
| 3:A:588:PRO:O     | 3:A:592:ARG:HG3   | 2.18                     | 0.43              |
| 3:A:593:ASP:OD2   | 3:A:1015:ALA:HB2  | 2.18                     | 0.43              |
| 3:A:604:HIS:HD2   | 3:A:696:HIS:CD2   | 2.36                     | 0.43              |
| 3:A:724:HIS:CD2   | 3:A:726:MET:H     | 2.36                     | 0.43              |
| 3:H:435:PHE:HB3   | 3:H:598:GLU:HG3   | 2.00                     | 0.43              |
| 3:H:490:TYR:OH    | 3:H:561:GLY:N     | 2.51                     | 0.43              |
| 3:H:643:ALA:N     | 4:h:78:MET:SD     | 2.91                     | 0.43              |
| 3:H:923:THR:O     | 3:H:926:MET:HG2   | 2.18                     | 0.43              |
| 4:l:42:HIS:CE1    | 4:l:44:HIS:HB2    | 2.52                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:N:119:TYR:HE2   | 3:D:42:VAL:HB     | 1.83                     | 0.43              |
| 3:N:762:GLU:HB3   | 3:N:763:PRO:HD2   | 2.00                     | 0.43              |
| 3:N:864:PRO:HB2   | 3:N:876:ASN:CG    | 2.43                     | 0.43              |
| 3:O:258:SER:OG    | 3:O:259:VAL:N     | 2.51                     | 0.43              |
| 3:O:486:PRO:O     | 3:O:509:TRP:HZ3   | 2.02                     | 0.43              |
| 3:O:1115:VAL:HG12 | 3:O:1116:ARG:O    | 2.17                     | 0.43              |
| 3:P:135:LEU:HD21  | 3:P:165:LEU:CD2   | 2.47                     | 0.43              |
| 3:P:457:ALA:O     | 3:P:460:THR:N     | 2.48                     | 0.43              |
| 3:P:1029:PHE:HB3  | 3:P:1039:GLN:HE21 | 1.77                     | 0.43              |
| 3:P:1319:GLU:OE1  | 3:P:1319:GLU:N    | 2.51                     | 0.43              |
| 3:B:595:ARG:HH11  | 3:B:1026:ALA:HB1  | 1.83                     | 0.43              |
| 3:B:1170:GLN:OE1  | 3:B:1170:GLN:N    | 2.48                     | 0.43              |
| 3:C:142:LEU:HD23  | 3:C:147:ALA:HB3   | 1.99                     | 0.43              |
| 3:C:405:PRO:HB3   | 3:C:1199:PHE:CE2  | 2.53                     | 0.43              |
| 3:C:469:ILE:HD11  | 3:C:547:PHE:CG    | 2.53                     | 0.43              |
| 3:D:873:ASN:OD1   | 4:c:92:PHE:N      | 2.51                     | 0.43              |
| 3:D:875:VAL:O     | 3:D:878:MET:HB3   | 2.19                     | 0.43              |
| 5:q:526:ARG:HG3   | 6:r:39:PRO:HD3    | 2.00                     | 0.43              |
| 3:F:1233:ASP:O    | 3:F:1237:PRO:HA   | 2.18                     | 0.43              |
| 3:G:110:HIS:CD2   | 3:G:110:HIS:H     | 2.36                     | 0.43              |
| 3:G:608:PRO:HA    | 3:G:611:ILE:HD12  | 2.00                     | 0.43              |
| 3:G:745:HIS:CD2   | 3:G:756:ILE:HD11  | 2.53                     | 0.43              |
| 2:V:285:LEU:HA    | 2:V:288:ILE:HD12  | 2.00                     | 0.43              |
| 1:W:29:GLY:N      | 3:H:145:GLY:HA3   | 2.33                     | 0.43              |
| 2:X:110:ASN:N     | 2:X:304:ALA:O     | 2.51                     | 0.43              |
| 1:1:192:ALA:HB2   | 1:1:207:VAL:HG12  | 2.00                     | 0.43              |
| 3:I:1227:TYR:CD1  | 3:I:1249:ARG:HB2  | 2.54                     | 0.43              |
| 3:I:1335:THR:N    | 3:I:1365:ASP:HB3  | 2.33                     | 0.43              |
| 3:K:82:THR:HG22   | 3:K:307:GLY:HA3   | 2.01                     | 0.43              |
| 3:K:222:GLU:O     | 3:K:225:ARG:N     | 2.51                     | 0.43              |
| 3:K:493:ALA:CA    | 3:K:559:PRO:HB2   | 2.49                     | 0.43              |
| 3:K:724:HIS:HE1   | 3:K:1025:MET:O    | 2.00                     | 0.43              |
| 3:L:231:SER:O     | 3:L:1112:THR:OG1  | 2.36                     | 0.43              |
| 3:M:20:THR:OG1    | 3:C:61:TYR:HE1    | 2.02                     | 0.43              |
| 3:M:50:TYR:HE2    | 3:C:139:ALA:HB2   | 1.83                     | 0.43              |
| 3:M:962:ALA:N     | 3:M:990:VAL:HG21  | 2.33                     | 0.43              |
| 3:A:82:THR:HG22   | 3:A:307:GLY:HA3   | 2.01                     | 0.43              |
| 3:A:494:PRO:HG2   | 3:A:760:GLY:CA    | 2.48                     | 0.43              |
| 3:H:627:PHE:HD1   | 3:H:664:PHE:CZ    | 2.36                     | 0.43              |
| 4:m:76:GLN:OE1    | 4:m:98:TYR:OH     | 2.25                     | 0.43              |
| 3:N:469:ILE:HD11  | 3:N:547:PHE:CD2   | 2.53                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:N:715:GLY:HA3   | 3:N:916:ALA:HB2   | 2.00                     | 0.43              |
| 3:O:255:THR:OG1   | 3:O:1067:GLU:OE2  | 2.26                     | 0.43              |
| 3:O:864:PRO:O     | 3:O:876:ASN:ND2   | 2.52                     | 0.43              |
| 3:P:435:PHE:CG    | 3:P:598:GLU:HG2   | 2.54                     | 0.43              |
| 3:P:467:MET:SD    | 3:P:918:ALA:HB1   | 2.58                     | 0.43              |
| 3:P:1198:TYR:HD1  | 3:P:1236:ARG:NH1  | 2.16                     | 0.43              |
| 3:B:197:LEU:HA    | 3:B:197:LEU:HD23  | 1.79                     | 0.43              |
| 3:B:426:ALA:HB3   | 3:B:429:HIS:CD2   | 2.53                     | 0.43              |
| 3:B:714:LEU:HD22  | 3:B:1143:ALA:HA   | 2.00                     | 0.43              |
| 3:B:766:ALA:H     | 3:B:783:LEU:C     | 2.26                     | 0.43              |
| 3:B:994:LEU:HD23  | 3:B:994:LEU:HA    | 1.70                     | 0.43              |
| 3:B:1206:ARG:HH21 | 3:B:1210:ALA:HB2  | 1.82                     | 0.43              |
| 3:B:1255:LEU:HD23 | 3:B:1255:LEU:HA   | 1.71                     | 0.43              |
| 3:C:277:VAL:CG1   | 3:C:279:VAL:HG23  | 2.48                     | 0.43              |
| 3:C:1175:ALA:O    | 3:D:213:ARG:NH2   | 2.52                     | 0.43              |
| 3:C:1289:LEU:HA   | 3:C:1289:LEU:HD23 | 1.72                     | 0.43              |
| 3:D:180:THR:HG22  | 3:D:1097:ARG:NH2  | 2.33                     | 0.43              |
| 5:q:123:VAL:HG11  | 5:q:422:LEU:H     | 1.83                     | 0.43              |
| 5:q:405:SER:O     | 5:q:410:GLY:HA3   | 2.19                     | 0.43              |
| 3:E:63:ASN:HD21   | 3:F:99:VAL:HG13   | 1.83                     | 0.43              |
| 6:r:85:ARG:HE     | 7:u:3100:ARG:HH21 | 1.65                     | 0.43              |
| 3:F:86:GLU:HB2    | 3:F:89:TYR:HD2    | 1.82                     | 0.43              |
| 3:F:227:PHE:CE2   | 3:F:1324:PRO:HB3  | 2.53                     | 0.43              |
| 3:F:266:HIS:HE1   | 3:F:302:VAL:HG13  | 1.82                     | 0.43              |
| 3:F:603:ARG:HD3   | 3:F:703:LEU:HD21  | 1.99                     | 0.43              |
| 3:G:405:PRO:CG    | 3:G:1363:ILE:CD1  | 2.97                     | 0.43              |
| 3:G:547:PHE:HB3   | 3:G:549:PHE:HE2   | 1.81                     | 0.43              |
| 1:Q:270:PRO:HA    | 1:Q:456:VAL:HA    | 2.00                     | 0.43              |
| 2:3:90:LEU:O      | 2:3:93:THR:OG1    | 2.35                     | 0.43              |
| 2:2:52:VAL:HG23   | 2:2:57:SER:HA     | 2.00                     | 0.43              |
| 3:I:625:ALA:HB3   | 3:I:878:MET:HE3   | 1.99                     | 0.43              |
| 3:I:837:ALA:HA    | 4:i:57:GLN:OE1    | 2.19                     | 0.43              |
| 3:I:877:ALA:O     | 3:I:881:ASN:N     | 2.44                     | 0.43              |
| 3:I:1020:LEU:HA   | 3:I:1020:LEU:HD23 | 1.83                     | 0.43              |
| 3:J:606:MET:HG3   | 3:J:692:ASP:HB3   | 2.00                     | 0.43              |
| 3:J:834:ARG:HB3   | 4:i:90:PRO:HG3    | 2.00                     | 0.43              |
| 3:K:196:ALA:HB1   | 3:K:227:PHE:HA    | 1.99                     | 0.43              |
| 3:K:765:TYR:CE1   | 3:K:783:LEU:HD12  | 2.53                     | 0.43              |
| 3:K:880:HIS:NE2   | 4:j:95:LYS:O      | 2.52                     | 0.43              |
| 3:K:1208:ARG:NE   | 3:K:1225:LEU:O    | 2.49                     | 0.43              |
| 3:K:1357:HIS:O    | 3:K:1358:PHE:C    | 2.60                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:L:216:ARG:HH22  | 3:L:1287:ARG:HB3  | 1.82                     | 0.43              |
| 3:L:668:TYR:HD2   | 3:L:809:HIS:CE1   | 2.36                     | 0.43              |
| 3:L:732:LEU:HD12  | 3:L:910:CYS:SG    | 2.58                     | 0.43              |
| 3:L:764:VAL:O     | 3:L:783:LEU:N     | 2.36                     | 0.43              |
| 3:M:130:ASN:OD1   | 3:M:1094:THR:HG22 | 2.18                     | 0.43              |
| 3:M:164:GLN:HE21  | 3:C:49:LEU:HD13   | 1.78                     | 0.43              |
| 3:M:438:ARG:HB2   | 3:M:454:MET:CG    | 2.49                     | 0.43              |
| 3:M:858:VAL:HG12  | 3:M:859:THR:HG23  | 1.99                     | 0.43              |
| 3:M:920:THR:HG22  | 3:M:921:ALA:H     | 1.82                     | 0.43              |
| 3:M:944:HIS:HB2   | 3:M:951:ASN:ND2   | 2.33                     | 0.43              |
| 3:M:945:LEU:HA    | 3:M:945:LEU:HD23  | 1.73                     | 0.43              |
| 3:M:1127:GLN:HG2  | 3:M:1128:ASN:O    | 2.18                     | 0.43              |
| 3:A:662:ALA:HB1   | 3:A:690:TYR:CE1   | 2.53                     | 0.43              |
| 3:H:79:CYS:HB3    | 3:H:81:CYS:SG     | 2.59                     | 0.43              |
| 3:H:831:ARG:HD2   | 3:H:834:ARG:HD2   | 2.01                     | 0.43              |
| 3:N:1038:HIS:O    | 3:N:1042:THR:OG1  | 2.33                     | 0.43              |
| 3:N:1209:ALA:HB1  | 3:N:1214:TYR:CE2  | 2.54                     | 0.43              |
| 3:O:591:PHE:CE2   | 3:O:595:ARG:HD2   | 2.53                     | 0.43              |
| 3:P:469:ILE:HD11  | 3:P:547:PHE:CG    | 2.54                     | 0.43              |
| 3:P:753:ASP:HB3   | 3:P:755:ARG:NH2   | 2.33                     | 0.43              |
| 3:P:888:GLY:N     | 3:P:889:PRO:HD2   | 2.34                     | 0.43              |
| 3:B:87:LEU:O      | 3:B:90:MET:N      | 2.43                     | 0.43              |
| 3:B:212:THR:HG21  | 3:G:1306:ALA:HA   | 2.01                     | 0.43              |
| 3:B:866:HIS:O     | 3:B:870:LEU:HG    | 2.17                     | 0.43              |
| 3:C:524:CYS:CB    | 3:C:1008:GLN:HE22 | 2.31                     | 0.43              |
| 3:C:646:ARG:NH2   | 3:C:889:PRO:HG2   | 2.34                     | 0.43              |
| 3:C:1004:GLN:HE21 | 3:C:1007:VAL:HB   | 1.82                     | 0.43              |
| 3:D:234:LEU:HD23  | 3:D:234:LEU:HA    | 1.85                     | 0.43              |
| 3:D:310:VAL:HG12  | 3:D:312:ASN:H     | 1.82                     | 0.43              |
| 3:D:311:LEU:O     | 3:D:316:LEU:HB2   | 2.18                     | 0.43              |
| 3:D:765:TYR:CE1   | 3:D:783:LEU:HD12  | 2.54                     | 0.43              |
| 3:D:1178:ASP:O    | 3:E:217:ALA:HB1   | 2.18                     | 0.43              |
| 3:D:1202:PRO:HB3  | 3:D:1332:TYR:CD1  | 2.53                     | 0.43              |
| 5:q:39:PRO:HD2    | 5:q:136:TRP:CZ2   | 2.53                     | 0.43              |
| 5:q:116:VAL:HG13  | 5:q:150:TYR:CE1   | 2.53                     | 0.43              |
| 5:q:610:ILE:HG12  | 5:q:622:CYS:SG    | 2.59                     | 0.43              |
| 3:E:507:ASN:HA    | 3:E:510:ARG:HE    | 1.82                     | 0.43              |
| 6:r:3:PRO:HG2     | 6:r:5:TYR:CE2     | 2.53                     | 0.43              |
| 3:F:188:LEU:HD23  | 3:F:188:LEU:HA    | 1.80                     | 0.43              |
| 3:F:374:LEU:HA    | 3:F:374:LEU:HD23  | 1.69                     | 0.43              |
| 3:F:472:ALA:O     | 3:F:476:VAL:HG23  | 2.17                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:F:739:CYS:HB3   | 3:F:765:TYR:CD1   | 2.53                     | 0.43              |
| 3:F:873:ASN:CA    | 4:e:92:PHE:CD2    | 2.98                     | 0.43              |
| 3:F:1208:ARG:HD3  | 3:F:1226:MET:O    | 2.19                     | 0.43              |
| 3:F:1221:ASP:O    | 3:F:1222:VAL:C    | 2.61                     | 0.43              |
| 3:F:1347:ARG:NH1  | 3:G:1350:GLU:OE2  | 2.52                     | 0.43              |
| 3:G:32:HIS:HB3    | 3:G:52:VAL:HA     | 2.01                     | 0.43              |
| 3:G:489:ALA:CB    | 3:G:551:ALA:O     | 2.66                     | 0.43              |
| 1:w:281:ARG:HD2   | 3:N:53:GLU:OE2    | 2.18                     | 0.43              |
| 3:I:280:THR:HG22  | 3:I:1063:VAL:HG13 | 2.00                     | 0.43              |
| 3:J:755:ARG:O     | 3:J:910:CYS:HA    | 2.18                     | 0.43              |
| 3:J:908:LEU:O     | 3:J:931:GLY:HA2   | 2.18                     | 0.43              |
| 3:J:1115:VAL:HG12 | 3:J:1116:ARG:O    | 2.18                     | 0.43              |
| 3:J:1121:ASP:HB3  | 3:J:1181:GLN:O    | 2.19                     | 0.43              |
| 3:K:749:ASP:OD1   | 3:K:749:ASP:N     | 2.50                     | 0.43              |
| 3:L:27:ILE:HG22   | 3:L:28:GLU:N      | 2.33                     | 0.43              |
| 3:L:835:VAL:O     | 3:L:839:LEU:N     | 2.49                     | 0.43              |
| 3:M:24:LEU:HD11   | 3:D:260:ALA:CB    | 2.39                     | 0.43              |
| 3:M:452:LEU:HD12  | 3:M:456:ASN:ND2   | 2.30                     | 0.43              |
| 3:M:533:GLN:C     | 3:M:535:ASP:H     | 2.27                     | 0.43              |
| 3:M:738:ASP:HB3   | 3:M:740:ASP:H     | 1.83                     | 0.43              |
| 3:H:301:ASP:OD1   | 3:H:362:ARG:NE    | 2.49                     | 0.43              |
| 3:H:405:PRO:O     | 3:H:440:LEU:HD11  | 2.19                     | 0.43              |
| 3:H:721:GLU:HA    | 3:H:727:ARG:HB2   | 2.00                     | 0.43              |
| 3:H:1129:PHE:O    | 3:H:1132:GLY:N    | 2.52                     | 0.43              |
| 3:N:77:VAL:HG22   | 3:N:266:HIS:CD2   | 2.54                     | 0.43              |
| 3:N:775:ASP:OD2   | 3:N:778:ARG:NH2   | 2.50                     | 0.43              |
| 3:N:1304:THR:HG21 | 3:N:1314:PRO:HD3  | 1.99                     | 0.43              |
| 3:O:405:PRO:HB3   | 3:O:1199:PHE:CE2  | 2.54                     | 0.43              |
| 3:P:523:GLU:OE2   | 3:P:538:ASN:ND2   | 2.52                     | 0.43              |
| 3:P:1147:LEU:O    | 3:P:1150:ALA:N    | 2.49                     | 0.43              |
| 3:B:227:PHE:CE2   | 3:B:1324:PRO:HB3  | 2.54                     | 0.43              |
| 3:B:402:PHE:HA    | 3:B:1332:TYR:O    | 2.19                     | 0.43              |
| 3:B:634:ILE:HG22  | 3:B:636:GLY:H     | 1.84                     | 0.43              |
| 3:C:229:ASP:O     | 3:C:236:LYS:NZ    | 2.42                     | 0.43              |
| 3:C:463:HIS:CD2   | 3:C:465:SER:HB3   | 2.52                     | 0.43              |
| 3:C:485:ASN:HD21  | 3:C:516:GLY:H     | 1.67                     | 0.43              |
| 3:C:624:PRO:HB2   | 3:C:627:PHE:CD2   | 2.54                     | 0.43              |
| 3:D:165:LEU:HA    | 3:D:165:LEU:HD23  | 1.75                     | 0.43              |
| 3:D:738:ASP:C     | 3:D:934:HIS:HE1   | 2.26                     | 0.43              |
| 3:D:961:HIS:CD2   | 3:D:963:LEU:H     | 2.35                     | 0.43              |
| 3:E:691:ARG:NH1   | 3:F:620:ASP:OD1   | 2.52                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:r:80:ILE:CG2    | 7:u:3100:ARG:HG2  | 2.48                     | 0.43              |
| 3:F:469:ILE:HD11  | 3:F:547:PHE:CG    | 2.54                     | 0.43              |
| 3:F:558:LEU:HA    | 3:F:559:PRO:C     | 2.44                     | 0.43              |
| 3:F:879:PHE:HE2   | 3:F:891:MET:HE1   | 1.82                     | 0.43              |
| 3:G:466:LEU:O     | 3:G:544:HIS:NE2   | 2.51                     | 0.43              |
| 3:G:624:PRO:HB3   | 3:G:882:GLY:HA3   | 2.00                     | 0.43              |
| 2:R:173:LEU:CA    | 5:q:371:GLY:CA    | 2.92                     | 0.43              |
| 2:S:53:SER:OG     | 2:S:54:GLY:N      | 2.52                     | 0.43              |
| 1:T:283:ARG:HG2   | 1:T:284:SER:N     | 2.34                     | 0.43              |
| 3:I:84:PHE:O      | 3:I:1076:GLY:HA2  | 2.19                     | 0.43              |
| 3:I:325:ALA:O     | 3:H:56:ALA:HA     | 2.19                     | 0.43              |
| 3:I:704:VAL:O     | 3:I:708:THR:HG23  | 2.18                     | 0.43              |
| 3:I:1125:LEU:HD22 | 3:I:1184:VAL:HG22 | 2.00                     | 0.43              |
| 3:I:1174:ARG:NH1  | 3:I:1182:ASP:OD2  | 2.51                     | 0.43              |
| 3:J:201:MET:O     | 3:J:204:TYR:N     | 2.48                     | 0.43              |
| 3:J:367:LEU:HD23  | 3:J:367:LEU:HA    | 1.82                     | 0.43              |
| 3:J:923:THR:HA    | 3:J:926:MET:HE3   | 2.01                     | 0.43              |
| 3:K:784:LEU:HD13  | 3:K:786:ASN:ND2   | 2.34                     | 0.43              |
| 3:K:888:GLY:N     | 3:K:889:PRO:HD2   | 2.32                     | 0.43              |
| 3:L:580:GLY:HA2   | 3:L:592:ARG:NH1   | 2.28                     | 0.43              |
| 3:L:994:LEU:HA    | 3:L:994:LEU:HD23  | 1.79                     | 0.43              |
| 3:L:1026:ALA:HA   | 3:L:1029:PHE:HE2  | 1.83                     | 0.43              |
| 3:M:326:VAL:HG21  | 3:O:321:VAL:CG1   | 2.49                     | 0.43              |
| 3:M:426:ALA:HA    | 3:H:1358:PHE:CE1  | 2.54                     | 0.43              |
| 3:A:257:PRO:HA    | 3:A:1067:GLU:OE1  | 2.19                     | 0.43              |
| 4:h:88:LEU:HD12   | 4:h:89:ARG:H      | 1.84                     | 0.43              |
| 4:o:89:ARG:NH1    | 3:P:873:ASN:ND2   | 2.65                     | 0.43              |
| 3:N:87:LEU:O      | 3:N:89:TYR:N      | 2.51                     | 0.43              |
| 3:N:469:ILE:HD11  | 3:N:547:PHE:CE2   | 2.54                     | 0.43              |
| 3:N:588:PRO:O     | 3:N:591:PHE:HB3   | 2.19                     | 0.43              |
| 3:O:124:ILE:HG12  | 3:O:1100:VAL:HG21 | 2.00                     | 0.43              |
| 3:O:1054:ARG:CZ   | 3:O:1122:MET:HB3  | 2.48                     | 0.43              |
| 3:O:1269:VAL:O    | 3:O:1312:LYS:NZ   | 2.42                     | 0.43              |
| 3:P:463:HIS:HA    | 3:P:1130:TYR:OH   | 2.19                     | 0.43              |
| 3:P:550:PHE:O     | 3:P:571:ILE:HA    | 2.18                     | 0.43              |
| 3:P:841:ASN:O     | 3:P:875:VAL:HG23  | 2.18                     | 0.43              |
| 3:B:651:CYS:O     | 3:B:654:SER:OG    | 2.36                     | 0.43              |
| 3:B:756:ILE:O     | 3:B:762:GLU:HA    | 2.19                     | 0.43              |
| 3:B:861:PRO:HA    | 3:B:866:HIS:CG    | 2.54                     | 0.43              |
| 3:C:463:HIS:HD2   | 3:C:465:SER:CB    | 2.31                     | 0.43              |
| 3:D:130:ASN:HB3   | 3:E:112:VAL:HG22  | 2.01                     | 0.43              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:D:439:GLN:HE21 | 3:D:451:ARG:NH2   | 2.17                     | 0.43              |
| 5:q:152:GLU:C    | 5:q:388:ARG:HH21  | 2.26                     | 0.43              |
| 3:E:784:LEU:HD22 | 3:E:786:ASN:ND2   | 2.34                     | 0.43              |
| 3:E:1078:LEU:HA  | 3:E:1094:THR:O    | 2.19                     | 0.43              |
| 3:F:13:TYR:CE2   | 3:F:49:LEU:HA     | 2.54                     | 0.43              |
| 3:F:469:ILE:HD13 | 3:F:469:ILE:HG21  | 1.76                     | 0.43              |
| 3:F:866:HIS:C    | 3:F:870:LEU:HG    | 2.42                     | 0.43              |
| 3:F:873:ASN:OD1  | 4:e:92:PHE:CA     | 2.67                     | 0.43              |
| 3:F:920:THR:HG22 | 3:F:921:ALA:N     | 2.34                     | 0.43              |
| 3:F:1275:LYS:HG3 | 3:F:1276:PHE:CD1  | 2.54                     | 0.43              |
| 3:G:898:ALA:HA   | 3:G:901:MET:HE2   | 2.00                     | 0.43              |
| 2:R:219:LEU:HD13 | 2:R:275:LEU:HD23  | 2.00                     | 0.43              |
| 1:T:115:THR:O    | 1:T:261:ALA:N     | 2.52                     | 0.43              |
| 2:U:300:PHE:CE2  | 3:I:1083:HIS:CD2  | 2.94                     | 0.43              |
| 2:X:284:GLN:CB   | 3:H:1166:PHE:HZ   | 2.25                     | 0.43              |
| 3:I:399:ASP:HB2  | 3:I:1323:ASP:OD1  | 2.18                     | 0.43              |
| 3:I:642:CYS:SG   | 4:i:95:LYS:HG2    | 2.59                     | 0.43              |
| 3:J:63:ASN:ND2   | 3:K:100:HIS:H     | 2.16                     | 0.43              |
| 3:J:947:HIS:HB2  | 4:i:79:PHE:CD1    | 2.54                     | 0.43              |
| 3:K:380:LEU:O    | 3:K:382:LYS:N     | 2.51                     | 0.43              |
| 3:K:707:PHE:CE2  | 3:K:1044:LEU:HD13 | 2.54                     | 0.43              |
| 3:K:790:ARG:NH2  | 4:k:81:GLY:O      | 2.52                     | 0.43              |
| 3:L:866:HIS:HD2  | 3:L:868:ALA:HB3   | 1.84                     | 0.43              |
| 3:M:9:PRO:HG2    | 3:D:94:ARG:NH2    | 2.29                     | 0.43              |
| 3:M:784:LEU:HG   | 3:M:934:HIS:HE2   | 1.84                     | 0.43              |
| 3:A:112:VAL:O    | 3:A:113:GLU:HB2   | 2.19                     | 0.43              |
| 3:A:635:HIS:CE1  | 3:A:640:VAL:HG21  | 2.54                     | 0.43              |
| 3:A:721:GLU:HG2  | 3:A:727:ARG:O     | 2.19                     | 0.43              |
| 4:k:21:GLY:O     | 4:k:25:LEU:N      | 2.51                     | 0.43              |
| 4:p:80:ALA:HA    | 4:p:92:PHE:O      | 2.18                     | 0.43              |
| 3:N:578:VAL:HB   | 3:N:1027:GLY:O    | 2.18                     | 0.43              |
| 3:N:836:TYR:O    | 3:N:840:GLN:N     | 2.47                     | 0.43              |
| 3:N:842:MET:HE1  | 3:N:891:MET:HE3   | 2.00                     | 0.43              |
| 3:O:787:THR:O    | 3:O:788:GLN:HG3   | 2.19                     | 0.43              |
| 3:P:79:CYS:HB3   | 3:P:81:CYS:SG     | 2.59                     | 0.43              |
| 3:P:469:ILE:HD11 | 3:P:547:PHE:CE1   | 2.54                     | 0.43              |
| 3:P:619:GLU:HG2  | 3:P:824:ARG:HH21  | 1.83                     | 0.43              |
| 3:B:220:VAL:HG11 | 3:B:1214:TYR:CE1  | 2.50                     | 0.43              |
| 3:B:399:ASP:HB2  | 3:B:1323:ASP:OD1  | 2.19                     | 0.43              |
| 3:B:440:LEU:HA   | 3:B:440:LEU:HD23  | 1.76                     | 0.43              |
| 3:B:865:LEU:HD22 | 3:B:879:PHE:HB2   | 2.00                     | 0.43              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:C:232:PHE:O    | 3:C:236:LYS:HD3   | 2.19                     | 0.43              |
| 3:C:775:ASP:HB2  | 3:C:778:ARG:HH21  | 1.84                     | 0.43              |
| 3:C:888:GLY:N    | 3:C:889:PRO:HD2   | 2.33                     | 0.43              |
| 3:D:42:VAL:HG13  | 3:D:43:ARG:O      | 2.15                     | 0.43              |
| 3:D:223:LEU:HD23 | 3:D:223:LEU:HA    | 1.76                     | 0.43              |
| 3:D:637:SER:HB3  | 3:D:640:VAL:HB    | 2.00                     | 0.43              |
| 3:E:69:ARG:HD2   | 3:E:72:GLU:OE2    | 2.19                     | 0.43              |
| 3:E:469:ILE:O    | 3:E:470:ASP:C     | 2.60                     | 0.43              |
| 3:E:630:LEU:O    | 3:E:634:ILE:HD12  | 2.18                     | 0.43              |
| 3:E:700:LEU:HD23 | 3:E:700:LEU:HA    | 1.80                     | 0.43              |
| 3:E:864:PRO:HB2  | 3:E:876:ASN:OD1   | 2.18                     | 0.43              |
| 3:E:1020:LEU:HA  | 3:E:1020:LEU:HD23 | 1.87                     | 0.43              |
| 3:E:1201:ARG:HB2 | 3:E:1202:PRO:HD2  | 2.01                     | 0.43              |
| 3:F:77:VAL:HG22  | 3:F:266:HIS:CG    | 2.54                     | 0.43              |
| 3:F:263:ARG:HH12 | 3:F:307:GLY:HA2   | 1.83                     | 0.43              |
| 3:F:961:HIS:CD2  | 3:F:963:LEU:H     | 2.36                     | 0.43              |
| 3:F:1140:ASP:O   | 3:F:1143:ALA:N    | 2.52                     | 0.43              |
| 2:2:18:ARG:NH2   | 3:N:91:ASN:HD22   | 2.17                     | 0.43              |
| 3:I:137:THR:O    | 3:I:140:ILE:N     | 2.48                     | 0.43              |
| 3:J:739:CYS:O    | 3:J:743:MET:HG2   | 2.19                     | 0.43              |
| 3:J:778:ARG:O    | 3:J:778:ARG:HG3   | 2.19                     | 0.43              |
| 3:K:784:LEU:HG   | 3:K:934:HIS:NE2   | 2.34                     | 0.43              |
| 3:K:958:LEU:HD23 | 3:K:958:LEU:HA    | 1.88                     | 0.43              |
| 3:L:646:ARG:CZ   | 3:L:890:ALA:HB2   | 2.48                     | 0.43              |
| 3:L:740:ASP:OD1  | 3:L:741:GLY:N     | 2.51                     | 0.43              |
| 3:M:84:PHE:O     | 3:M:1076:GLY:HA2  | 2.19                     | 0.43              |
| 3:M:86:GLU:OE2   | 3:M:311:LEU:HG    | 2.19                     | 0.43              |
| 3:M:163:GLN:O    | 3:M:167:ARG:HG2   | 2.18                     | 0.43              |
| 3:M:296:GLU:OE1  | 3:M:374:LEU:HD21  | 2.18                     | 0.43              |
| 3:M:606:MET:HG3  | 3:M:692:ASP:HB3   | 2.01                     | 0.43              |
| 3:M:852:GLU:HA   | 4:m:101:PHE:CZ    | 2.54                     | 0.43              |
| 3:A:621:ARG:O    | 3:A:943:GLN:HG2   | 2.18                     | 0.43              |
| 3:A:871:VAL:O    | 3:A:877:ALA:HB2   | 2.19                     | 0.43              |
| 3:H:788:GLN:NE2  | 3:H:794:ALA:HA    | 2.33                     | 0.43              |
| 3:N:87:LEU:O     | 3:N:90:MET:N      | 2.52                     | 0.43              |
| 3:N:820:PHE:HA   | 3:N:1017:GLU:OE1  | 2.19                     | 0.43              |
| 3:N:1206:ARG:NH1 | 3:N:1208:ARG:HB3  | 2.34                     | 0.43              |
| 3:O:280:THR:HG22 | 3:O:1063:VAL:HG22 | 2.00                     | 0.43              |
| 3:O:790:ARG:HG3  | 3:O:792:ALA:H     | 1.83                     | 0.43              |
| 3:O:910:CYS:SG   | 3:O:930:ASP:HB2   | 2.59                     | 0.43              |
| 3:P:180:THR:OG1  | 3:P:181:ALA:N     | 2.51                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:P:280:THR:HG22  | 3:P:1063:VAL:HG22 | 1.99                     | 0.43              |
| 3:P:643:ALA:HB1   | 3:P:896:VAL:HG21  | 2.01                     | 0.43              |
| 3:P:784:LEU:O     | 3:P:934:HIS:NE2   | 2.52                     | 0.43              |
| 3:B:432:PRO:HB2   | 3:C:413:MET:SD    | 2.59                     | 0.43              |
| 3:B:785:HIS:HD2   | 3:B:788:GLN:HE21  | 1.67                     | 0.43              |
| 3:B:1236:ARG:O    | 3:B:1238:PHE:N    | 2.52                     | 0.43              |
| 3:C:63:ASN:HD21   | 3:D:99:VAL:HG13   | 1.82                     | 0.43              |
| 3:C:176:PHE:O     | 3:C:180:THR:HG23  | 2.19                     | 0.43              |
| 3:C:289:LEU:HA    | 3:C:289:LEU:HD23  | 1.81                     | 0.43              |
| 3:C:765:TYR:HD1   | 3:C:783:LEU:HB2   | 1.84                     | 0.43              |
| 3:C:1040:LEU:HD23 | 3:C:1040:LEU:HA   | 1.78                     | 0.43              |
| 3:D:86:GLU:HB2    | 3:D:89:TYR:HD2    | 1.84                     | 0.43              |
| 3:D:184:MET:HE3   | 3:D:184:MET:HB3   | 1.79                     | 0.43              |
| 3:D:383:ARG:HB2   | 3:D:384:ILE:HD12  | 2.01                     | 0.43              |
| 3:D:390:VAL:HG22  | 3:E:106:ARG:HH11  | 1.82                     | 0.43              |
| 3:D:1067:GLU:O    | 3:D:1068:ARG:C    | 2.62                     | 0.43              |
| 5:q:13:LEU:O      | 5:q:14:THR:HG22   | 2.19                     | 0.43              |
| 5:q:254:THR:HA    | 5:q:257:ASN:HB2   | 2.00                     | 0.43              |
| 5:q:459:PRO:HB2   | 5:q:470:PHE:CE2   | 2.53                     | 0.43              |
| 5:q:611:ASP:HB2   | 5:q:620:SER:HB2   | 2.00                     | 0.43              |
| 3:E:268:ASP:OD1   | 3:E:367:LEU:HD13  | 2.19                     | 0.43              |
| 3:E:880:HIS:HE1   | 3:E:883:ARG:HH11  | 1.66                     | 0.43              |
| 6:r:79:ASP:O      | 6:r:83:ARG:N      | 2.50                     | 0.43              |
| 3:F:750:ARG:CA    | 3:F:753:ASP:HB3   | 2.43                     | 0.43              |
| 3:F:861:PRO:HB3   | 3:F:866:HIS:CE1   | 2.53                     | 0.43              |
| 3:F:1125:LEU:HD21 | 3:F:1157:LEU:HD22 | 2.01                     | 0.43              |
| 3:G:106:ARG:HB3   | 3:G:110:HIS:CB    | 2.49                     | 0.43              |
| 3:G:466:LEU:HD21  | 3:G:1033:PRO:HD3  | 2.00                     | 0.43              |
| 4:f:89:ARG:HH21   | 4:g:29:THR:C      | 2.27                     | 0.43              |
| 2:R:59:ASP:OD1    | 2:R:62:GLY:N      | 2.45                     | 0.43              |
| 2:R:101:ARG:HA    | 2:R:311:MET:HA    | 2.01                     | 0.43              |
| 2:Y:53:SER:OG     | 2:Y:54:GLY:N      | 2.52                     | 0.43              |
| 1:1:191:VAL:HB    | 1:1:207:VAL:HG11  | 2.01                     | 0.43              |
| 3:I:879:PHE:CE1   | 3:I:886:VAL:HG21  | 2.54                     | 0.43              |
| 3:I:1115:VAL:HG12 | 3:I:1116:ARG:O    | 2.19                     | 0.43              |
| 3:J:550:PHE:O     | 3:J:571:ILE:HA    | 2.19                     | 0.43              |
| 3:K:834:ARG:NH1   | 3:K:953:GLU:HA    | 2.34                     | 0.43              |
| 3:K:1336:CYS:SG   | 3:K:1337:ALA:N    | 2.92                     | 0.43              |
| 3:L:244:ILE:HG21  | 3:L:292:PHE:CD2   | 2.54                     | 0.43              |
| 3:L:1032:SER:O    | 3:L:1035:ALA:N    | 2.52                     | 0.43              |
| 3:L:1354:ARG:HG3  | 3:L:1354:ARG:O    | 2.19                     | 0.43              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:M:81:CYS:HG    | 3:M:1073:TYR:HD2  | 1.65                     | 0.43              |
| 3:M:492:ALA:O    | 3:M:559:PRO:HB3   | 2.19                     | 0.43              |
| 3:M:496:GLY:HA3  | 3:M:504:ARG:NH2   | 2.34                     | 0.43              |
| 3:M:628:TYR:HB3  | 3:M:955:PHE:HE2   | 1.83                     | 0.43              |
| 3:M:958:LEU:HD23 | 3:M:958:LEU:HA    | 1.87                     | 0.43              |
| 3:A:265:THR:HG21 | 3:A:1068:ARG:HH21 | 1.83                     | 0.43              |
| 3:A:438:ARG:O    | 3:A:454:MET:HG2   | 2.19                     | 0.43              |
| 3:A:580:GLY:HA3  | 3:A:1006:VAL:HG22 | 2.01                     | 0.43              |
| 3:A:863:HIS:CD2  | 3:A:865:LEU:H     | 2.37                     | 0.43              |
| 3:A:1055:GLN:HB2 | 3:A:1272:PRO:HB3  | 2.01                     | 0.43              |
| 3:H:709:LEU:C    | 3:H:709:LEU:CD1   | 2.92                     | 0.43              |
| 3:H:778:ARG:HG2  | 3:H:904:ARG:NH1   | 2.34                     | 0.43              |
| 3:H:840:GLN:HE21 | 3:H:897:LEU:HB2   | 1.84                     | 0.43              |
| 3:H:1058:PHE:HE2 | 3:H:1369:LEU:HD11 | 1.77                     | 0.43              |
| 4:p:88:LEU:HD12  | 4:p:89:ARG:N      | 2.34                     | 0.43              |
| 3:N:103:LEU:HD11 | 3:N:115:PRO:HA    | 2.00                     | 0.43              |
| 3:O:73:LEU:HD23  | 3:O:383:ARG:NH1   | 2.33                     | 0.43              |
| 3:O:435:PHE:CG   | 3:O:598:GLU:HG3   | 2.53                     | 0.43              |
| 3:P:184:MET:HE1  | 3:P:1071:GLU:OE1  | 2.19                     | 0.43              |
| 3:B:1198:TYR:HD1 | 3:B:1236:ARG:HH11 | 1.67                     | 0.43              |
| 3:C:462:CYS:SG   | 3:C:1147:LEU:HD22 | 2.59                     | 0.43              |
| 3:C:677:TYR:HA   | 4:c:95:LYS:HZ3    | 1.81                     | 0.43              |
| 5:q:65:HIS:HE1   | 5:q:470:PHE:N     | 2.09                     | 0.43              |
| 3:E:520:TRP:CD1  | 3:E:1004:GLN:HB2  | 2.53                     | 0.43              |
| 3:E:601:VAL:O    | 3:E:601:VAL:HG12  | 2.19                     | 0.43              |
| 3:E:790:ARG:CZ   | 4:e:80:ALA:O      | 2.66                     | 0.43              |
| 3:E:1301:SER:HB3 | 3:E:1321:VAL:CG2  | 2.46                     | 0.43              |
| 3:F:198:LEU:O    | 3:F:199:LEU:C     | 2.61                     | 0.43              |
| 3:G:279:VAL:HG12 | 3:G:394:LEU:HD22  | 2.01                     | 0.43              |
| 3:G:914:PRO:HG3  | 3:G:923:THR:HG22  | 1.99                     | 0.43              |
| 1:w:141:PRO:CB   | 3:O:1165:VAL:HG11 | 2.48                     | 0.42              |
| 3:I:300:ALA:O    | 3:I:362:ARG:HD3   | 2.18                     | 0.42              |
| 3:J:193:PRO:HG2  | 3:J:198:LEU:HD11  | 2.00                     | 0.42              |
| 3:J:481:VAL:HG21 | 3:J:571:ILE:HD11  | 2.00                     | 0.42              |
| 3:K:244:ILE:HG21 | 3:K:292:PHE:CE2   | 2.53                     | 0.42              |
| 3:K:382:LYS:HA   | 3:K:382:LYS:HD2   | 1.87                     | 0.42              |
| 3:K:610:THR:HA   | 3:K:689:VAL:HG22  | 2.01                     | 0.42              |
| 3:K:746:ALA:HA   | 3:K:754:CYS:SG    | 2.60                     | 0.42              |
| 3:L:38:PHE:HB3   | 3:O:121:THR:OG1   | 2.19                     | 0.42              |
| 3:L:915:ASP:O    | 3:L:919:ASN:N     | 2.52                     | 0.42              |
| 3:M:123:VAL:HG23 | 3:N:37:ASP:OD2    | 2.19                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:M:433:ARG:NH1   | 3:H:413:MET:HE3   | 2.34                     | 0.42              |
| 3:M:584:LEU:HD22  | 3:M:589:VAL:HG22  | 2.01                     | 0.42              |
| 3:A:344:LEU:HD21  | 3:B:340:GLN:CB    | 2.48                     | 0.42              |
| 3:A:461:VAL:O     | 3:A:466:LEU:HD23  | 2.19                     | 0.42              |
| 3:A:1115:VAL:HG12 | 3:A:1116:ARG:O    | 2.19                     | 0.42              |
| 3:H:404:LEU:HB3   | 3:H:440:LEU:CD1   | 2.48                     | 0.42              |
| 3:H:725:LEU:HD23  | 3:H:1028:TYR:CD1  | 2.54                     | 0.42              |
| 3:N:195:LEU:HA    | 3:N:195:LEU:HD23  | 1.80                     | 0.42              |
| 3:N:448:GLN:HE21  | 3:O:1201:ARG:NH1  | 2.16                     | 0.42              |
| 3:O:224:LYS:HA    | 3:O:1328:PHE:CE2  | 2.53                     | 0.42              |
| 3:O:520:TRP:CD1   | 3:O:521:VAL:HG23  | 2.54                     | 0.42              |
| 3:O:742:LEU:HD13  | 3:O:783:LEU:HD13  | 2.01                     | 0.42              |
| 3:O:784:LEU:HD22  | 3:O:786:ASN:ND2   | 2.34                     | 0.42              |
| 3:P:383:ARG:HB2   | 3:P:384:ILE:HD12  | 2.00                     | 0.42              |
| 3:P:724:HIS:CD2   | 3:P:726:MET:HB2   | 2.53                     | 0.42              |
| 3:P:1085:THR:O    | 3:P:1088:GLY:N    | 2.51                     | 0.42              |
| 3:P:1335:THR:N    | 3:P:1365:ASP:HB3  | 2.34                     | 0.42              |
| 3:B:463:HIS:HD2   | 3:B:465:SER:CB    | 2.30                     | 0.42              |
| 3:B:644:LEU:HD22  | 3:B:647:LEU:HD12  | 2.01                     | 0.42              |
| 3:B:1366:ALA:HA   | 3:B:1370:LYS:HZ3  | 1.84                     | 0.42              |
| 3:C:634:ILE:HA    | 3:C:640:VAL:CG1   | 2.49                     | 0.42              |
| 3:C:1124:ASN:OD1  | 3:C:1124:ASN:N    | 2.44                     | 0.42              |
| 3:D:577:VAL:H     | 3:D:581:ASN:HD22  | 1.67                     | 0.42              |
| 3:D:595:ARG:O     | 3:D:598:GLU:HB3   | 2.19                     | 0.42              |
| 3:D:633:ALA:HB1   | 3:D:897:LEU:HD21  | 2.00                     | 0.42              |
| 3:D:983:LEU:O     | 3:D:987:VAL:HG22  | 2.19                     | 0.42              |
| 3:E:65:LEU:HD23   | 3:E:65:LEU:HA     | 1.84                     | 0.42              |
| 3:E:739:CYS:O     | 3:E:743:MET:HG2   | 2.19                     | 0.42              |
| 3:E:842:MET:HE3   | 3:E:842:MET:HB3   | 1.58                     | 0.42              |
| 3:F:67:LEU:HA     | 3:F:67:LEU:HD23   | 1.79                     | 0.42              |
| 3:F:1248:GLN:HB2  | 3:F:1251:SER:OG   | 2.19                     | 0.42              |
| 3:G:489:ALA:HB1   | 3:G:552:GLY:HA2   | 2.01                     | 0.42              |
| 3:G:701:ALA:O     | 3:G:727:ARG:NH2   | 2.51                     | 0.42              |
| 3:G:866:HIS:CD2   | 3:G:868:ALA:H     | 2.37                     | 0.42              |
| 7:u:3113:SER:O    | 7:u:3117:VAL:HG23 | 2.18                     | 0.42              |
| 2:S:205:LEU:HD23  | 2:S:285:LEU:HD21  | 2.00                     | 0.42              |
| 2:S:247:THR:HA    | 2:S:250:ALA:HB3   | 2.01                     | 0.42              |
| 2:V:197:SER:O     | 2:V:200:THR:OG1   | 2.36                     | 0.42              |
| 1:W:257:GLN:CD    | 3:D:109:PRO:HD2   | 2.40                     | 0.42              |
| 2:X:33:PHE:HZ     | 2:X:116:LEU:HD13  | 1.84                     | 0.42              |
| 2:X:116:LEU:H     | 2:X:116:LEU:HG    | 1.64                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:I:28:ALA:HB3    | 3:D:144:THR:HG23  | 1.70                     | 0.42              |
| 2:y:10:ILE:HG12   | 2:y:46:VAL:HG21   | 2.00                     | 0.42              |
| 3:I:44:SER:O      | 3:I:45:ASP:HB2    | 2.18                     | 0.42              |
| 3:I:79:CYS:HB3    | 3:I:81:CYS:SG     | 2.59                     | 0.42              |
| 3:I:390:VAL:HG21  | 3:J:104:ILE:CG1   | 2.49                     | 0.42              |
| 3:I:401:THR:HA    | 3:I:1054:ARG:O    | 2.20                     | 0.42              |
| 3:I:784:LEU:CD2   | 3:I:903:GLU:H     | 2.33                     | 0.42              |
| 3:I:861:PRO:HA    | 3:I:866:HIS:CG    | 2.54                     | 0.42              |
| 3:J:219:LEU:HA    | 3:J:219:LEU:HD23  | 1.76                     | 0.42              |
| 3:J:718:ALA:HB3   | 3:J:721:GLU:HG3   | 2.00                     | 0.42              |
| 3:J:840:GLN:NE2   | 4:j:58:ALA:HB2    | 2.35                     | 0.42              |
| 3:J:945:LEU:HA    | 3:J:945:LEU:HD23  | 1.68                     | 0.42              |
| 3:K:263:ARG:NH1   | 3:K:307:GLY:HA2   | 2.33                     | 0.42              |
| 3:K:705:ASP:OD2   | 3:L:985:ARG:HD3   | 2.19                     | 0.42              |
| 3:K:765:TYR:HD1   | 3:K:783:LEU:HB2   | 1.83                     | 0.42              |
| 3:K:1054:ARG:NH2  | 3:K:1122:MET:HB3  | 2.33                     | 0.42              |
| 3:L:80:VAL:HG23   | 3:L:1069:ALA:HB1  | 2.02                     | 0.42              |
| 3:L:136:ALA:H     | 3:L:139:ALA:HB3   | 1.83                     | 0.42              |
| 3:L:524:CYS:SG    | 3:L:1008:GLN:NE2  | 2.93                     | 0.42              |
| 3:L:670:LEU:O     | 3:L:674:ILE:HG13  | 2.19                     | 0.42              |
| 3:L:1314:PRO:HA   | 3:L:1315:PRO:HD3  | 1.89                     | 0.42              |
| 3:M:833:ASP:HA    | 4:m:54:LEU:HD11   | 2.00                     | 0.42              |
| 3:M:915:ASP:O     | 3:M:919:ASN:HB2   | 2.19                     | 0.42              |
| 3:M:1020:LEU:HD23 | 3:M:1020:LEU:HA   | 1.73                     | 0.42              |
| 3:A:822:ARG:HB2   | 3:A:824:ARG:NH1   | 2.35                     | 0.42              |
| 3:H:302:VAL:HG12  | 3:H:303:PRO:O     | 2.20                     | 0.42              |
| 3:H:606:MET:HE1   | 3:H:820:PHE:HZ    | 1.84                     | 0.42              |
| 4:n:90:PRO:HD3    | 3:O:834:ARG:HD3   | 2.01                     | 0.42              |
| 3:N:384:ILE:HG22  | 3:N:385:TYR:N     | 2.34                     | 0.42              |
| 3:N:756:ILE:HA    | 3:N:909:LEU:O     | 2.19                     | 0.42              |
| 3:N:767:ALA:HA    | 3:N:796:ASP:OD1   | 2.19                     | 0.42              |
| 3:N:907:ALA:HA    | 3:N:933:LEU:HD23  | 2.01                     | 0.42              |
| 3:N:1176:GLY:HA3  | 3:O:1225:LEU:HD21 | 2.01                     | 0.42              |
| 3:O:204:TYR:HB2   | 3:O:219:LEU:HD21  | 2.01                     | 0.42              |
| 3:O:244:ILE:HG21  | 3:O:292:PHE:CE2   | 2.54                     | 0.42              |
| 3:O:388:THR:HG23  | 3:P:102:PRO:HG2   | 2.00                     | 0.42              |
| 3:O:745:HIS:CE1   | 3:O:910:CYS:HB2   | 2.54                     | 0.42              |
| 3:O:1335:THR:N    | 3:O:1365:ASP:HB3  | 2.33                     | 0.42              |
| 3:P:458:VAL:O     | 3:P:462:CYS:HB3   | 2.19                     | 0.42              |
| 3:P:624:PRO:HB2   | 3:P:627:PHE:CE2   | 2.54                     | 0.42              |
| 3:P:790:ARG:HG3   | 3:P:792:ALA:H     | 1.83                     | 0.42              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:B:417:ALA:HB2  | 3:B:1358:PHE:CE1  | 2.54                     | 0.42              |
| 3:B:787:THR:C    | 3:B:788:GLN:HG3   | 2.44                     | 0.42              |
| 3:B:804:ASP:HB3  | 3:B:808:HIS:CD2   | 2.55                     | 0.42              |
| 3:B:978:PRO:HA   | 3:B:981:ARG:CZ    | 2.49                     | 0.42              |
| 3:B:1188:ILE:O   | 3:B:1190:THR:HG23 | 2.19                     | 0.42              |
| 3:C:550:PHE:O    | 3:C:571:ILE:HA    | 2.19                     | 0.42              |
| 3:D:106:ARG:HH21 | 3:D:110:HIS:HB3   | 1.83                     | 0.42              |
| 5:q:406:VAL:HA   | 5:q:412:ARG:O     | 2.20                     | 0.42              |
| 3:E:85:PRO:HD2   | 3:E:309:MET:O     | 2.19                     | 0.42              |
| 3:E:614:VAL:HG21 | 3:E:693:LEU:HD21  | 2.01                     | 0.42              |
| 3:E:778:ARG:NH1  | 3:E:782:ARG:HH11  | 2.17                     | 0.42              |
| 3:E:1191:PRO:HG2 | 3:E:1194:THR:CG2  | 2.48                     | 0.42              |
| 3:E:1255:LEU:HA  | 3:E:1255:LEU:HD23 | 1.65                     | 0.42              |
| 3:E:1354:ARG:O   | 3:E:1354:ARG:HG3  | 2.19                     | 0.42              |
| 3:E:1357:HIS:O   | 3:E:1358:PHE:C    | 2.62                     | 0.42              |
| 6:r:83:ARG:O     | 6:r:86:PRO:HD2    | 2.19                     | 0.42              |
| 3:F:639:HIS:HD2  | 4:f:78:MET:SD     | 2.42                     | 0.42              |
| 3:F:801:ARG:HD3  | 3:F:805:TRP:CD1   | 2.53                     | 0.42              |
| 3:F:866:HIS:HD2  | 3:F:868:ALA:HB3   | 1.84                     | 0.42              |
| 3:F:970:VAL:HG11 | 3:F:989:LEU:HB2   | 2.01                     | 0.42              |
| 6:s:26:PHE:CG    | 6:s:27:ILE:N      | 2.86                     | 0.42              |
| 6:s:26:PHE:HZ    | 6:s:29:PRO:HD3    | 1.84                     | 0.42              |
| 3:G:350:THR:HG22 | 3:G:352:ASP:H     | 1.83                     | 0.42              |
| 3:G:1314:PRO:HA  | 3:G:1315:PRO:HD3  | 1.90                     | 0.42              |
| 2:S:300:PHE:HD2  | 3:A:111:PRO:HG3   | 1.67                     | 0.42              |
| 1:T:145:ARG:HG2  | 1:T:154:THR:HB    | 2.01                     | 0.42              |
| 1:W:210:HIS:HB3  | 1:W:445:VAL:HB    | 2.01                     | 0.42              |
| 1:1:210:HIS:HB3  | 1:1:445:VAL:HB    | 2.01                     | 0.42              |
| 2:y:180:TYR:OH   | 2:y:185:ARG:NH1   | 2.52                     | 0.42              |
| 3:I:440:LEU:HD13 | 3:I:1336:CYS:SG   | 2.60                     | 0.42              |
| 3:I:544:HIS:CG   | 3:I:545:PRO:HD2   | 2.53                     | 0.42              |
| 3:I:947:HIS:O    | 4:h:79:PHE:HB3    | 2.19                     | 0.42              |
| 3:I:1218:LYS:HB3 | 3:I:1221:ASP:CG   | 2.45                     | 0.42              |
| 3:J:446:ASP:O    | 3:J:447:HIS:HB2   | 2.19                     | 0.42              |
| 3:J:834:ARG:HB3  | 4:i:90:PRO:HD3    | 2.01                     | 0.42              |
| 3:J:861:PRO:HA   | 3:J:866:HIS:CD2   | 2.54                     | 0.42              |
| 3:K:463:HIS:HD2  | 3:K:465:SER:HB3   | 1.84                     | 0.42              |
| 3:L:448:GLN:HG2  | 3:M:1201:ARG:HD3  | 2.01                     | 0.42              |
| 3:L:460:THR:HA   | 3:L:1129:PHE:CD2  | 2.54                     | 0.42              |
| 3:L:600:GLY:C    | 3:L:602:GLY:H     | 2.28                     | 0.42              |
| 3:L:706:ASP:O    | 3:M:525:GLN:NE2   | 2.52                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:L:1157:LEU:O    | 3:L:1171:VAL:HG13 | 2.18                     | 0.42              |
| 3:M:11:TYR:HB2    | 3:D:96:GLN:HG2    | 2.00                     | 0.42              |
| 3:M:32:HIS:HB3    | 3:D:1290:GLU:HG3  | 2.01                     | 0.42              |
| 3:M:195:LEU:HD23  | 3:M:195:LEU:HA    | 1.86                     | 0.42              |
| 3:A:494:PRO:HG2   | 3:A:760:GLY:HA2   | 2.02                     | 0.42              |
| 3:A:742:LEU:HD13  | 3:A:756:ILE:HG21  | 2.01                     | 0.42              |
| 3:A:748:LEU:HB2   | 3:A:754:CYS:SG    | 2.59                     | 0.42              |
| 3:H:293:LEU:HD13  | 3:H:368:VAL:HG11  | 2.01                     | 0.42              |
| 3:H:752:ARG:HG3   | 3:H:913:ALA:N     | 2.33                     | 0.42              |
| 3:H:1291:ARG:HH12 | 3:C:35:LEU:CD1    | 2.30                     | 0.42              |
| 3:H:1333:PRO:HG2  | 3:H:1366:ALA:H    | 1.85                     | 0.42              |
| 4:I:73:PHE:HE2    | 4:I:100:PRO:HA    | 1.84                     | 0.42              |
| 3:N:106:ARG:HE    | 3:N:110:HIS:CB    | 2.32                     | 0.42              |
| 3:N:831:ARG:O     | 3:N:835:VAL:HG23  | 2.19                     | 0.42              |
| 3:O:133:PHE:O     | 3:O:133:PHE:CG    | 2.72                     | 0.42              |
| 3:O:318:THR:O     | 3:O:322:MET:HB2   | 2.20                     | 0.42              |
| 3:O:521:VAL:HG21  | 3:O:987:VAL:HG12  | 2.00                     | 0.42              |
| 3:O:756:ILE:HB    | 3:O:763:PRO:HD3   | 2.01                     | 0.42              |
| 3:P:193:PRO:CB    | 3:P:1293:ILE:HG22 | 2.49                     | 0.42              |
| 3:P:1342:LEU:CD2  | 3:P:1362:LEU:HB2  | 2.50                     | 0.42              |
| 3:C:499:ALA:HA    | 3:C:956:TYR:CD1   | 2.55                     | 0.42              |
| 3:C:669:SER:O     | 3:C:672:SER:OG    | 2.23                     | 0.42              |
| 3:C:994:LEU:HD23  | 3:C:994:LEU:HA    | 1.82                     | 0.42              |
| 3:C:1020:LEU:O    | 3:C:1023:ALA:N    | 2.52                     | 0.42              |
| 3:D:54:PHE:CE1    | 3:E:319:ALA:HB1   | 2.54                     | 0.42              |
| 3:D:219:LEU:HD23  | 3:D:219:LEU:HA    | 1.81                     | 0.42              |
| 3:D:876:ASN:HA    | 3:D:879:PHE:CD2   | 2.50                     | 0.42              |
| 3:D:1147:LEU:O    | 3:D:1148:ARG:C    | 2.60                     | 0.42              |
| 5:q:39:PRO:HD2    | 5:q:136:TRP:CH2   | 2.54                     | 0.42              |
| 3:E:1100:VAL:HG12 | 3:E:1101:ASP:N    | 2.34                     | 0.42              |
| 3:F:888:GLY:N     | 3:F:889:PRO:HD2   | 2.34                     | 0.42              |
| 3:G:106:ARG:NH1   | 3:G:113:GLU:CD    | 2.76                     | 0.42              |
| 2:S:241:LEU:HD12  | 2:S:248:ARG:HH21  | 1.84                     | 0.42              |
| 2:Y:31:VAL:HG11   | 2:Y:116:LEU:HD22  | 2.00                     | 0.42              |
| 2:Y:147:LEU:HD23  | 2:Y:147:LEU:HA    | 1.88                     | 0.42              |
| 2:2:1:MET:O       | 2:2:5:CYS:N       | 2.46                     | 0.42              |
| 3:I:724:HIS:CD2   | 3:I:726:MET:HB2   | 2.54                     | 0.42              |
| 3:I:953:GLU:HB3   | 4:h:90:PRO:HG3    | 2.01                     | 0.42              |
| 3:I:1304:THR:HG21 | 3:I:1314:PRO:HD2  | 2.00                     | 0.42              |
| 3:J:655:TYR:CE2   | 3:J:663:ALA:HB2   | 2.54                     | 0.42              |
| 3:K:438:ARG:O     | 3:K:454:MET:HG2   | 2.18                     | 0.42              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:K:752:ARG:HA   | 3:K:913:ALA:H     | 1.85                     | 0.42              |
| 3:K:946:ASP:HB3  | 3:K:949:ILE:N     | 2.25                     | 0.42              |
| 3:L:17:MET:HE2   | 3:O:339:MET:HE2   | 2.01                     | 0.42              |
| 3:L:414:GLU:CG   | 3:L:1356:THR:HG21 | 2.50                     | 0.42              |
| 3:L:472:ALA:O    | 3:L:475:GLY:N     | 2.52                     | 0.42              |
| 3:M:21:GLY:O     | 3:C:61:TYR:HD1    | 1.99                     | 0.42              |
| 3:M:27:ILE:HG22  | 3:M:28:GLU:N      | 2.35                     | 0.42              |
| 3:M:505:PHE:O    | 3:M:509:TRP:HD1   | 2.02                     | 0.42              |
| 3:M:578:VAL:HB   | 3:M:1027:GLY:O    | 2.19                     | 0.42              |
| 3:M:1227:TYR:CD1 | 3:M:1249:ARG:HB2  | 2.54                     | 0.42              |
| 3:A:195:LEU:O    | 3:A:198:LEU:N     | 2.35                     | 0.42              |
| 3:A:637:SER:HA   | 3:A:787:THR:HB    | 2.02                     | 0.42              |
| 3:H:311:LEU:HD23 | 3:H:311:LEU:HA    | 1.87                     | 0.42              |
| 3:H:524:CYS:HB3  | 3:H:1008:GLN:HE22 | 1.84                     | 0.42              |
| 3:H:708:THR:HG22 | 3:H:723:ASN:HD22  | 1.83                     | 0.42              |
| 3:N:103:LEU:HD11 | 3:N:115:PRO:CA    | 2.50                     | 0.42              |
| 3:N:1155:ASN:C   | 3:N:1157:LEU:H    | 2.27                     | 0.42              |
| 3:O:367:LEU:HD23 | 3:O:367:LEU:HA    | 1.75                     | 0.42              |
| 3:O:402:PHE:O    | 3:O:1053:VAL:HA   | 2.20                     | 0.42              |
| 3:O:447:HIS:CD2  | 3:P:225:ARG:HH22  | 2.38                     | 0.42              |
| 3:O:1181:GLN:OE1 | 3:O:1307:SER:OG   | 2.37                     | 0.42              |
| 3:O:1340:PRO:O   | 3:O:1344:ARG:HG3  | 2.19                     | 0.42              |
| 3:P:86:GLU:OE1   | 3:P:86:GLU:N      | 2.48                     | 0.42              |
| 3:P:443:TRP:HA   | 3:P:448:GLN:O     | 2.19                     | 0.42              |
| 3:P:712:PRO:HD2  | 3:P:1146:TYR:CE1  | 2.54                     | 0.42              |
| 3:B:62:CYS:SG    | 3:B:63:ASN:N      | 2.93                     | 0.42              |
| 3:B:163:GLN:HG2  | 3:C:344:LEU:HD11  | 2.01                     | 0.42              |
| 3:B:713:GLU:HG2  | 3:B:718:ALA:HA    | 2.00                     | 0.42              |
| 3:B:763:PRO:HB2  | 3:B:765:TYR:CZ    | 2.53                     | 0.42              |
| 3:B:961:HIS:O    | 3:B:964:PHE:N     | 2.38                     | 0.42              |
| 3:C:84:PHE:HD1   | 3:C:84:PHE:HA     | 1.73                     | 0.42              |
| 3:C:1301:SER:HB3 | 3:C:1321:VAL:HB   | 2.01                     | 0.42              |
| 3:D:54:PHE:HD2   | 3:E:90:MET:HA     | 1.85                     | 0.42              |
| 3:D:133:PHE:CD2  | 3:D:1091:PHE:HD2  | 2.37                     | 0.42              |
| 3:D:400:LEU:HD12 | 3:D:1058:PHE:CE2  | 2.55                     | 0.42              |
| 3:D:463:HIS:ND1  | 3:D:464:PRO:HD2   | 2.34                     | 0.42              |
| 5:q:69:ASP:OD1   | 5:q:685:ARG:NH1   | 2.52                     | 0.42              |
| 5:q:86:VAL:O     | 5:q:90:LEU:HG     | 2.19                     | 0.42              |
| 5:q:594:THR:CB   | 5:q:647:ALA:HA    | 2.50                     | 0.42              |
| 3:E:71:LEU:O     | 3:E:302:VAL:HG11  | 2.19                     | 0.42              |
| 3:E:615:ARG:HE   | 3:E:1017:GLU:HG3  | 1.84                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:E:946:ASP:HB3   | 3:E:949:ILE:N     | 2.32                     | 0.42              |
| 6:r:66:LEU:O      | 6:r:70:ALA:N      | 2.38                     | 0.42              |
| 3:F:643:ALA:HB2   | 4:f:78:MET:HE1    | 2.02                     | 0.42              |
| 3:F:863:HIS:ND1   | 3:F:864:PRO:HD2   | 2.35                     | 0.42              |
| 3:F:1335:THR:HA   | 3:F:1363:ILE:O    | 2.19                     | 0.42              |
| 3:G:23:ILE:CG2    | 3:G:167:ARG:NH1   | 2.81                     | 0.42              |
| 3:G:592:ARG:HB2   | 3:G:1009:HIS:CE1  | 2.54                     | 0.42              |
| 4:d:21:GLY:O      | 4:d:25:LEU:N      | 2.50                     | 0.42              |
| 2:R:90:LEU:O      | 2:R:93:THR:OG1    | 2.35                     | 0.42              |
| 2:2:295:VAL:HG13  | 2:2:314:VAL:HG13  | 2.02                     | 0.42              |
| 3:I:205:LEU:HD21  | 3:I:1290:GLU:OE2  | 2.20                     | 0.42              |
| 3:J:318:THR:O     | 3:J:323:GLY:N     | 2.37                     | 0.42              |
| 3:J:426:ALA:HB3   | 3:J:429:HIS:CD2   | 2.54                     | 0.42              |
| 3:J:1166:PHE:CD1  | 3:J:1167:GLY:N    | 2.88                     | 0.42              |
| 3:K:443:TRP:CE2   | 3:K:1343:LEU:HD21 | 2.55                     | 0.42              |
| 3:K:508:ALA:HB1   | 3:K:563:VAL:HG23  | 2.02                     | 0.42              |
| 3:K:539:LEU:HA    | 3:K:539:LEU:HD23  | 1.77                     | 0.42              |
| 3:K:1227:TYR:OH   | 3:K:1279:ALA:HB2  | 2.20                     | 0.42              |
| 3:L:414:GLU:HG2   | 3:L:1356:THR:HG21 | 2.00                     | 0.42              |
| 3:L:539:LEU:HD23  | 3:L:539:LEU:HA    | 1.87                     | 0.42              |
| 3:L:630:LEU:O     | 3:L:634:ILE:HD12  | 2.20                     | 0.42              |
| 3:L:871:VAL:O     | 3:L:874:THR:OG1   | 2.22                     | 0.42              |
| 3:L:1190:THR:HG22 | 3:L:1243:ASN:ND2  | 2.35                     | 0.42              |
| 3:M:164:GLN:NE2   | 3:C:49:LEU:CD1    | 2.81                     | 0.42              |
| 3:M:745:HIS:NE2   | 3:M:910:CYS:HB2   | 2.35                     | 0.42              |
| 3:M:811:ILE:O     | 3:M:815:VAL:HB    | 2.19                     | 0.42              |
| 3:M:1251:SER:O    | 3:M:1255:LEU:HG   | 2.20                     | 0.42              |
| 3:M:1336:CYS:O    | 3:M:1362:LEU:HG   | 2.20                     | 0.42              |
| 3:A:125:ASP:O     | 3:A:1098:GLY:HA2  | 2.19                     | 0.42              |
| 3:A:187:VAL:HG11  | 3:A:1071:GLU:OE2  | 2.18                     | 0.42              |
| 3:A:544:HIS:CG    | 3:A:545:PRO:HD2   | 2.55                     | 0.42              |
| 3:A:708:THR:HG21  | 3:A:720:ALA:HA    | 2.01                     | 0.42              |
| 3:A:1208:ARG:HD3  | 3:A:1226:MET:O    | 2.19                     | 0.42              |
| 3:H:350:THR:HG21  | 3:C:21:GLY:HA2    | 2.00                     | 0.42              |
| 3:H:989:LEU:HD23  | 3:H:989:LEU:HA    | 1.87                     | 0.42              |
| 4:j:76:GLN:CB     | 4:j:94:LEU:HD12   | 2.50                     | 0.42              |
| 4:n:79:PHE:CZ     | 3:N:639:HIS:HA    | 2.54                     | 0.42              |
| 4:o:94:LEU:HD22   | 3:P:880:HIS:HD2   | 1.85                     | 0.42              |
| 3:N:96:GLN:NE2    | 3:D:11:TYR:CB     | 2.83                     | 0.42              |
| 3:N:244:ILE:O     | 3:N:247:TRP:N     | 2.46                     | 0.42              |
| 3:N:1208:ARG:NE   | 3:N:1225:LEU:O    | 2.52                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:O:274:VAL:HG11  | 3:O:376:PHE:CE2   | 2.55                     | 0.42              |
| 3:O:1020:LEU:O    | 3:O:1023:ALA:N    | 2.53                     | 0.42              |
| 3:O:1080:VAL:HG22 | 3:O:1093:LEU:CD2  | 2.49                     | 0.42              |
| 3:B:84:PHE:HD2    | 3:B:87:LEU:HD12   | 1.84                     | 0.42              |
| 3:B:262:PRO:CA    | 3:G:60:SER:HA     | 2.48                     | 0.42              |
| 3:B:809:HIS:O     | 3:B:810:LYS:C     | 2.62                     | 0.42              |
| 3:B:836:TYR:CE1   | 3:B:897:LEU:HD22  | 2.54                     | 0.42              |
| 3:D:188:LEU:HD23  | 3:D:188:LEU:HA    | 1.76                     | 0.42              |
| 3:D:741:GLY:O     | 3:D:745:HIS:HB3   | 2.20                     | 0.42              |
| 3:D:1093:LEU:HD23 | 3:D:1093:LEU:HA   | 1.85                     | 0.42              |
| 5:q:510:TYR:CE1   | 5:q:644:GLU:HA    | 2.55                     | 0.42              |
| 3:E:56:ALA:HA     | 3:F:325:ALA:O     | 2.19                     | 0.42              |
| 3:E:154:SER:C     | 3:E:157:ARG:H     | 2.27                     | 0.42              |
| 3:E:463:HIS:O     | 3:E:465:SER:N     | 2.49                     | 0.42              |
| 3:F:301:ASP:OD1   | 3:F:362:ARG:NE    | 2.52                     | 0.42              |
| 3:F:410:ASN:ND2   | 3:F:1359:THR:C    | 2.77                     | 0.42              |
| 3:F:438:ARG:O     | 3:F:454:MET:HG2   | 2.19                     | 0.42              |
| 3:F:539:LEU:O     | 3:F:541:LEU:N     | 2.53                     | 0.42              |
| 3:F:778:ARG:HH11  | 3:F:782:ARG:HD2   | 1.85                     | 0.42              |
| 3:F:983:LEU:O     | 3:F:987:VAL:HG22  | 2.20                     | 0.42              |
| 3:F:1034:VAL:HG22 | 3:F:1147:LEU:HD21 | 2.00                     | 0.42              |
| 3:F:1050:PHE:CD1  | 3:F:1187:PHE:HB3  | 2.55                     | 0.42              |
| 6:s:83:ARG:HG3    | 7:u:3103:LEU:HD21 | 2.02                     | 0.42              |
| 3:G:454:MET:HE2   | 3:G:1040:LEU:CD2  | 2.50                     | 0.42              |
| 2:U:10:ILE:N      | 2:U:83:ILE:O      | 2.49                     | 0.42              |
| 2:U:109:CYS:SG    | 2:U:182:ASN:ND2   | 2.91                     | 0.42              |
| 1:w:197:ALA:HB2   | 1:w:324:LEU:HD22  | 2.01                     | 0.42              |
| 3:I:103:LEU:HB3   | 3:H:175:ALA:HB2   | 2.02                     | 0.42              |
| 3:I:331:ASP:O     | 3:I:335:HIS:HD2   | 2.03                     | 0.42              |
| 3:J:58:LEU:HD13   | 3:K:1074:PHE:CZ   | 2.55                     | 0.42              |
| 3:J:469:ILE:O     | 3:J:469:ILE:CG2   | 2.67                     | 0.42              |
| 3:K:408:LEU:HD23  | 3:K:408:LEU:HA    | 1.85                     | 0.42              |
| 3:K:853:CYS:HB2   | 4:k:101:PHE:CD1   | 2.54                     | 0.42              |
| 3:K:1024:LEU:O    | 3:K:1027:GLY:N    | 2.45                     | 0.42              |
| 3:L:337:LEU:O     | 3:L:340:GLN:HB3   | 2.19                     | 0.42              |
| 3:L:411:PRO:O     | 3:L:415:ARG:NH1   | 2.52                     | 0.42              |
| 3:L:488:GLY:HA2   | 3:L:996:ALA:HB1   | 2.02                     | 0.42              |
| 3:L:892:LEU:HD21  | 4:l:68:HIS:CD2    | 2.54                     | 0.42              |
| 3:L:950:GLN:H     | 3:L:953:GLU:CD    | 2.27                     | 0.42              |
| 3:M:71:LEU:HD23   | 3:M:71:LEU:HA     | 1.85                     | 0.42              |
| 3:M:1072:ALA:HB3  | 3:M:1100:VAL:HB   | 2.01                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:M:1081:ALA:HB3  | 3:M:1092:THR:OG1  | 2.19                     | 0.42              |
| 3:A:532:MET:HE1   | 3:A:1194:THR:HG22 | 2.01                     | 0.42              |
| 3:H:86:GLU:OE1    | 3:H:86:GLU:N      | 2.52                     | 0.42              |
| 3:H:98:GLU:OE2    | 3:C:11:TYR:HE2    | 2.02                     | 0.42              |
| 3:H:252:THR:HB    | 3:H:373:ARG:HD2   | 2.02                     | 0.42              |
| 3:H:724:HIS:HD2   | 3:H:726:MET:HB2   | 1.84                     | 0.42              |
| 3:H:875:VAL:HG12  | 3:H:879:PHE:HE2   | 1.83                     | 0.42              |
| 4:j:4:PRO:HD3     | 4:j:16:ASN:HB3    | 2.01                     | 0.42              |
| 3:N:1340:PRO:O    | 3:N:1344:ARG:HG3  | 2.19                     | 0.42              |
| 3:O:128:ALA:HA    | 3:O:1095:GLN:O    | 2.20                     | 0.42              |
| 3:O:463:HIS:CG    | 3:O:464:PRO:HD2   | 2.55                     | 0.42              |
| 3:P:403:VAL:HG21  | 3:P:1205:PRO:HG3  | 2.00                     | 0.42              |
| 3:P:834:ARG:HD2   | 3:P:953:GLU:O     | 2.20                     | 0.42              |
| 3:P:1339:ASP:OD2  | 3:P:1360:GLN:HG3  | 2.20                     | 0.42              |
| 3:B:86:GLU:O      | 3:B:86:GLU:HG2    | 2.20                     | 0.42              |
| 3:B:266:HIS:HE1   | 3:B:302:VAL:HG13  | 1.81                     | 0.42              |
| 3:B:706:ASP:O     | 3:C:525:GLN:NE2   | 2.52                     | 0.42              |
| 3:B:1132:GLY:HA2  | 3:B:1266:ALA:HB3  | 2.01                     | 0.42              |
| 3:C:264:LEU:C     | 3:C:265:THR:HG1   | 2.21                     | 0.42              |
| 3:C:279:VAL:HG12  | 3:C:394:LEU:HD22  | 2.00                     | 0.42              |
| 3:C:910:CYS:SG    | 3:C:930:ASP:HB2   | 2.60                     | 0.42              |
| 3:C:1171:VAL:HG11 | 3:C:1309:VAL:HG21 | 2.01                     | 0.42              |
| 3:C:1259:GLY:HA3  | 3:C:1274:PHE:HE1  | 1.85                     | 0.42              |
| 3:D:600:GLY:C     | 3:D:602:GLY:N     | 2.77                     | 0.42              |
| 3:D:842:MET:CE    | 3:D:891:MET:HE3   | 2.49                     | 0.42              |
| 3:D:863:HIS:CG    | 3:D:864:PRO:HD2   | 2.55                     | 0.42              |
| 3:D:1024:LEU:HD23 | 3:D:1024:LEU:HA   | 1.83                     | 0.42              |
| 3:D:1248:GLN:O    | 3:D:1251:SER:OG   | 2.32                     | 0.42              |
| 3:E:408:LEU:HA    | 3:E:408:LEU:HD23  | 1.75                     | 0.42              |
| 3:E:864:PRO:HB2   | 3:E:876:ASN:CG    | 2.45                     | 0.42              |
| 3:E:879:PHE:CE2   | 3:E:891:MET:HE1   | 2.54                     | 0.42              |
| 3:E:1227:TYR:CD1  | 3:E:1249:ARG:HB2  | 2.54                     | 0.42              |
| 3:F:258:SER:HB3   | 3:F:1069:ALA:O    | 2.19                     | 0.42              |
| 3:F:336:LEU:HD23  | 3:F:336:LEU:HA    | 1.76                     | 0.42              |
| 3:F:754:CYS:O     | 3:F:755:ARG:C     | 2.63                     | 0.42              |
| 3:F:854:PRO:HG3   | 3:F:862:ALA:HB3   | 2.02                     | 0.42              |
| 3:F:1366:ALA:HA   | 3:F:1370:LYS:NZ   | 2.35                     | 0.42              |
| 3:G:548:ASP:C     | 3:G:549:PHE:HD2   | 2.28                     | 0.42              |
| 1:T:286:VAL:HB    | 1:T:452:LEU:HB2   | 2.02                     | 0.42              |
| 1:W:125:GLU:OE2   | 1:W:215:TYR:OH    | 2.31                     | 0.42              |
| 1:w:288:ILE:O     | 1:w:450:VAL:N     | 2.53                     | 0.42              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:I:189:LEU:HD23 | 3:I:1064:LEU:HD21 | 2.01                     | 0.42              |
| 3:I:491:VAL:HG11 | 3:I:929:PHE:HD2   | 1.83                     | 0.42              |
| 3:I:496:GLY:HA3  | 3:I:504:ARG:NH1   | 2.34                     | 0.42              |
| 3:J:195:LEU:O    | 3:J:197:LEU:N     | 2.53                     | 0.42              |
| 3:J:833:ASP:HA   | 4:j:54:LEU:HD11   | 2.00                     | 0.42              |
| 3:J:1215:ALA:C   | 3:J:1287:ARG:HH21 | 2.26                     | 0.42              |
| 3:K:887:ASP:O    | 3:K:891:MET:HG2   | 2.19                     | 0.42              |
| 3:L:219:LEU:O    | 3:L:223:LEU:N     | 2.49                     | 0.42              |
| 3:L:367:LEU:HD23 | 3:L:367:LEU:HA    | 1.73                     | 0.42              |
| 3:L:384:ILE:HG22 | 3:L:385:TYR:N     | 2.34                     | 0.42              |
| 3:M:485:ASN:ND2  | 3:M:512:ARG:O     | 2.52                     | 0.42              |
| 3:M:499:ALA:HA   | 3:M:956:TYR:CD1   | 2.54                     | 0.42              |
| 3:M:778:ARG:NH1  | 3:M:782:ARG:HD2   | 2.35                     | 0.42              |
| 3:A:329:LEU:CD1  | 3:G:61:TYR:CE2    | 2.84                     | 0.42              |
| 3:A:381:GLU:HB3  | 3:A:392:TYR:CD1   | 2.55                     | 0.42              |
| 3:A:1026:ALA:HA  | 3:A:1029:PHE:CE2  | 2.55                     | 0.42              |
| 3:A:1031:MET:HE2 | 3:A:1048:PHE:HZ   | 1.78                     | 0.42              |
| 3:H:108:GLY:HA2  | 3:H:110:HIS:N     | 2.33                     | 0.42              |
| 3:H:440:LEU:HD23 | 3:H:440:LEU:HA    | 1.87                     | 0.42              |
| 3:H:743:MET:HE2  | 3:H:797:ASP:O     | 2.20                     | 0.42              |
| 3:H:892:LEU:HD13 | 4:h:68:HIS:HB2    | 2.01                     | 0.42              |
| 3:N:133:PHE:O    | 3:N:133:PHE:CG    | 2.73                     | 0.42              |
| 3:N:771:VAL:CG2  | 3:N:898:ALA:HA    | 2.49                     | 0.42              |
| 3:N:1072:ALA:HB3 | 3:N:1100:VAL:HB   | 2.01                     | 0.42              |
| 3:O:417:ALA:HB2  | 3:O:1358:PHE:CE1  | 2.55                     | 0.42              |
| 3:P:129:LEU:O    | 3:P:1094:THR:HA   | 2.20                     | 0.42              |
| 3:P:293:LEU:HD23 | 3:P:293:LEU:HA    | 1.82                     | 0.42              |
| 3:P:392:TYR:CE2  | 3:P:394:LEU:HB3   | 2.55                     | 0.42              |
| 3:P:665:VAL:O    | 3:P:812:TYR:OH    | 2.29                     | 0.42              |
| 3:B:589:VAL:O    | 3:B:592:ARG:N     | 2.52                     | 0.42              |
| 3:B:1076:GLY:HA3 | 3:B:1096:PRO:HG2  | 2.01                     | 0.42              |
| 3:C:634:ILE:HG22 | 3:C:636:GLY:N     | 2.34                     | 0.42              |
| 3:C:1346:ALA:HA  | 3:C:1353:ALA:HB2  | 2.02                     | 0.42              |
| 3:D:54:PHE:HB2   | 3:E:90:MET:HG3    | 2.01                     | 0.42              |
| 3:D:57:LEU:O     | 3:D:58:LEU:HD23   | 2.19                     | 0.42              |
| 3:D:593:ASP:OD1  | 3:D:1009:HIS:HE1  | 2.02                     | 0.42              |
| 3:D:896:VAL:HA   | 3:D:899:HIS:CD2   | 2.53                     | 0.42              |
| 3:D:1339:ASP:HB2 | 3:D:1342:LEU:HB2  | 2.01                     | 0.42              |
| 3:E:199:LEU:HA   | 3:E:199:LEU:HD23  | 1.67                     | 0.42              |
| 3:E:231:SER:O    | 3:E:1112:THR:OG1  | 2.38                     | 0.42              |
| 3:E:1026:ALA:HA  | 3:E:1029:PHE:CE2  | 2.55                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:E:1256:LEU:HA   | 3:E:1256:LEU:HD23 | 1.82                     | 0.42              |
| 6:r:77:PRO:HA     | 7:u:3104:PHE:HD1  | 1.84                     | 0.42              |
| 3:F:107:ASP:O     | 3:F:110:HIS:CD2   | 2.70                     | 0.42              |
| 3:F:159:LEU:HD13  | 3:G:339:MET:O     | 2.18                     | 0.42              |
| 3:F:842:MET:HB3   | 3:F:842:MET:HE3   | 1.65                     | 0.42              |
| 3:F:1080:VAL:HG22 | 3:F:1093:LEU:HD22 | 2.02                     | 0.42              |
| 3:G:985:ARG:CZ    | 3:G:985:ARG:HB2   | 2.49                     | 0.42              |
| 2:S:158:ARG:HH21  | 2:S:193:GLN:HE21  | 1.68                     | 0.42              |
| 1:T:317:ARG:HB3   | 1:T:324:LEU:H     | 1.84                     | 0.42              |
| 2:U:223:LEU:HD12  | 2:U:271:LEU:HD21  | 2.02                     | 0.42              |
| 1:W:130:LEU:HB2   | 1:W:187:PHE:HB2   | 2.02                     | 0.42              |
| 3:I:599:LEU:HD23  | 3:I:599:LEU:HA    | 1.89                     | 0.42              |
| 3:I:1013:SER:OG   | 3:I:1020:LEU:HD21 | 2.19                     | 0.42              |
| 3:I:1372:LEU:HD23 | 3:I:1372:LEU:HA   | 1.82                     | 0.42              |
| 3:J:397:ALA:HA    | 3:J:1058:PHE:O    | 2.20                     | 0.42              |
| 3:J:411:PRO:O     | 3:J:415:ARG:NH1   | 2.52                     | 0.42              |
| 3:J:866:HIS:CG    | 3:J:867:PRO:HD2   | 2.55                     | 0.42              |
| 3:J:1204:ASN:ND2  | 3:J:1209:ALA:HA   | 2.32                     | 0.42              |
| 3:K:469:ILE:HD13  | 3:K:469:ILE:HG21  | 1.83                     | 0.42              |
| 3:K:743:MET:HE2   | 3:K:797:ASP:O     | 2.20                     | 0.42              |
| 3:K:842:MET:O     | 4:k:22:MET:HG3    | 2.20                     | 0.42              |
| 3:K:1292:LEU:HB3  | 3:K:1327:LEU:CD2  | 2.50                     | 0.42              |
| 3:M:61:TYR:CD1    | 3:C:21:GLY:C      | 2.91                     | 0.42              |
| 3:M:133:PHE:CG    | 3:M:133:PHE:O     | 2.73                     | 0.42              |
| 3:A:492:ALA:HA    | 3:A:561:GLY:O     | 2.20                     | 0.42              |
| 3:A:854:PRO:HG3   | 3:A:862:ALA:C     | 2.45                     | 0.42              |
| 3:H:198:LEU:O     | 3:H:199:LEU:C     | 2.62                     | 0.42              |
| 3:N:27:ILE:HG22   | 3:N:28:GLU:N      | 2.35                     | 0.42              |
| 3:N:218:THR:O     | 3:N:222:GLU:HG2   | 2.20                     | 0.42              |
| 3:N:258:SER:OG    | 3:N:259:VAL:N     | 2.44                     | 0.42              |
| 3:N:857:PRO:HA    | 3:N:863:HIS:HD2   | 1.85                     | 0.42              |
| 3:O:632:ALA:HB3   | 3:O:835:VAL:HG11  | 2.01                     | 0.42              |
| 3:O:1080:VAL:HG22 | 3:O:1093:LEU:HD22 | 2.02                     | 0.42              |
| 3:O:1257:TYR:HB2  | 3:O:1277:PHE:CD2  | 2.42                     | 0.42              |
| 3:B:764:VAL:O     | 3:B:783:LEU:N     | 2.50                     | 0.42              |
| 3:B:784:LEU:CD2   | 3:B:903:GLU:H     | 2.32                     | 0.42              |
| 3:B:945:LEU:HD23  | 3:B:945:LEU:HA    | 1.74                     | 0.42              |
| 3:C:163:GLN:O     | 3:C:166:ALA:N     | 2.52                     | 0.42              |
| 3:C:1174:ARG:NH1  | 3:D:1232:SER:OG   | 2.30                     | 0.42              |
| 3:C:1191:PRO:HG2  | 3:C:1194:THR:CG2  | 2.49                     | 0.42              |
| 3:D:194:PRO:HA    | 3:D:1110:ALA:O    | 2.20                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:578:VAL:HB    | 3:D:1027:GLY:O    | 2.18                     | 0.42              |
| 3:D:682:LEU:HB2   | 3:D:687:MET:HG2   | 2.01                     | 0.42              |
| 3:D:746:ALA:O     | 3:D:748:LEU:O     | 2.37                     | 0.42              |
| 3:D:836:TYR:O     | 3:D:840:GLN:N     | 2.52                     | 0.42              |
| 3:D:959:PRO:HG2   | 3:D:991:PRO:HD3   | 2.01                     | 0.42              |
| 5:q:61:GLN:HE22   | 5:q:690:ARG:HA    | 1.84                     | 0.42              |
| 3:E:201:MET:HE1   | 3:E:1290:GLU:OE2  | 2.20                     | 0.42              |
| 3:E:533:GLN:O     | 3:E:535:ASP:N     | 2.51                     | 0.42              |
| 3:E:1342:LEU:CD2  | 3:E:1362:LEU:HB2  | 2.50                     | 0.42              |
| 3:F:390:VAL:HG21  | 3:G:104:ILE:HG13  | 1.86                     | 0.42              |
| 3:F:467:MET:O     | 3:F:922:SER:OG    | 2.37                     | 0.42              |
| 3:F:752:ARG:NH2   | 3:F:915:ASP:OD1   | 2.52                     | 0.42              |
| 3:F:830:VAL:HG13  | 3:F:955:PHE:HE1   | 1.85                     | 0.42              |
| 3:G:77:VAL:HG22   | 3:G:266:HIS:CD2   | 2.55                     | 0.42              |
| 3:G:958:LEU:HD23  | 3:G:958:LEU:HA    | 1.83                     | 0.42              |
| 4:b:21:GLY:O      | 4:b:25:LEU:N      | 2.49                     | 0.42              |
| 1:T:166:GLU:CD    | 3:I:1262:HIS:NE2  | 2.77                     | 0.42              |
| 1:W:221:GLY:HA2   | 1:W:224:LEU:HD12  | 2.01                     | 0.42              |
| 1:I:273:ALA:HB2   | 3:N:137:THR:HB    | 2.02                     | 0.42              |
| 3:I:497:PRO:HD2   | 3:I:504:ARG:NH2   | 2.35                     | 0.42              |
| 3:I:631:GLN:HE22  | 3:I:666:ASN:CG    | 2.26                     | 0.42              |
| 3:I:745:HIS:NE2   | 3:I:910:CYS:HB2   | 2.35                     | 0.42              |
| 3:I:873:ASN:CB    | 4:h:89:ARG:HH12   | 2.23                     | 0.42              |
| 3:I:1064:LEU:HA   | 3:I:1064:LEU:HD23 | 1.87                     | 0.42              |
| 3:I:1116:ARG:HB3  | 3:I:1117:ASN:H    | 1.70                     | 0.42              |
| 3:J:491:VAL:HG22  | 3:J:996:ALA:H     | 1.84                     | 0.42              |
| 3:J:591:PHE:CZ    | 3:J:1045:HIS:CD2  | 3.08                     | 0.42              |
| 3:J:1248:GLN:N    | 3:J:1251:SER:HG   | 2.18                     | 0.42              |
| 3:K:512:ARG:NH1   | 3:K:564:PRO:HG2   | 2.35                     | 0.42              |
| 3:K:809:HIS:O     | 3:K:813:TYR:N     | 2.42                     | 0.42              |
| 3:K:1256:LEU:HD23 | 3:K:1256:LEU:HA   | 1.77                     | 0.42              |
| 3:L:440:LEU:HD22  | 3:L:1336:CYS:SG   | 2.59                     | 0.42              |
| 3:L:490:TYR:OH    | 3:L:561:GLY:N     | 2.53                     | 0.42              |
| 3:L:550:PHE:O     | 3:L:571:ILE:HA    | 2.20                     | 0.42              |
| 3:L:749:ASP:OD2   | 3:L:751:HIS:HB2   | 2.20                     | 0.42              |
| 3:M:895:GLN:HE22  | 4:m:65:GLY:HA3    | 1.84                     | 0.42              |
| 3:A:505:PHE:CG    | 3:A:991:PRO:HB3   | 2.54                     | 0.42              |
| 3:H:380:LEU:HD23  | 3:H:380:LEU:HA    | 1.85                     | 0.42              |
| 3:H:635:HIS:CE1   | 3:H:640:VAL:HG21  | 2.55                     | 0.42              |
| 3:H:1054:ARG:NH2  | 3:H:1122:MET:HB3  | 2.35                     | 0.42              |
| 4:n:78:MET:HG2    | 4:n:94:LEU:O      | 2.20                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:o:61:LEU:C      | 3:O:895:GLN:HE21  | 2.23                     | 0.42              |
| 3:N:863:HIS:CG    | 3:N:864:PRO:HD2   | 2.55                     | 0.42              |
| 3:O:646:ARG:NH2   | 3:O:889:PRO:HG2   | 2.35                     | 0.42              |
| 3:O:906:THR:OG1   | 3:O:934:HIS:HB3   | 2.20                     | 0.42              |
| 3:O:1357:HIS:O    | 3:O:1358:PHE:C    | 2.63                     | 0.42              |
| 3:P:727:ARG:O     | 3:P:729:PRO:HD3   | 2.19                     | 0.42              |
| 3:P:1115:VAL:HG12 | 3:P:1116:ARG:O    | 2.20                     | 0.42              |
| 3:B:137:THR:HA    | 3:B:140:ILE:HD12  | 2.02                     | 0.42              |
| 3:B:475:GLY:HA2   | 3:B:478:HIS:CD2   | 2.54                     | 0.42              |
| 3:B:707:PHE:N     | 3:B:707:PHE:CD1   | 2.87                     | 0.42              |
| 3:B:778:ARG:O     | 3:B:904:ARG:NE    | 2.53                     | 0.42              |
| 3:C:801:ARG:HB3   | 3:C:802:PRO:HD2   | 2.02                     | 0.42              |
| 3:C:1004:GLN:O    | 3:C:1007:VAL:N    | 2.47                     | 0.42              |
| 3:D:33:ARG:HD3    | 3:D:39:PHE:HD2    | 1.83                     | 0.42              |
| 3:D:159:LEU:HA    | 3:D:159:LEU:HD23  | 1.74                     | 0.42              |
| 3:D:275:ASP:HB2   | 3:D:373:ARG:HB2   | 2.01                     | 0.42              |
| 3:D:293:LEU:HA    | 3:D:293:LEU:HD23  | 1.85                     | 0.42              |
| 3:D:1128:ASN:ND2  | 3:D:1155:ASN:ND2  | 2.66                     | 0.42              |
| 5:q:23:LEU:HD12   | 5:q:114:LEU:O     | 2.20                     | 0.42              |
| 3:E:715:GLY:HA3   | 3:E:916:ALA:HB2   | 2.02                     | 0.42              |
| 3:E:1271:SER:OG   | 3:E:1274:PHE:HB2  | 2.20                     | 0.42              |
| 3:F:634:ILE:O     | 3:F:635:HIS:ND1   | 2.52                     | 0.42              |
| 3:F:786:ASN:HD21  | 3:F:902:ALA:HA    | 1.85                     | 0.42              |
| 3:F:802:PRO:HG3   | 3:G:945:LEU:CD2   | 2.48                     | 0.42              |
| 6:s:79:ASP:HA     | 6:s:82:ARG:CZ     | 2.50                     | 0.42              |
| 3:G:709:LEU:HD12  | 3:G:1037:TYR:CE1  | 2.55                     | 0.42              |
| 4:c:21:GLY:O      | 4:c:25:LEU:N      | 2.49                     | 0.42              |
| 4:g:21:GLY:O      | 4:g:25:LEU:N      | 2.49                     | 0.42              |
| 1:T:318:GLN:N     | 1:T:354:ASN:OD1   | 2.41                     | 0.42              |
| 2:3:80:PRO:CD     | 3:C:53:GLU:OE2    | 2.68                     | 0.42              |
| 2:3:300:PHE:CG    | 3:M:1083:HIS:NE2  | 2.87                     | 0.42              |
| 2:2:39:ARG:HH22   | 3:N:1085:THR:HG21 | 0.60                     | 0.42              |
| 3:I:197:LEU:O     | 3:I:201:MET:HG2   | 2.20                     | 0.42              |
| 3:I:198:LEU:O     | 3:I:199:LEU:C     | 2.63                     | 0.42              |
| 3:I:738:ASP:HB3   | 3:I:740:ASP:H     | 1.85                     | 0.42              |
| 3:I:959:PRO:HB2   | 3:I:990:VAL:HG22  | 2.01                     | 0.42              |
| 3:I:1208:ARG:HD3  | 3:I:1226:MET:O    | 2.20                     | 0.42              |
| 3:I:1234:PRO:HA   | 3:H:1174:ARG:NH2  | 2.34                     | 0.42              |
| 3:K:837:ALA:HA    | 4:k:57:GLN:NE2    | 2.34                     | 0.42              |
| 3:K:1081:ALA:O    | 3:K:1091:PHE:HA   | 2.20                     | 0.42              |
| 3:L:293:LEU:HD23  | 3:L:293:LEU:HA    | 1.90                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:L:350:THR:HG22  | 3:L:352:ASP:H     | 1.83                     | 0.42              |
| 3:L:397:ALA:HB3   | 3:L:1321:VAL:HG22 | 2.01                     | 0.42              |
| 3:L:778:ARG:HD2   | 3:L:782:ARG:HB2   | 2.02                     | 0.42              |
| 3:L:828:ALA:HA    | 3:L:958:LEU:H     | 1.85                     | 0.42              |
| 3:L:873:ASN:O     | 4:k:89:ARG:NH1    | 2.51                     | 0.42              |
| 3:L:881:ASN:HD21  | 3:L:948:THR:CG2   | 2.33                     | 0.42              |
| 3:L:1208:ARG:NE   | 3:L:1225:LEU:O    | 2.40                     | 0.42              |
| 3:M:11:TYR:HB3    | 3:D:121:THR:HG21  | 1.99                     | 0.42              |
| 3:M:390:VAL:HG11  | 3:H:104:ILE:HD11  | 2.02                     | 0.42              |
| 3:M:740:ASP:HB3   | 3:M:799:PRO:HB3   | 2.01                     | 0.42              |
| 3:M:765:TYR:HE1   | 3:M:783:LEU:HD12  | 1.84                     | 0.42              |
| 3:M:1339:ASP:HB2  | 3:M:1342:LEU:CB   | 2.50                     | 0.42              |
| 3:A:511:GLN:HA    | 3:A:514:ALA:HB3   | 2.02                     | 0.42              |
| 3:A:577:VAL:H     | 3:A:581:ASN:HD22  | 1.67                     | 0.42              |
| 3:A:721:GLU:O     | 3:A:1030:LYS:NZ   | 2.45                     | 0.42              |
| 3:A:944:HIS:CD2   | 3:A:972:ASN:ND2   | 2.88                     | 0.42              |
| 3:H:487:TYR:HD2   | 3:H:520:TRP:HH2   | 1.68                     | 0.42              |
| 3:H:714:LEU:HD12  | 3:H:722:LEU:HD22  | 2.00                     | 0.42              |
| 3:H:742:LEU:HB3   | 3:H:765:TYR:OH    | 2.20                     | 0.42              |
| 4:n:5:GLN:HB3     | 4:n:7:HIS:CE1     | 2.55                     | 0.42              |
| 4:n:80:ALA:N      | 3:O:948:THR:HA    | 2.33                     | 0.42              |
| 3:N:229:ASP:O     | 3:N:236:LYS:NZ    | 2.33                     | 0.42              |
| 3:N:445:LYS:NZ    | 3:N:1179:HIS:O    | 2.44                     | 0.42              |
| 3:N:578:VAL:O     | 3:N:1031:MET:HE2  | 2.20                     | 0.42              |
| 3:N:706:ASP:O     | 3:O:525:GLN:NE2   | 2.53                     | 0.42              |
| 3:N:724:HIS:CE1   | 3:N:1028:TYR:HB2  | 2.54                     | 0.42              |
| 3:N:1003:ARG:HB2  | 3:N:1005:PRO:HD2  | 2.02                     | 0.42              |
| 3:N:1054:ARG:NH2  | 3:N:1122:MET:HB3  | 2.34                     | 0.42              |
| 3:O:406:LEU:HD12  | 3:O:1050:PHE:HB2  | 2.02                     | 0.42              |
| 3:O:755:ARG:NH1   | 3:O:911:SER:OG    | 2.53                     | 0.42              |
| 3:O:1334:ILE:HG22 | 3:O:1335:THR:H    | 1.84                     | 0.42              |
| 3:P:128:ALA:HA    | 3:P:1095:GLN:O    | 2.20                     | 0.42              |
| 3:P:744:ARG:HA    | 3:P:747:ALA:HB3   | 2.01                     | 0.42              |
| 3:P:749:ASP:N     | 3:P:749:ASP:OD1   | 2.52                     | 0.42              |
| 3:P:1177:MET:HE2  | 3:P:1177:MET:HB3  | 1.77                     | 0.42              |
| 3:P:1262:HIS:O    | 3:P:1262:HIS:CG   | 2.72                     | 0.42              |
| 3:B:87:LEU:HD22   | 3:B:1096:PRO:HB2  | 2.01                     | 0.42              |
| 3:B:399:ASP:CG    | 3:B:1321:VAL:HG11 | 2.45                     | 0.42              |
| 3:B:454:MET:O     | 3:B:456:ASN:N     | 2.53                     | 0.42              |
| 3:B:836:TYR:CD1   | 3:B:897:LEU:HD22  | 2.55                     | 0.42              |
| 3:B:845:PRO:HG3   | 3:B:869:ASN:HD21  | 1.85                     | 0.42              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:B:1181:GLN:HB2 | 3:B:1309:VAL:O    | 2.20                     | 0.42              |
| 3:C:302:VAL:HG12 | 3:C:303:PRO:O     | 2.20                     | 0.42              |
| 3:C:783:LEU:HA   | 3:C:783:LEU:HD23  | 1.87                     | 0.42              |
| 3:C:915:ASP:O    | 3:C:919:ASN:N     | 2.53                     | 0.42              |
| 3:C:1054:ARG:NH1 | 3:C:1123:GLY:O    | 2.53                     | 0.42              |
| 3:D:180:THR:HG22 | 3:D:1097:ARG:HH22 | 1.85                     | 0.42              |
| 3:D:398:MET:O    | 3:D:1057:ARG:HA   | 2.19                     | 0.42              |
| 3:D:481:VAL:HG12 | 3:D:570:ALA:HA    | 2.02                     | 0.42              |
| 3:D:873:ASN:CA   | 4:c:92:PHE:HD2    | 2.24                     | 0.42              |
| 3:D:989:LEU:O    | 3:D:990:VAL:C     | 2.62                     | 0.42              |
| 5:q:475:GLU:O    | 5:q:478:PHE:HB3   | 2.20                     | 0.42              |
| 3:E:255:THR:OG1  | 3:E:1067:GLU:OE2  | 2.24                     | 0.42              |
| 3:E:610:THR:HA   | 3:E:689:VAL:HG22  | 2.01                     | 0.42              |
| 3:F:85:PRO:HG2   | 3:F:86:GLU:OE1    | 2.20                     | 0.42              |
| 3:F:493:ALA:N    | 3:F:559:PRO:HB2   | 2.35                     | 0.42              |
| 3:F:1289:LEU:HA  | 3:F:1289:LEU:HD23 | 1.79                     | 0.42              |
| 1:W:85:GLN:HA    | 1:W:88:ASP:HB2    | 2.01                     | 0.41              |
| 1:1:125:GLU:OE1  | 1:1:186:SER:OG    | 2.32                     | 0.41              |
| 2:3:38:ARG:HH22  | 3:E:110:HIS:C     | 2.27                     | 0.41              |
| 3:I:382:LYS:HD2  | 3:I:382:LYS:HA    | 1.81                     | 0.41              |
| 3:I:728:ASP:HB3  | 3:I:730:ALA:N     | 2.34                     | 0.41              |
| 3:I:884:VAL:HG12 | 3:I:886:VAL:HG23  | 2.01                     | 0.41              |
| 3:J:167:ARG:HE   | 3:K:346:ALA:HB1   | 1.85                     | 0.41              |
| 3:J:581:ASN:O    | 3:J:1005:PRO:HG2  | 2.20                     | 0.41              |
| 3:J:724:HIS:CD2  | 3:J:726:MET:HB2   | 2.55                     | 0.41              |
| 3:J:801:ARG:HB3  | 3:J:802:PRO:CD    | 2.46                     | 0.41              |
| 3:J:857:PRO:HA   | 3:J:863:HIS:CD2   | 2.54                     | 0.41              |
| 3:J:1185:CYS:O   | 3:J:1186:GLU:HG3  | 2.20                     | 0.41              |
| 3:K:845:PRO:HG3  | 3:K:869:ASN:ND2   | 2.35                     | 0.41              |
| 3:K:1296:THR:O   | 3:K:1322:GLU:HB2  | 2.20                     | 0.41              |
| 3:L:469:ILE:HD11 | 3:L:547:PHE:CZ    | 2.55                     | 0.41              |
| 3:M:56:ALA:HA    | 3:H:325:ALA:O     | 2.20                     | 0.41              |
| 3:M:81:CYS:HB2   | 3:M:306:TYR:HD1   | 1.85                     | 0.41              |
| 3:M:124:ILE:HA   | 3:M:1100:VAL:HG22 | 2.01                     | 0.41              |
| 3:M:463:HIS:CD2  | 3:M:465:SER:HB3   | 2.54                     | 0.41              |
| 3:M:623:TYR:HA   | 3:M:624:PRO:HD3   | 1.86                     | 0.41              |
| 3:A:293:LEU:O    | 3:A:294:LYS:HD2   | 2.20                     | 0.41              |
| 3:A:518:VAL:HG21 | 3:A:987:VAL:HG11  | 2.02                     | 0.41              |
| 3:H:128:ALA:HA   | 3:H:1095:GLN:O    | 2.19                     | 0.41              |
| 3:N:162:ILE:O    | 3:N:165:LEU:HB2   | 2.20                     | 0.41              |
| 3:O:56:ALA:HA    | 3:P:325:ALA:O     | 2.20                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:O:83:LYS:HE3    | 3:O:306:TYR:HB2   | 2.01                     | 0.41              |
| 3:O:469:ILE:O     | 3:O:472:ALA:N     | 2.53                     | 0.41              |
| 3:O:718:ALA:HB1   | 3:P:982:ASP:OD2   | 2.19                     | 0.41              |
| 3:O:1226:MET:HE3  | 3:O:1226:MET:HB3  | 1.98                     | 0.41              |
| 3:P:826:CYS:HB3   | 3:P:966:GLY:N     | 2.35                     | 0.41              |
| 3:P:918:ALA:HB2   | 3:P:1032:SER:OG   | 2.20                     | 0.41              |
| 3:P:1149:ASN:O    | 3:P:1153:ALA:HB2  | 2.20                     | 0.41              |
| 3:B:133:PHE:O     | 3:B:133:PHE:CG    | 2.73                     | 0.41              |
| 3:B:223:LEU:HA    | 3:B:223:LEU:HD23  | 1.76                     | 0.41              |
| 3:B:725:LEU:HA    | 3:B:725:LEU:HD12  | 1.85                     | 0.41              |
| 3:B:790:ARG:HG3   | 3:B:792:ALA:H     | 1.84                     | 0.41              |
| 3:B:1035:ALA:O    | 3:B:1039:GLN:HG3  | 2.19                     | 0.41              |
| 3:C:124:ILE:HG12  | 3:C:1100:VAL:CG2  | 2.50                     | 0.41              |
| 3:C:248:LEU:HD23  | 3:C:248:LEU:HA    | 1.83                     | 0.41              |
| 3:C:789:ALA:O     | 4:c:79:PHE:CE2    | 2.73                     | 0.41              |
| 3:C:866:HIS:O     | 3:C:870:LEU:HG    | 2.20                     | 0.41              |
| 3:D:866:HIS:O     | 3:D:870:LEU:HG    | 2.20                     | 0.41              |
| 3:D:917:GLY:O     | 3:D:1138:LEU:HD22 | 2.19                     | 0.41              |
| 5:q:510:TYR:CE1   | 5:q:644:GLU:HG2   | 2.55                     | 0.41              |
| 3:E:63:ASN:HD21   | 3:F:99:VAL:HG22   | 1.84                     | 0.41              |
| 3:E:493:ALA:N     | 3:E:559:PRO:HB2   | 2.35                     | 0.41              |
| 3:E:838:THR:HA    | 3:E:841:ASN:ND2   | 2.34                     | 0.41              |
| 3:E:1334:ILE:HG22 | 3:E:1335:THR:O    | 2.19                     | 0.41              |
| 3:F:338:GLU:C     | 3:F:340:GLN:N     | 2.77                     | 0.41              |
| 3:F:423:LEU:HD23  | 3:F:423:LEU:HA    | 1.85                     | 0.41              |
| 3:F:1208:ARG:NH1  | 3:F:1240:ALA:O    | 2.52                     | 0.41              |
| 3:G:435:PHE:CE1   | 3:G:598:GLU:HA    | 2.55                     | 0.41              |
| 3:G:469:ILE:HD12  | 3:G:547:PHE:CZ    | 2.55                     | 0.41              |
| 3:G:625:ALA:HA    | 3:G:628:TYR:HD2   | 1.85                     | 0.41              |
| 1:T:428:MET:HE1   | 1:T:452:LEU:HD22  | 2.01                     | 0.41              |
| 2:U:63:LEU:HD11   | 2:U:138:ARG:HH21  | 1.85                     | 0.41              |
| 1:W:259:GLU:OE2   | 3:C:1313:ARG:NH1  | 2.54                     | 0.41              |
| 2:3:47:ALA:HA     | 2:3:137:LEU:HD23  | 2.02                     | 0.41              |
| 2:x:25:GLN:NE2    | 2:x:28:GLU:OE2    | 2.52                     | 0.41              |
| 2:y:219:LEU:O     | 2:y:222:THR:OG1   | 2.37                     | 0.41              |
| 2:y:254:ILE:HG22  | 2:y:256:PRO:HD3   | 2.02                     | 0.41              |
| 3:I:668:TYR:HD2   | 3:I:809:HIS:CE1   | 2.38                     | 0.41              |
| 3:I:1269:VAL:HG12 | 3:I:1270:LEU:O    | 2.20                     | 0.41              |
| 3:J:405:PRO:HB3   | 3:J:1199:PHE:CE2  | 2.55                     | 0.41              |
| 3:K:266:HIS:CE1   | 3:K:303:PRO:HD2   | 2.55                     | 0.41              |
| 3:K:508:ALA:HB1   | 3:K:563:VAL:CG2   | 2.50                     | 0.41              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:K:599:LEU:HA   | 3:K:599:LEU:HD23  | 1.81                     | 0.41              |
| 3:K:653:THR:HG22 | 3:K:683:PRO:HD3   | 2.02                     | 0.41              |
| 3:K:1227:TYR:CG  | 3:K:1249:ARG:HB2  | 2.54                     | 0.41              |
| 3:L:1332:TYR:HB3 | 3:L:1367:SER:HG   | 1.85                     | 0.41              |
| 3:M:417:ALA:HB2  | 3:M:1358:PHE:CE1  | 2.55                     | 0.41              |
| 3:M:769:CYS:N    | 3:M:786:ASN:OD1   | 2.53                     | 0.41              |
| 3:A:463:HIS:NE2  | 3:A:1135:ALA:HB2  | 2.33                     | 0.41              |
| 3:A:630:LEU:O    | 3:A:634:ILE:HD12  | 2.19                     | 0.41              |
| 3:H:873:ASN:HD22 | 4:m:89:ARG:NH1    | 2.18                     | 0.41              |
| 3:H:1185:CYS:O   | 3:H:1186:GLU:HG3  | 2.20                     | 0.41              |
| 3:N:43:ARG:O     | 3:N:44:SER:C      | 2.64                     | 0.41              |
| 3:N:543:LEU:HB2  | 3:N:549:PHE:HE2   | 1.84                     | 0.41              |
| 3:N:697:VAL:O    | 3:N:700:LEU:N     | 2.53                     | 0.41              |
| 3:N:1257:TYR:HB2 | 3:N:1277:PHE:CD2  | 2.42                     | 0.41              |
| 3:N:1342:LEU:CD2 | 3:N:1362:LEU:HB2  | 2.50                     | 0.41              |
| 3:O:827:THR:HA   | 3:O:938:LEU:HA    | 2.02                     | 0.41              |
| 3:O:863:HIS:CD2  | 3:O:865:LEU:HB2   | 2.55                     | 0.41              |
| 3:O:1124:ASN:OD1 | 3:O:1124:ASN:N    | 2.52                     | 0.41              |
| 3:O:1301:SER:HB3 | 3:O:1321:VAL:HG21 | 2.01                     | 0.41              |
| 3:P:334:ARG:O    | 3:P:337:LEU:N     | 2.40                     | 0.41              |
| 3:P:767:ALA:O    | 3:P:786:ASN:HA    | 2.21                     | 0.41              |
| 3:B:158:GLN:O    | 3:B:162:ILE:N     | 2.53                     | 0.41              |
| 3:B:182:ASP:OD1  | 3:B:385:TYR:OH    | 2.36                     | 0.41              |
| 3:B:608:PRO:O    | 3:B:611:ILE:N     | 2.53                     | 0.41              |
| 3:C:58:LEU:HD12  | 3:D:124:ILE:HD11  | 2.01                     | 0.41              |
| 3:D:194:PRO:HG2  | 3:D:197:LEU:HB2   | 2.01                     | 0.41              |
| 3:D:724:HIS:HE1  | 3:D:1028:TYR:HB2  | 1.84                     | 0.41              |
| 3:D:1205:PRO:HG2 | 3:D:1276:PHE:CE2  | 2.55                     | 0.41              |
| 3:E:73:LEU:HA    | 3:E:73:LEU:HD23   | 1.87                     | 0.41              |
| 3:E:687:MET:HE3  | 3:E:687:MET:HB3   | 1.90                     | 0.41              |
| 3:E:1166:PHE:CG  | 3:E:1167:GLY:N    | 2.89                     | 0.41              |
| 3:F:108:GLY:HA2  | 3:F:110:HIS:N     | 2.32                     | 0.41              |
| 3:F:302:VAL:HG13 | 3:F:303:PRO:HD2   | 2.02                     | 0.41              |
| 3:F:843:VAL:HB   | 3:F:876:ASN:HD22  | 1.84                     | 0.41              |
| 3:F:1155:ASN:OD1 | 3:F:1156:ARG:N    | 2.52                     | 0.41              |
| 6:s:83:ARG:HD2   | 7:u:3099:THR:HG22 | 2.02                     | 0.41              |
| 3:G:502:GLN:HE22 | 3:G:970:VAL:HG13  | 1.85                     | 0.41              |
| 3:G:1229:HIS:CE1 | 3:G:1248:GLN:HG2  | 2.55                     | 0.41              |
| 1:1:466:ALA:HB3  | 2:2:281:HIS:NE2   | 2.36                     | 0.41              |
| 2:2:65:LEU:HD23  | 2:2:65:LEU:HA     | 1.91                     | 0.41              |
| 2:x:110:ASN:N    | 2:x:304:ALA:O     | 2.54                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:I:114:GLN:NE2   | 3:H:134:SER:OG    | 2.53                     | 0.41              |
| 3:I:234:LEU:HA    | 3:I:234:LEU:HD23  | 1.88                     | 0.41              |
| 3:I:426:ALA:HA    | 3:J:1358:PHE:CE1  | 2.55                     | 0.41              |
| 3:J:63:ASN:ND2    | 3:K:99:VAL:HA     | 2.35                     | 0.41              |
| 3:J:390:VAL:HG21  | 3:K:104:ILE:CG1   | 2.50                     | 0.41              |
| 3:J:473:VAL:HG21  | 3:J:573:ALA:HB2   | 2.02                     | 0.41              |
| 3:J:606:MET:HE3   | 3:J:611:ILE:HG12  | 2.03                     | 0.41              |
| 3:J:829:GLY:HA2   | 3:J:905:THR:HG21  | 2.03                     | 0.41              |
| 3:J:954:TYR:OH    | 4:i:92:PHE:HE1    | 2.04                     | 0.41              |
| 3:K:279:VAL:HA    | 3:K:378:GLU:O     | 2.20                     | 0.41              |
| 3:K:512:ARG:HD3   | 3:K:515:HIS:HD2   | 1.84                     | 0.41              |
| 3:K:1073:TYR:OH   | 3:K:1097:ARG:NH1  | 2.54                     | 0.41              |
| 3:L:424:VAL:HG12  | 3:L:425:PRO:O     | 2.20                     | 0.41              |
| 3:L:450:LEU:HD13  | 3:L:1123:GLY:HA2  | 2.01                     | 0.41              |
| 3:L:1007:VAL:O    | 3:L:1010:ALA:HB3  | 2.20                     | 0.41              |
| 3:L:1051:THR:HG23 | 3:L:1190:THR:HG21 | 2.02                     | 0.41              |
| 3:M:43:ARG:O      | 3:M:45:ASP:N      | 2.50                     | 0.41              |
| 3:A:517:ARG:HD2   | 3:A:522:ALA:HB2   | 2.03                     | 0.41              |
| 3:H:496:GLY:HA3   | 3:H:504:ARG:HH12  | 1.84                     | 0.41              |
| 3:H:827:THR:OG1   | 3:H:960:VAL:HG23  | 2.20                     | 0.41              |
| 4:o:101:PHE:CE1   | 3:O:847:ILE:HG21  | 2.55                     | 0.41              |
| 3:N:505:PHE:CD1   | 3:N:509:TRP:CD1   | 3.08                     | 0.41              |
| 3:N:1081:ALA:HB3  | 3:N:1092:THR:OG1  | 2.20                     | 0.41              |
| 3:N:1292:LEU:HB3  | 3:N:1327:LEU:HD21 | 2.02                     | 0.41              |
| 3:O:511:GLN:HB3   | 3:O:515:HIS:CE1   | 2.56                     | 0.41              |
| 3:O:541:LEU:HA    | 3:O:541:LEU:HD23  | 1.86                     | 0.41              |
| 3:O:708:THR:HG21  | 3:O:720:ALA:HA    | 2.02                     | 0.41              |
| 3:O:767:ALA:HA    | 3:O:785:HIS:HB3   | 2.01                     | 0.41              |
| 3:P:148:LEU:HD21  | 3:P:158:GLN:CD    | 2.45                     | 0.41              |
| 3:P:195:LEU:HD23  | 3:P:1109:VAL:HG11 | 2.02                     | 0.41              |
| 3:P:201:MET:HE3   | 3:P:201:MET:HB3   | 1.86                     | 0.41              |
| 3:P:205:LEU:HD23  | 3:P:205:LEU:HA    | 1.88                     | 0.41              |
| 3:P:485:ASN:O     | 3:P:487:TYR:N     | 2.52                     | 0.41              |
| 3:P:614:VAL:O     | 3:P:617:ALA:N     | 2.49                     | 0.41              |
| 3:P:785:HIS:NE2   | 3:P:798:ARG:O     | 2.49                     | 0.41              |
| 3:P:863:HIS:ND1   | 3:P:864:PRO:HD2   | 2.35                     | 0.41              |
| 3:P:923:THR:HA    | 3:P:926:MET:HE3   | 2.01                     | 0.41              |
| 3:P:1165:VAL:HG13 | 3:P:1166:PHE:CD2  | 2.55                     | 0.41              |
| 3:P:1359:THR:OG1  | 3:P:1360:GLN:NE2  | 2.53                     | 0.41              |
| 3:B:260:ALA:HB1   | 3:G:60:SER:HB3    | 2.01                     | 0.41              |
| 3:B:600:GLY:C     | 3:B:602:GLY:H     | 2.28                     | 0.41              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:B:835:VAL:O    | 3:B:839:LEU:N     | 2.48                     | 0.41              |
| 3:B:1229:HIS:CE1 | 3:B:1248:GLN:HG2  | 2.55                     | 0.41              |
| 3:C:451:ARG:O    | 3:C:1124:ASN:ND2  | 2.52                     | 0.41              |
| 3:C:485:ASN:ND2  | 3:C:516:GLY:O     | 2.53                     | 0.41              |
| 3:C:784:LEU:HD13 | 3:C:786:ASN:ND2   | 2.36                     | 0.41              |
| 3:C:1176:GLY:N   | 3:D:1225:LEU:HD21 | 2.35                     | 0.41              |
| 3:D:24:LEU:HD23  | 3:D:24:LEU:HA     | 1.84                     | 0.41              |
| 3:D:67:LEU:HD23  | 3:D:67:LEU:HA     | 1.81                     | 0.41              |
| 3:D:93:GLY:HA3   | 3:D:124:ILE:HD12  | 2.03                     | 0.41              |
| 3:D:448:GLN:HG2  | 3:E:1201:ARG:HD3  | 2.02                     | 0.41              |
| 3:D:766:ALA:O    | 3:D:785:HIS:HB2   | 2.20                     | 0.41              |
| 3:D:1081:ALA:HB3 | 3:D:1092:THR:OG1  | 2.20                     | 0.41              |
| 3:E:289:LEU:HD23 | 3:E:289:LEU:HA    | 1.83                     | 0.41              |
| 3:E:384:ILE:HG22 | 3:E:385:TYR:N     | 2.35                     | 0.41              |
| 3:E:463:HIS:C    | 3:E:465:SER:H     | 2.28                     | 0.41              |
| 3:E:829:GLY:HA3  | 3:E:956:TYR:CE1   | 2.55                     | 0.41              |
| 3:E:920:THR:O    | 3:E:923:THR:N     | 2.53                     | 0.41              |
| 3:E:994:LEU:HD23 | 3:E:994:LEU:HA    | 1.85                     | 0.41              |
| 3:E:1031:MET:HE3 | 3:E:1048:PHE:HZ   | 1.85                     | 0.41              |
| 3:E:1292:LEU:HA  | 3:E:1292:LEU:HD23 | 1.78                     | 0.41              |
| 3:F:280:THR:HG22 | 3:F:1063:VAL:HG22 | 2.01                     | 0.41              |
| 3:F:638:GLU:CB   | 3:F:789:ALA:HA    | 2.42                     | 0.41              |
| 3:F:838:THR:HG21 | 3:F:954:TYR:OH    | 2.20                     | 0.41              |
| 3:G:812:TYR:HD1  | 3:G:816:LEU:CD1   | 2.31                     | 0.41              |
| 2:V:53:SER:OG    | 2:V:54:GLY:N      | 2.54                     | 0.41              |
| 1:W:256:THR:HA   | 1:W:261:ALA:HA    | 2.02                     | 0.41              |
| 1:1:193:ALA:HB1  | 1:1:228:SER:HB3   | 2.02                     | 0.41              |
| 2:2:232:ALA:HB1  | 3:D:1139:LEU:HD23 | 2.02                     | 0.41              |
| 1:w:311:TYR:HB2  | 1:w:330:VAL:HB    | 2.03                     | 0.41              |
| 2:x:163:LEU:HD23 | 2:y:223:LEU:HD21  | 2.02                     | 0.41              |
| 3:I:771:VAL:HG23 | 3:I:898:ALA:O     | 2.21                     | 0.41              |
| 3:I:1191:PRO:HG2 | 3:I:1194:THR:HG23 | 2.03                     | 0.41              |
| 3:I:1355:GLU:HB2 | 3:H:1344:ARG:NH1  | 2.35                     | 0.41              |
| 3:J:1063:VAL:O   | 3:J:1110:ALA:HA   | 2.20                     | 0.41              |
| 3:K:505:PHE:CD1  | 3:K:992:PRO:HD3   | 2.56                     | 0.41              |
| 3:K:634:ILE:HG21 | 3:K:670:LEU:HD21  | 2.02                     | 0.41              |
| 3:K:634:ILE:HA   | 3:K:640:VAL:HG11  | 2.02                     | 0.41              |
| 3:K:769:CYS:HB2  | 3:K:901:MET:O     | 2.20                     | 0.41              |
| 3:K:854:PRO:HG3  | 3:K:862:ALA:C     | 2.45                     | 0.41              |
| 3:K:866:HIS:CD2  | 3:K:868:ALA:HB3   | 2.56                     | 0.41              |
| 3:L:649:THR:HG22 | 3:L:678:LEU:HD13  | 2.03                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:L:656:TRP:O     | 3:L:660:ARG:HA    | 2.21                     | 0.41              |
| 3:L:708:THR:HG21  | 3:L:720:ALA:HA    | 2.02                     | 0.41              |
| 3:L:839:LEU:O     | 3:L:875:VAL:HG21  | 2.20                     | 0.41              |
| 3:M:128:ALA:HA    | 3:M:1095:GLN:O    | 2.20                     | 0.41              |
| 3:M:558:LEU:HD12  | 3:M:558:LEU:O     | 2.20                     | 0.41              |
| 3:M:611:ILE:O     | 3:M:614:VAL:N     | 2.51                     | 0.41              |
| 3:A:403:VAL:HG21  | 3:A:1205:PRO:HG3  | 2.01                     | 0.41              |
| 3:A:463:HIS:HA    | 3:A:1130:TYR:CZ   | 2.54                     | 0.41              |
| 3:A:467:MET:HE2   | 3:A:575:TRP:NE1   | 2.35                     | 0.41              |
| 3:H:278:LEU:HA    | 3:H:1064:LEU:O    | 2.20                     | 0.41              |
| 3:H:476:VAL:HG12  | 3:H:571:ILE:HD13  | 2.02                     | 0.41              |
| 3:H:581:ASN:HA    | 3:H:1005:PRO:HG2  | 2.02                     | 0.41              |
| 3:H:755:ARG:O     | 3:H:910:CYS:HA    | 2.20                     | 0.41              |
| 3:N:1139:LEU:HD23 | 3:N:1139:LEU:HA   | 1.88                     | 0.41              |
| 3:N:1181:GLN:HB2  | 3:N:1309:VAL:O    | 2.20                     | 0.41              |
| 3:N:1290:GLU:CB   | 3:D:32:HIS:HB3    | 2.51                     | 0.41              |
| 3:N:1335:THR:HA   | 3:N:1363:ILE:O    | 2.20                     | 0.41              |
| 3:O:58:LEU:HA     | 3:P:327:ARG:HB2   | 2.02                     | 0.41              |
| 3:O:165:LEU:O     | 3:O:168:ASN:N     | 2.53                     | 0.41              |
| 3:O:769:CYS:CB    | 3:O:786:ASN:HD21  | 2.32                     | 0.41              |
| 3:P:294:LYS:HA    | 3:P:294:LYS:HD2   | 1.84                     | 0.41              |
| 3:P:1024:LEU:HD23 | 3:P:1024:LEU:HA   | 1.79                     | 0.41              |
| 3:P:1165:VAL:HG13 | 3:P:1166:PHE:HD2  | 1.85                     | 0.41              |
| 3:P:1335:THR:H    | 3:P:1365:ASP:HB3  | 1.84                     | 0.41              |
| 3:B:158:GLN:O     | 3:B:159:LEU:C     | 2.61                     | 0.41              |
| 3:B:450:LEU:HA    | 3:B:450:LEU:HD23  | 1.72                     | 0.41              |
| 3:B:610:THR:HG21  | 3:B:692:ASP:OD2   | 2.20                     | 0.41              |
| 3:B:915:ASP:O     | 3:B:919:ASN:HB2   | 2.21                     | 0.41              |
| 3:C:765:TYR:CE1   | 3:C:783:LEU:HD12  | 2.56                     | 0.41              |
| 3:D:128:ALA:HA    | 3:D:1095:GLN:O    | 2.19                     | 0.41              |
| 3:D:923:THR:O     | 3:D:923:THR:HG22  | 2.19                     | 0.41              |
| 5:q:365:TRP:O     | 5:q:368:LEU:N     | 2.53                     | 0.41              |
| 3:E:244:ILE:HG21  | 3:E:292:PHE:CE2   | 2.55                     | 0.41              |
| 3:E:460:THR:HA    | 3:E:1129:PHE:CE2  | 2.55                     | 0.41              |
| 3:E:721:GLU:HG2   | 3:E:727:ARG:O     | 2.20                     | 0.41              |
| 3:E:959:PRO:HG2   | 3:E:991:PRO:HD3   | 2.02                     | 0.41              |
| 3:E:1017:GLU:O    | 3:E:1021:THR:HG23 | 2.20                     | 0.41              |
| 3:E:1320:LEU:HD23 | 3:E:1320:LEU:HA   | 1.87                     | 0.41              |
| 3:E:1362:LEU:HD23 | 3:E:1363:ILE:N    | 2.35                     | 0.41              |
| 3:F:10:GLY:HA2    | 3:F:38:PHE:CZ     | 2.55                     | 0.41              |
| 3:F:24:LEU:HD23   | 3:F:24:LEU:HA     | 1.87                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:F:244:ILE:O     | 3:F:245:GLU:C     | 2.61                     | 0.41              |
| 3:F:709:LEU:HD23  | 3:F:709:LEU:HA    | 1.87                     | 0.41              |
| 3:G:861:PRO:HA    | 3:G:866:HIS:CG    | 2.55                     | 0.41              |
| 3:G:1125:LEU:HD12 | 3:G:1184:VAL:HG22 | 2.02                     | 0.41              |
| 1:T:297:ASP:OD1   | 1:T:333:GLN:N     | 2.54                     | 0.41              |
| 2:X:147:LEU:HD11  | 2:X:181:TYR:CG    | 2.56                     | 0.41              |
| 2:3:114:VAL:HB    | 2:3:295:VAL:HB    | 2.02                     | 0.41              |
| 2:2:47:ALA:O      | 2:2:50:SER:OG     | 2.33                     | 0.41              |
| 1:w:147:ARG:NH2   | 2:x:150:GLU:OE2   | 2.52                     | 0.41              |
| 3:I:258:SER:OG    | 3:I:259:VAL:N     | 2.53                     | 0.41              |
| 3:I:467:MET:HE1   | 3:I:1032:SER:HA   | 2.03                     | 0.41              |
| 3:I:898:ALA:CB    | 4:i:58:ALA:HB1    | 2.47                     | 0.41              |
| 3:I:1007:VAL:O    | 3:I:1010:ALA:HB3  | 2.20                     | 0.41              |
| 3:J:463:HIS:CG    | 3:J:464:PRO:HD2   | 2.56                     | 0.41              |
| 3:J:684:GLU:CD    | 3:K:660:ARG:HB2   | 2.45                     | 0.41              |
| 3:J:840:GLN:C     | 3:J:842:MET:HG2   | 2.45                     | 0.41              |
| 3:J:1164:PRO:HG2  | 3:J:1167:GLY:O    | 2.21                     | 0.41              |
| 3:J:1289:LEU:HA   | 3:J:1289:LEU:HD23 | 1.80                     | 0.41              |
| 3:K:433:ARG:NH1   | 3:L:413:MET:HE3   | 2.35                     | 0.41              |
| 3:K:634:ILE:HG22  | 3:K:636:GLY:N     | 2.34                     | 0.41              |
| 3:K:771:VAL:HG23  | 3:K:898:ALA:HA    | 2.02                     | 0.41              |
| 3:K:784:LEU:HD22  | 3:K:786:ASN:ND2   | 2.35                     | 0.41              |
| 3:K:840:GLN:HE22  | 4:k:58:ALA:HB2    | 1.85                     | 0.41              |
| 3:L:394:LEU:HA    | 3:L:394:LEU:HD12  | 1.85                     | 0.41              |
| 3:M:668:TYR:HD2   | 3:M:809:HIS:CE1   | 2.39                     | 0.41              |
| 3:M:802:PRO:HB3   | 3:H:944:HIS:CD2   | 2.55                     | 0.41              |
| 3:M:829:GLY:HA3   | 3:M:956:TYR:CZ    | 2.56                     | 0.41              |
| 3:A:385:TYR:CE1   | 3:A:393:PRO:HD3   | 2.56                     | 0.41              |
| 3:A:1058:PHE:CD1  | 3:A:1118:PRO:HB3  | 2.56                     | 0.41              |
| 3:H:492:ALA:O     | 3:H:993:ALA:HA    | 2.20                     | 0.41              |
| 3:H:756:ILE:HG22  | 3:H:908:LEU:HD22  | 2.02                     | 0.41              |
| 4:i:95:LYS:HE2    | 4:i:95:LYS:HB2    | 1.83                     | 0.41              |
| 4:j:25:LEU:HD21   | 4:j:57:GLN:HE21   | 1.85                     | 0.41              |
| 3:N:87:LEU:HD22   | 3:N:1096:PRO:HB2  | 2.01                     | 0.41              |
| 3:N:205:LEU:HA    | 3:N:205:LEU:HD23  | 1.82                     | 0.41              |
| 3:N:509:TRP:CZ2   | 3:N:564:PRO:HD3   | 2.56                     | 0.41              |
| 3:N:669:SER:O     | 3:N:672:SER:OG    | 2.34                     | 0.41              |
| 3:O:84:PHE:HE1    | 3:O:309:MET:SD    | 2.43                     | 0.41              |
| 3:O:183:GLN:O     | 3:O:186:HIS:N     | 2.53                     | 0.41              |
| 3:O:185:LEU:HD23  | 3:O:185:LEU:HA    | 1.87                     | 0.41              |
| 3:O:198:LEU:HD23  | 3:O:198:LEU:HA    | 1.81                     | 0.41              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:O:298:THR:HG22 | 3:O:298:THR:O     | 2.20                     | 0.41              |
| 3:O:834:ARG:NH1  | 3:O:953:GLU:O     | 2.52                     | 0.41              |
| 3:O:875:VAL:O    | 3:O:878:MET:HB3   | 2.21                     | 0.41              |
| 3:O:1206:ARG:NH2 | 3:O:1208:ARG:O    | 2.53                     | 0.41              |
| 3:O:1344:ARG:O   | 3:O:1347:ARG:HG2  | 2.21                     | 0.41              |
| 3:B:1357:HIS:O   | 3:B:1358:PHE:C    | 2.63                     | 0.41              |
| 3:C:435:PHE:HB3  | 3:C:598:GLU:HG3   | 2.03                     | 0.41              |
| 3:C:462:CYS:SG   | 3:C:1037:TYR:HB2  | 2.60                     | 0.41              |
| 3:D:180:THR:HG22 | 3:D:1097:ARG:CZ   | 2.49                     | 0.41              |
| 3:D:374:LEU:HD23 | 3:D:374:LEU:HA    | 1.79                     | 0.41              |
| 3:D:481:VAL:HG11 | 3:D:571:ILE:HD12  | 2.03                     | 0.41              |
| 3:D:533:GLN:C    | 3:D:535:ASP:H     | 2.29                     | 0.41              |
| 3:D:769:CYS:HB2  | 3:D:901:MET:O     | 2.19                     | 0.41              |
| 3:D:836:TYR:HD1  | 3:D:897:LEU:HD13  | 1.86                     | 0.41              |
| 3:D:877:ALA:HB1  | 4:c:94:LEU:HD21   | 2.01                     | 0.41              |
| 3:D:1256:LEU:HA  | 3:D:1256:LEU:HD23 | 1.87                     | 0.41              |
| 5:q:257:ASN:O    | 5:q:261:LEU:HD22  | 2.20                     | 0.41              |
| 5:q:263:LEU:HB3  | 7:u:3084:VAL:HG13 | 2.02                     | 0.41              |
| 5:q:572:LEU:CD2  | 5:q:693:ARG:HB2   | 2.50                     | 0.41              |
| 3:E:87:LEU:O     | 3:E:89:TYR:N      | 2.53                     | 0.41              |
| 3:E:679:GLY:HA3  | 3:F:622:SER:OG    | 2.20                     | 0.41              |
| 3:E:703:LEU:HA   | 3:E:703:LEU:HD23  | 1.84                     | 0.41              |
| 3:E:826:CYS:SG   | 3:E:969:HIS:CG    | 3.13                     | 0.41              |
| 3:E:1003:ARG:HB2 | 3:E:1005:PRO:HD2  | 2.01                     | 0.41              |
| 3:E:1226:MET:HE2 | 3:E:1279:ALA:CB   | 2.51                     | 0.41              |
| 6:r:90:GLN:HB2   | 7:u:3093:GLN:NE2  | 2.35                     | 0.41              |
| 3:G:182:ASP:OD1  | 3:G:385:TYR:OH    | 2.28                     | 0.41              |
| 3:G:469:ILE:HD12 | 3:G:547:PHE:CE1   | 2.55                     | 0.41              |
| 3:G:966:GLY:HA3  | 3:G:969:HIS:HD2   | 1.85                     | 0.41              |
| 3:K:248:LEU:HD11 | 3:K:288:LEU:HD22  | 2.03                     | 0.41              |
| 3:K:840:GLN:HB3  | 4:k:57:GLN:HB3    | 2.02                     | 0.41              |
| 3:L:44:SER:OG    | 3:N:134:SER:O     | 2.30                     | 0.41              |
| 3:L:808:HIS:O    | 3:L:812:TYR:N     | 2.43                     | 0.41              |
| 3:L:825:CYS:HB2  | 3:L:939:LEU:O     | 2.21                     | 0.41              |
| 3:M:163:GLN:HE22 | 3:H:348:ARG:HH21  | 1.67                     | 0.41              |
| 3:M:839:LEU:O    | 3:M:875:VAL:HG21  | 2.21                     | 0.41              |
| 3:M:1004:GLN:NE2 | 3:M:1007:VAL:HB   | 2.35                     | 0.41              |
| 3:M:1037:TYR:CZ  | 3:M:1150:ALA:HB1  | 2.56                     | 0.41              |
| 3:M:1058:PHE:HE2 | 3:M:1369:LEU:HD11 | 1.81                     | 0.41              |
| 3:A:22:SER:OG    | 3:A:23:ILE:N      | 2.53                     | 0.41              |
| 3:A:182:ASP:OD1  | 3:A:385:TYR:OH    | 2.21                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:A:466:LEU:HD12  | 3:A:467:MET:HG3   | 2.02                     | 0.41              |
| 3:A:631:GLN:HE22  | 3:A:666:ASN:CG    | 2.19                     | 0.41              |
| 3:A:1024:LEU:HD23 | 3:A:1024:LEU:HA   | 1.82                     | 0.41              |
| 3:H:267:ALA:O     | 3:H:301:ASP:N     | 2.41                     | 0.41              |
| 3:H:484:ALA:O     | 3:H:485:ASN:C     | 2.63                     | 0.41              |
| 3:H:718:ALA:HB3   | 3:H:721:GLU:HG3   | 2.02                     | 0.41              |
| 3:H:884:VAL:HG12  | 3:H:886:VAL:HG23  | 2.01                     | 0.41              |
| 3:N:103:LEU:HD11  | 3:N:115:PRO:CB    | 2.49                     | 0.41              |
| 3:N:1218:LYS:HB3  | 3:N:1221:ASP:CG   | 2.46                     | 0.41              |
| 3:O:85:PRO:HG3    | 3:O:310:VAL:HG22  | 2.03                     | 0.41              |
| 3:P:786:ASN:O     | 3:P:788:GLN:HG3   | 2.21                     | 0.41              |
| 3:P:1013:SER:OG   | 3:P:1020:LEU:HD11 | 2.21                     | 0.41              |
| 3:B:582:LEU:HD23  | 3:B:582:LEU:HA    | 1.81                     | 0.41              |
| 3:B:1132:GLY:N    | 3:B:1267:SER:HB3  | 2.35                     | 0.41              |
| 3:D:656:TRP:O     | 3:D:660:ARG:HA    | 2.21                     | 0.41              |
| 3:D:767:ALA:HA    | 3:D:785:HIS:HB3   | 2.03                     | 0.41              |
| 3:D:784:LEU:HD22  | 3:D:902:ALA:HA    | 2.02                     | 0.41              |
| 3:D:864:PRO:HB2   | 3:D:876:ASN:CG    | 2.45                     | 0.41              |
| 3:E:126:ARG:HG3   | 3:E:1097:ARG:O    | 2.20                     | 0.41              |
| 3:E:178:ARG:CB    | 3:F:104:ILE:HG22  | 2.48                     | 0.41              |
| 3:E:367:LEU:HA    | 3:E:367:LEU:HD23  | 1.74                     | 0.41              |
| 3:E:524:CYS:HB3   | 3:E:1008:GLN:HE22 | 1.86                     | 0.41              |
| 3:F:86:GLU:HB2    | 3:F:89:TYR:CD2    | 2.56                     | 0.41              |
| 3:F:124:ILE:HG23  | 3:F:1100:VAL:HG23 | 2.02                     | 0.41              |
| 3:G:52:VAL:HG12   | 3:G:53:GLU:N      | 2.35                     | 0.41              |
| 3:G:1196:ILE:H    | 3:G:1196:ILE:HG13 | 1.71                     | 0.41              |
| 1:Q:91:LEU:O      | 1:Q:95:ARG:N      | 2.39                     | 0.41              |
| 2:X:211:TYR:OH    | 2:Y:241:LEU:O     | 2.39                     | 0.41              |
| 3:I:80:VAL:O      | 3:I:1073:TYR:N    | 2.50                     | 0.41              |
| 3:I:235:GLY:HA3   | 3:I:1372:LEU:HD21 | 2.03                     | 0.41              |
| 3:I:492:ALA:H     | 3:I:992:PRO:HB2   | 1.86                     | 0.41              |
| 3:I:683:PRO:HD2   | 3:I:686:CYS:HB3   | 2.01                     | 0.41              |
| 3:I:1208:ARG:NH1  | 3:I:1240:ALA:O    | 2.52                     | 0.41              |
| 3:J:784:LEU:HD13  | 3:J:786:ASN:HB2   | 2.02                     | 0.41              |
| 3:J:888:GLY:N     | 3:J:889:PRO:HD2   | 2.35                     | 0.41              |
| 3:J:1093:LEU:HA   | 3:J:1093:LEU:HD23 | 1.83                     | 0.41              |
| 3:K:326:VAL:O     | 3:K:327:ARG:C     | 2.63                     | 0.41              |
| 3:K:842:MET:HE2   | 3:K:891:MET:HB3   | 2.02                     | 0.41              |
| 3:L:646:ARG:NE    | 3:L:890:ALA:HB2   | 2.35                     | 0.41              |
| 3:L:684:GLU:CD    | 3:M:660:ARG:HG2   | 2.46                     | 0.41              |
| 3:L:887:ASP:O     | 3:L:891:MET:HG2   | 2.20                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:M:382:LYS:HA    | 3:M:382:LYS:HD2   | 1.87                     | 0.41              |
| 3:M:490:TYR:OH    | 3:M:561:GLY:O     | 2.38                     | 0.41              |
| 3:M:544:HIS:CG    | 3:M:545:PRO:HD2   | 2.55                     | 0.41              |
| 3:M:645:ALA:O     | 3:M:649:THR:HG23  | 2.21                     | 0.41              |
| 3:M:842:MET:HB2   | 4:m:22:MET:HG2    | 2.01                     | 0.41              |
| 3:A:85:PRO:HG2    | 3:A:86:GLU:OE1    | 2.20                     | 0.41              |
| 3:A:944:HIS:CD2   | 3:A:972:ASN:HD22  | 2.38                     | 0.41              |
| 3:A:1227:TYR:O    | 3:A:1229:HIS:ND1  | 2.53                     | 0.41              |
| 3:H:84:PHE:HD2    | 3:H:87:LEU:HA     | 1.85                     | 0.41              |
| 3:H:335:HIS:HB2   | 3:C:18:VAL:HG21   | 2.03                     | 0.41              |
| 3:H:1083:HIS:CD2  | 3:H:1085:THR:HG23 | 2.56                     | 0.41              |
| 3:H:1340:PRO:O    | 3:H:1344:ARG:HG3  | 2.20                     | 0.41              |
| 4:o:88:LEU:HD12   | 4:o:89:ARG:N      | 2.36                     | 0.41              |
| 3:N:324:LYS:O     | 3:E:322:MET:HE2   | 2.20                     | 0.41              |
| 3:N:339:MET:SD    | 3:N:339:MET:O     | 2.79                     | 0.41              |
| 3:N:481:VAL:HG22  | 3:N:482:GLU:O     | 2.21                     | 0.41              |
| 3:N:624:PRO:HG2   | 3:N:627:PHE:HE2   | 1.86                     | 0.41              |
| 3:O:125:ASP:O     | 3:O:1098:GLY:HA2  | 2.21                     | 0.41              |
| 3:O:263:ARG:HH12  | 3:O:307:GLY:HA2   | 1.86                     | 0.41              |
| 3:O:398:MET:O     | 3:O:1057:ARG:HA   | 2.20                     | 0.41              |
| 3:O:487:TYR:HE1   | 3:O:505:PHE:HZ    | 1.68                     | 0.41              |
| 3:O:635:HIS:CD2   | 3:O:787:THR:HG22  | 2.56                     | 0.41              |
| 3:O:1148:ARG:NH2  | 3:O:1163:LEU:HG   | 2.34                     | 0.41              |
| 3:P:475:GLY:HA3   | 3:P:1250:PHE:CE2  | 2.56                     | 0.41              |
| 3:P:627:PHE:HD1   | 3:P:664:PHE:CZ    | 2.39                     | 0.41              |
| 3:P:734:PRO:HD3   | 3:P:814:TYR:CE2   | 2.55                     | 0.41              |
| 3:B:563:VAL:HG13  | 3:B:564:PRO:HD2   | 2.02                     | 0.41              |
| 3:B:1248:GLN:C    | 3:B:1251:SER:HG   | 2.26                     | 0.41              |
| 3:C:687:MET:O     | 3:C:688:ALA:C     | 2.64                     | 0.41              |
| 3:C:808:HIS:O     | 3:C:812:TYR:N     | 2.47                     | 0.41              |
| 3:D:54:PHE:HE1    | 3:E:319:ALA:HB1   | 1.86                     | 0.41              |
| 3:D:177:GLU:OE1   | 3:D:177:GLU:N     | 2.40                     | 0.41              |
| 3:D:887:ASP:O     | 3:D:891:MET:HG2   | 2.21                     | 0.41              |
| 3:E:227:PHE:CZ    | 3:E:1324:PRO:HB3  | 2.55                     | 0.41              |
| 3:E:877:ALA:O     | 3:E:881:ASN:N     | 2.50                     | 0.41              |
| 3:F:32:HIS:HD2    | 3:F:35:LEU:HD13   | 1.84                     | 0.41              |
| 3:F:745:HIS:CE1   | 3:F:910:CYS:HB2   | 2.56                     | 0.41              |
| 3:F:1024:LEU:HD23 | 3:F:1024:LEU:HA   | 1.77                     | 0.41              |
| 3:F:1339:ASP:OD2  | 3:F:1360:GLN:HG3  | 2.21                     | 0.41              |
| 3:G:549:PHE:N     | 3:G:549:PHE:CD2   | 2.88                     | 0.41              |
| 3:G:934:HIS:CD2   | 3:G:934:HIS:C     | 2.99                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:T:195:ALA:HB1   | 1:T:204:ALA:HB1   | 2.03                     | 0.41              |
| 2:U:114:VAL:HB    | 2:U:295:VAL:HG12  | 2.02                     | 0.41              |
| 3:I:348:ARG:NH2   | 3:H:163:GLN:HE22  | 2.18                     | 0.41              |
| 3:I:600:GLY:C     | 3:I:602:GLY:H     | 2.29                     | 0.41              |
| 3:J:466:LEU:HD12  | 3:J:466:LEU:C     | 2.46                     | 0.41              |
| 3:J:726:MET:HE3   | 3:J:1028:TYR:CD1  | 2.56                     | 0.41              |
| 3:J:1059:VAL:HG23 | 3:J:1119:VAL:HG23 | 2.02                     | 0.41              |
| 3:K:156:HIS:O     | 3:K:156:HIS:CG    | 2.74                     | 0.41              |
| 3:K:884:VAL:HG12  | 3:K:886:VAL:HG23  | 2.02                     | 0.41              |
| 3:K:945:LEU:HD23  | 3:K:945:LEU:HA    | 1.55                     | 0.41              |
| 3:L:263:ARG:NH2   | 3:L:306:TYR:O     | 2.53                     | 0.41              |
| 3:M:159:LEU:CD1   | 3:H:340:GLN:HA    | 2.51                     | 0.41              |
| 3:M:161:ALA:HA    | 3:C:50:TYR:CZ     | 2.55                     | 0.41              |
| 3:M:1139:LEU:HA   | 3:M:1139:LEU:HD23 | 1.80                     | 0.41              |
| 3:A:452:LEU:HD13  | 3:A:1124:ASN:HD22 | 1.85                     | 0.41              |
| 3:H:463:HIS:CD2   | 3:H:465:SER:HB3   | 2.56                     | 0.41              |
| 3:H:521:VAL:HG21  | 3:H:987:VAL:HG12  | 2.03                     | 0.41              |
| 3:H:950:GLN:HB2   | 3:H:953:GLU:HG3   | 2.02                     | 0.41              |
| 4:k:25:LEU:HD11   | 4:k:53:PHE:CZ     | 2.55                     | 0.41              |
| 4:k:60:ALA:HA     | 4:k:63:ASP:HB2    | 2.01                     | 0.41              |
| 4:n:62:THR:HA     | 3:N:895:GLN:NE2   | 2.35                     | 0.41              |
| 3:N:122:LYS:HE3   | 3:D:36:PHE:CE1    | 2.56                     | 0.41              |
| 3:N:195:LEU:O     | 3:N:198:LEU:N     | 2.39                     | 0.41              |
| 3:N:277:VAL:HG22  | 3:N:376:PHE:HB2   | 2.03                     | 0.41              |
| 3:N:641:PHE:O     | 3:N:645:ALA:N     | 2.53                     | 0.41              |
| 3:N:888:GLY:N     | 3:N:889:PRO:HD2   | 2.35                     | 0.41              |
| 3:N:909:LEU:HD23  | 3:N:909:LEU:HA    | 1.82                     | 0.41              |
| 3:N:989:LEU:HD23  | 3:N:989:LEU:HA    | 1.77                     | 0.41              |
| 3:N:1218:LYS:HB3  | 3:N:1221:ASP:OD2  | 2.19                     | 0.41              |
| 3:O:43:ARG:C      | 3:O:45:ASP:H      | 2.29                     | 0.41              |
| 3:O:439:GLN:HE21  | 3:O:451:ARG:NH2   | 2.19                     | 0.41              |
| 3:O:1128:ASN:HD22 | 3:O:1158:GLY:HA3  | 1.86                     | 0.41              |
| 3:P:124:ILE:HG12  | 3:P:1100:VAL:HG23 | 2.02                     | 0.41              |
| 3:P:599:LEU:HD23  | 3:P:599:LEU:HA    | 1.84                     | 0.41              |
| 3:P:989:LEU:HD23  | 3:P:989:LEU:HA    | 1.68                     | 0.41              |
| 3:B:187:VAL:HG11  | 3:B:1071:GLU:OE2  | 2.21                     | 0.41              |
| 3:B:330:ASP:O     | 3:B:334:ARG:HG2   | 2.20                     | 0.41              |
| 3:B:485:ASN:HA    | 3:B:486:PRO:HD3   | 1.83                     | 0.41              |
| 3:B:669:SER:O     | 3:B:672:SER:OG    | 2.33                     | 0.41              |
| 3:B:1020:LEU:HD23 | 3:B:1020:LEU:HA   | 1.71                     | 0.41              |
| 3:C:143:LEU:HD23  | 3:C:143:LEU:HA    | 1.89                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:C:406:LEU:HD23  | 3:C:406:LEU:HA    | 1.85                     | 0.41              |
| 3:C:469:ILE:HD11  | 3:C:547:PHE:CD1   | 2.56                     | 0.41              |
| 3:C:708:THR:HG22  | 3:C:723:ASN:ND2   | 2.27                     | 0.41              |
| 3:C:866:HIS:HD2   | 3:C:868:ALA:HB3   | 1.85                     | 0.41              |
| 3:C:1147:LEU:HD23 | 3:C:1147:LEU:HA   | 1.75                     | 0.41              |
| 3:D:264:LEU:HD23  | 3:D:264:LEU:HA    | 1.86                     | 0.41              |
| 3:D:286:GLN:O     | 3:D:287:ARG:C     | 2.63                     | 0.41              |
| 3:D:390:VAL:HG22  | 3:E:106:ARG:NH1   | 2.36                     | 0.41              |
| 3:D:524:CYS:HB3   | 3:D:1008:GLN:HE22 | 1.86                     | 0.41              |
| 3:D:704:VAL:O     | 3:D:708:THR:HG23  | 2.21                     | 0.41              |
| 3:D:793:ASP:CG    | 3:D:800:HIS:HD1   | 2.24                     | 0.41              |
| 3:D:1128:ASN:HD22 | 3:D:1158:GLY:CA   | 2.33                     | 0.41              |
| 3:D:1224:ALA:HA   | 3:D:1228:ASP:OD2  | 2.20                     | 0.41              |
| 5:q:65:HIS:HB2    | 5:q:128:THR:HG22  | 2.02                     | 0.41              |
| 5:q:169:ARG:HH11  | 5:q:232:ILE:HA    | 1.85                     | 0.41              |
| 5:q:576:ILE:HG23  | 5:q:580:PHE:HB3   | 2.03                     | 0.41              |
| 3:E:1058:PHE:CD1  | 3:E:1118:PRO:HB3  | 2.56                     | 0.41              |
| 3:E:1221:ASP:O    | 3:E:1222:VAL:C    | 2.63                     | 0.41              |
| 6:r:83:ARG:HE     | 7:t:3099:THR:HG22 | 1.86                     | 0.41              |
| 3:F:1155:ASN:OD1  | 3:F:1157:LEU:N    | 2.52                     | 0.41              |
| 3:G:410:ASN:O     | 3:G:415:ARG:NH1   | 2.53                     | 0.41              |
| 2:U:219:LEU:HD13  | 2:U:275:LEU:HD23  | 2.03                     | 0.41              |
| 2:V:116:LEU:H     | 2:V:116:LEU:HG    | 1.73                     | 0.41              |
| 1:W:125:GLU:OE1   | 1:W:186:SER:OG    | 2.27                     | 0.41              |
| 2:X:47:ALA:HA     | 2:X:137:LEU:HD23  | 2.03                     | 0.41              |
| 2:3:284:GLN:CG    | 3:D:1166:PHE:HZ   | 2.21                     | 0.41              |
| 2:2:147:LEU:HD23  | 2:2:147:LEU:HA    | 1.92                     | 0.41              |
| 1:w:130:LEU:HD22  | 1:w:247:PHE:HE1   | 1.86                     | 0.41              |
| 3:I:133:PHE:O     | 3:I:133:PHE:CG    | 2.73                     | 0.41              |
| 3:I:183:GLN:O     | 3:I:187:VAL:N     | 2.47                     | 0.41              |
| 3:I:185:LEU:HA    | 3:I:185:LEU:HD23  | 1.79                     | 0.41              |
| 3:I:298:THR:HG22  | 3:I:299:GLU:HG3   | 2.03                     | 0.41              |
| 3:I:467:MET:SD    | 3:I:918:ALA:HB1   | 2.61                     | 0.41              |
| 3:I:646:ARG:HG3   | 3:I:647:LEU:N     | 2.36                     | 0.41              |
| 3:I:721:GLU:HG2   | 3:I:727:ARG:O     | 2.21                     | 0.41              |
| 3:I:756:ILE:HA    | 3:I:909:LEU:O     | 2.21                     | 0.41              |
| 3:I:840:GLN:HB2   | 4:i:57:GLN:OE1    | 2.21                     | 0.41              |
| 3:I:843:VAL:HG23  | 4:i:26:VAL:HG11   | 2.03                     | 0.41              |
| 3:I:915:ASP:CG    | 3:I:1030:LYS:HZ3  | 2.29                     | 0.41              |
| 3:I:1049:GLY:O    | 3:I:1190:THR:N    | 2.48                     | 0.41              |
| 3:I:1139:LEU:HD23 | 3:I:1139:LEU:HA   | 1.61                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:I:1205:PRO:HG2  | 3:I:1276:PHE:CE2  | 2.56                     | 0.41              |
| 3:J:266:HIS:CE1   | 3:J:302:VAL:HG13  | 2.56                     | 0.41              |
| 3:J:496:GLY:HA3   | 3:J:504:ARG:NH1   | 2.36                     | 0.41              |
| 3:J:1186:GLU:CD   | 3:J:1272:PRO:HD2  | 2.46                     | 0.41              |
| 3:K:129:LEU:HD11  | 3:K:1097:ARG:NH1  | 2.36                     | 0.41              |
| 3:K:421:GLY:O     | 3:K:424:VAL:HG23  | 2.20                     | 0.41              |
| 3:K:463:HIS:CD2   | 3:K:465:SER:HB3   | 2.56                     | 0.41              |
| 3:K:837:ALA:HA    | 4:k:57:GLN:OE1    | 2.21                     | 0.41              |
| 3:K:840:GLN:CB    | 4:k:57:GLN:HB3    | 2.51                     | 0.41              |
| 3:L:544:HIS:CG    | 3:L:545:PRO:HD2   | 2.56                     | 0.41              |
| 3:L:873:ASN:HB3   | 4:k:89:ARG:HH12   | 1.85                     | 0.41              |
| 3:L:1291:ARG:O    | 3:L:1294:VAL:N    | 2.54                     | 0.41              |
| 3:M:896:VAL:HA    | 3:M:899:HIS:HD2   | 1.85                     | 0.41              |
| 3:M:1075:LEU:O    | 3:M:1075:LEU:HD12 | 2.20                     | 0.41              |
| 3:M:1218:LYS:N    | 3:M:1221:ASP:OD2  | 2.53                     | 0.41              |
| 3:A:98:GLU:HG2    | 3:A:119:TYR:CE1   | 2.55                     | 0.41              |
| 3:A:319:ALA:HA    | 3:G:24:LEU:O      | 2.21                     | 0.41              |
| 3:A:1197:ASN:OD1  | 3:A:1200:ARG:NH1  | 2.54                     | 0.41              |
| 3:H:130:ASN:OD1   | 3:H:1094:THR:HG22 | 2.21                     | 0.41              |
| 3:H:398:MET:HE3   | 3:H:398:MET:HB3   | 1.95                     | 0.41              |
| 3:H:405:PRO:HB3   | 3:H:1199:PHE:CD2  | 2.56                     | 0.41              |
| 3:H:425:PRO:HG3   | 3:H:431:GLU:HG2   | 2.03                     | 0.41              |
| 3:H:467:MET:O     | 3:H:922:SER:OG    | 2.39                     | 0.41              |
| 3:H:1020:LEU:HD23 | 3:H:1020:LEU:HA   | 1.75                     | 0.41              |
| 4:l:7:HIS:CD2     | 4:l:8:ARG:HG3     | 2.55                     | 0.41              |
| 3:N:309:MET:HE3   | 3:N:327:ARG:HA    | 2.02                     | 0.41              |
| 3:N:367:LEU:HA    | 3:N:367:LEU:HD23  | 1.84                     | 0.41              |
| 3:N:495:ALA:C     | 3:N:504:ARG:HH12  | 2.29                     | 0.41              |
| 3:N:769:CYS:HB2   | 3:N:786:ASN:ND2   | 2.36                     | 0.41              |
| 3:N:827:THR:OG1   | 3:N:960:VAL:HG23  | 2.20                     | 0.41              |
| 3:N:1209:ALA:HB1  | 3:N:1214:TYR:HE2  | 1.86                     | 0.41              |
| 3:O:289:LEU:HD23  | 3:O:289:LEU:HA    | 1.95                     | 0.41              |
| 3:O:742:LEU:HD22  | 3:O:756:ILE:HD13  | 2.03                     | 0.41              |
| 3:O:766:ALA:HB3   | 3:O:783:LEU:O     | 2.20                     | 0.41              |
| 3:O:1177:MET:HE2  | 3:O:1177:MET:HB3  | 1.88                     | 0.41              |
| 3:O:1344:ARG:HH12 | 3:P:1356:THR:CG2  | 2.34                     | 0.41              |
| 3:P:127:ARG:NH1   | 3:P:187:VAL:HG22  | 2.35                     | 0.41              |
| 3:P:234:LEU:HD23  | 3:P:234:LEU:HA    | 1.87                     | 0.41              |
| 3:P:266:HIS:HE1   | 3:P:302:VAL:HG13  | 1.85                     | 0.41              |
| 3:P:892:LEU:O     | 3:P:895:GLN:HG3   | 2.20                     | 0.41              |
| 3:P:951:ASN:HD22  | 3:P:974:PRO:HD3   | 1.86                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:P:1258:ASN:OD1  | 3:P:1259:GLY:N    | 2.54                     | 0.41              |
| 3:P:1357:HIS:O    | 3:P:1358:PHE:C    | 2.63                     | 0.41              |
| 3:B:251:LEU:HA    | 3:B:251:LEU:HD23  | 1.77                     | 0.41              |
| 3:B:301:ASP:OD1   | 3:B:362:ARG:NE    | 2.51                     | 0.41              |
| 3:B:731:LEU:HA    | 3:B:731:LEU:HD23  | 1.86                     | 0.41              |
| 3:B:827:THR:HA    | 3:B:938:LEU:HA    | 2.03                     | 0.41              |
| 3:B:920:THR:HG22  | 3:B:921:ALA:N     | 2.36                     | 0.41              |
| 3:B:1168:CYS:HB2  | 3:B:1268:PRO:HD3  | 2.02                     | 0.41              |
| 3:C:24:LEU:HD23   | 3:C:24:LEU:HA     | 1.82                     | 0.41              |
| 3:C:496:GLY:HA3   | 3:C:504:ARG:NH1   | 2.36                     | 0.41              |
| 3:C:753:ASP:HB3   | 3:C:755:ARG:NH2   | 2.36                     | 0.41              |
| 3:C:873:ASN:CA    | 4:b:92:PHE:HB2    | 2.44                     | 0.41              |
| 3:D:399:ASP:HB2   | 3:D:1323:ASP:OD1  | 2.20                     | 0.41              |
| 3:D:838:THR:HG21  | 3:D:954:TYR:OH    | 2.21                     | 0.41              |
| 3:D:842:MET:CE    | 3:D:891:MET:HB3   | 2.51                     | 0.41              |
| 3:D:944:HIS:CE1   | 3:D:972:ASN:ND2   | 2.88                     | 0.41              |
| 3:D:1177:MET:HB3  | 3:D:1177:MET:HE2  | 1.84                     | 0.41              |
| 5:q:84:ASP:HB3    | 5:q:106:SER:N     | 2.33                     | 0.41              |
| 3:E:83:LYS:HE2    | 3:E:83:LYS:HB3    | 1.91                     | 0.41              |
| 3:E:399:ASP:OD1   | 3:E:1057:ARG:HG2  | 2.21                     | 0.41              |
| 3:E:404:LEU:HB2   | 3:E:1052:VAL:HB   | 2.03                     | 0.41              |
| 3:E:584:LEU:HA    | 3:E:584:LEU:HD23  | 1.78                     | 0.41              |
| 3:E:697:VAL:O     | 3:E:700:LEU:N     | 2.54                     | 0.41              |
| 3:E:724:HIS:CE1   | 3:E:1028:TYR:HB2  | 2.56                     | 0.41              |
| 3:E:1013:SER:OG   | 3:E:1020:LEU:HD11 | 2.21                     | 0.41              |
| 3:E:1335:THR:N    | 3:E:1365:ASP:HB3  | 2.36                     | 0.41              |
| 3:F:124:ILE:HG12  | 3:F:1100:VAL:HG21 | 2.03                     | 0.41              |
| 3:F:623:TYR:HA    | 3:F:624:PRO:HD3   | 1.91                     | 0.41              |
| 3:F:1270:LEU:CD2  | 3:F:1303:ALA:HB2  | 2.43                     | 0.41              |
| 3:F:1291:ARG:O    | 3:F:1294:VAL:N    | 2.54                     | 0.41              |
| 3:F:1362:LEU:HD23 | 3:F:1363:ILE:N    | 2.36                     | 0.41              |
| 6:s:76:LEU:N      | 6:s:77:PRO:HD2    | 2.36                     | 0.41              |
| 3:G:23:ILE:HB     | 3:G:64:THR:OG1    | 2.20                     | 0.41              |
| 3:G:405:PRO:CG    | 3:G:1363:ILE:HD11 | 2.50                     | 0.41              |
| 3:G:496:GLY:HA3   | 3:G:504:ARG:NH1   | 2.36                     | 0.41              |
| 3:G:1225:LEU:HD22 | 3:G:1234:PRO:HG3  | 2.03                     | 0.41              |
| 1:Q:428:MET:HE1   | 1:Q:452:LEU:HD22  | 2.03                     | 0.41              |
| 2:U:78:VAL:HG13   | 2:U:83:ILE:HG12   | 2.03                     | 0.41              |
| 1:1:149:PRO:HD2   | 1:1:152:ARG:HD2   | 2.03                     | 0.41              |
| 1:1:335:PRO:HG3   | 2:2:71:PHE:CE1    | 2.56                     | 0.41              |
| 2:2:232:ALA:HB1   | 3:D:1139:LEU:CD2  | 2.51                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:x:10:ILE:HD13   | 2:x:46:VAL:HG21   | 2.02                     | 0.41              |
| 2:y:264:ASP:OD2   | 2:y:267:ARG:NH2   | 2.54                     | 0.41              |
| 3:I:191:LYS:HD2   | 3:I:1101:ASP:OD2  | 2.21                     | 0.41              |
| 3:I:436:PRO:HD3   | 3:I:594:ALA:HB1   | 2.03                     | 0.41              |
| 3:I:783:LEU:HA    | 3:I:783:LEU:HD23  | 1.78                     | 0.41              |
| 3:I:841:ASN:HD21  | 4:h:89:ARG:HD3    | 1.86                     | 0.41              |
| 3:I:1024:LEU:HD23 | 3:I:1024:LEU:HA   | 1.86                     | 0.41              |
| 3:J:439:GLN:CD    | 3:J:451:ARG:HH21  | 2.29                     | 0.41              |
| 3:J:487:TYR:HE1   | 3:J:505:PHE:HZ    | 1.67                     | 0.41              |
| 3:K:1334:ILE:HG22 | 3:K:1335:THR:N    | 2.36                     | 0.41              |
| 3:L:541:LEU:HD23  | 3:L:541:LEU:HA    | 1.90                     | 0.41              |
| 3:L:591:PHE:O     | 3:L:594:ALA:HB3   | 2.20                     | 0.41              |
| 3:L:1139:LEU:HA   | 3:L:1139:LEU:HD23 | 1.75                     | 0.41              |
| 3:M:52:VAL:HG22   | 3:C:160:ARG:HH12  | 1.86                     | 0.41              |
| 3:M:61:TYR:HB3    | 3:C:23:ILE:HG13   | 2.02                     | 0.41              |
| 3:M:685:GLU:O     | 3:M:688:ALA:N     | 2.49                     | 0.41              |
| 3:M:895:GLN:HG2   | 4:m:61:LEU:C      | 2.46                     | 0.41              |
| 3:M:1354:ARG:O    | 3:M:1354:ARG:HG3  | 2.21                     | 0.41              |
| 3:A:367:LEU:HA    | 3:A:375:VAL:O     | 2.21                     | 0.41              |
| 3:A:461:VAL:HG12  | 3:A:1036:LEU:HD12 | 2.00                     | 0.41              |
| 3:A:491:VAL:HG21  | 3:A:929:PHE:CD2   | 2.46                     | 0.41              |
| 3:A:863:HIS:ND1   | 3:A:864:PRO:HD2   | 2.36                     | 0.41              |
| 3:A:1252:TYR:CZ   | 3:A:1256:LEU:HD11 | 2.55                     | 0.41              |
| 3:H:320:LEU:HD23  | 3:H:320:LEU:HA    | 1.89                     | 0.41              |
| 3:H:730:ALA:HB2   | 3:H:752:ARG:NH1   | 2.26                     | 0.41              |
| 3:H:906:THR:OG1   | 3:H:934:HIS:HB3   | 2.20                     | 0.41              |
| 3:H:1119:VAL:HG11 | 3:H:1305:ALA:HB1  | 2.03                     | 0.41              |
| 3:H:1218:LYS:HB3  | 3:H:1221:ASP:CG   | 2.46                     | 0.41              |
| 3:N:279:VAL:O     | 3:N:394:LEU:HD21  | 2.20                     | 0.41              |
| 3:N:405:PRO:O     | 3:N:440:LEU:HD11  | 2.20                     | 0.41              |
| 3:O:158:GLN:O     | 3:O:162:ILE:N     | 2.47                     | 0.41              |
| 3:O:738:ASP:OD1   | 3:O:787:THR:OG1   | 2.40                     | 0.41              |
| 3:P:201:MET:HG3   | 3:P:1293:ILE:HD13 | 2.02                     | 0.41              |
| 3:P:403:VAL:HA    | 3:P:1052:VAL:O    | 2.21                     | 0.41              |
| 3:P:1004:GLN:N    | 3:P:1005:PRO:HD2  | 2.35                     | 0.41              |
| 3:B:130:ASN:OD1   | 3:B:1094:THR:HG22 | 2.20                     | 0.41              |
| 3:B:195:LEU:O     | 3:B:196:ALA:C     | 2.62                     | 0.41              |
| 3:B:541:LEU:HD23  | 3:B:541:LEU:HA    | 1.79                     | 0.41              |
| 3:B:700:LEU:O     | 3:B:1025:MET:HE2  | 2.21                     | 0.41              |
| 3:B:778:ARG:HH11  | 3:B:782:ARG:HD2   | 1.85                     | 0.41              |
| 3:C:137:THR:HG22  | 3:C:1087:GLY:C    | 2.46                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:C:703:LEU:O     | 3:C:704:VAL:C     | 2.64                     | 0.41              |
| 3:C:1013:SER:OG   | 3:C:1020:LEU:HD21 | 2.21                     | 0.41              |
| 3:C:1333:PRO:HG2  | 3:C:1366:ALA:H    | 1.86                     | 0.41              |
| 3:D:156:HIS:O     | 3:D:156:HIS:CG    | 2.74                     | 0.41              |
| 3:D:465:SER:HB3   | 3:D:1135:ALA:HB1  | 2.03                     | 0.41              |
| 3:D:505:PHE:CD1   | 3:D:992:PRO:HD2   | 2.54                     | 0.41              |
| 5:q:62:THR:H      | 5:q:71:THR:HB     | 1.85                     | 0.41              |
| 3:E:258:SER:OG    | 3:E:259:VAL:N     | 2.49                     | 0.41              |
| 3:E:311:LEU:O     | 3:E:316:LEU:HB2   | 2.21                     | 0.41              |
| 3:E:441:PHE:CE2   | 3:E:1340:PRO:HD3  | 2.56                     | 0.41              |
| 3:E:448:GLN:NE2   | 3:F:1201:ARG:NH1  | 2.65                     | 0.41              |
| 3:E:513:LEU:HD23  | 3:E:513:LEU:HA    | 1.84                     | 0.41              |
| 3:E:668:TYR:O     | 3:E:672:SER:N     | 2.43                     | 0.41              |
| 3:E:753:ASP:CB    | 3:E:755:ARG:HH12  | 2.32                     | 0.41              |
| 3:F:129:LEU:O     | 3:F:1094:THR:HA   | 2.21                     | 0.41              |
| 3:F:630:LEU:O     | 3:F:634:ILE:HD12  | 2.21                     | 0.41              |
| 3:F:769:CYS:O     | 3:F:901:MET:N     | 2.28                     | 0.41              |
| 3:F:1036:LEU:HD23 | 3:F:1039:GLN:OE1  | 2.20                     | 0.41              |
| 3:G:106:ARG:HB3   | 3:G:110:HIS:HB2   | 2.03                     | 0.41              |
| 3:G:432:PRO:HA    | 3:G:435:PHE:CD2   | 2.56                     | 0.41              |
| 3:G:712:PRO:HD2   | 3:G:1146:TYR:CZ   | 2.56                     | 0.41              |
| 7:u:3116:HIS:ND1  | 7:u:3119:MET:SD   | 2.89                     | 0.41              |
| 2:R:220:ILE:HG12  | 2:S:209:MET:HB3   | 2.01                     | 0.40              |
| 2:S:32:VAL:HG13   | 2:S:46:VAL:HG13   | 2.03                     | 0.40              |
| 2:S:300:PHE:CD2   | 3:A:111:PRO:HG3   | 2.45                     | 0.40              |
| 2:U:306:VAL:HG11  | 2:U:312:ALA:HB2   | 2.03                     | 0.40              |
| 2:V:10:ILE:HG12   | 2:V:46:VAL:HG21   | 2.03                     | 0.40              |
| 1:w:282:PRO:CG    | 3:L:138:GLU:OE2   | 2.67                     | 0.40              |
| 3:I:71:LEU:HD23   | 3:I:71:LEU:HA     | 1.80                     | 0.40              |
| 3:I:219:LEU:HD23  | 3:I:219:LEU:HA    | 1.93                     | 0.40              |
| 3:I:266:HIS:CE1   | 3:I:303:PRO:HD2   | 2.57                     | 0.40              |
| 3:I:509:TRP:CZ2   | 3:I:564:PRO:HD3   | 2.57                     | 0.40              |
| 3:I:745:HIS:CD2   | 3:I:754:CYS:SG    | 3.14                     | 0.40              |
| 3:I:895:GLN:NE2   | 4:i:62:THR:HA     | 2.36                     | 0.40              |
| 3:I:1054:ARG:NH2  | 3:I:1122:MET:HB3  | 2.36                     | 0.40              |
| 3:J:251:LEU:HD23  | 3:J:251:LEU:HA    | 1.90                     | 0.40              |
| 3:J:1034:VAL:HG22 | 3:J:1147:LEU:HD21 | 2.03                     | 0.40              |
| 3:K:493:ALA:N     | 3:K:559:PRO:HB2   | 2.35                     | 0.40              |
| 3:K:745:HIS:CE1   | 3:K:754:CYS:HA    | 2.57                     | 0.40              |
| 3:K:961:HIS:HD2   | 3:K:963:LEU:HB2   | 1.86                     | 0.40              |
| 3:L:39:PHE:CD1    | 3:O:120:MET:HG2   | 2.52                     | 0.40              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:L:542:GLU:OE2  | 3:L:576:ARG:NH2   | 2.54                     | 0.40              |
| 3:L:545:PRO:HB2  | 3:L:1048:PHE:HE1  | 1.86                     | 0.40              |
| 3:L:578:VAL:HB   | 3:L:1028:TYR:HA   | 2.03                     | 0.40              |
| 3:L:739:CYS:HB3  | 3:L:765:TYR:CD1   | 2.56                     | 0.40              |
| 3:L:1074:PHE:O   | 3:L:1098:GLY:N    | 2.49                     | 0.40              |
| 3:M:97:PHE:HD1   | 3:N:23:ILE:HD11   | 1.86                     | 0.40              |
| 3:M:120:MET:HB3  | 3:N:36:PHE:CD1    | 2.56                     | 0.40              |
| 3:M:124:ILE:HG12 | 3:M:1100:VAL:CG2  | 2.51                     | 0.40              |
| 3:M:272:ARG:HD3  | 3:M:374:LEU:HD11  | 2.03                     | 0.40              |
| 3:A:510:ARG:CZ   | 3:A:977:PRO:HG3   | 2.51                     | 0.40              |
| 3:A:517:ARG:HD2  | 3:A:522:ALA:CB    | 2.50                     | 0.40              |
| 3:A:1075:LEU:HA  | 3:A:1097:ARG:HG2  | 2.03                     | 0.40              |
| 3:H:198:LEU:HA   | 3:H:198:LEU:HD23  | 1.64                     | 0.40              |
| 3:H:241:ARG:NE   | 3:H:245:GLU:OE2   | 2.52                     | 0.40              |
| 3:H:438:ARG:O    | 3:H:454:MET:HG3   | 2.21                     | 0.40              |
| 3:H:746:ALA:HA   | 3:H:754:CYS:CB    | 2.51                     | 0.40              |
| 3:H:835:VAL:O    | 3:H:839:LEU:N     | 2.48                     | 0.40              |
| 3:H:1201:ARG:HB2 | 3:H:1202:PRO:HD2  | 2.03                     | 0.40              |
| 4:j:64:LEU:HG    | 4:j:68:HIS:HD2    | 1.85                     | 0.40              |
| 4:k:76:GLN:OE1   | 4:k:98:TYR:OH     | 2.18                     | 0.40              |
| 3:N:724:HIS:HE1  | 3:N:1025:MET:O    | 2.04                     | 0.40              |
| 3:O:296:GLU:OE1  | 3:O:374:LEU:HD21  | 2.20                     | 0.40              |
| 3:O:915:ASP:O    | 3:O:919:ASN:HB2   | 2.21                     | 0.40              |
| 3:O:1007:VAL:O   | 3:O:1010:ALA:HB3  | 2.21                     | 0.40              |
| 3:P:133:PHE:O    | 3:P:133:PHE:CG    | 2.73                     | 0.40              |
| 3:P:544:HIS:CG   | 3:P:545:PRO:HD2   | 2.55                     | 0.40              |
| 3:P:793:ASP:OD2  | 3:P:800:HIS:ND1   | 2.53                     | 0.40              |
| 3:P:1166:PHE:CD1 | 3:P:1167:GLY:N    | 2.89                     | 0.40              |
| 3:B:742:LEU:HA   | 3:B:745:HIS:HB3   | 2.03                     | 0.40              |
| 3:C:604:HIS:CD2  | 3:C:696:HIS:HA    | 2.56                     | 0.40              |
| 3:D:193:PRO:CB   | 3:D:1293:ILE:HG22 | 2.51                     | 0.40              |
| 3:D:300:ALA:N    | 3:D:363:VAL:O     | 2.51                     | 0.40              |
| 3:D:469:ILE:HD11 | 3:D:547:PHE:CE2   | 2.56                     | 0.40              |
| 3:D:475:GLY:O    | 3:D:478:HIS:CD2   | 2.74                     | 0.40              |
| 3:D:584:LEU:HD23 | 3:D:584:LEU:HA    | 1.94                     | 0.40              |
| 3:D:740:ASP:O    | 3:D:743:MET:HB2   | 2.20                     | 0.40              |
| 3:D:829:GLY:HA2  | 3:D:905:THR:HG21  | 2.03                     | 0.40              |
| 3:D:874:THR:H    | 3:D:877:ALA:HB3   | 1.86                     | 0.40              |
| 5:q:430:CYS:SG   | 5:q:438:PRO:HA    | 2.60                     | 0.40              |
| 3:E:173:LEU:HD23 | 3:E:173:LEU:HA    | 1.85                     | 0.40              |
| 3:E:469:ILE:HD11 | 3:E:547:PHE:CD2   | 2.55                     | 0.40              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:E:469:ILE:HG21 | 3:E:469:ILE:HD13  | 1.77                     | 0.40              |
| 3:F:129:LEU:HD12 | 3:F:1097:ARG:NH1  | 2.36                     | 0.40              |
| 3:F:149:ASP:HB3  | 3:F:151:THR:HG23  | 2.03                     | 0.40              |
| 3:F:187:VAL:HG11 | 3:F:1071:GLU:OE2  | 2.21                     | 0.40              |
| 3:F:644:LEU:HA   | 3:F:644:LEU:HD23  | 1.82                     | 0.40              |
| 6:s:80:ILE:HD13  | 7:t:3103:LEU:HB3  | 2.03                     | 0.40              |
| 6:s:92:HIS:HA    | 7:t:3093:GLN:NE2  | 2.36                     | 0.40              |
| 3:G:103:LEU:CD2  | 3:G:113:GLU:C     | 2.81                     | 0.40              |
| 3:G:665:VAL:O    | 3:G:812:TYR:OH    | 2.29                     | 0.40              |
| 2:R:276:VAL:HG21 | 2:S:154:ARG:HD3   | 2.02                     | 0.40              |
| 2:S:147:LEU:HD21 | 2:S:181:TYR:HB2   | 2.02                     | 0.40              |
| 1:T:258:ASP:CB   | 3:I:1318:ARG:HD2  | 2.52                     | 0.40              |
| 1:T:259:GLU:OE1  | 3:I:1315:PRO:C    | 2.63                     | 0.40              |
| 1:W:29:GLY:HA2   | 3:H:144:THR:N     | 2.35                     | 0.40              |
| 2:X:38:ARG:NH2   | 3:I:109:PRO:HA    | 2.36                     | 0.40              |
| 1:1:25:ARG:O     | 1:1:28:ALA:HB3    | 2.21                     | 0.40              |
| 2:3:10:ILE:HD13  | 2:3:46:VAL:HG21   | 2.04                     | 0.40              |
| 3:I:133:PHE:HZ   | 3:I:165:LEU:HD22  | 1.87                     | 0.40              |
| 3:I:469:ILE:HD11 | 3:I:547:PHE:CD2   | 2.56                     | 0.40              |
| 3:I:834:ARG:NH1  | 3:I:953:GLU:HA    | 2.37                     | 0.40              |
| 3:I:950:GLN:HB2  | 3:I:953:GLU:CG    | 2.51                     | 0.40              |
| 3:J:108:GLY:HA2  | 3:J:110:HIS:N     | 2.36                     | 0.40              |
| 3:J:865:LEU:HD21 | 3:J:879:PHE:CD2   | 2.56                     | 0.40              |
| 3:K:148:LEU:HD21 | 3:K:158:GLN:HG3   | 2.03                     | 0.40              |
| 3:K:198:LEU:HD23 | 3:K:198:LEU:HA    | 1.74                     | 0.40              |
| 3:K:724:HIS:HD2  | 3:K:726:MET:HB2   | 1.86                     | 0.40              |
| 3:L:630:LEU:HD23 | 3:L:630:LEU:HA    | 1.92                     | 0.40              |
| 3:L:854:PRO:HG3  | 3:L:862:ALA:O     | 2.21                     | 0.40              |
| 3:M:27:ILE:CG1   | 3:D:256:GLN:CD    | 2.93                     | 0.40              |
| 3:M:44:SER:O     | 3:M:45:ASP:HB2    | 2.21                     | 0.40              |
| 3:M:71:LEU:O     | 3:M:302:VAL:HG11  | 2.21                     | 0.40              |
| 3:M:248:LEU:HD23 | 3:M:248:LEU:HA    | 1.84                     | 0.40              |
| 3:M:258:SER:OG   | 3:M:259:VAL:N     | 2.54                     | 0.40              |
| 3:M:932:ALA:O    | 3:M:933:LEU:HD23  | 2.21                     | 0.40              |
| 3:A:627:PHE:HD1  | 3:A:664:PHE:CE2   | 2.39                     | 0.40              |
| 3:A:1118:PRO:HG3 | 3:A:1122:MET:HE3  | 2.03                     | 0.40              |
| 3:A:1122:MET:HE1 | 3:A:1374:LEU:HD22 | 2.02                     | 0.40              |
| 3:H:616:GLY:HA3  | 3:H:661:CYS:SG    | 2.62                     | 0.40              |
| 3:H:753:ASP:HB3  | 3:H:755:ARG:NH2   | 2.36                     | 0.40              |
| 3:H:845:PRO:HG3  | 3:H:869:ASN:HD21  | 1.86                     | 0.40              |
| 3:H:863:HIS:CD2  | 3:H:865:LEU:HB2   | 2.56                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:H:1082:ARG:HG3  | 3:H:1091:PHE:CE1  | 2.56                     | 0.40              |
| 4:h:94:LEU:HD23   | 4:h:94:LEU:HA     | 1.87                     | 0.40              |
| 4:n:68:HIS:O      | 4:n:71:ASN:N      | 2.48                     | 0.40              |
| 4:o:79:PHE:HB3    | 3:P:947:HIS:O     | 2.21                     | 0.40              |
| 3:N:914:PRO:HG3   | 3:N:923:THR:HG22  | 2.03                     | 0.40              |
| 3:O:438:ARG:O     | 3:O:454:MET:HG2   | 2.22                     | 0.40              |
| 3:O:1232:SER:HB2  | 3:O:1237:PRO:O    | 2.21                     | 0.40              |
| 3:P:137:THR:HG22  | 3:P:1087:GLY:O    | 2.21                     | 0.40              |
| 3:P:903:GLU:HB3   | 3:P:904:ARG:NH1   | 2.36                     | 0.40              |
| 3:B:222:GLU:HG2   | 3:G:1117:ASN:ND2  | 2.36                     | 0.40              |
| 3:B:1117:ASN:HB3  | 3:C:222:GLU:OE2   | 2.21                     | 0.40              |
| 3:C:331:ASP:O     | 3:C:334:ARG:N     | 2.53                     | 0.40              |
| 3:C:380:LEU:HD23  | 3:C:380:LEU:HA    | 1.89                     | 0.40              |
| 3:C:485:ASN:HD21  | 3:C:516:GLY:CA    | 2.34                     | 0.40              |
| 3:C:1024:LEU:HD23 | 3:C:1024:LEU:HA   | 1.85                     | 0.40              |
| 3:D:591:PHE:HE2   | 3:D:595:ARG:HH21  | 1.69                     | 0.40              |
| 3:D:604:HIS:CG    | 3:D:605:ALA:N     | 2.89                     | 0.40              |
| 3:D:623:TYR:CE1   | 3:D:940:MET:HE1   | 2.55                     | 0.40              |
| 3:D:1036:LEU:HA   | 3:D:1036:LEU:HD23 | 1.68                     | 0.40              |
| 5:q:557:ALA:HB2   | 5:q:576:ILE:HD11  | 2.02                     | 0.40              |
| 3:E:83:LYS:HG2    | 3:E:308:GLU:HG2   | 2.03                     | 0.40              |
| 3:E:198:LEU:O     | 3:E:201:MET:HB2   | 2.22                     | 0.40              |
| 3:E:402:PHE:HA    | 3:E:1332:TYR:O    | 2.20                     | 0.40              |
| 3:E:677:TYR:HA    | 4:e:95:LYS:HZ3    | 1.83                     | 0.40              |
| 3:E:836:TYR:CE1   | 3:E:897:LEU:HD22  | 2.57                     | 0.40              |
| 3:E:1207:GLY:HA2  | 3:E:1242:ALA:HB3  | 2.03                     | 0.40              |
| 3:G:440:LEU:N     | 3:G:452:LEU:O     | 2.54                     | 0.40              |
| 1:T:116:LEU:HA    | 1:T:260:LEU:HA    | 2.03                     | 0.40              |
| 2:U:287:ASP:OD2   | 2:V:149:ARG:NH1   | 2.54                     | 0.40              |
| 1:W:122:PRO:HB2   | 1:W:254:TRP:CG    | 2.57                     | 0.40              |
| 3:I:162:ILE:HG22  | 3:J:344:LEU:CD1   | 2.50                     | 0.40              |
| 3:I:309:MET:SD    | 3:I:327:ARG:HG3   | 2.61                     | 0.40              |
| 3:I:467:MET:O     | 3:I:922:SER:OG    | 2.38                     | 0.40              |
| 3:I:502:GLN:O     | 3:I:505:PHE:HB3   | 2.21                     | 0.40              |
| 3:J:765:TYR:CD1   | 3:J:783:LEU:HB2   | 2.57                     | 0.40              |
| 3:J:1065:PHE:CG   | 3:J:1066:SER:N    | 2.89                     | 0.40              |
| 3:K:506:LEU:O     | 3:K:510:ARG:HG3   | 2.20                     | 0.40              |
| 3:K:718:ALA:HB1   | 3:L:982:ASP:OD2   | 2.21                     | 0.40              |
| 3:L:310:VAL:HG12  | 3:L:312:ASN:H     | 1.86                     | 0.40              |
| 3:L:469:ILE:HD13  | 3:L:469:ILE:HG21  | 1.86                     | 0.40              |
| 3:L:646:ARG:HD3   | 3:L:890:ALA:HB2   | 2.03                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:L:1004:GLN:O    | 3:L:1007:VAL:N    | 2.41                     | 0.40              |
| 3:L:1138:LEU:HD21 | 3:L:1147:LEU:HD12 | 2.03                     | 0.40              |
| 3:L:1292:LEU:HA   | 3:L:1292:LEU:HD23 | 1.90                     | 0.40              |
| 3:M:558:LEU:H     | 3:M:558:LEU:HG    | 1.73                     | 0.40              |
| 3:A:1335:THR:N    | 3:A:1365:ASP:HB3  | 2.35                     | 0.40              |
| 3:A:1343:LEU:O    | 3:A:1346:ALA:N    | 2.51                     | 0.40              |
| 3:H:408:LEU:HA    | 3:H:408:LEU:HD23  | 1.77                     | 0.40              |
| 3:H:460:THR:HA    | 3:H:1129:PHE:CE2  | 2.57                     | 0.40              |
| 3:H:462:CYS:O     | 3:H:1033:PRO:HB3  | 2.21                     | 0.40              |
| 3:H:1072:ALA:HB2  | 3:H:1102:LEU:HD23 | 2.03                     | 0.40              |
| 3:H:1190:THR:HG22 | 3:H:1243:ASN:ND2  | 2.37                     | 0.40              |
| 4:n:65:GLY:HA3    | 3:N:895:GLN:HE22  | 1.87                     | 0.40              |
| 3:N:66:SER:OG     | 3:N:178:ARG:NH2   | 2.54                     | 0.40              |
| 3:N:400:LEU:HD12  | 3:N:1058:PHE:HE2  | 1.86                     | 0.40              |
| 3:N:463:HIS:HD2   | 3:N:465:SER:CB    | 2.29                     | 0.40              |
| 3:O:79:CYS:SG     | 3:O:184:MET:HG3   | 2.62                     | 0.40              |
| 3:O:193:PRO:HD2   | 3:O:1108:ALA:O    | 2.21                     | 0.40              |
| 3:O:1173:ARG:HH12 | 3:P:1218:LYS:HB2  | 1.87                     | 0.40              |
| 3:O:1292:LEU:HB3  | 3:O:1327:LEU:HD21 | 2.03                     | 0.40              |
| 3:P:165:LEU:O     | 3:P:166:ALA:C     | 2.64                     | 0.40              |
| 3:P:989:LEU:O     | 3:P:990:VAL:C     | 2.65                     | 0.40              |
| 3:P:1139:LEU:HD23 | 3:P:1139:LEU:HA   | 1.89                     | 0.40              |
| 3:B:65:LEU:HD22   | 3:C:102:PRO:HB3   | 2.02                     | 0.40              |
| 3:B:141:ALA:HB1   | 3:B:147:ALA:HB2   | 2.03                     | 0.40              |
| 3:B:250:ASP:O     | 3:B:251:LEU:C     | 2.65                     | 0.40              |
| 3:B:441:PHE:N     | 3:B:1337:ALA:O    | 2.55                     | 0.40              |
| 3:B:539:LEU:HA    | 3:B:539:LEU:HD23  | 1.68                     | 0.40              |
| 3:B:888:GLY:O     | 3:B:892:LEU:HG    | 2.21                     | 0.40              |
| 3:B:1217:ASP:O    | 3:B:1218:LYS:HG3  | 2.20                     | 0.40              |
| 3:C:375:VAL:HG12  | 3:C:376:PHE:O     | 2.21                     | 0.40              |
| 3:C:390:VAL:HG21  | 3:D:104:ILE:CD1   | 2.44                     | 0.40              |
| 3:C:848:ALA:HB3   | 3:C:851:GLU:HB2   | 2.04                     | 0.40              |
| 3:C:1075:LEU:HA   | 3:C:1097:ARG:HG2  | 2.03                     | 0.40              |
| 3:C:1291:ARG:HA   | 3:C:1291:ARG:HD3  | 1.82                     | 0.40              |
| 3:D:85:PRO:HG2    | 3:D:86:GLU:OE1    | 2.21                     | 0.40              |
| 3:D:520:TRP:CG    | 3:D:997:ASN:ND2   | 2.89                     | 0.40              |
| 3:D:521:VAL:HG21  | 3:D:987:VAL:HG12  | 2.03                     | 0.40              |
| 3:D:543:LEU:HD12  | 3:D:549:PHE:CE2   | 2.56                     | 0.40              |
| 3:D:593:ASP:OD2   | 3:D:1015:ALA:HB2  | 2.21                     | 0.40              |
| 3:D:1013:SER:OG   | 3:D:1020:LEU:HD21 | 2.22                     | 0.40              |
| 5:q:133:ARG:HE    | 5:q:143:ALA:HB1   | 1.87                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 5:q:163:ASP:OD2  | 5:q:382:SER:HA   | 2.22                     | 0.40              |
| 3:E:172:VAL:C    | 3:E:174:GLY:N    | 2.80                     | 0.40              |
| 3:E:788:GLN:NE2  | 3:E:794:ALA:HA   | 2.35                     | 0.40              |
| 3:E:1202:PRO:HA  | 3:E:1333:PRO:HD3 | 2.03                     | 0.40              |
| 3:F:187:VAL:HG21 | 3:F:1099:ASN:ND2 | 2.36                     | 0.40              |
| 3:F:604:HIS:CG   | 3:F:605:ALA:N    | 2.89                     | 0.40              |
| 3:F:873:ASN:CA   | 4:e:92:PHE:HD2   | 2.34                     | 0.40              |
| 3:F:1129:PHE:O   | 3:F:1132:GLY:N   | 2.55                     | 0.40              |
| 6:s:90:GLN:HB3   | 7:u:3092:ILE:CD1 | 2.52                     | 0.40              |
| 3:G:475:GLY:HA3  | 3:G:1250:PHE:CE2 | 2.54                     | 0.40              |
| 1:Q:133:ALA:N    | 1:Q:246:ARG:O    | 2.55                     | 0.40              |
| 2:U:300:PHE:CG   | 3:I:1083:HIS:NE2 | 2.90                     | 0.40              |
| 2:2:20:ASP:HB3   | 2:2:130:LEU:HD22 | 2.02                     | 0.40              |
| 3:I:124:ILE:HG12 | 3:I:1100:VAL:CG2 | 2.50                     | 0.40              |
| 3:I:403:VAL:HA   | 3:I:1052:VAL:O   | 2.21                     | 0.40              |
| 3:I:406:LEU:HD11 | 3:I:1187:PHE:HE1 | 1.87                     | 0.40              |
| 3:I:744:ARG:HH12 | 3:I:799:PRO:HG3  | 1.85                     | 0.40              |
| 3:I:861:PRO:HA   | 3:I:866:HIS:CD2  | 2.57                     | 0.40              |
| 3:J:600:GLY:C    | 3:J:602:GLY:H    | 2.28                     | 0.40              |
| 3:J:634:ILE:O    | 3:J:635:HIS:CG   | 2.75                     | 0.40              |
| 3:K:84:PHE:O     | 3:K:1076:GLY:HA2 | 2.21                     | 0.40              |
| 3:K:130:ASN:HA   | 3:K:1093:LEU:O   | 2.21                     | 0.40              |
| 3:K:241:ARG:NE   | 3:K:245:GLU:OE2  | 2.38                     | 0.40              |
| 3:K:485:ASN:HD21 | 3:K:516:GLY:CA   | 2.34                     | 0.40              |
| 3:K:753:ASP:OD1  | 3:K:753:ASP:N    | 2.54                     | 0.40              |
| 3:L:12:ARG:H     | 3:O:96:GLN:NE2   | 2.20                     | 0.40              |
| 3:L:467:MET:HE1  | 3:L:1032:SER:HA  | 2.03                     | 0.40              |
| 3:L:769:CYS:SG   | 3:L:786:ASN:ND2  | 2.87                     | 0.40              |
| 3:M:870:LEU:HD22 | 3:M:877:ALA:N    | 2.36                     | 0.40              |
| 3:M:1032:SER:O   | 3:M:1035:ALA:N   | 2.54                     | 0.40              |
| 3:M:1342:LEU:CD2 | 3:M:1362:LEU:HB2 | 2.50                     | 0.40              |
| 3:A:578:VAL:H    | 3:A:581:ASN:ND2  | 2.19                     | 0.40              |
| 3:A:784:LEU:CD2  | 3:A:903:GLU:H    | 2.34                     | 0.40              |
| 3:H:384:ILE:HG22 | 3:H:385:TYR:N    | 2.37                     | 0.40              |
| 3:H:864:PRO:HB2  | 3:H:876:ASN:CG   | 2.47                     | 0.40              |
| 4:n:22:MET:HE2   | 4:n:60:ALA:HB3   | 2.03                     | 0.40              |
| 4:n:100:PRO:HD2  | 3:N:646:ARG:HH12 | 1.86                     | 0.40              |
| 3:N:84:PHE:HB3   | 3:N:86:GLU:O     | 2.21                     | 0.40              |
| 3:N:606:MET:HE3  | 3:N:611:ILE:HG12 | 2.04                     | 0.40              |
| 3:N:637:SER:HB2  | 3:N:787:THR:HA   | 2.02                     | 0.40              |
| 3:N:812:TYR:CD1  | 3:N:816:LEU:HD12 | 2.56                     | 0.40              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:N:858:VAL:O    | 3:N:866:HIS:ND1   | 2.51                     | 0.40              |
| 3:O:1155:ASN:C   | 3:O:1157:LEU:H    | 2.30                     | 0.40              |
| 3:B:406:LEU:HD23 | 3:B:406:LEU:HA    | 1.83                     | 0.40              |
| 3:B:575:TRP:O    | 3:B:1003:ARG:NH2  | 2.55                     | 0.40              |
| 3:B:816:LEU:HD23 | 3:B:816:LEU:HA    | 1.77                     | 0.40              |
| 3:C:58:LEU:HA    | 3:C:58:LEU:HD23   | 1.75                     | 0.40              |
| 3:C:143:LEU:HD21 | 3:C:162:ILE:HG12  | 2.03                     | 0.40              |
| 3:C:266:HIS:CE1  | 3:C:303:PRO:HD2   | 2.56                     | 0.40              |
| 3:C:392:TYR:HE2  | 3:C:394:LEU:HB3   | 1.86                     | 0.40              |
| 3:C:656:TRP:O    | 3:C:660:ARG:HA    | 2.22                     | 0.40              |
| 3:C:842:MET:HB3  | 3:C:842:MET:HE3   | 1.88                     | 0.40              |
| 3:C:923:THR:HG22 | 3:C:923:THR:O     | 2.22                     | 0.40              |
| 3:C:1049:GLY:O   | 3:C:1190:THR:OG1  | 2.27                     | 0.40              |
| 3:D:127:ARG:NH1  | 3:D:187:VAL:HG22  | 2.36                     | 0.40              |
| 3:D:309:MET:CE   | 3:D:327:ARG:HA    | 2.52                     | 0.40              |
| 3:D:336:LEU:HD23 | 3:D:336:LEU:HA    | 1.85                     | 0.40              |
| 3:D:639:HIS:HB2  | 3:D:789:ALA:O     | 2.22                     | 0.40              |
| 3:D:652:ILE:O    | 3:D:653:THR:C     | 2.64                     | 0.40              |
| 3:D:920:THR:H    | 3:D:923:THR:HB    | 1.86                     | 0.40              |
| 5:q:22:SER:HB2   | 5:q:116:VAL:HB    | 2.03                     | 0.40              |
| 5:q:669:PHE:HE1  | 5:q:671:ILE:HD11  | 1.85                     | 0.40              |
| 3:E:509:TRP:CZ2  | 3:E:564:PRO:HD3   | 2.57                     | 0.40              |
| 3:E:714:LEU:HA   | 3:E:714:LEU:HD23  | 1.78                     | 0.40              |
| 3:E:861:PRO:HA   | 3:E:866:HIS:CD2   | 2.55                     | 0.40              |
| 6:r:76:LEU:N     | 6:r:77:PRO:HD2    | 2.37                     | 0.40              |
| 3:F:293:LEU:HD23 | 3:F:293:LEU:HA    | 1.85                     | 0.40              |
| 3:F:610:THR:HG21 | 3:F:692:ASP:OD2   | 2.22                     | 0.40              |
| 3:F:775:ASP:HB2  | 3:F:778:ARG:HH21  | 1.86                     | 0.40              |
| 3:F:804:ASP:O    | 3:F:805:TRP:C     | 2.64                     | 0.40              |
| 3:F:866:HIS:O    | 3:F:870:LEU:HG    | 2.22                     | 0.40              |
| 3:G:280:THR:HG22 | 3:G:1063:VAL:HG13 | 2.04                     | 0.40              |
| 3:G:550:PHE:CD1  | 3:G:998:TYR:CE2   | 3.00                     | 0.40              |
| 3:G:871:VAL:O    | 3:G:874:THR:OG1   | 2.36                     | 0.40              |
| 2:S:260:MET:HG2  | 5:q:412:ARG:HH11  | 1.85                     | 0.40              |
| 2:U:147:LEU:HD23 | 2:U:147:LEU:HA    | 1.95                     | 0.40              |
| 2:y:205:LEU:HD22 | 2:y:209:MET:HE3   | 2.03                     | 0.40              |
| 3:I:232:PHE:O    | 3:I:236:LYS:HD3   | 2.22                     | 0.40              |
| 3:I:652:ILE:O    | 3:I:655:TYR:N     | 2.54                     | 0.40              |
| 3:I:1056:ASP:HA  | 3:I:1120:THR:OG1  | 2.21                     | 0.40              |
| 3:J:524:CYS:CB   | 3:J:1008:GLN:HE22 | 2.34                     | 0.40              |
| 3:K:244:ILE:O    | 3:K:247:TRP:N     | 2.49                     | 0.40              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 3:K:775:ASP:CB    | 3:K:778:ARG:HH21 | 2.34                     | 0.40              |
| 3:L:623:TYR:HA    | 3:L:624:PRO:HD3  | 1.92                     | 0.40              |
| 3:M:160:ARG:HD2   | 3:C:49:LEU:O     | 2.15                     | 0.40              |
| 3:M:336:LEU:HD23  | 3:M:336:LEU:HA   | 1.83                     | 0.40              |
| 3:M:381:GLU:HB3   | 3:M:392:TYR:CD1  | 2.57                     | 0.40              |
| 3:M:467:MET:O     | 3:M:922:SER:OG   | 2.40                     | 0.40              |
| 3:M:726:MET:HE3   | 3:M:1028:TYR:CD1 | 2.56                     | 0.40              |
| 3:A:490:TYR:CE2   | 3:A:564:PRO:HD3  | 2.57                     | 0.40              |
| 3:A:826:CYS:SG    | 3:A:939:LEU:HB2  | 2.62                     | 0.40              |
| 3:A:1245:TRP:C    | 3:A:1251:SER:HB3 | 2.46                     | 0.40              |
| 3:A:1283:THR:O    | 3:A:1287:ARG:HG2 | 2.22                     | 0.40              |
| 3:H:133:PHE:O     | 3:H:133:PHE:CG   | 2.74                     | 0.40              |
| 3:H:878:MET:HE2   | 4:m:92:PHE:CE2   | 2.56                     | 0.40              |
| 3:H:1017:GLU:O    | 3:H:1020:LEU:N   | 2.54                     | 0.40              |
| 3:N:238:GLY:HA2   | 3:N:244:ILE:HD11 | 2.02                     | 0.40              |
| 3:N:400:LEU:HD23  | 3:N:400:LEU:HA   | 1.90                     | 0.40              |
| 3:N:499:ALA:HA    | 3:N:956:TYR:CD1  | 2.56                     | 0.40              |
| 3:N:950:GLN:HB2   | 3:N:953:GLU:CG   | 2.43                     | 0.40              |
| 3:O:801:ARG:HD3   | 3:O:805:TRP:CD1  | 2.57                     | 0.40              |
| 3:P:98:GLU:HG2    | 3:P:119:TYR:CD1  | 2.57                     | 0.40              |
| 3:P:124:ILE:HG12  | 3:P:1100:VAL:CG2 | 2.52                     | 0.40              |
| 3:P:176:PHE:HD1   | 3:P:176:PHE:HA   | 1.76                     | 0.40              |
| 3:P:582:LEU:HD13  | 3:P:587:CYS:SG   | 2.60                     | 0.40              |
| 3:P:639:HIS:HB2   | 3:P:789:ALA:O    | 2.22                     | 0.40              |
| 3:P:861:PRO:HA    | 3:P:866:HIS:CD2  | 2.56                     | 0.40              |
| 3:B:197:LEU:HD22  | 3:B:223:LEU:HD22 | 2.02                     | 0.40              |
| 3:B:544:HIS:ND1   | 3:B:545:PRO:HD2  | 2.36                     | 0.40              |
| 3:B:547:PHE:CD1   | 3:B:575:TRP:HA   | 2.57                     | 0.40              |
| 3:C:219:LEU:HD23  | 3:C:219:LEU:HA   | 1.76                     | 0.40              |
| 3:C:227:PHE:CE2   | 3:C:1324:PRO:HB3 | 2.56                     | 0.40              |
| 3:C:315:ASN:ND2   | 3:C:326:VAL:O    | 2.54                     | 0.40              |
| 3:C:505:PHE:HD1   | 3:C:509:TRP:CD1  | 2.40                     | 0.40              |
| 3:C:958:LEU:HD23  | 3:C:958:LEU:HA   | 1.84                     | 0.40              |
| 3:C:1067:GLU:O    | 3:C:1068:ARG:C   | 2.64                     | 0.40              |
| 3:C:1270:LEU:HD12 | 3:C:1271:SER:N   | 2.36                     | 0.40              |
| 3:D:756:ILE:HG12  | 3:D:910:CYS:CB   | 2.52                     | 0.40              |
| 3:D:1369:LEU:O    | 3:D:1370:LYS:C   | 2.64                     | 0.40              |
| 5:q:100:LEU:HD23  | 5:q:101:LEU:HG   | 2.03                     | 0.40              |
| 5:q:159:ARG:O     | 5:q:159:ARG:HG3  | 2.21                     | 0.40              |
| 3:E:201:MET:HB3   | 3:E:201:MET:HE3  | 1.74                     | 0.40              |
| 3:F:646:ARG:HD3   | 3:F:890:ALA:HB2  | 2.03                     | 0.40              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:F:731:LEU:HB2  | 3:F:810:LYS:HZ1   | 1.86                     | 0.40              |
| 3:F:783:LEU:HD22 | 3:F:934:HIS:CG    | 2.56                     | 0.40              |
| 3:G:24:LEU:HD23  | 3:G:62:CYS:O      | 2.21                     | 0.40              |
| 3:G:195:LEU:HD21 | 3:G:251:LEU:HD23  | 2.03                     | 0.40              |
| 3:G:666:ASN:CG   | 3:G:938:LEU:HD22  | 2.42                     | 0.40              |
| 3:G:724:HIS:CD2  | 3:G:726:MET:H     | 2.40                     | 0.40              |
| 3:G:983:LEU:CD2  | 3:G:987:VAL:HG22  | 2.51                     | 0.40              |
| 7:t:3095:GLN:O   | 7:t:3099:THR:HG23 | 2.21                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

There are no protein backbone outliers to report in this entry.

### 5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

### 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](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

The following chains have linkage breaks:

| Mol | Chain | Number of breaks |
|-----|-------|------------------|
| 3   | E     | 1                |
| 3   | F     | 1                |
| 3   | L     | 1                |
| 3   | P     | 1                |
| 3   | C     | 1                |
| 3   | B     | 1                |

All chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1     | E     | 1312:LYS  | C      | 1313:ARG  | N      | 1.16         |
| 1     | F     | 1116:ARG  | C      | 1117:ASN  | N      | 1.11         |
| 1     | L     | 485:ASN   | C      | 486:PRO   | N      | 0.98         |
| 1     | P     | 485:ASN   | C      | 486:PRO   | N      | 0.98         |
| 1     | C     | 485:ASN   | C      | 486:PRO   | N      | 0.97         |
| 1     | B     | 485:ASN   | C      | 486:PRO   | N      | 0.93         |

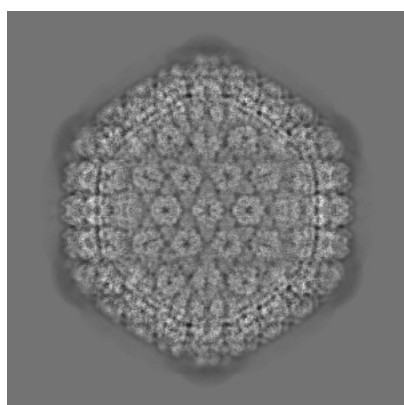
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-6976. These allow visual inspection of the internal detail of the map and identification of artifacts.

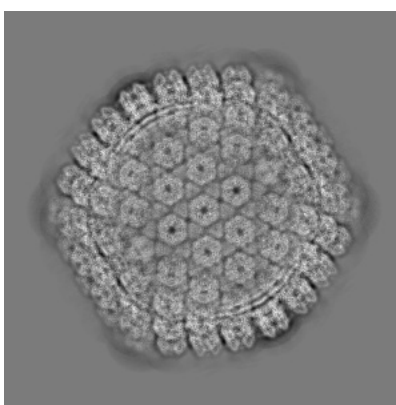
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

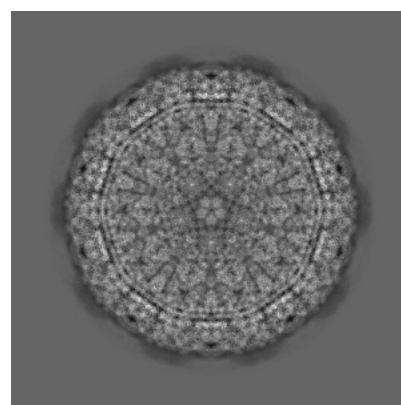
#### 6.1.1 Primary map



X



Y



Z

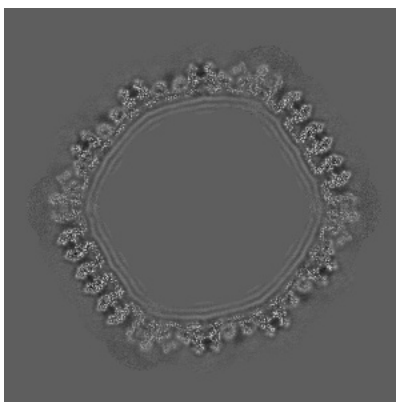
The images above show the map projected in three orthogonal directions.

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

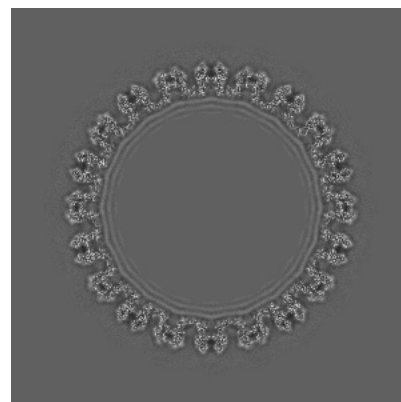
#### 6.2.1 Primary map



X Index: 600



Y Index: 600

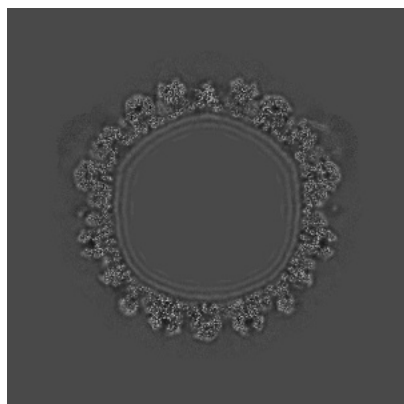


Z Index: 600

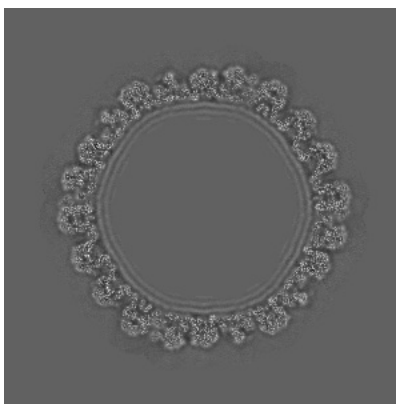
The images above show central slices of the map in three orthogonal directions.

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

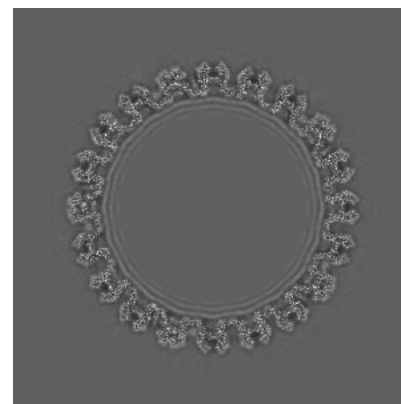
### 6.3.1 Primary map



X Index: 775



Y Index: 502

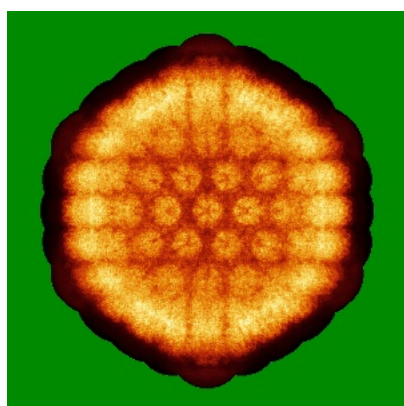


Z Index: 595

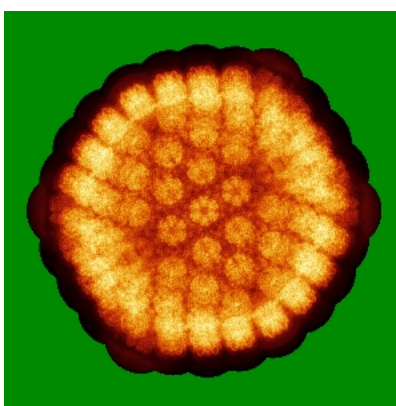
The images above show the largest variance slices of the map in three orthogonal directions.

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

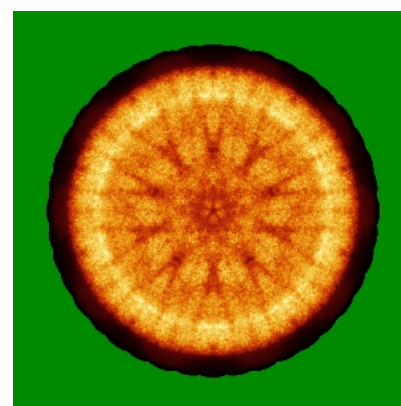
### 6.4.1 Primary map



X



Y



Z

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

## 6.5 Orthogonal surface views

This section was not generated.

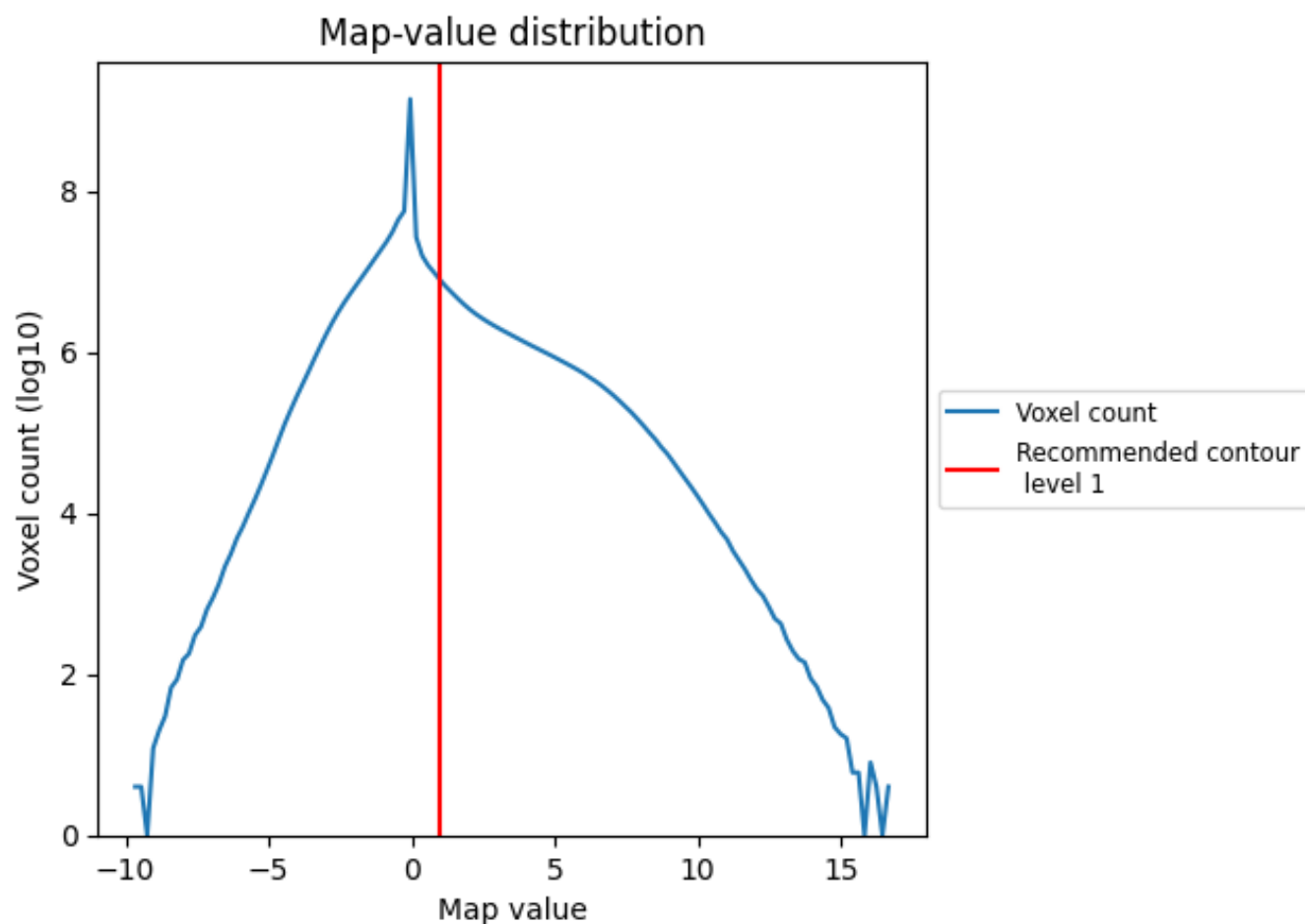
## 6.6 Mask visualisation

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.

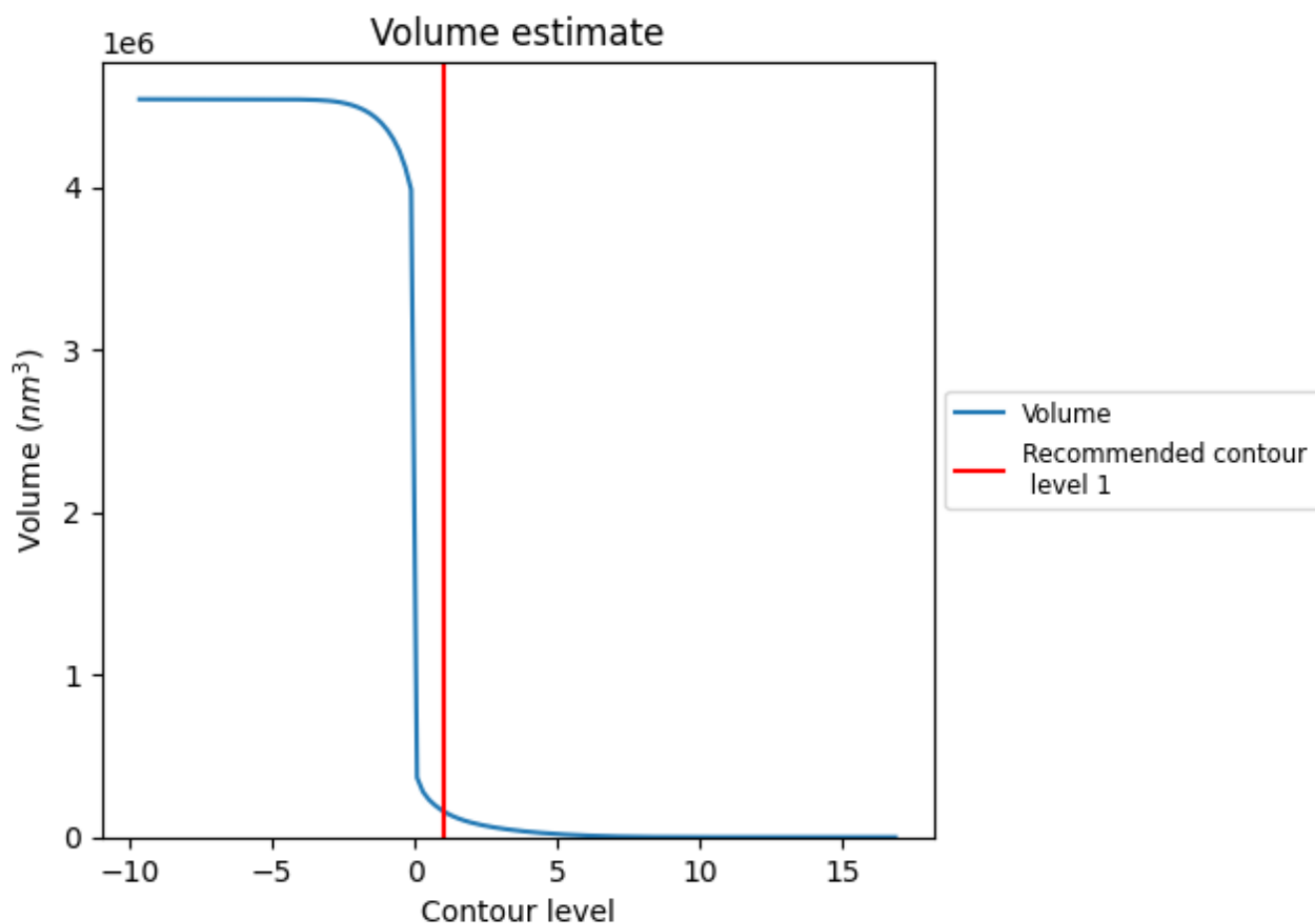
### 7.1 Map-value distribution [i](#)



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.



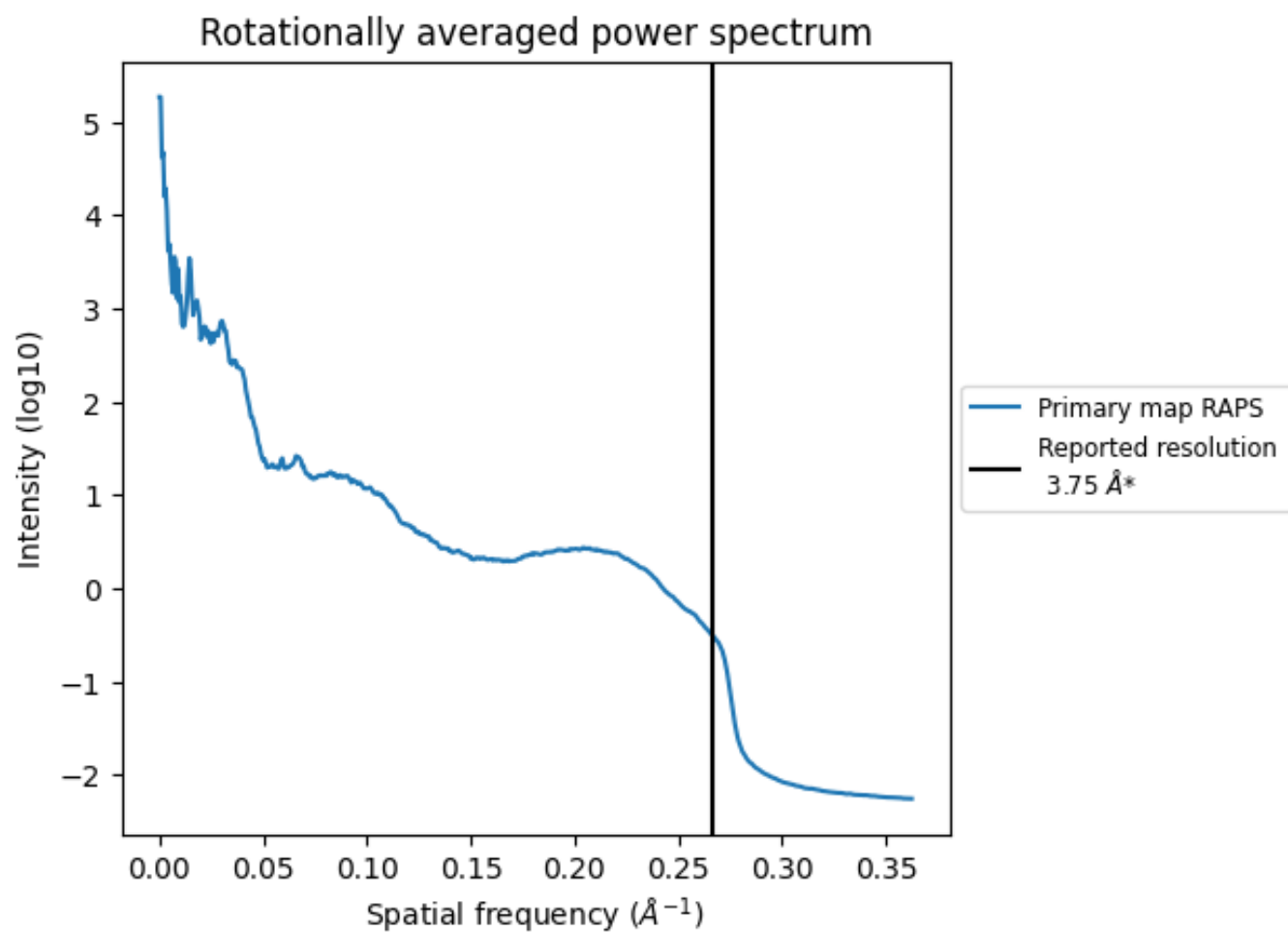
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is  $160951 \text{ nm}^3$ ; this corresponds to an approximate mass of 145391 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 0.267 Å<sup>-1</sup>

## 8 Fourier-Shell correlation

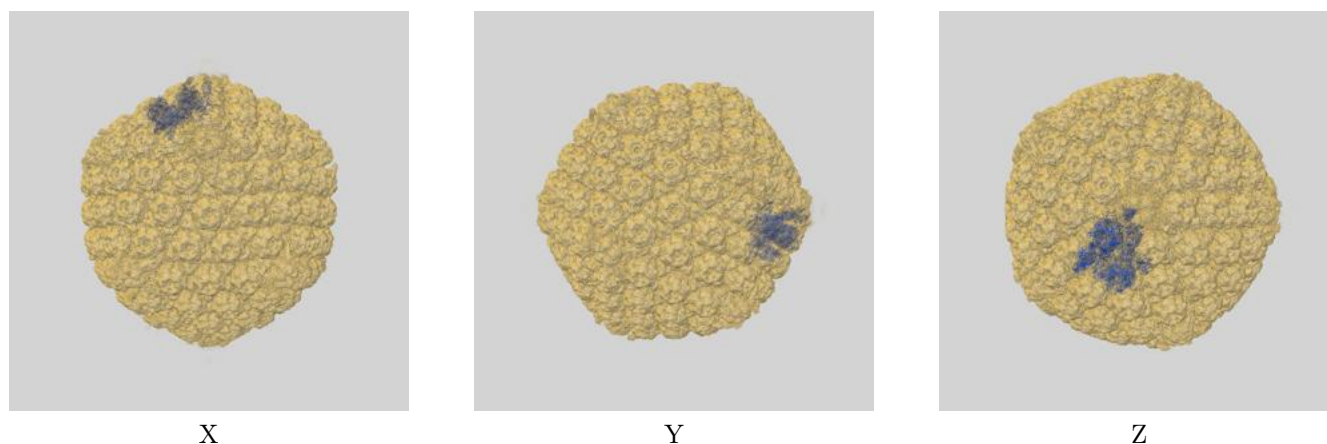
This section was not generated. No FSC curve or half-maps provided.

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

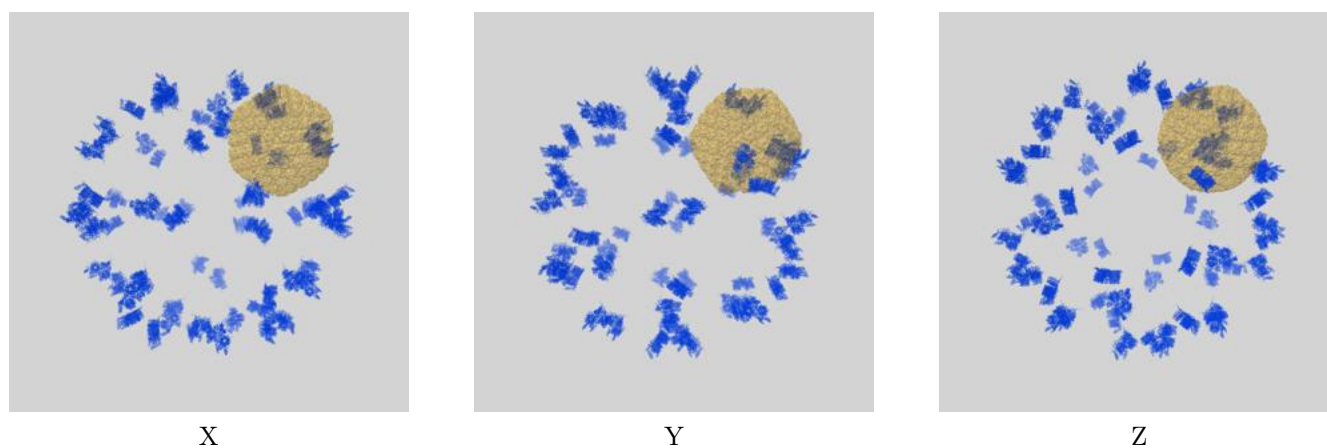
This section contains information regarding the fit between EMDB map EMD-6976 and PDB model 5ZZ8. Per-residue inclusion information can be found in section 3 on page 9.

### 9.1 Map-model overlays

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

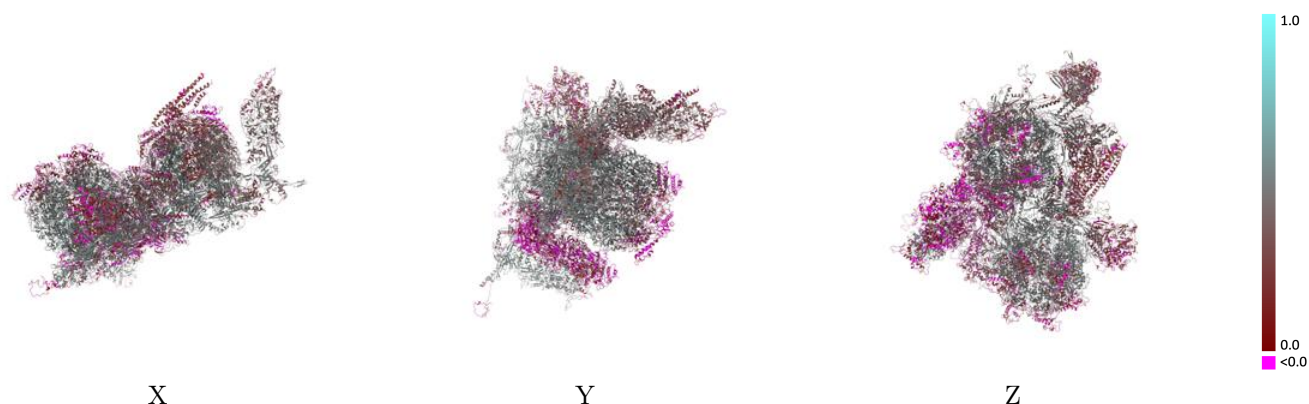


#### 9.1.2 Map-model assembly overlay [i](#)



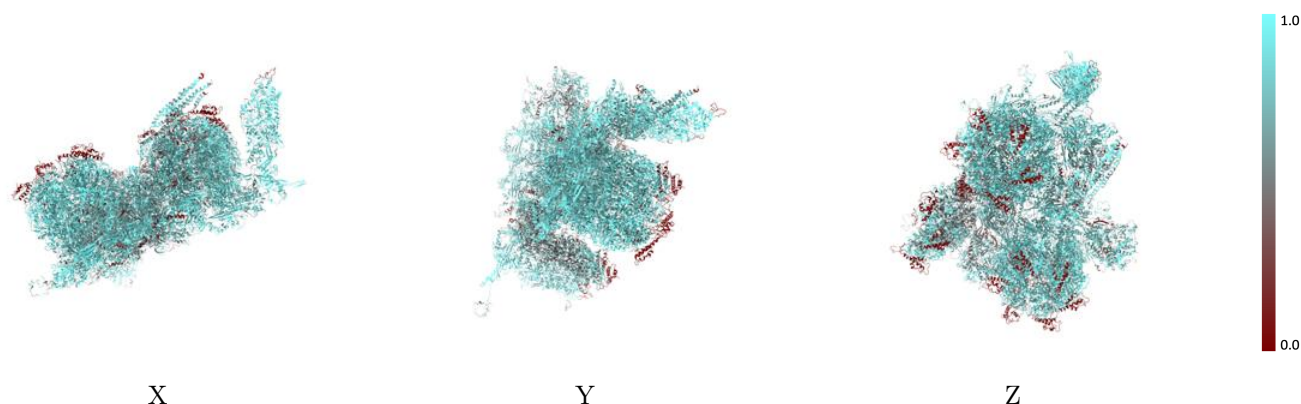
The images above show the 3D surface view of the map at the recommended contour level 1.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



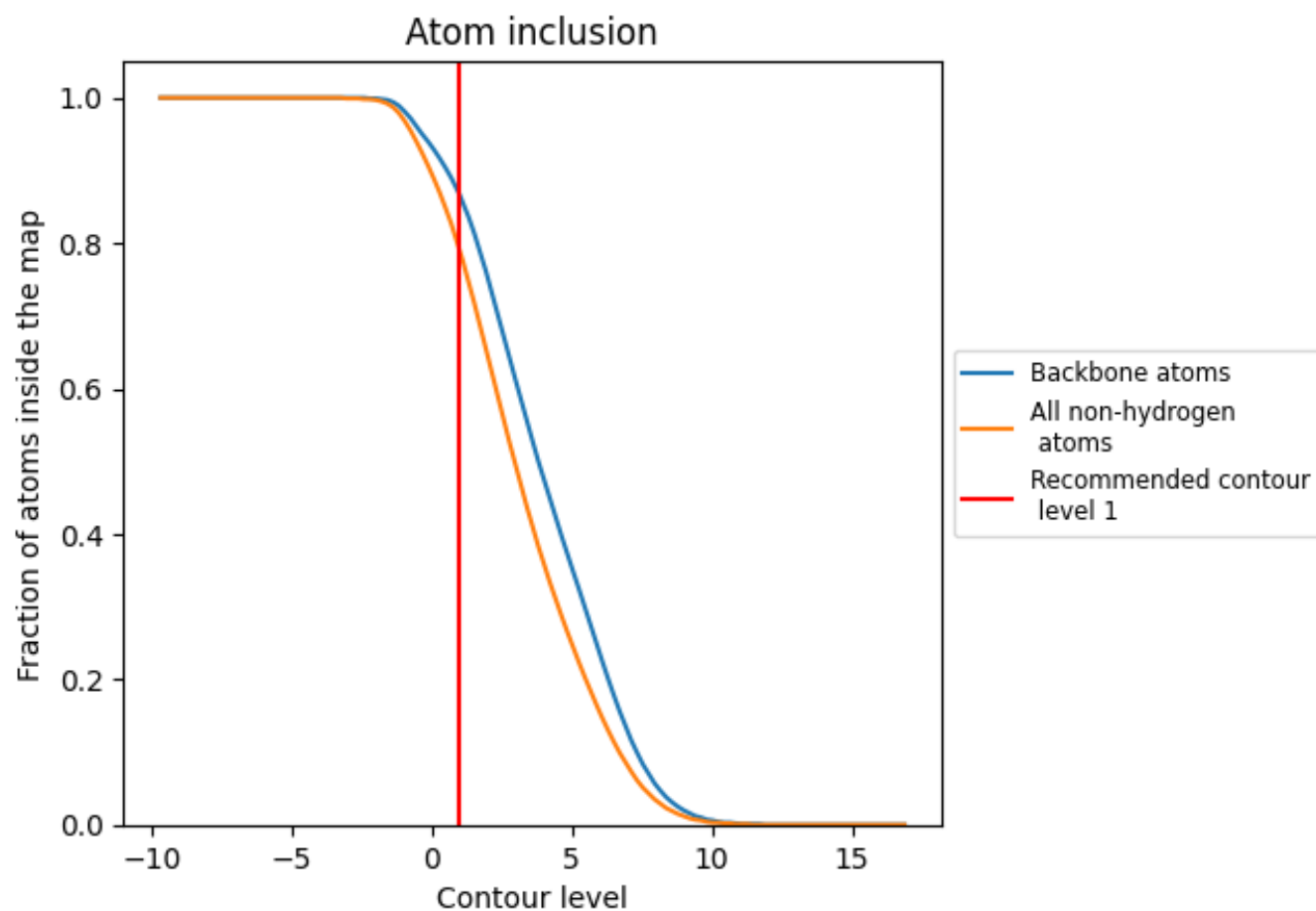
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (1).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 79% 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 (1) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion                                                                             | Q-score                                                                                     |
|-------|--------------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------------|
| All   |  0.7910   |  0.3500    |
| 1     |  0.6180   |  0.1710    |
| 2     |  0.7910   |  0.3110    |
| 3     |  0.8980   |  0.4270    |
| A     |  0.8460   |  0.3780    |
| B     |  0.8810   |  0.4450    |
| C     |  0.9040   |  0.4570    |
| D     |  0.8840   |  0.4460    |
| E     |  0.8840   |  0.4510    |
| F     |  0.8990   |  0.4480    |
| G     |  0.8300   |  0.3650    |
| H     |  0.8950   |  0.4480    |
| I     |  0.8940   |  0.4440    |
| J     |  0.8920   |  0.4470    |
| K     |  0.8890  |  0.4450   |
| L     |  0.8840 |  0.4400  |
| M     |  0.9030 |  0.4530  |
| N     |  0.6140 |  0.0620  |
| O     |  0.6470 |  0.0930  |
| P     |  0.8940 |  0.4520  |
| Q     |  0.6400 |  0.2530  |
| R     |  0.8020 |  0.3460  |
| S     |  0.8050 |  0.3830  |
| T     |  0.6450 |  0.2260  |
| U     |  0.7140 |  0.1450  |
| V     |  0.6880 |  0.1630  |
| W     |  0.6000 |  0.2500  |
| X     |  0.8970 |  0.4290  |
| Y     |  0.8290 |  0.3740  |
| b     |  0.1180 |  0.0060  |
| c     |  0.1340 |  -0.0140 |
| d     |  0.1380 |  -0.0000 |
| e     |  0.1310 |  -0.0240 |
| f     |  0.1310 |  -0.0100 |
| g     |  0.1200 |  0.0070  |



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| Chain | Atom inclusion                                                                           | Q-score                                                                                   |
|-------|------------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------------|
| h     |  0.1920 |  0.0870  |
| i     |  0.2090 |  0.0920  |
| j     |  0.2250 |  0.1070  |
| k     |  0.2090 |  0.0860  |
| l     |  0.1940 |  0.1280  |
| m     |  0.2200 |  0.1180  |
| n     |  0.1430 |  -0.0060 |
| o     |  0.1570 |  0.0230  |
| p     |  0.1790 |  0.1130  |
| q     |  0.6840 |  0.2560  |
| r     |  0.6540 |  0.1910  |
| s     |  0.6770 |  0.2030  |
| t     |  0.7300 |  0.2140  |
| u     |  0.8600 |  0.2120  |
| w     |  0.6040 |  0.1840  |
| x     |  0.6980 |  0.1760  |
| y     |  0.7180 |  0.2490  |