



## Full wwPDB EM Validation Report ⓘ

Mar 26, 2026 – 09:35 PM UTC

PDB ID : 6NHJ / pdb\_00006nhj  
EMDB ID : EMD-9366  
Title : Atomic structures and deletion mutant reveal different capsid-binding patterns and functional significance of tegument protein pp150 in murine and human cytomegaloviruses with implications for therapeutic development  
Authors : Liu, W.; Dai, X.H.; Jih, J.; Chan, K.; Trang, P.; Yu, X.K.; Balogun, R.; Mei, Y.; Liu, F.Y.; Zhou, Z.H.  
Deposited on : 2018-12-22  
Resolution : 5.00 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:

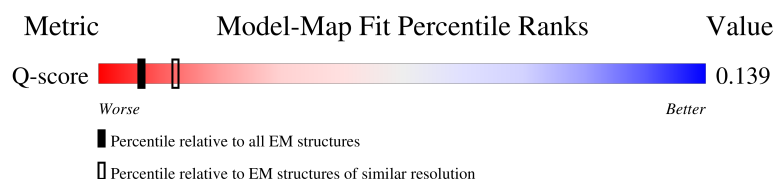
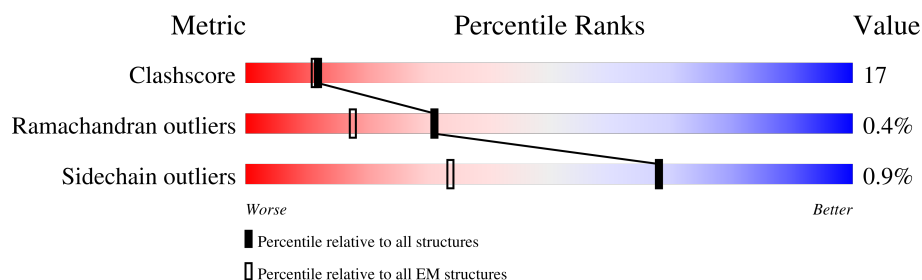
EMDB validation analysis : 0.0.1.dev132  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : 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 5.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



| Metric                | Whole archive<br>(#Entries) | EM structures<br>(#Entries) | Similar EM resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-----------------------------|----------------------------------------------------------|
| Clashscore            | 229148                      | 23984                       | -                                                        |
| Ramachandran outliers | 224038                      | 23583                       | -                                                        |
| Sidechain outliers    | 223484                      | 23102                       | -                                                        |
| Q-score               | -                           | 25397                       | 1057 ( 4.50 - 5.50 )                                     |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain                                                        |
|-----|-------|--------|-------------------------------------------------------------------------|
| 1   | A     | 1353   | <div> <div>28%</div> <div>69%</div> <div>29%</div> <div>..</div> </div> |
| 1   | B     | 1353   | <div> <div>27%</div> <div>68%</div> <div>28%</div> <div>.</div> </div>  |
| 1   | C     | 1353   | <div> <div>30%</div> <div>67%</div> <div>29%</div> <div>..</div> </div> |
| 1   | D     | 1353   | <div> <div>30%</div> <div>64%</div> <div>32%</div> <div>..</div> </div> |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | E     | 1353   |                  |
| 1   | F     | 1353   |                  |
| 1   | G     | 1353   |                  |
| 1   | H     | 1353   |                  |
| 1   | I     | 1353   |                  |
| 1   | k     | 1353   |                  |
| 1   | l     | 1353   |                  |
| 1   | m     | 1353   |                  |
| 1   | n     | 1353   |                  |
| 1   | o     | 1353   |                  |
| 1   | p     | 1353   |                  |
| 1   | q     | 1353   |                  |
| 2   | 2     | 718    |                  |
| 2   | 3     | 718    |                  |
| 2   | e     | 718    |                  |
| 2   | f     | 718    |                  |
| 2   | g     | 718    |                  |
| 2   | h     | 718    |                  |
| 2   | i     | 718    |                  |
| 2   | j     | 718    |                  |
| 3   | J     | 98     |                  |
| 3   | K     | 98     |                  |
| 3   | L     | 98     |                  |
| 3   | M     | 98     |                  |
| 3   | N     | 98     |                  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 3   | O     | 98     |                  |
| 3   | P     | 98     |                  |
| 3   | Q     | 98     |                  |
| 3   | R     | 98     |                  |
| 3   | r     | 98     |                  |
| 3   | s     | 98     |                  |
| 3   | t     | 98     |                  |
| 3   | u     | 98     |                  |
| 3   | v     | 98     |                  |
| 3   | w     | 98     |                  |
| 3   | x     | 98     |                  |
| 4   | S     | 294    |                  |
| 4   | T     | 294    |                  |
| 4   | U     | 294    |                  |
| 4   | V     | 294    |                  |
| 4   | y     | 294    |                  |
| 5   | 1     | 311    |                  |
| 5   | W     | 311    |                  |
| 5   | X     | 311    |                  |
| 5   | Y     | 311    |                  |
| 5   | Z     | 311    |                  |
| 5   | a     | 311    |                  |
| 5   | b     | 311    |                  |
| 5   | c     | 311    |                  |
| 5   | d     | 311    |                  |

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| Mol | Chain | Length | Quality of chain                                                              |
|-----|-------|--------|-------------------------------------------------------------------------------|
| 5   | z     | 311    | <div><div></div><div>53%</div><div>55%</div><div>33%</div><div>9%</div></div> |

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 218639 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 Major capsid protein.

| Mol | Chain | Residues | Atoms |      |      |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
| 1   | A     | 1335     | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 10537 | 6666 | 1856 | 1962 | 53 |         |       |
| 1   | B     | 1310     | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 10351 | 6550 | 1822 | 1926 | 53 |         |       |
| 1   | C     | 1310     | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 10350 | 6551 | 1822 | 1924 | 53 |         |       |
| 1   | D     | 1314     | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 10375 | 6567 | 1826 | 1929 | 53 |         |       |
| 1   | E     | 1330     | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 10495 | 6635 | 1852 | 1955 | 53 |         |       |
| 1   | F     | 1319     | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 10407 | 6585 | 1831 | 1938 | 53 |         |       |
| 1   | G     | 1341     | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 10580 | 6692 | 1864 | 1971 | 53 |         |       |
| 1   | H     | 1341     | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 10580 | 6692 | 1864 | 1971 | 53 |         |       |
| 1   | I     | 1321     | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 10421 | 6593 | 1834 | 1941 | 53 |         |       |
| 1   | k     | 1295     | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 10209 | 6465 | 1795 | 1896 | 53 |         |       |
| 1   | l     | 1336     | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 10548 | 6673 | 1859 | 1963 | 53 |         |       |
| 1   | m     | 1312     | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 10364 | 6559 | 1824 | 1928 | 53 |         |       |
| 1   | n     | 1335     | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 10538 | 6663 | 1858 | 1964 | 53 |         |       |
| 1   | o     | 1313     | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 10368 | 6558 | 1828 | 1929 | 53 |         |       |
| 1   | p     | 1301     | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 10252 | 6477 | 1813 | 1910 | 52 |         |       |
| 1   | q     | 1219     | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 9621  | 6090 | 1690 | 1791 | 50 |         |       |

- Molecule 2 is a protein called Tegument protein.

| Mol | Chain | Residues | Atoms         |           |          |          |        | AltConf | Trace |
|-----|-------|----------|---------------|-----------|----------|----------|--------|---------|-------|
| 2   | 2     | 174      | Total<br>1469 | C<br>929  | N<br>279 | O<br>255 | S<br>6 | 0       | 0     |
| 2   | 3     | 200      | Total<br>1665 | C<br>1052 | N<br>314 | O<br>291 | S<br>8 | 0       | 0     |
| 2   | e     | 174      | Total<br>1469 | C<br>929  | N<br>279 | O<br>255 | S<br>6 | 0       | 0     |
| 2   | h     | 200      | Total<br>1665 | C<br>1052 | N<br>314 | O<br>291 | S<br>8 | 0       | 0     |
| 2   | f     | 174      | Total<br>1469 | C<br>929  | N<br>279 | O<br>255 | S<br>6 | 0       | 0     |
| 2   | i     | 200      | Total<br>1665 | C<br>1052 | N<br>314 | O<br>291 | S<br>8 | 0       | 0     |
| 2   | g     | 174      | Total<br>1469 | C<br>929  | N<br>279 | O<br>255 | S<br>6 | 0       | 0     |
| 2   | j     | 200      | Total<br>1665 | C<br>1052 | N<br>314 | O<br>291 | S<br>8 | 0       | 0     |

- Molecule 3 is a protein called Small capsomere-interacting protein.

| Mol | Chain | Residues | Atoms        |          |         |         |        | AltConf | Trace |
|-----|-------|----------|--------------|----------|---------|---------|--------|---------|-------|
| 3   | J     | 60       | Total<br>471 | C<br>300 | N<br>83 | O<br>83 | S<br>5 | 0       | 0     |
| 3   | K     | 59       | Total<br>462 | C<br>294 | N<br>81 | O<br>82 | S<br>5 | 0       | 0     |
| 3   | L     | 59       | Total<br>462 | C<br>294 | N<br>81 | O<br>82 | S<br>5 | 0       | 0     |
| 3   | M     | 59       | Total<br>462 | C<br>294 | N<br>81 | O<br>82 | S<br>5 | 0       | 0     |
| 3   | N     | 59       | Total<br>462 | C<br>294 | N<br>81 | O<br>82 | S<br>5 | 0       | 0     |
| 3   | O     | 59       | Total<br>462 | C<br>294 | N<br>81 | O<br>82 | S<br>5 | 0       | 0     |
| 3   | P     | 59       | Total<br>462 | C<br>294 | N<br>81 | O<br>82 | S<br>5 | 0       | 0     |
| 3   | Q     | 59       | Total<br>462 | C<br>294 | N<br>81 | O<br>82 | S<br>5 | 0       | 0     |
| 3   | R     | 59       | Total<br>462 | C<br>294 | N<br>81 | O<br>82 | S<br>5 | 0       | 0     |
| 3   | r     | 60       | Total<br>471 | C<br>300 | N<br>83 | O<br>83 | S<br>5 | 0       | 0     |
| 3   | s     | 59       | Total<br>462 | C<br>294 | N<br>81 | O<br>82 | S<br>5 | 0       | 0     |
| 3   | t     | 59       | Total<br>462 | C<br>294 | N<br>81 | O<br>82 | S<br>5 | 0       | 0     |

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| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 3   | u     | 60       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 471   | 300 | 83 | 83 | 5 |         |       |
| 3   | v     | 60       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 471   | 300 | 83 | 83 | 5 |         |       |
| 3   | w     | 60       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 471   | 300 | 83 | 83 | 5 |         |       |
| 3   | x     | 57       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 450   | 287 | 79 | 79 | 5 |         |       |

- Molecule 4 is a protein called Minor capsid protein.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 4   | y     | 249      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1977  | 1261 | 350 | 356 | 10 |         |       |
| 4   | S     | 289      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2305  | 1470 | 406 | 416 | 13 |         |       |
| 4   | T     | 289      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2305  | 1470 | 406 | 416 | 13 |         |       |
| 4   | U     | 289      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2305  | 1470 | 406 | 416 | 13 |         |       |
| 4   | V     | 289      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2305  | 1470 | 406 | 416 | 13 |         |       |

- Molecule 5 is a protein called Triplex capsid protein 2.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 5   | z     | 284      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2224  | 1403 | 382 | 419 | 20 |         |       |
| 5   | W     | 281      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2201  | 1390 | 378 | 414 | 19 |         |       |
| 5   | X     | 277      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2166  | 1367 | 373 | 407 | 19 |         |       |
| 5   | Y     | 282      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2209  | 1395 | 379 | 415 | 20 |         |       |
| 5   | Z     | 281      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2201  | 1390 | 378 | 414 | 19 |         |       |
| 5   | 1     | 257      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2009  | 1268 | 350 | 374 | 17 |         |       |
| 5   | a     | 267      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2085  | 1314 | 363 | 389 | 19 |         |       |
| 5   | b     | 270      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2109  | 1330 | 366 | 394 | 19 |         |       |

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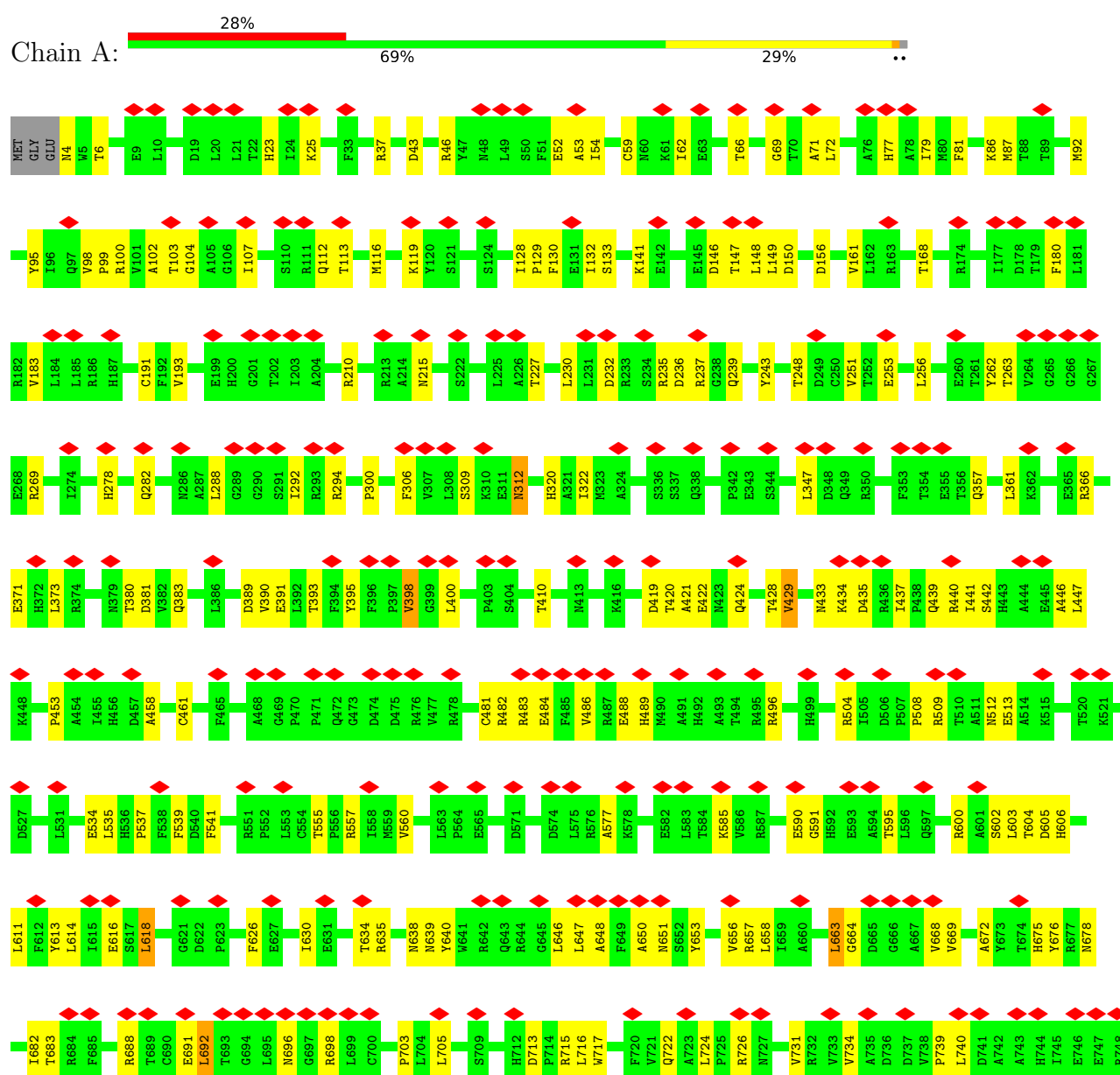
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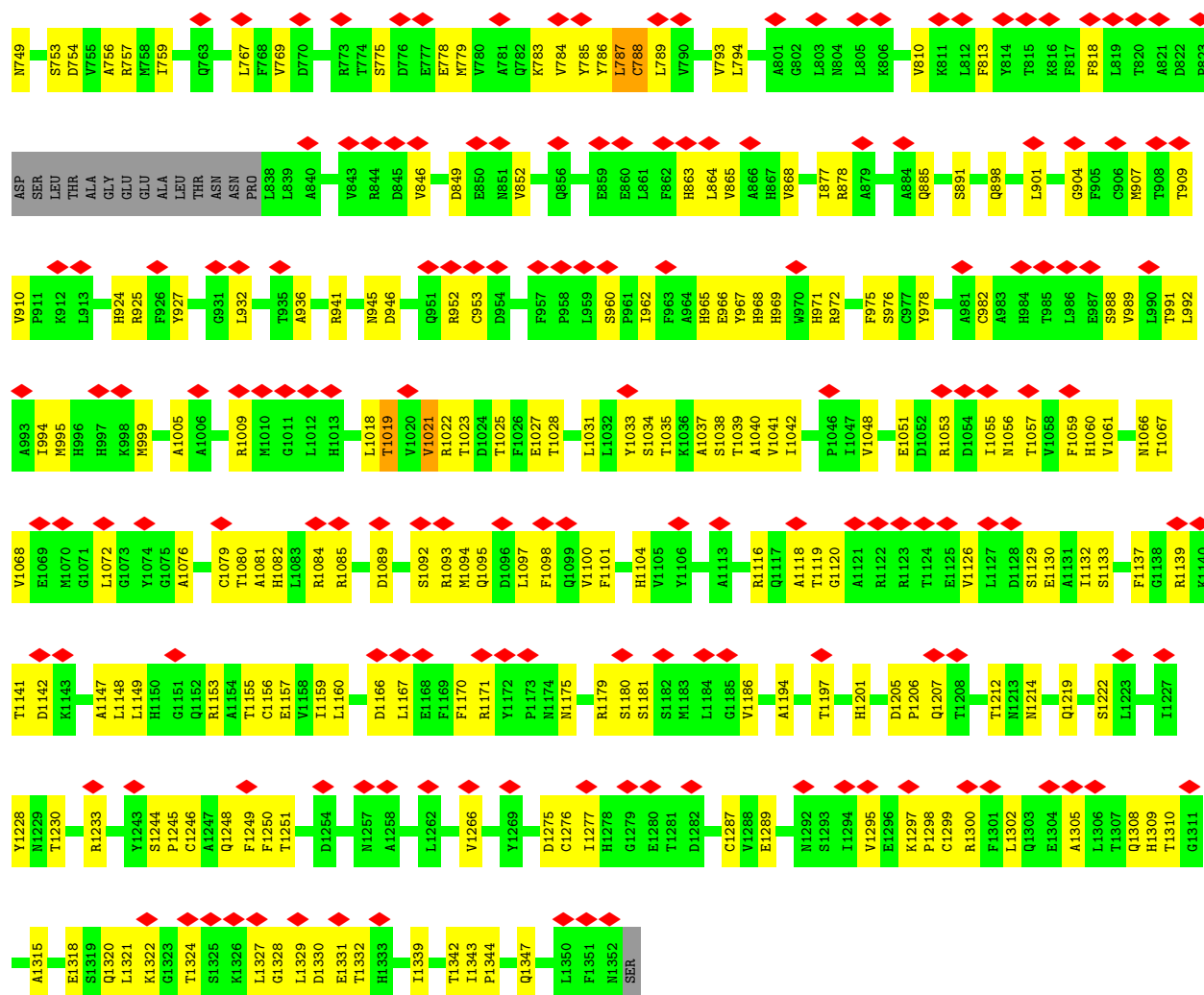
| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 5   | c     | 274      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2141  | 1349 | 371 | 401 | 20 |         |       |
| 5   | d     | 274      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2140  | 1351 | 370 | 399 | 20 |         |       |

### 3 Residue-property plots

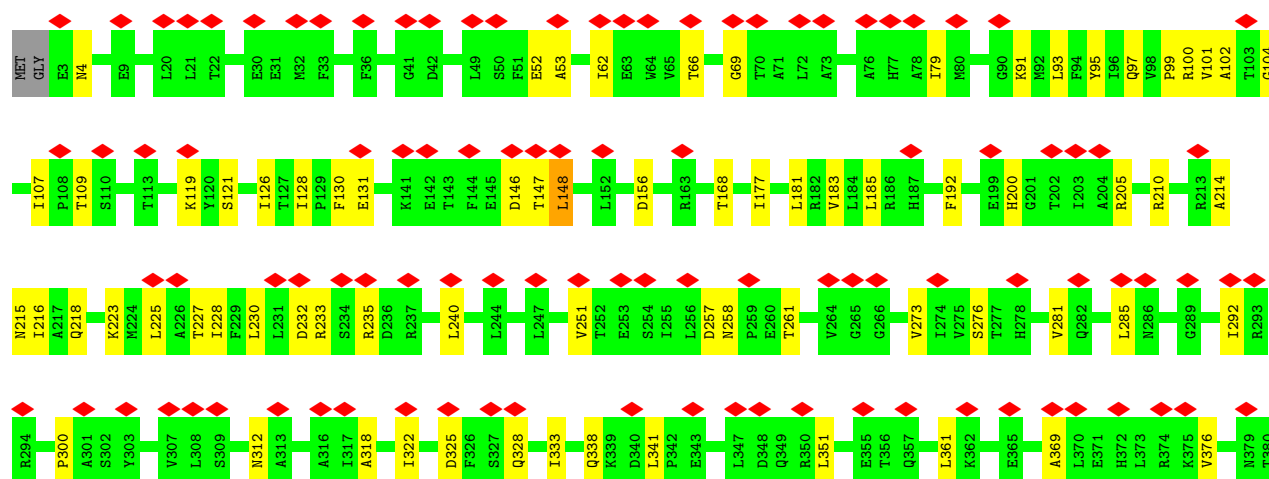
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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.

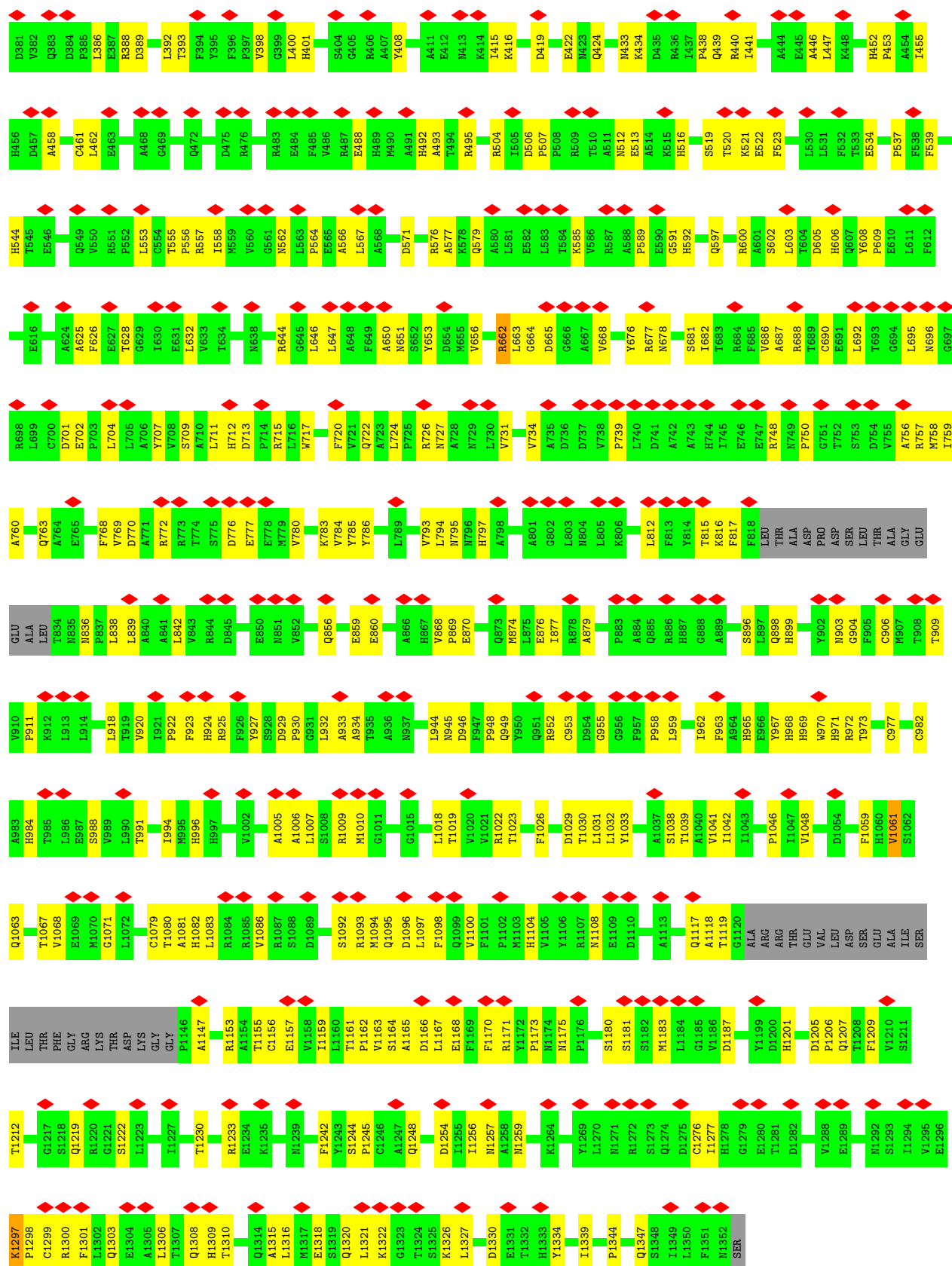
#### • Molecule 1: Major capsid protein



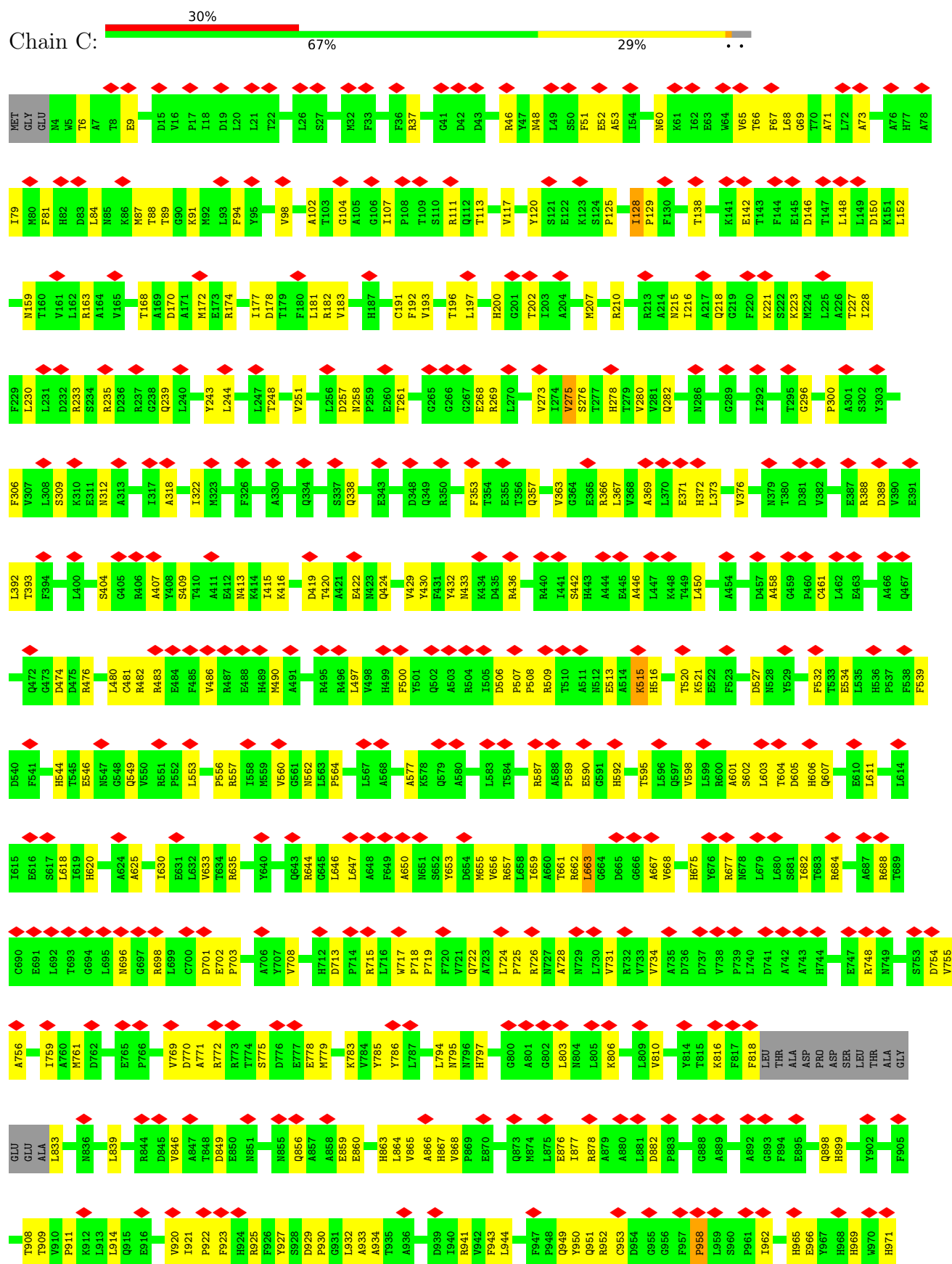


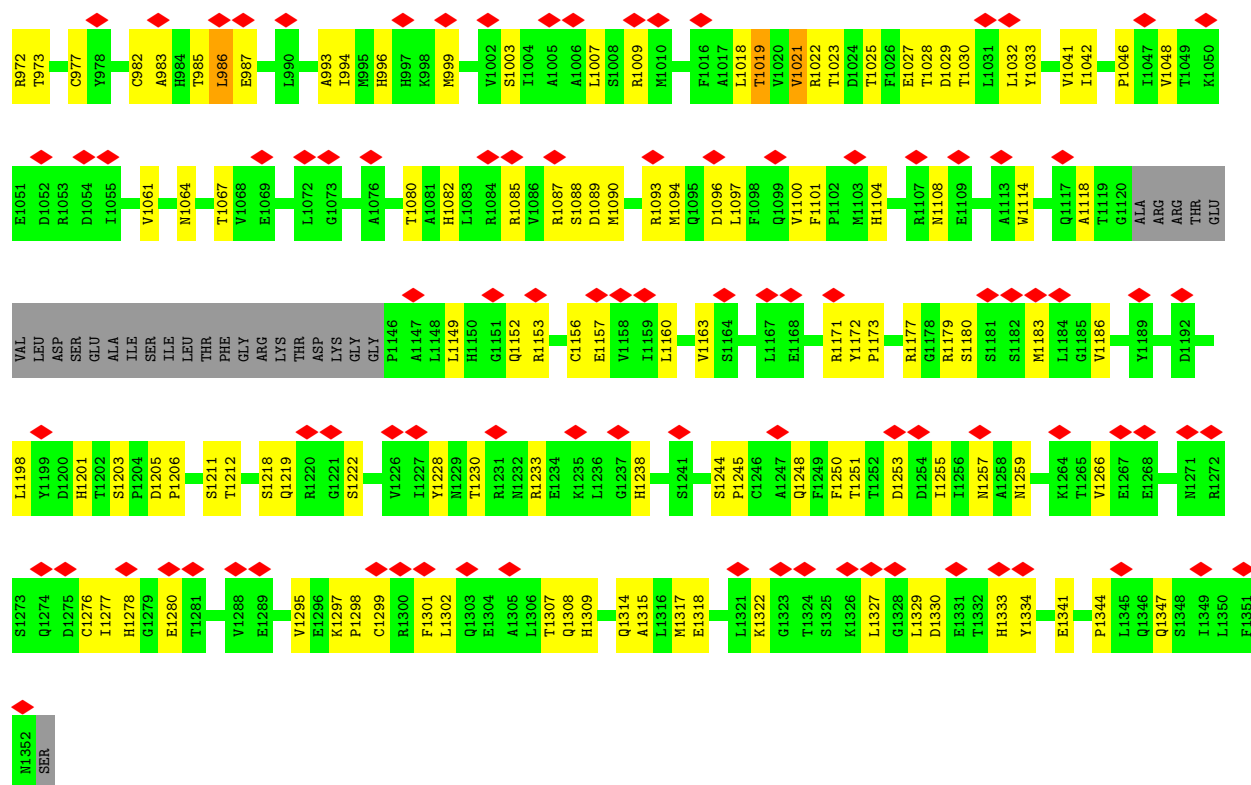
• Molecule 1: Major capsid protein



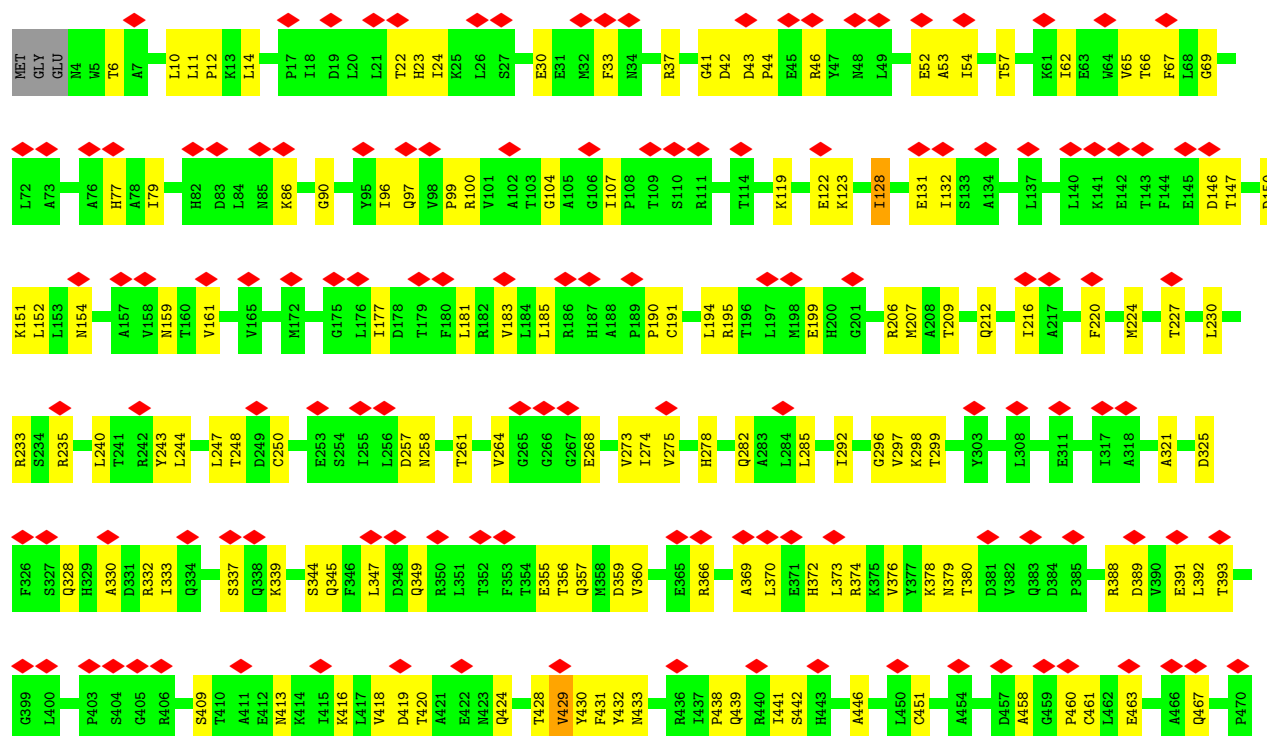


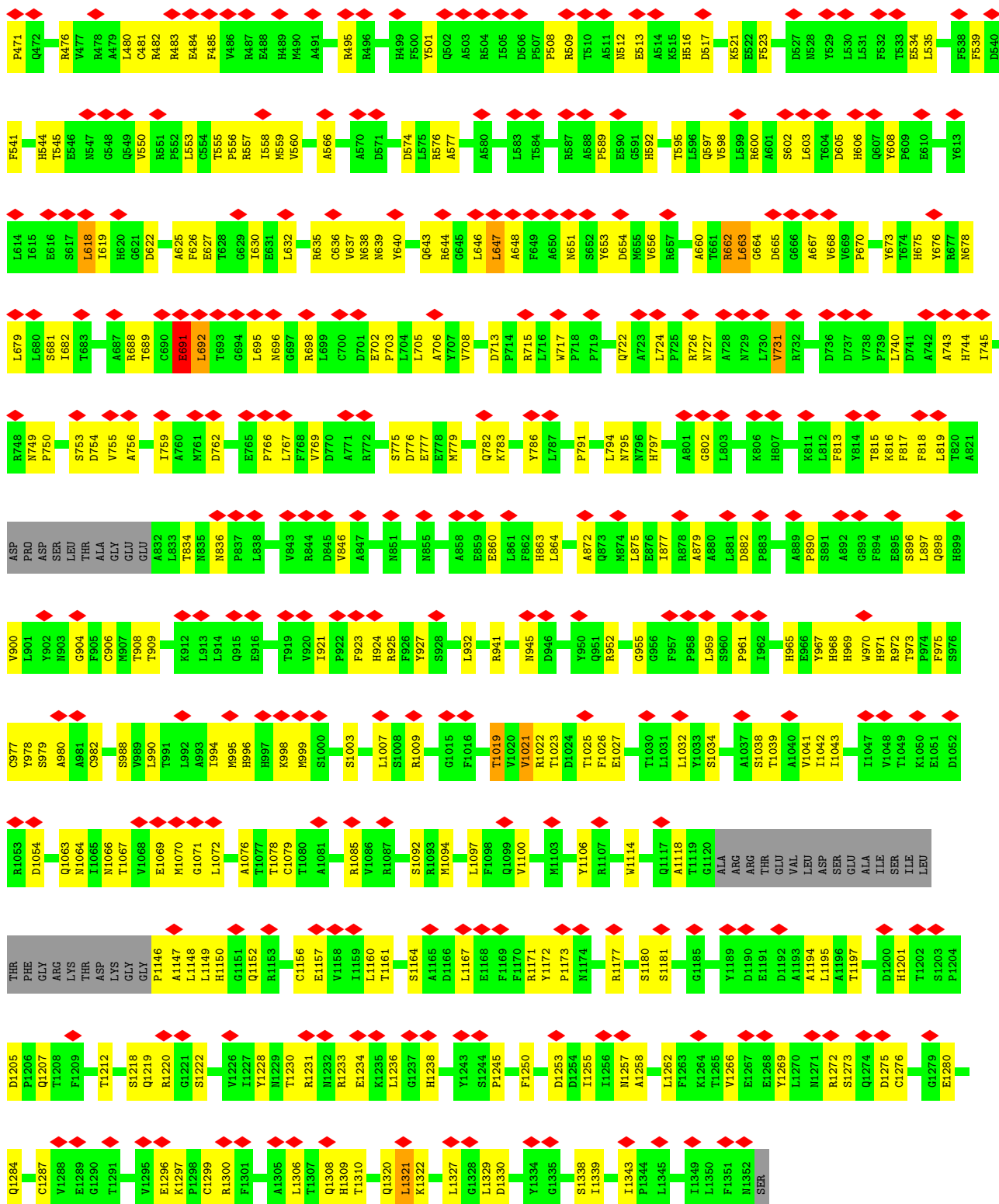
• Molecule 1: Major capsid protein





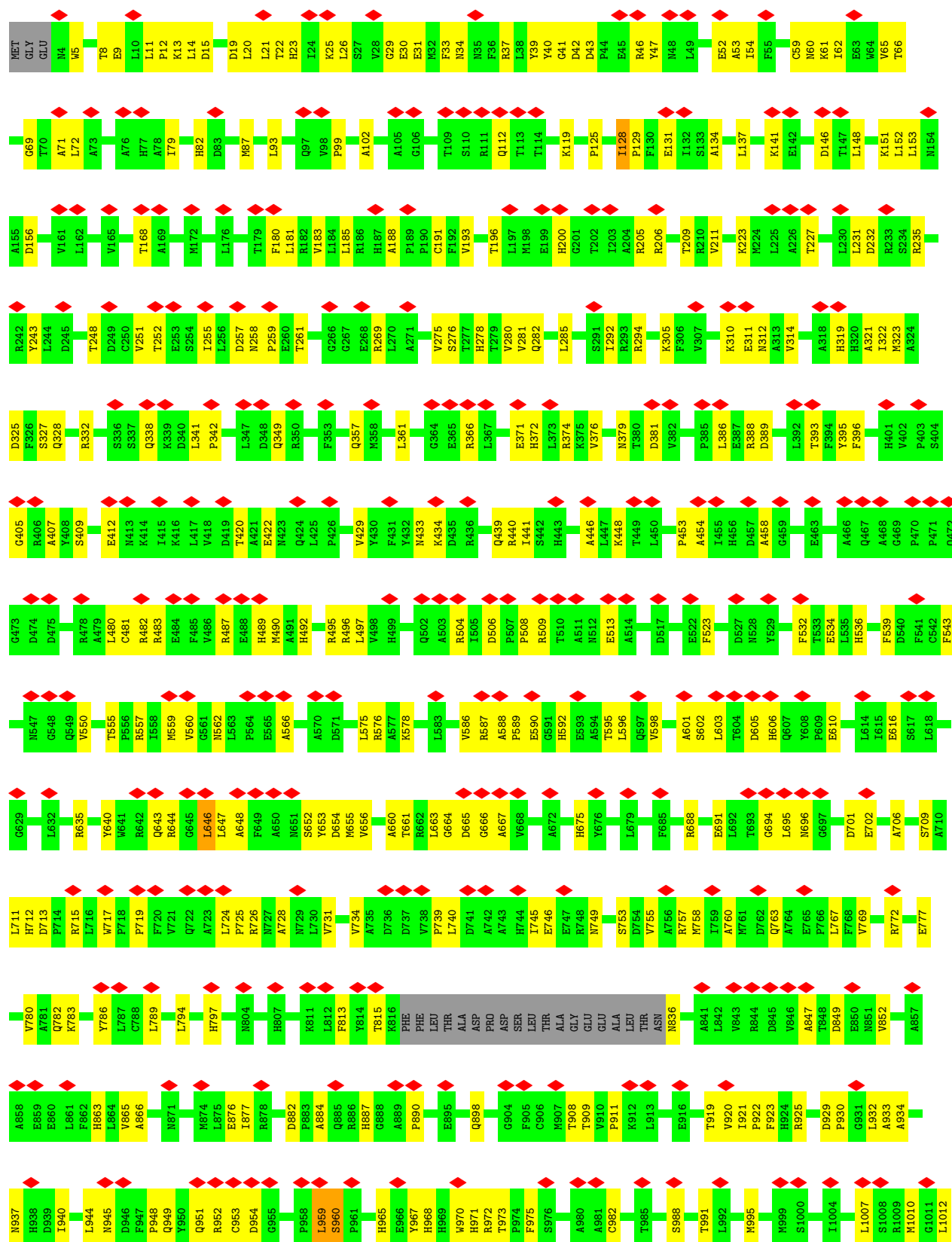
• Molecule 1: Major capsid protein

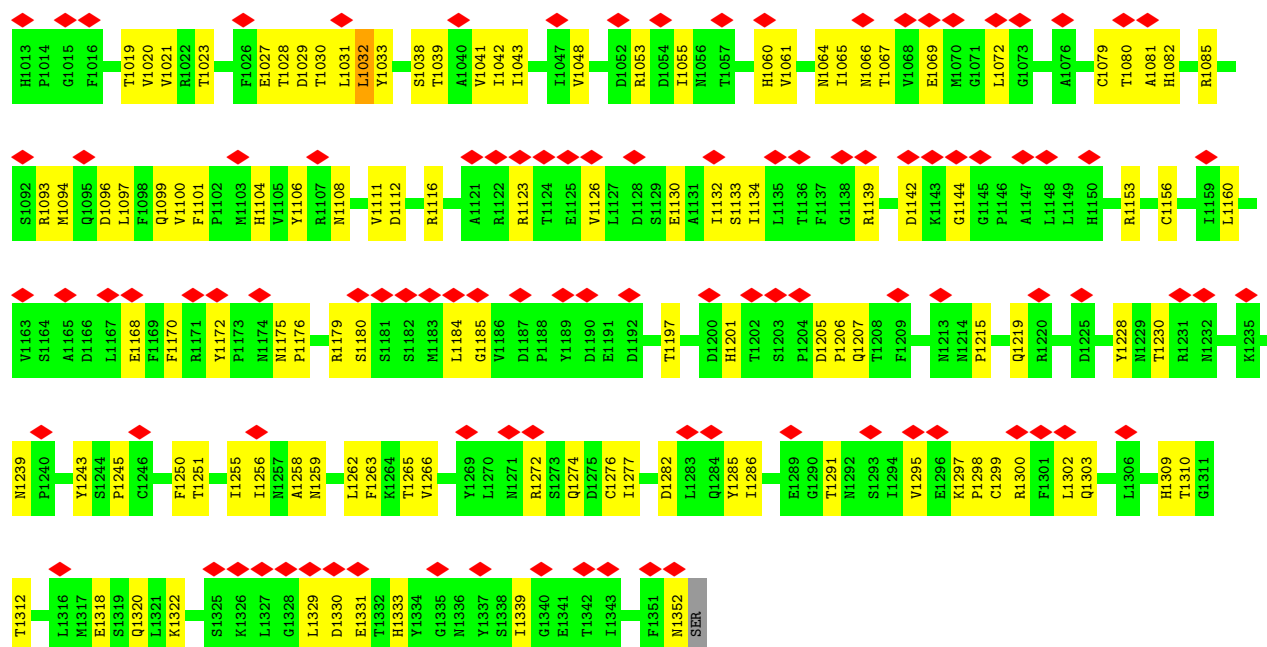




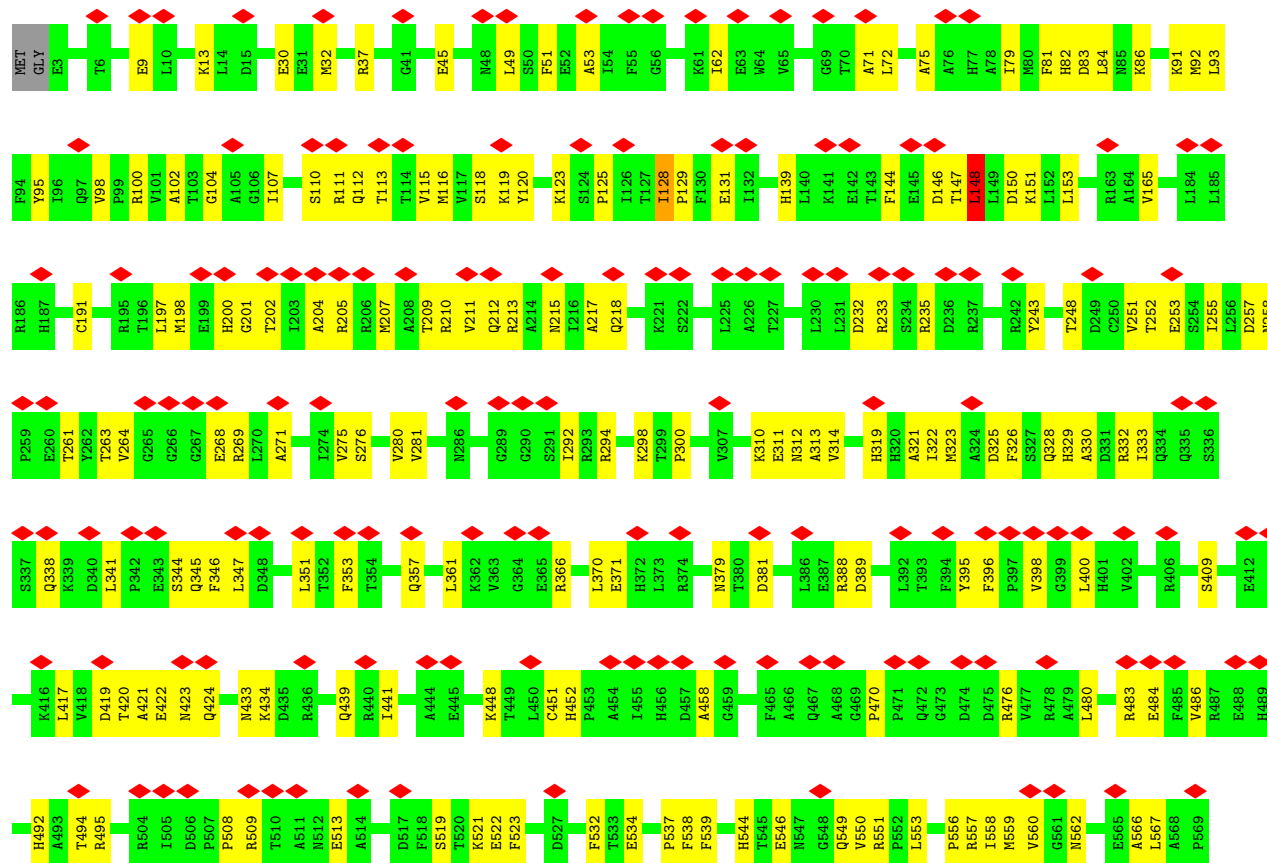
• Molecule 1: Major capsid protein

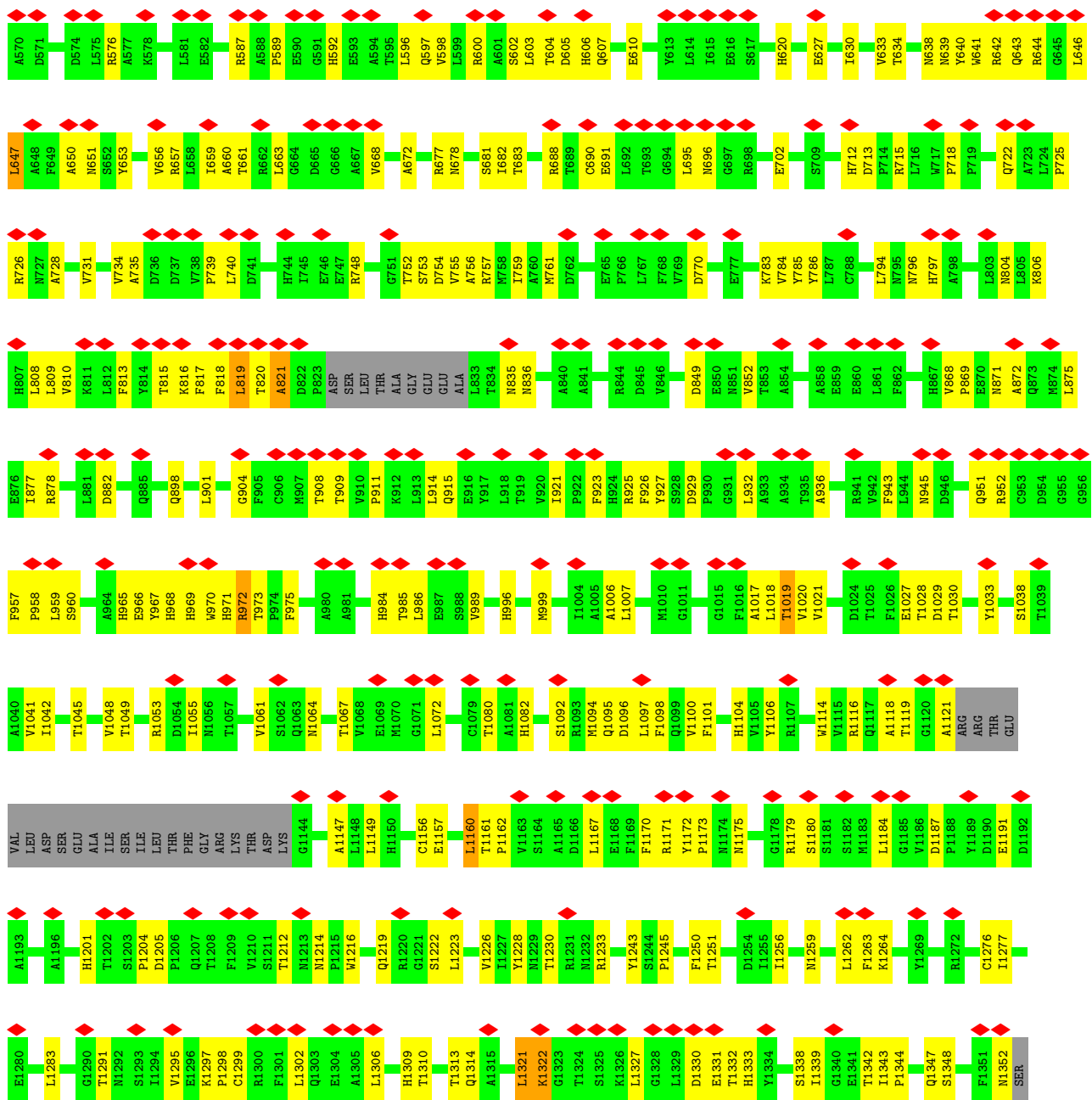




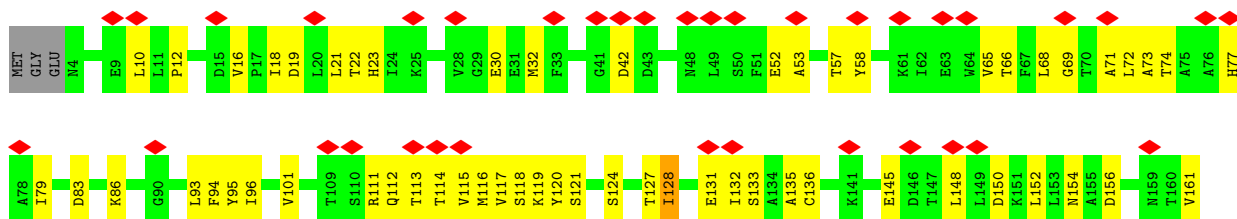


• Molecule 1: Major capsid protein

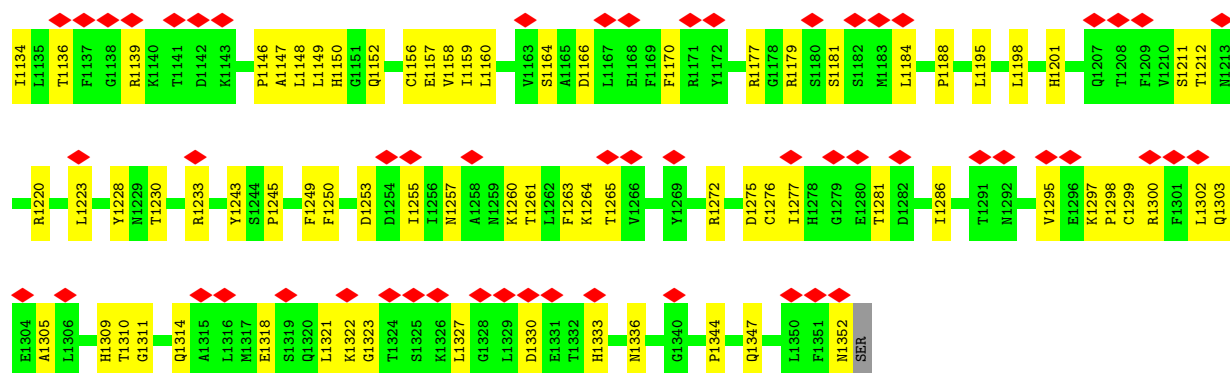




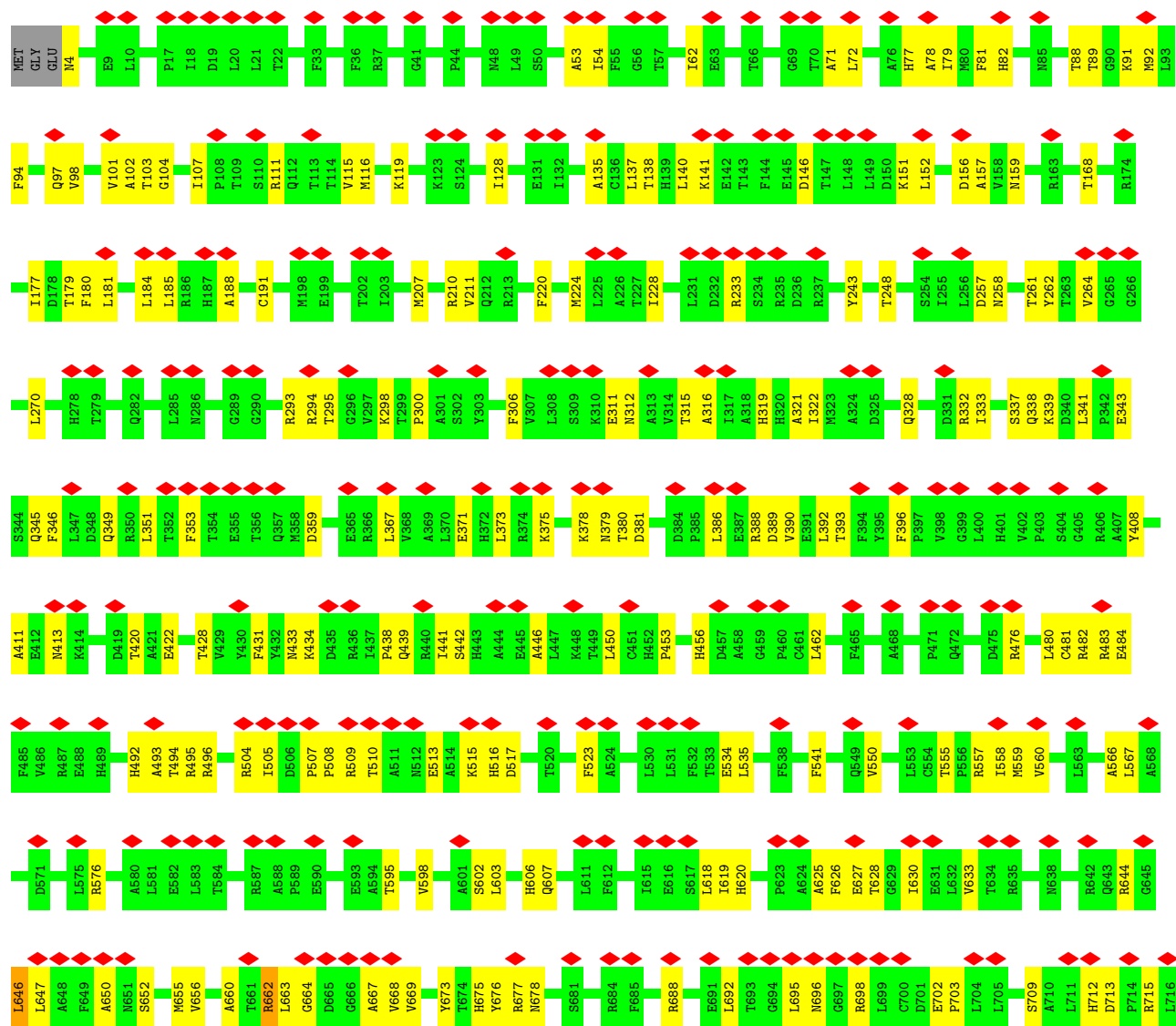
• Molecule 1: Major capsid protein

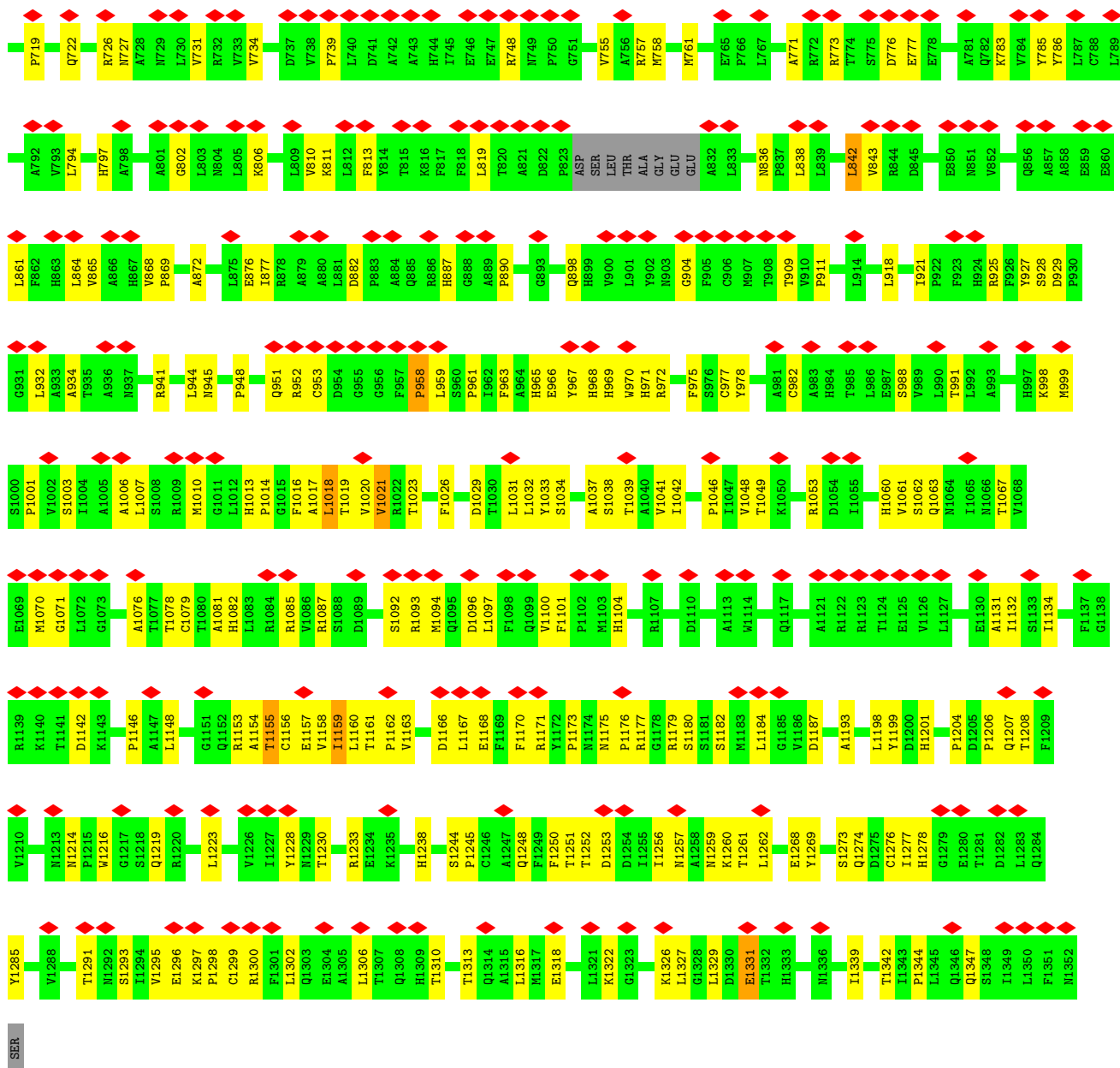


|       |       |      |      |      |      |      |      |      |      |      |      |      |
|-------|-------|------|------|------|------|------|------|------|------|------|------|------|
| V1061 | C982  | M907 | N835 | F766 | L699 | E627 | N563 | V477 | F396 | A324 | T248 | L162 |
| M1064 | A983  | T908 | N836 | L767 | C700 | E630 | L563 | R478 | P397 | D325 | D249 | R163 |
| I1065 | H984  | T909 | A840 | R772 | D701 | E631 | E565 | A479 | V398 | F326 | T252 | K166 |
| T1067 | T985  | V910 | A841 | R773 | E702 | E632 | E566 | L480 | G399 | H329 | E253 | R174 |
| V1068 | L986  | P911 | A842 | T774 | P703 | L632 | A566 | C481 | L400 | A330 | E254 | I177 |
| E1069 | E987  | K912 | R844 | S775 | L704 | V633 | A567 | R482 | S404 | D331 | S255 | F180 |
| G1070 | S988  | L914 | D845 | D776 | L705 | T634 | A570 | E483 | G405 | Q332 | L256 | L181 |
| G1071 | T991  | L915 | V846 | E777 | V707 | R635 | D571 | E484 | R406 | Q334 | D257 | L184 |
| L1072 | L992  | T919 | A847 | E778 | V708 | N638 | F572 | F485 | N413 | Q335 | N258 | L185 |
| G1073 | A993  | V920 | T848 | V780 | S709 | N639 | H573 | V486 | N414 | G336 | P259 | A188 |
| Y1074 | N995  | P922 | D849 | A781 | A710 | N640 | D574 | R487 | K414 | S337 | E260 | C191 |
| G1075 | H996  | F923 | E850 | K782 | L711 | H641 | L575 | E488 | L417 | Q338 | T261 | F192 |
| A1076 | H997  | H924 | N851 | K783 | H712 | R642 | R576 | H489 | L418 | G339 | Y262 | L197 |
| C1079 | K998  | H925 | A854 | V784 | D713 | G643 | K578 | T494 | D419 | L341 | G265 | M198 |
| T1080 | N999  | F926 | A857 | V785 | L716 | R644 | E582 | R495 | T420 | P342 | G266 | E199 |
| H1082 | V1002 | S928 | A857 | V786 | W717 | G645 | L583 | R496 | Q424 | L347 | G267 | H200 |
| L1083 | S1003 | D929 | E860 | L787 | P718 | L646 | L584 | L497 | F500 | D348 | E268 | G201 |
| R1084 | T1004 | P930 | L861 | C788 | P719 | A648 | K585 | F501 | V429 | Q349 | R269 | T202 |
| R1085 | A1005 | G931 | F862 | L789 | F720 | F649 | V586 | R504 | Y430 | R350 | L270 | I203 |
| S1088 | L1006 | L932 | H863 | V790 | W721 | A650 | R587 | I505 | F431 | L351 | V275 | R206 |
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| G1095 | P1014 | P948 | L803 | L803 | V733 | R662 | T595 | D517 | Q439 | L285 | L286 | S222 |
| D1096 | G1015 | Q949 | N804 | L804 | W734 | L663 | L596 | F518 | R440 | V363 | N286 | K223 |
| L1097 | F1016 | Y950 | L805 | L805 | A735 | G664 | Q597 | S519 | I441 | G364 | A287 | M224 |
| V1100 | A1017 | Q951 | K806 | K806 | A735 | D665 | V598 | T520 | A444 | E365 | L288 | L225 |
| V1105 | L1018 | R952 | W810 | W810 | P739 | G666 | L599 | K521 | A445 | A369 | G289 | A226 |
| T1106 | V1020 | C953 | K811 | K811 | L740 | A667 | R600 | E522 | A446 | L370 | G290 | F229 |
| R1107 | G955  | D954 | L812 | L812 | D741 | V668 | S602 | D527 | T449 | E371 | G291 | L230 |
| M1108 | T1023 | G956 | F813 | F813 | A742 | V669 | L603 | L530 | L450 | H372 | I292 | L231 |
| W1114 | D1024 | P957 | V814 | V814 | H744 | A671 | T604 | L531 | P453 | L373 | R293 | D232 |
| V1115 | F1026 | P958 | T815 | T815 | I745 | A672 | D605 | E534 | A454 | R374 | R294 | R233 |
| R1116 | E1027 | L959 | K816 | K816 | E746 | V673 | H606 | P609 | A455 | K375 | F306 | S234 |
| Q1117 | T1028 | S960 | F817 | F817 | E747 | T674 | Q607 | E610 | I456 | V376 | V307 | L236 |
| A1118 | Y1033 | P961 | L818 | L818 | R748 | T677 | Y608 | E511 | D457 | N379 | L308 | R237 |
| A1121 | S1034 | P962 | L819 | L819 | P750 | H678 | L611 | D540 | A458 | T380 | S309 | Y243 |
| R1122 | A1037 | E966 | T820 | T820 | G751 | R684 | F612 | H544 | C461 | Q383 | K310 | L247 |
| R1123 | S1038 | Y967 | A821 | A821 | T752 | R688 | T615 | L553 | F465 | D384 | N312 |      |
| T1124 | T1039 | H968 | D822 | D822 | S753 | C690 | E616 | L553 | A468 | E387 | A313 |      |
| T1125 | H969  | L969 | P823 | P823 | D754 | R691 | S617 | L553 | P471 | R388 | V314 |      |
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| V1126 | I1042 | H971 | SER  | SER  | W756 | C690 | L618 | L553 | G473 | H319 | H319 |      |
| L1127 | I1043 | R972 | LEU  | LEU  | R757 | C690 | L618 | L553 | D474 | T393 | I322 |      |
| D1128 | I1044 | R972 | THR  | THR  | W758 | C690 | L618 | L553 | D475 | F394 | M323 |      |
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| E1130 | H1060 | A980 | GLY  | GLY  | D762 | C690 | L618 | L553 | R476 | F394 | M323 |      |
| S1133 |       | A981 | GLU  | GLU  | Q763 | C690 | L618 | L553 | R476 | F394 | M323 |      |
|       |       |      | A832 | A832 | E765 | C690 | L618 | L553 | R476 | F394 | M323 |      |
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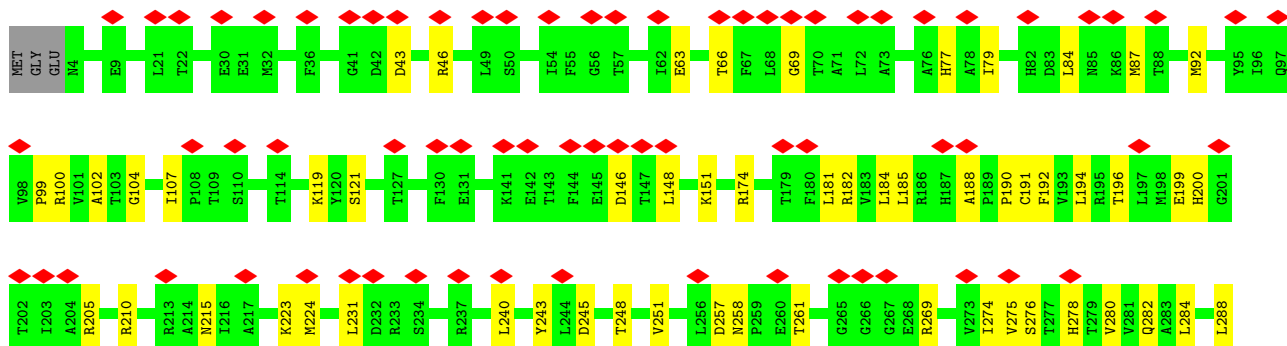


• Molecule 1: Major capsid protein

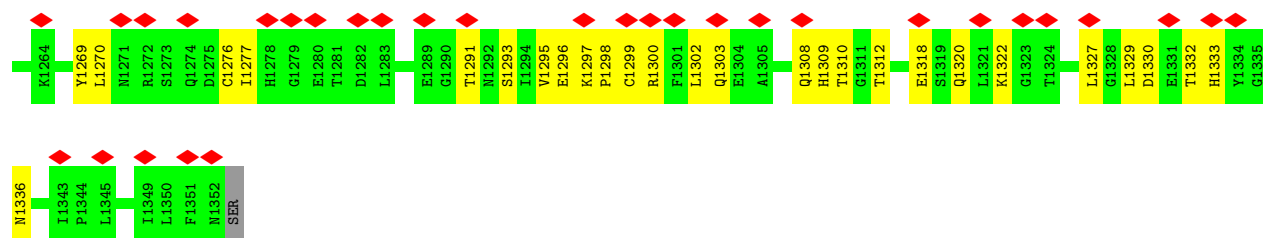




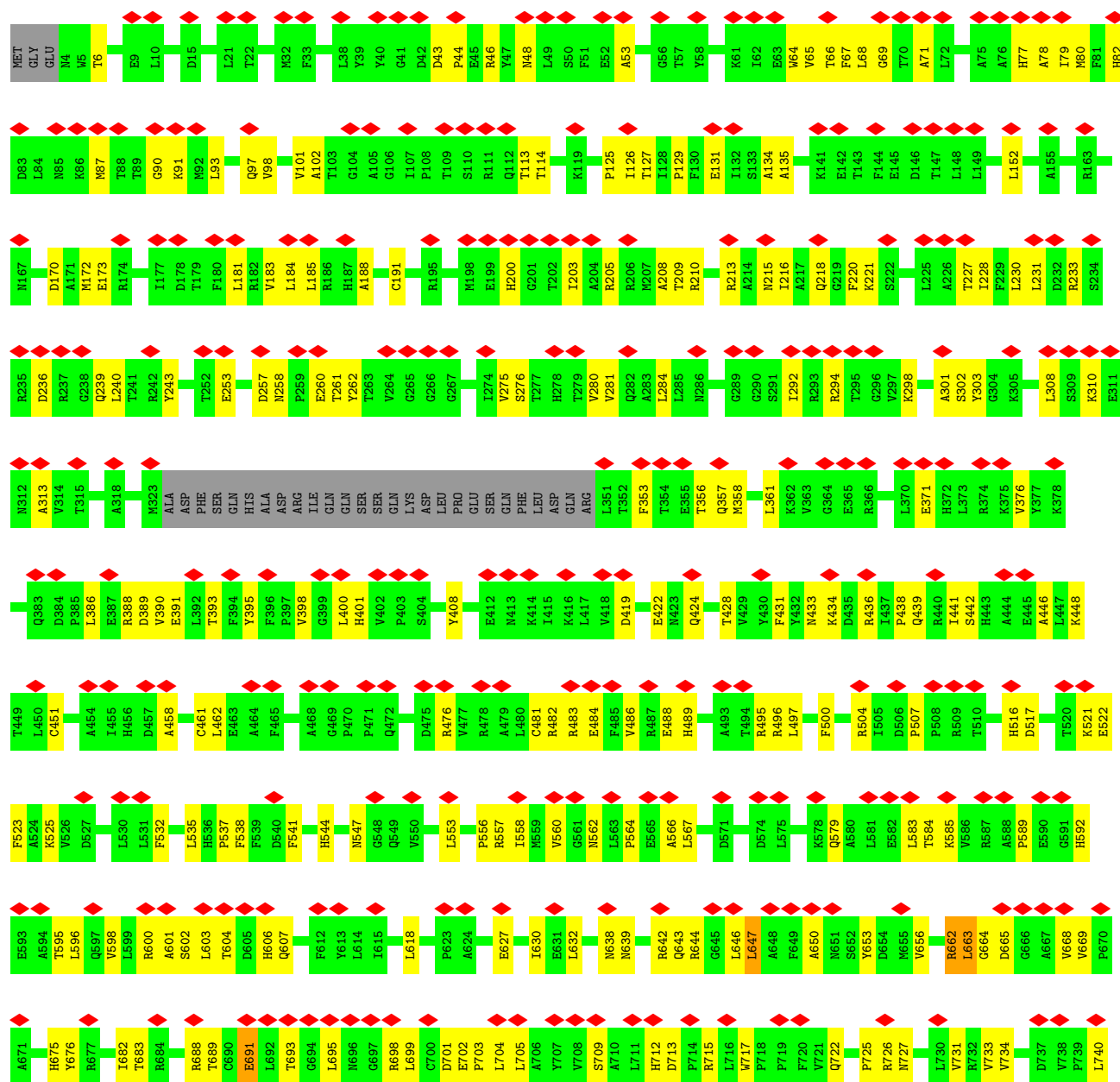
• Molecule 1: Major capsid protein

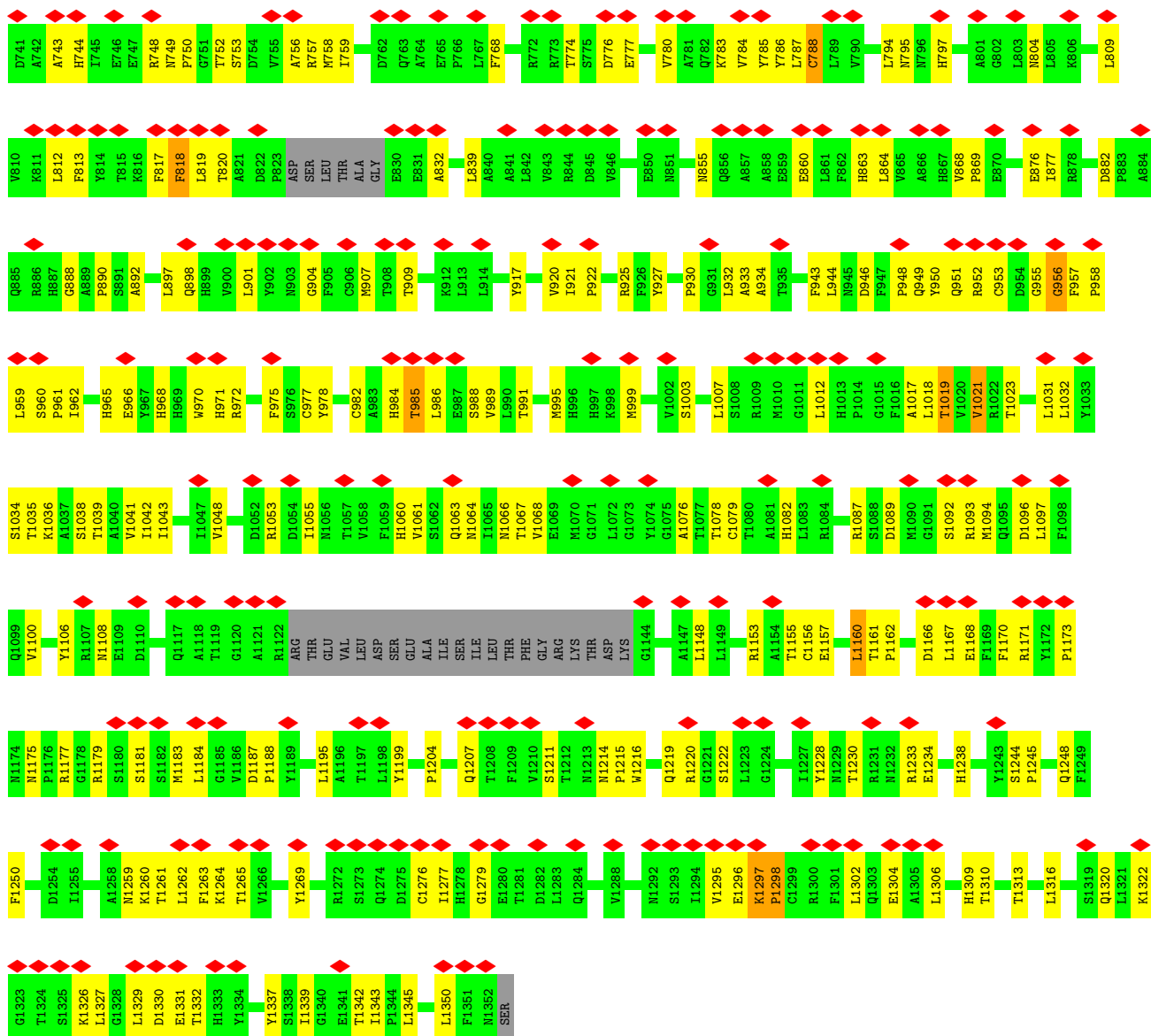




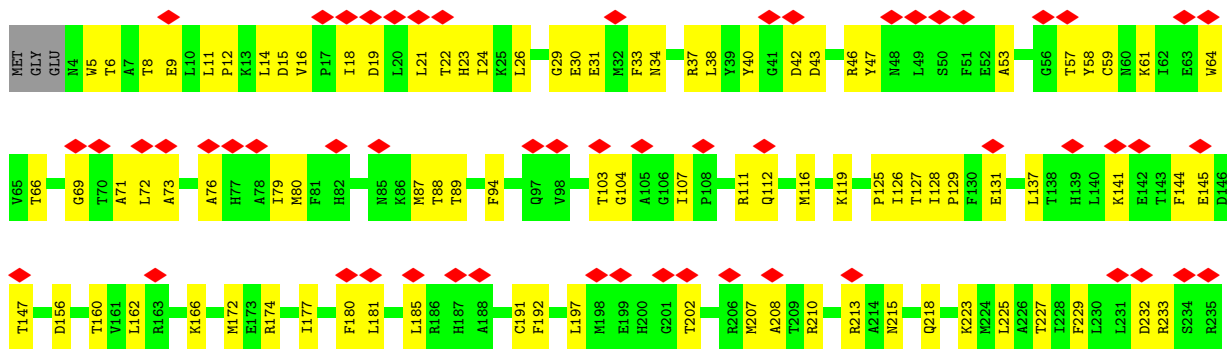


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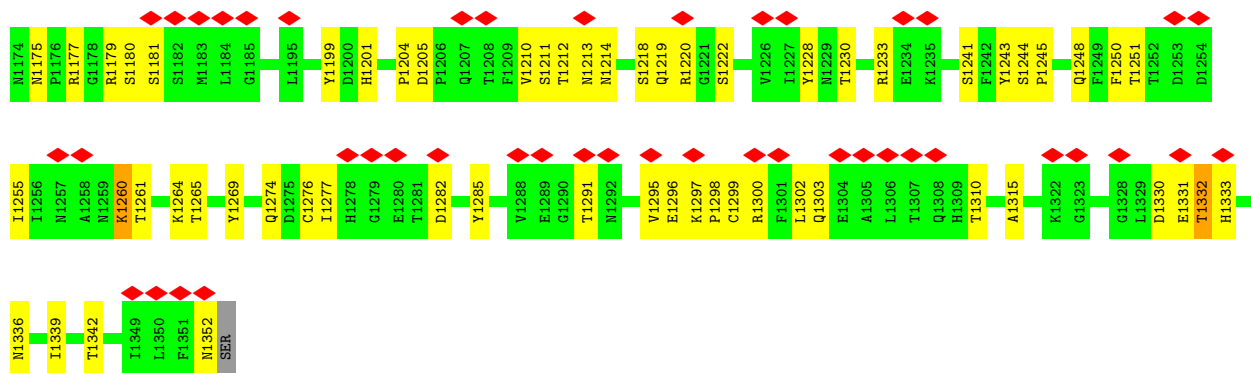




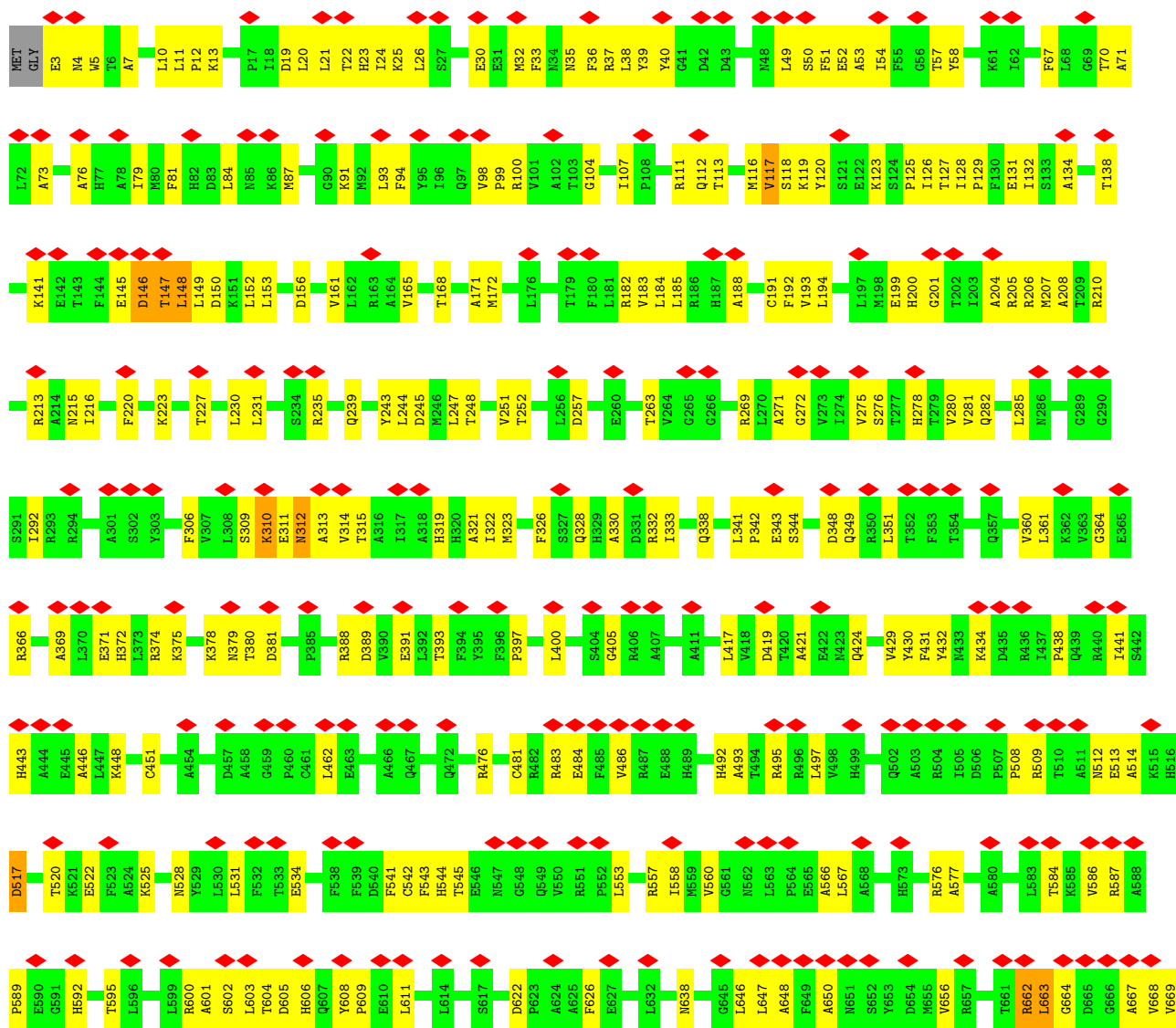
• Molecule 1: Major capsid protein

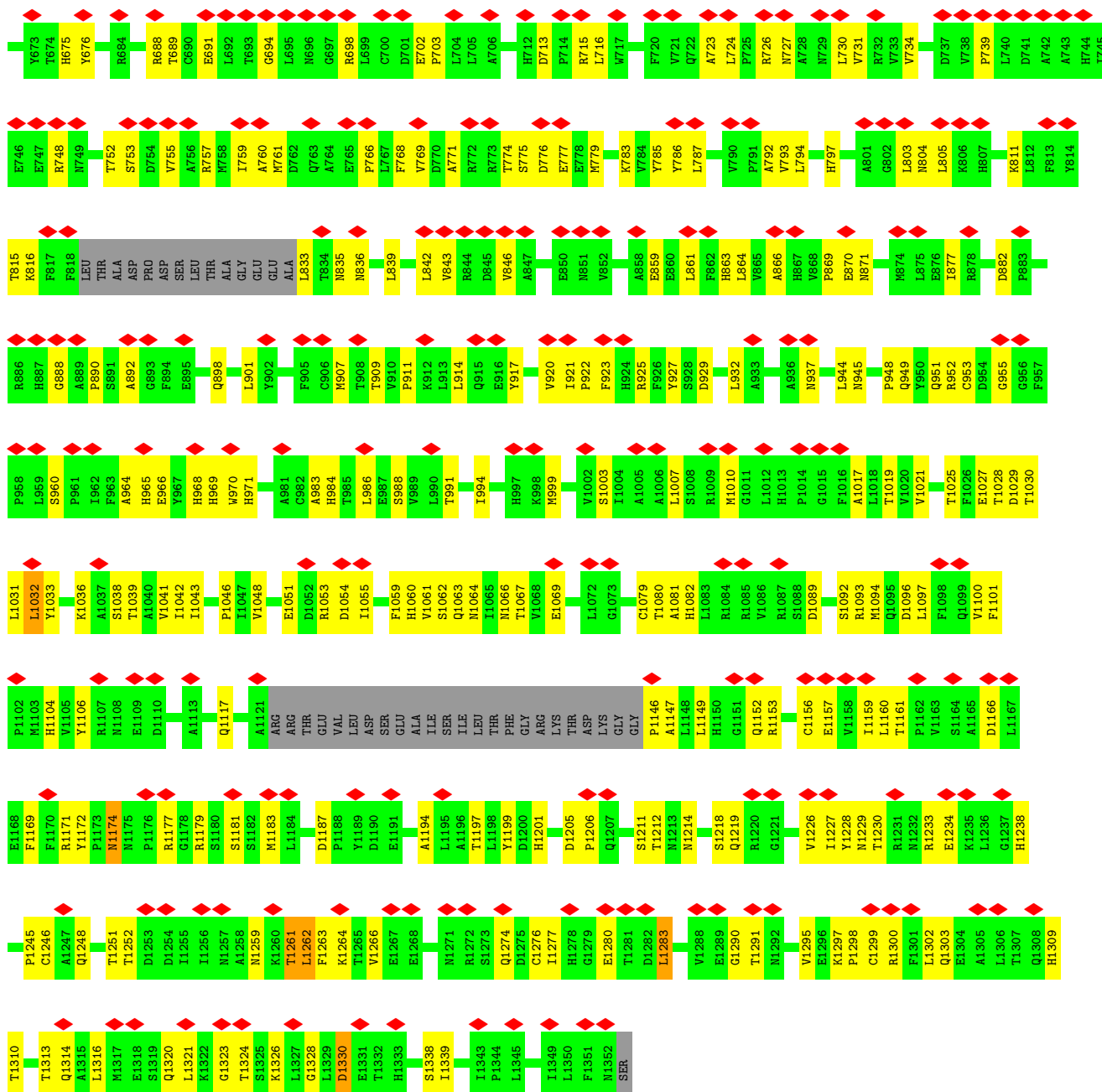


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| T1039 | E109 | R972 | F905  | ALA  | D769 | D701 | T628 | E546 | G399 | K310 | R237 |
| A1040 | D110 |      | C906  | L833 | V770 | E702 | G629 | N547 | L400 | E311 | L240 |
| V1041 |      |      | M907  | T834 | A771 | L704 | P630 | G548 | H401 | N312 |      |
| I1042 | A113 | C977 | T908  |      | R772 | L705 | E631 | V550 | V402 | A313 | Y243 |
|       |      |      | T909  | L839 | R773 | A706 |      | R551 | P403 | V314 |      |
|       |      |      | V910  | A840 | T774 |      |      | R561 | R482 | T315 | L244 |
|       |      |      |       | A841 | S775 |      |      | P552 | S404 | A316 |      |
|       |      |      | L913  | L842 | D776 |      |      | L553 | G405 |      |      |
|       |      |      | L914  | W843 | E777 | S709 |      | R557 | R406 |      |      |
|       |      |      |       | R844 | R778 |      |      | F485 | A407 |      |      |
|       |      |      | Y917  | D845 | W779 | H712 | N638 | I558 | H320 |      |      |
|       |      |      | L918  | D846 | V780 | P714 |      | H559 | A321 |      |      |
|       |      |      | T919  | V846 | A781 | R715 | Q643 | V560 | M413 |      |      |
|       |      |      | V920  | A847 | Q782 | L716 | R644 |      | R487 |      |      |
|       |      |      | I921  | T848 | K783 | W717 | G645 |      | K414 |      |      |
|       |      |      | P922  | D849 | V784 | P718 | L646 |      | I415 |      |      |
|       |      |      | F923  | E850 | Y785 | P719 | L647 |      | D419 |      |      |
|       |      |      | H924  | N851 | Y786 | F720 | A648 |      | M423 |      |      |
|       |      |      | R925  | V852 | L787 | F720 | F649 |      | Q424 |      |      |
|       |      |      | F926  |      | C788 | A723 | A650 |      | R495 |      |      |
|       |      |      | Y927  | Q856 | L789 | L724 | N651 |      | R496 |      |      |
|       |      |      | S928  | A857 |      | R726 |      |      | I428 |      |      |
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|       |      |      | P930  | E860 | L794 | A728 | V656 |      | Y432 |      |      |
|       |      |      | G931  | L861 | W796 | N729 | R657 |      | M433 |      |      |
|       |      |      | L932  | R862 | H797 | N729 | L658 |      | K434 |      |      |
|       |      |      | A933  | H863 | A798 | L730 | T659 |      | D435 |      |      |
|       |      |      | A934  | L864 | C799 | V731 | A680 |      | R436 |      |      |
|       |      |      | T935  |      | G799 | R732 | T681 |      | P507 |      |      |
|       |      |      | A936  | H867 | G800 | V733 | L682 |      | P438 |      |      |
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|       |      |      | V942  | E870 | G802 | D737 | L683 |      | R440 |      |      |
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|       |      |      | N945  | A872 | N804 | P739 | D665 |      | S442 |      |      |
|       |      |      |       | Q873 | L805 | L740 | G666 |      | H443 |      |      |
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|       |      |      | Y950  | I877 | L808 | A742 | R600 |      | L447 |      |      |
|       |      |      | Q951  | R878 | L809 | A743 | A601 |      | H372 |      |      |
|       |      |      | R952  |      | V810 | H744 | G602 |      | L373 |      |      |
|       |      |      | C953  | L881 | R811 | T674 | L603 |      | R374 |      |      |
|       |      |      | D954  | D882 | L812 | E745 | T604 |      | L450 |      |      |
|       |      |      | G955  | P883 | F813 | E747 | P605 |      | C451 |      |      |
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|       |      |      | F957  | A884 | T815 | N749 | Q607 |      | P453 |      |      |
|       |      |      | P958  | Q885 | R815 |      | Y608 |      | A454 |      |      |
|       |      |      | L959  | R866 | K816 | P750 | P609 |      | L455 |      |      |
|       |      |      | S960  | H857 | F817 | G751 | R610 |      | R456 |      |      |
|       |      |      | P961  | C888 | F818 | T752 | L611 |      | D457 |      |      |
|       |      |      | P962  | A889 | L819 | S753 | F612 |      | A458 |      |      |
|       |      |      | F963  | P890 | L819 | T754 | F532 |      | E387 |      |      |
|       |      |      | Q964  | S891 | THR  | V755 | T533 |      | G459 |      |      |
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|       |      |      | P967  | Q898 | ASP  | R757 | L618 |      | L462 |      |      |
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|       |      |      |       |      | LEU  |      | F465 |      | T393 |      |      |
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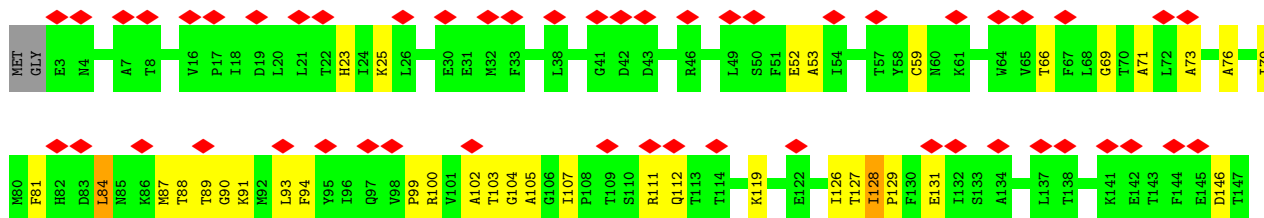
• Molecule 1: Major capsid protein



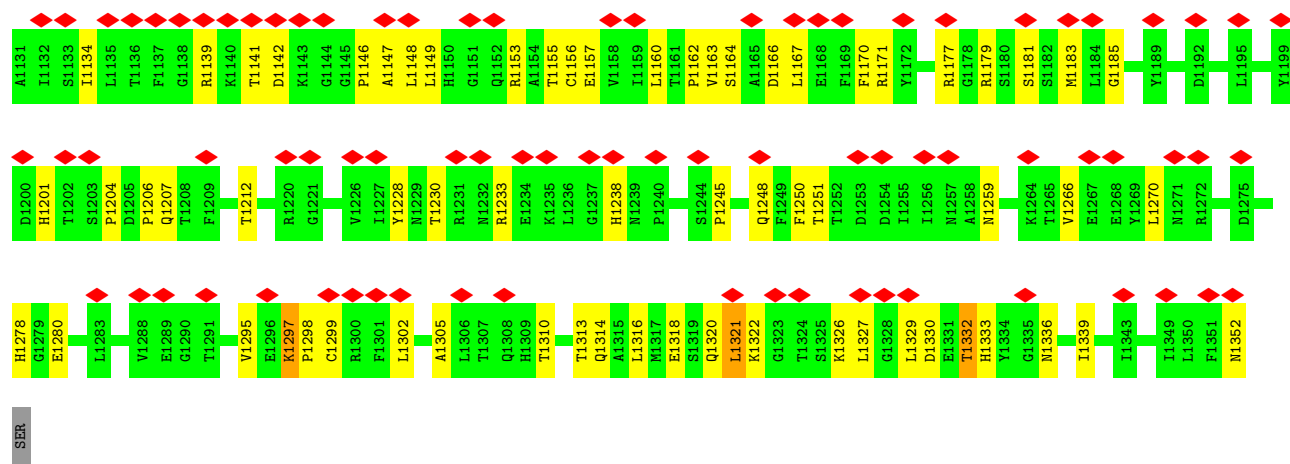


• Molecule 1: Major capsid protein

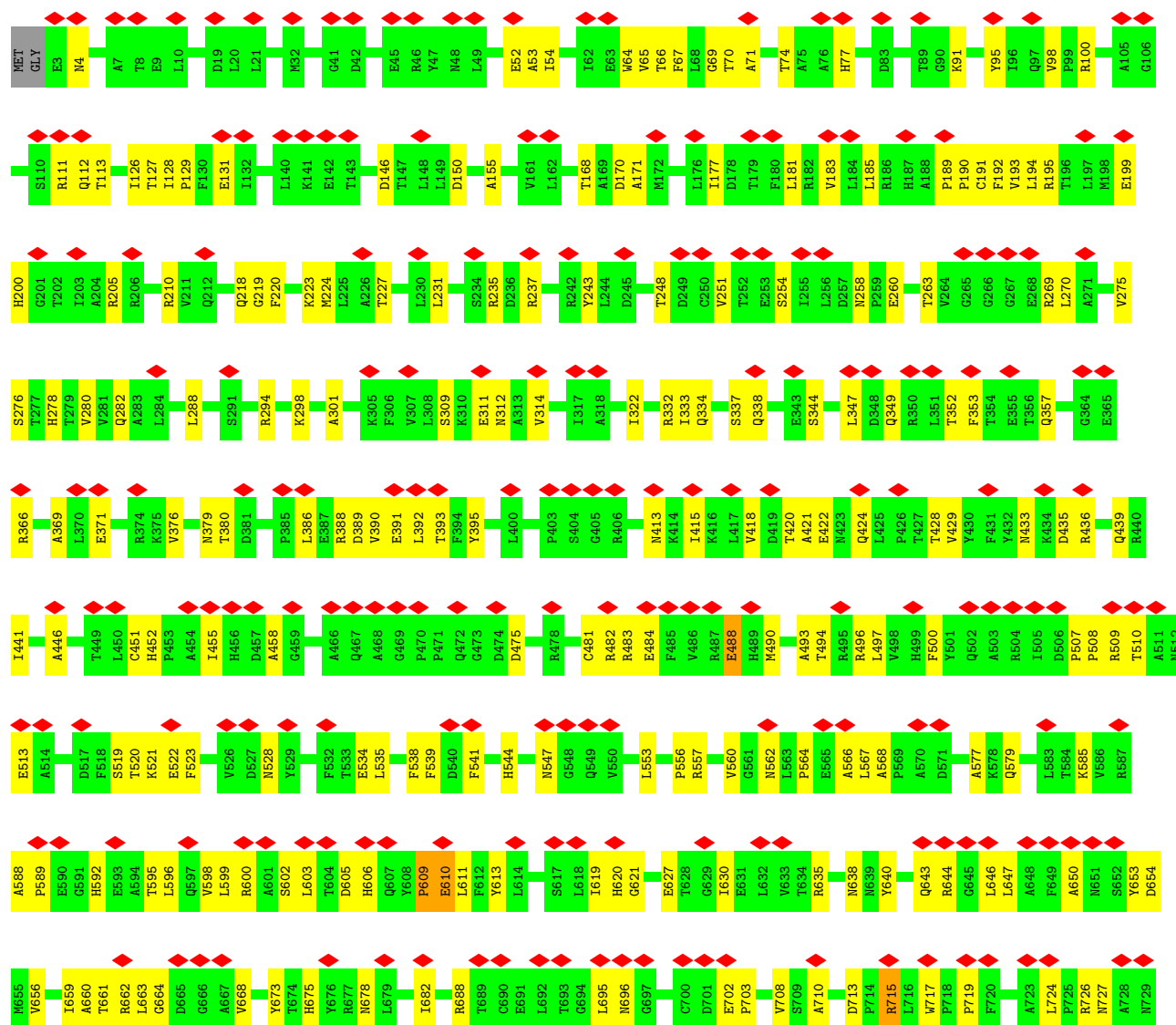
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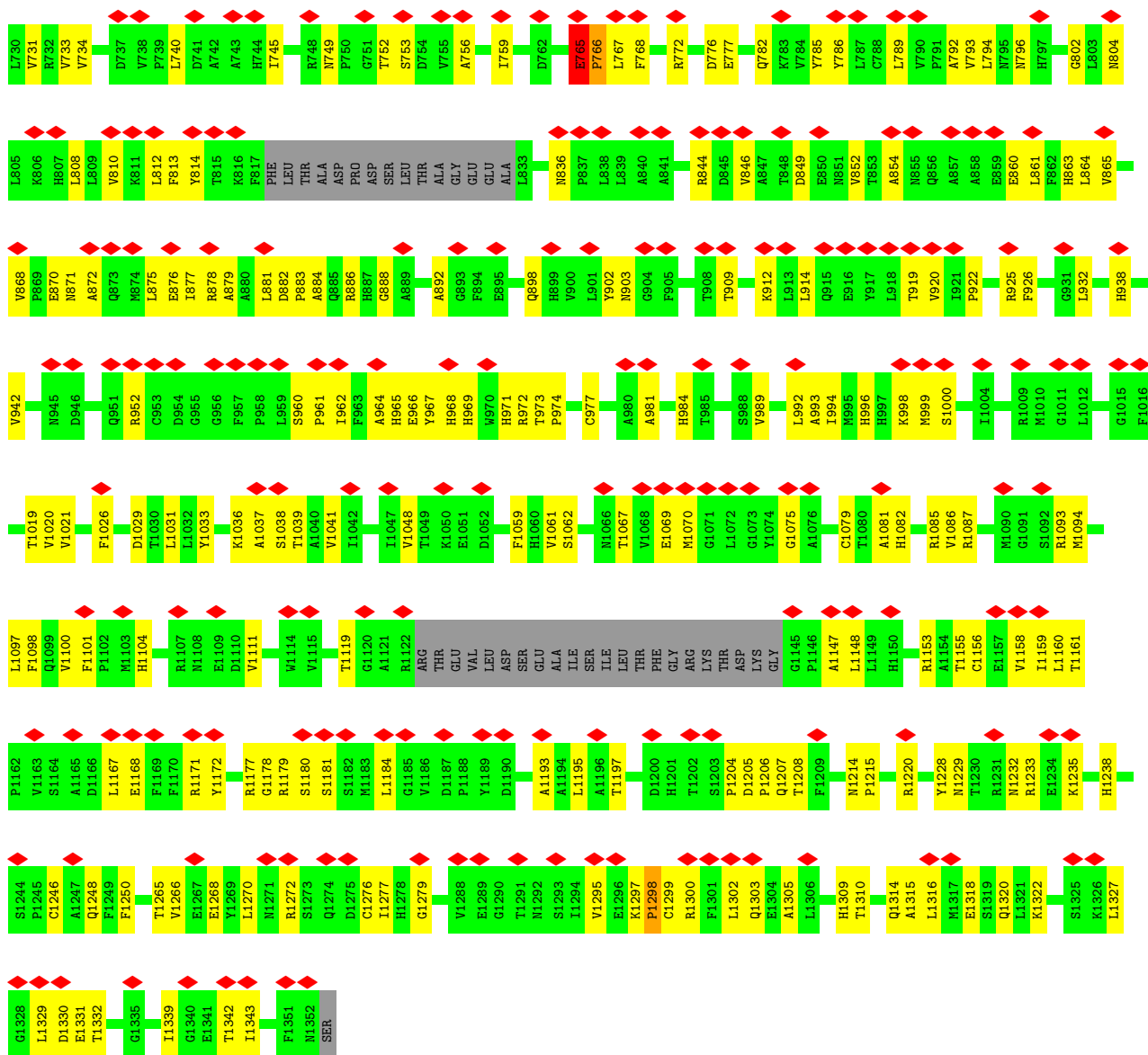


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| C1079 | H996  | Y917 | T848 | E777 | Y707 | N638 | R557 | E484 | L417 | D249 | M172 |
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| H1082 | M999  | V920 | N851 | Q782 | S709 | R642 | N562 | D487 | A421 | Q338 |      |
|       | S1003 | I921 |      | W783 | A710 | Q643 | L563 | E488 | E422 | E343 |      |
| R1085 | L1007 | P922 | N855 | V784 | L711 | R644 | A566 | H489 | N423 | E344 |      |
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| M1090 | R1009 | H924 | E859 | Y786 | F714 | R715 | A570 | A491 | L425 | D257 |      |
| G1091 | M1010 | R925 | E860 | L787 | R716 | L646 |      | A491 | L425 | N258 | F180 |
| S1092 | G1011 | Y927 | L861 |      | W717 | A648 |      | H492 | P426 | D348 |      |
| R1093 | L1012 | P930 | F862 | V790 | P718 | A648 | L575 | R495 | V429 | Q349 | V183 |
| D1096 | G1015 | G931 | H863 | F791 | F719 | F649 | R576 | R496 | Y430 | T352 | L184 |
| F1016 | F1016 | L932 | L864 | L794 | F720 | A650 |      | L497 | F431 | F353 | L185 |
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|       |       |      | A866 |      | Q722 | Y653 | T584 | H499 |      | G266 | H187 |
|       |       |      |      |      | A723 | D654 | K585 |      |      | G267 | P189 |
|       |       |      |      |      | L724 | M655 | V586 |      |      | E268 |      |
|       |       |      |      |      | F725 | R587 | R587 |      |      | R269 | F192 |
|       |       |      |      |      | R726 | A588 | P589 |      |      | A271 | V193 |
|       |       |      |      |      | N727 | R657 | E590 |      |      | V273 | L197 |
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|       |       |      |      |      |      |      | T595 |      |      | S276 | H200 |
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|       |       |      |      |      |      |      |      |      |      | T292 | R210 |
|       |       |      |      |      |      |      |      |      |      | R293 | V211 |
|       |       |      |      |      |      |      |      |      |      | R294 | Q212 |
|       |       |      |      |      |      |      |      |      |      | V382 | R213 |
|       |       |      |      |      |      |      |      |      |      |      |      |
|       |       |      |      |      |      |      |      |      |      | Y303 | T216 |
|       |       |      |      |      |      |      |      |      |      | G304 | A217 |
|       |       |      |      |      |      |      |      |      |      | K305 | Q218 |
|       |       |      |      |      |      |      |      |      |      | F306 | G219 |
|       |       |      |      |      |      |      |      |      |      | V307 | F220 |
|       |       |      |      |      |      |      |      |      |      |      | K223 |

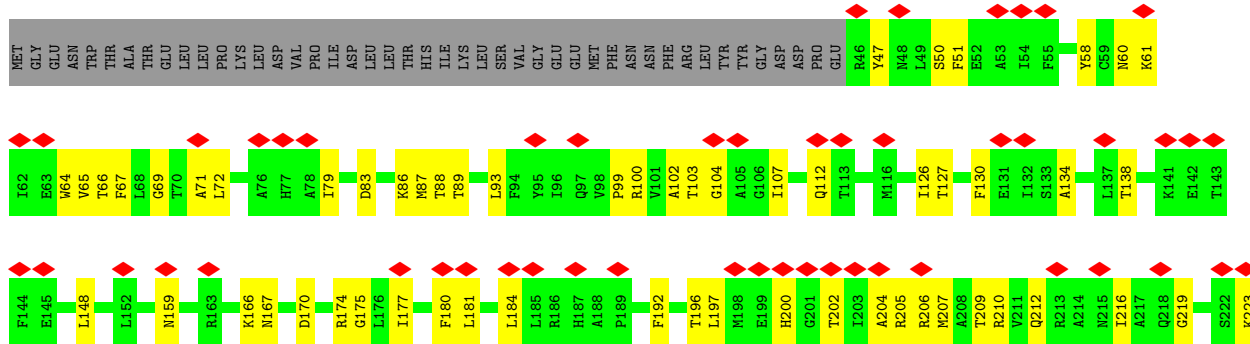


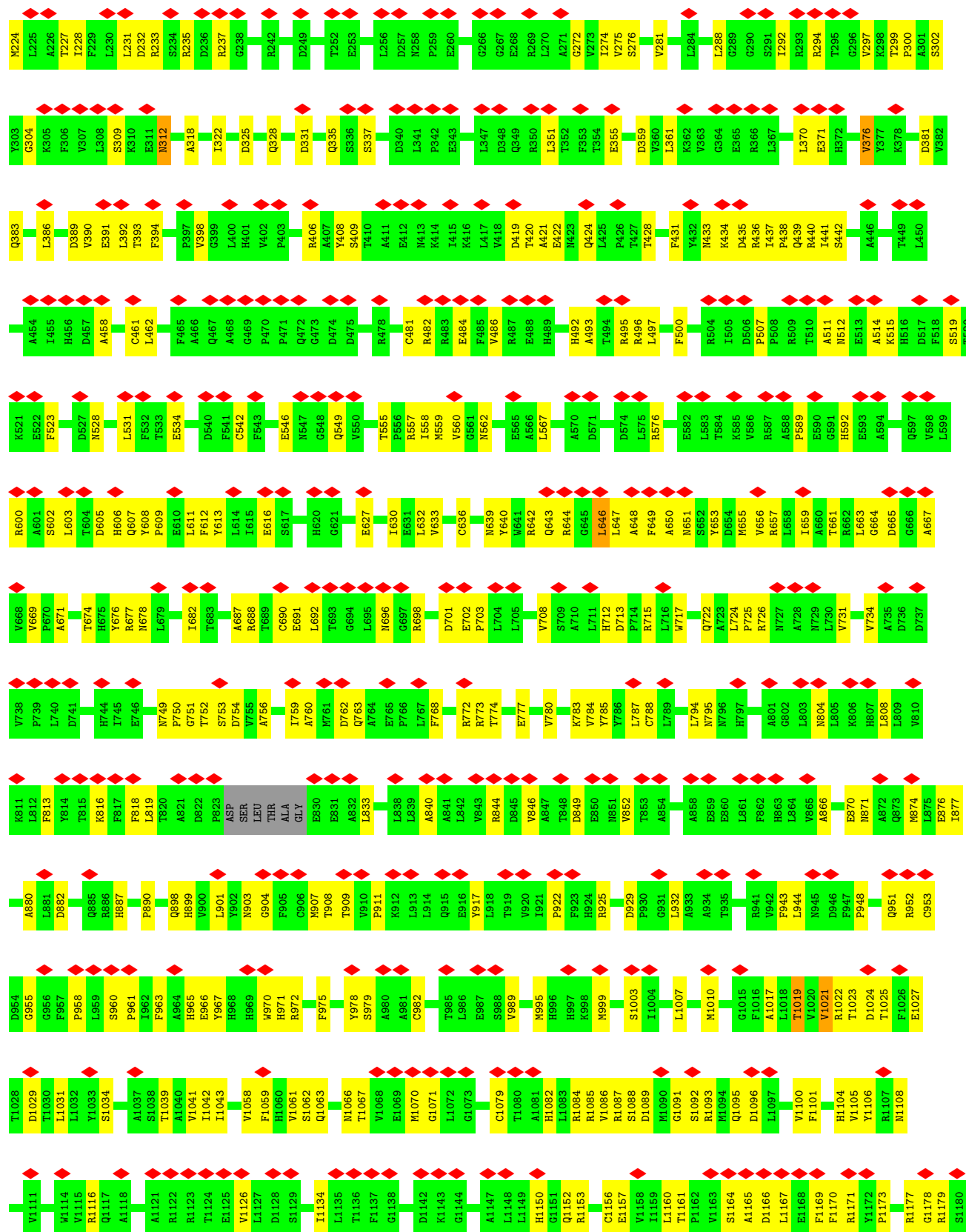
• Molecule 1: Major capsid protein

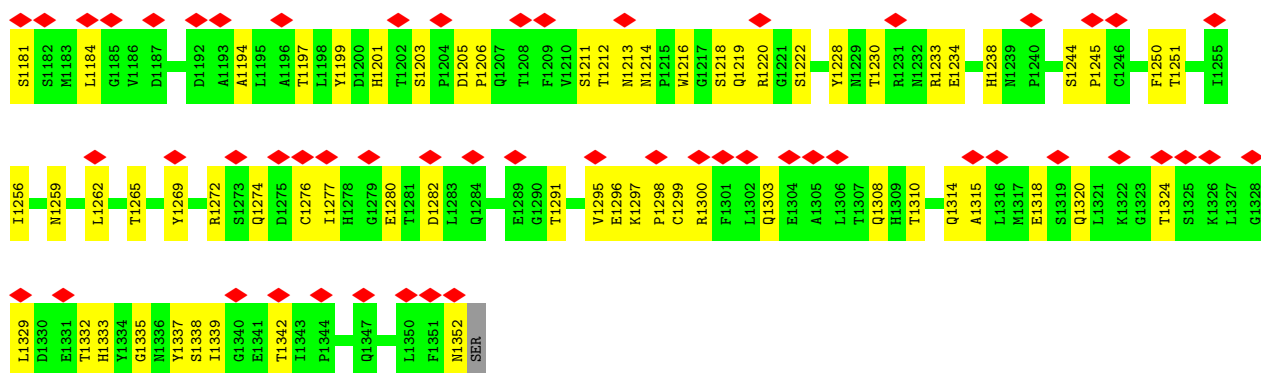




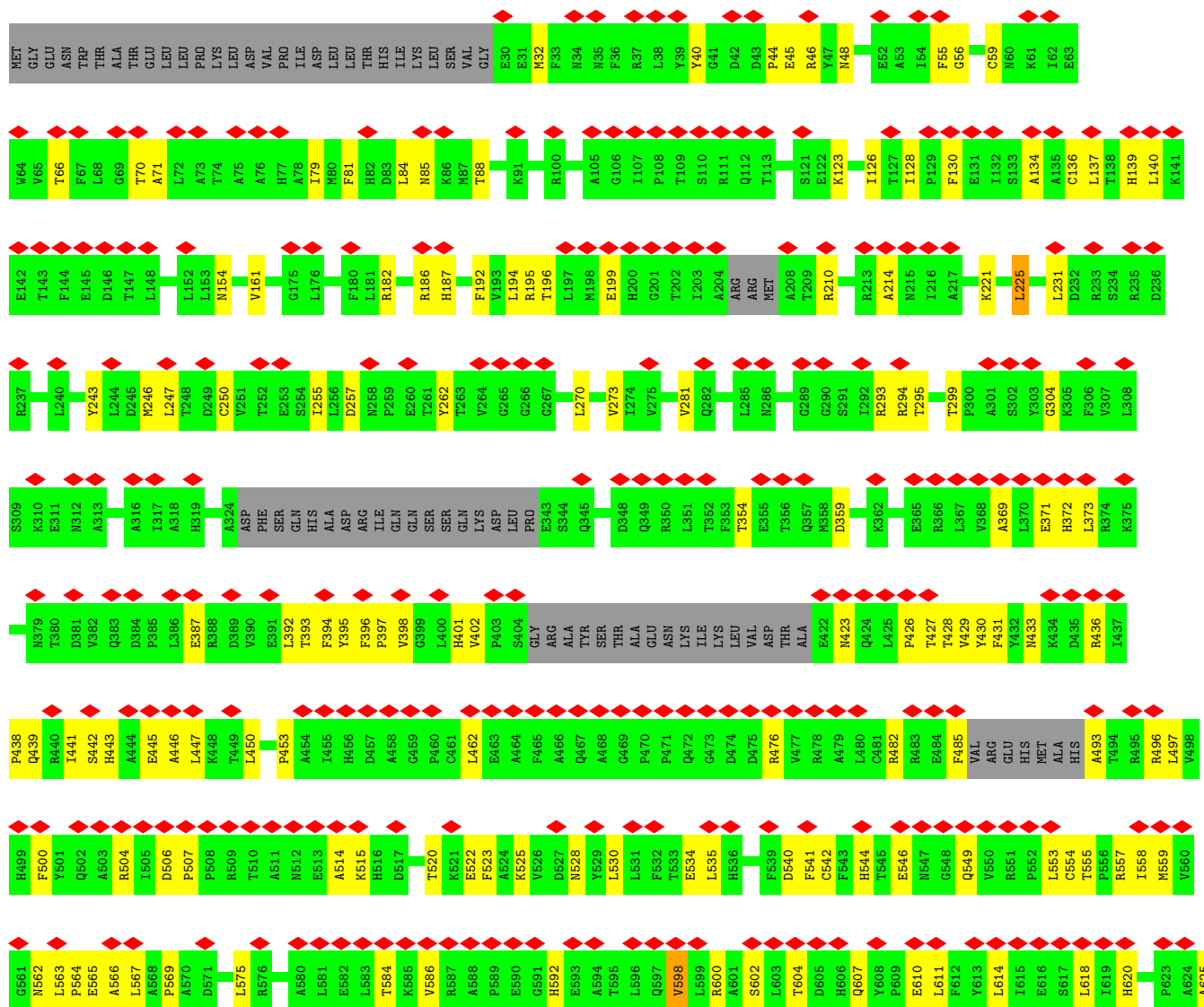
• Molecule 1: Major capsid protein







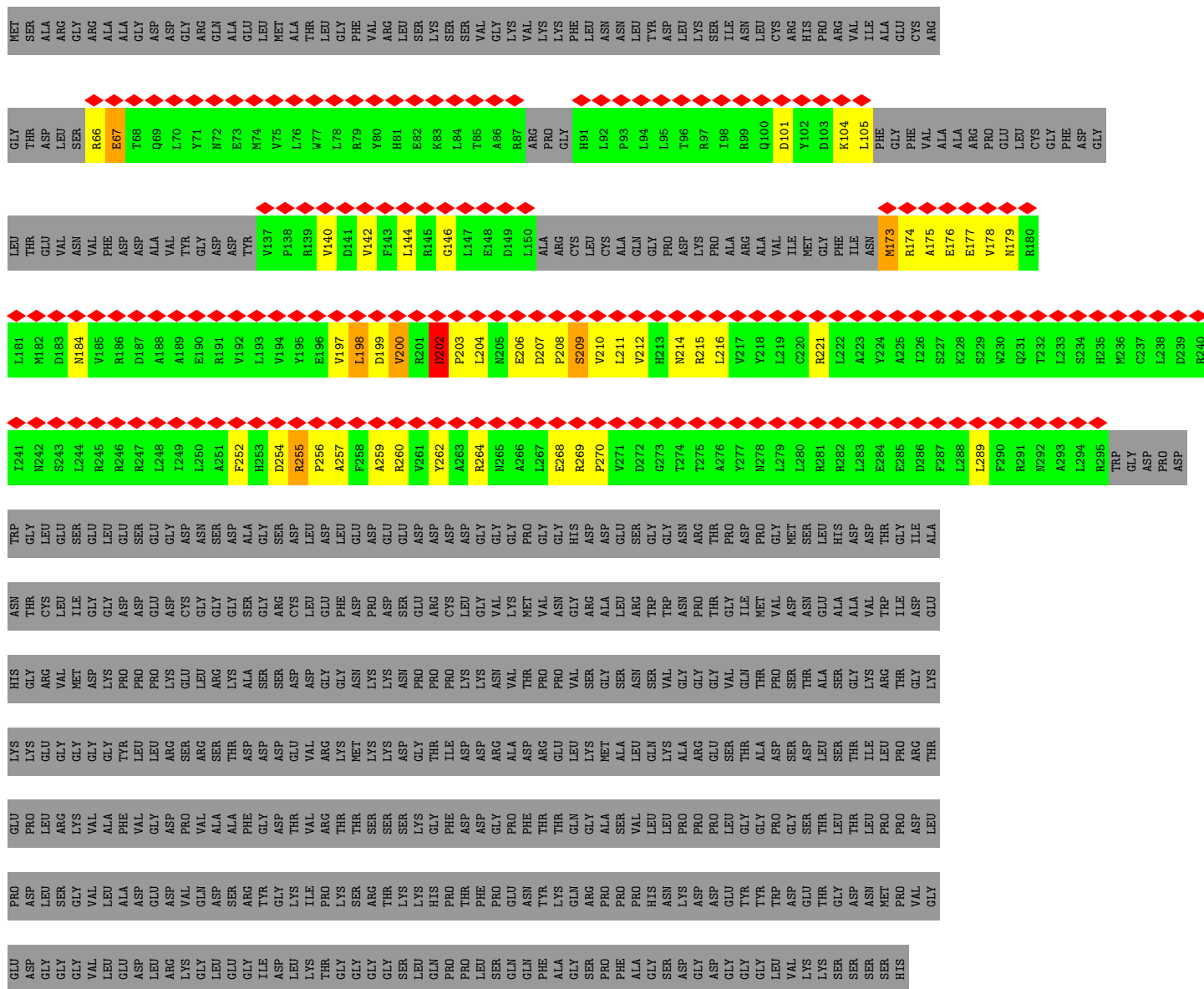
• Molecule 1: Major capsid protein



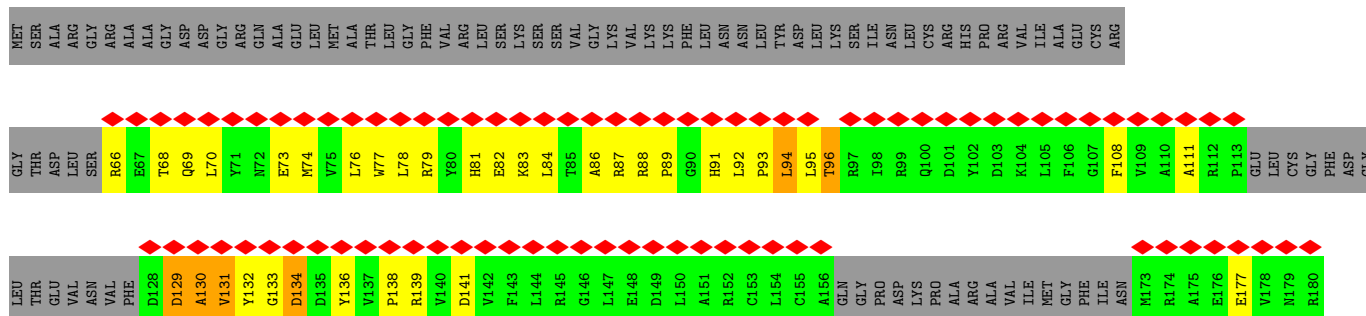


• Molecule 2: Tegument protein





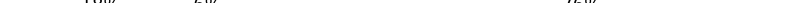
- Molecule 2: Tegument protein

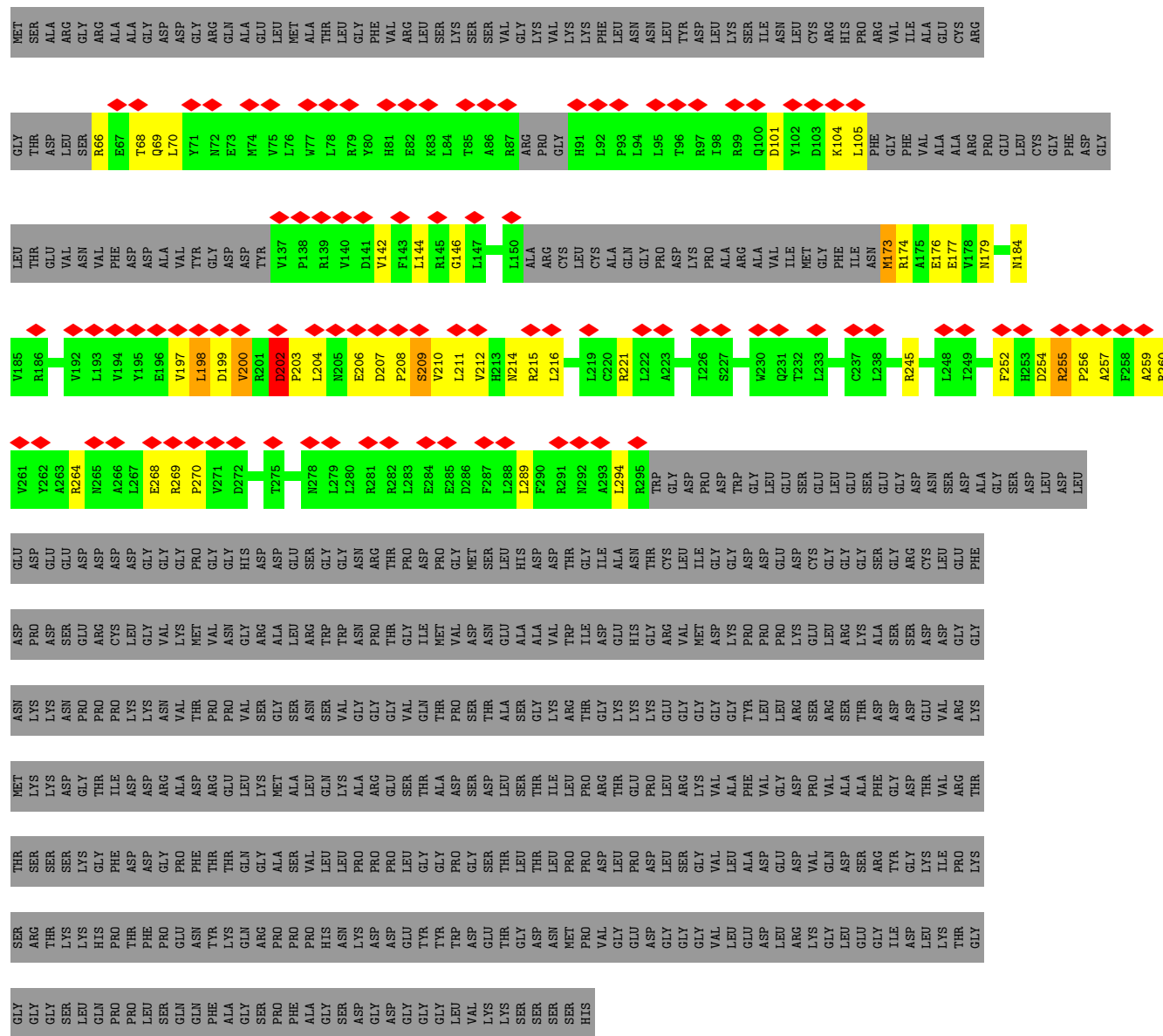


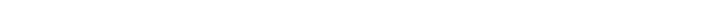


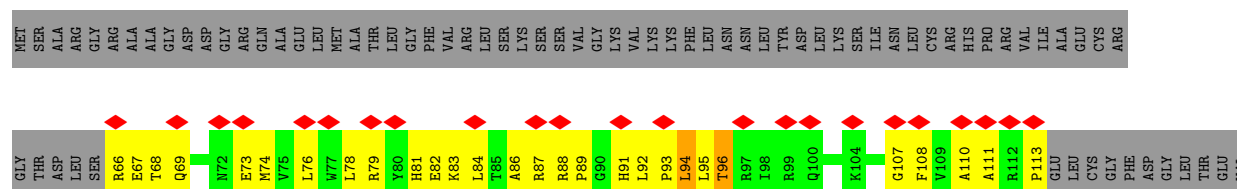
- Molecule 2: Tegument protein

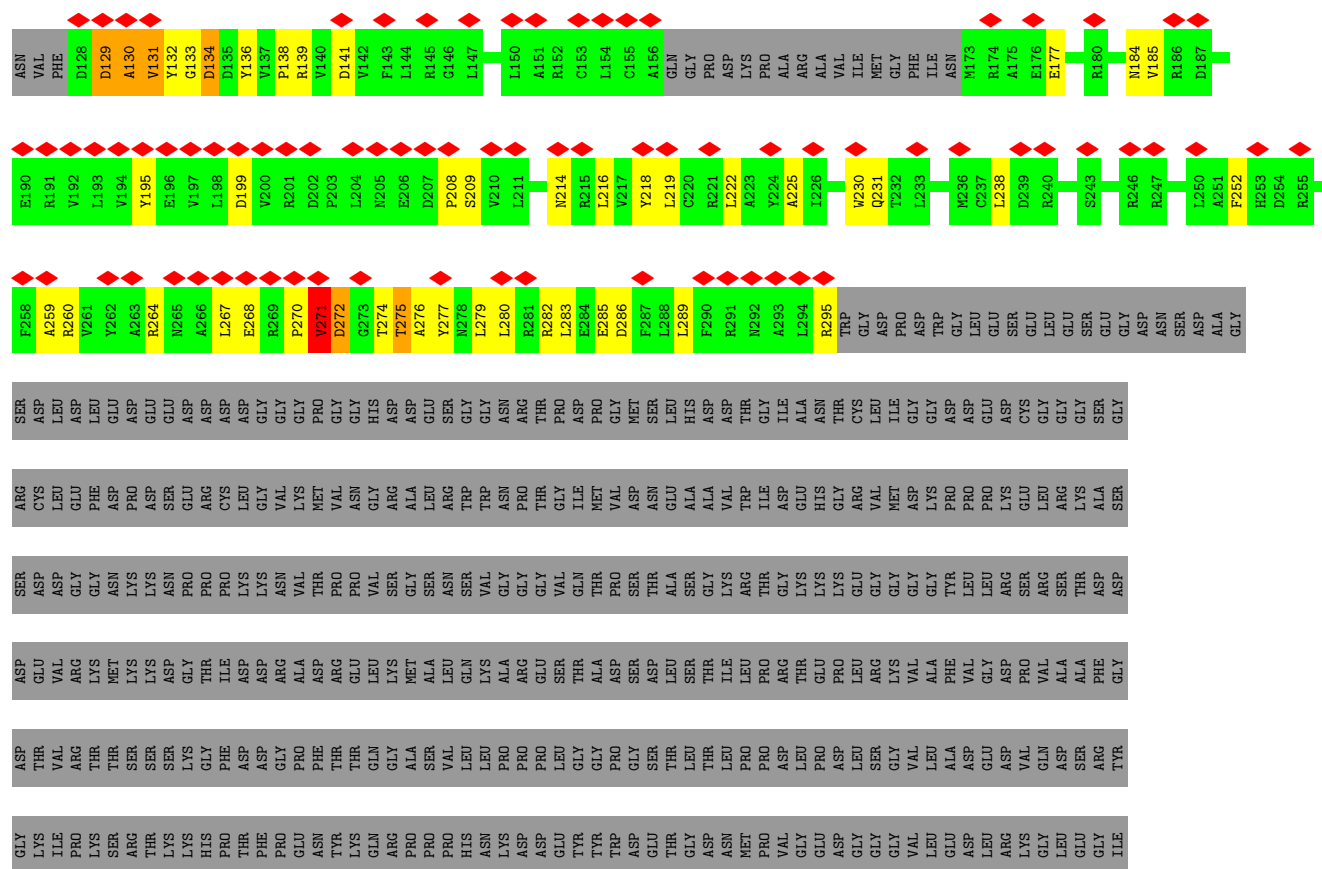
[illegible]

Chain f: 

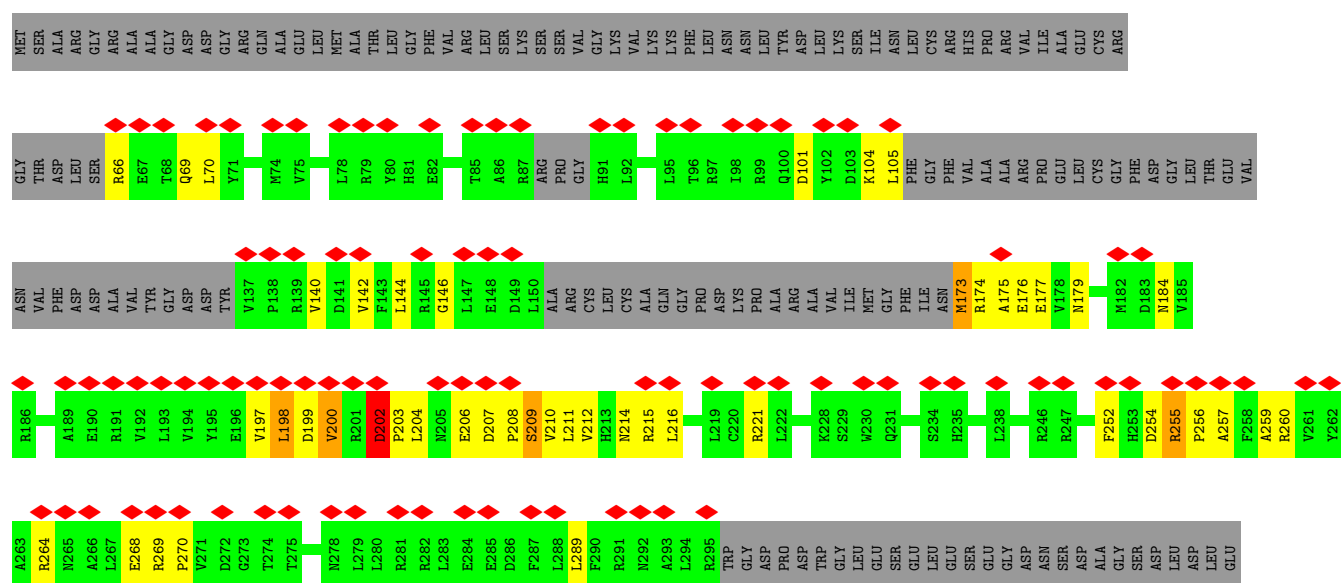


Chain i: 



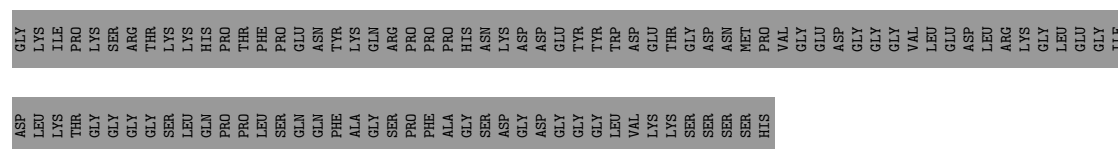


### • Molecule 2: Tegument protein

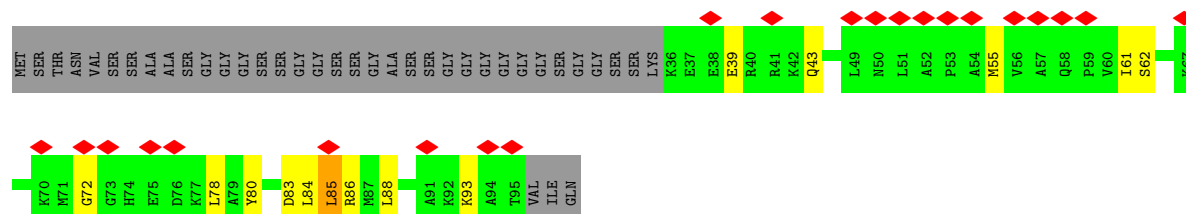


- Molecule 2: Tegument protein

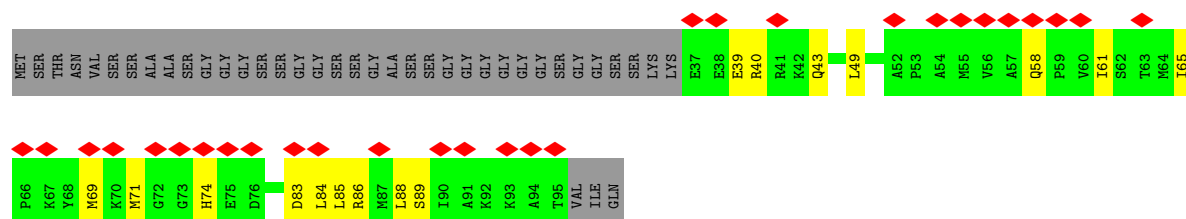
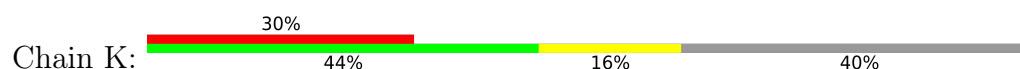
[illegible]



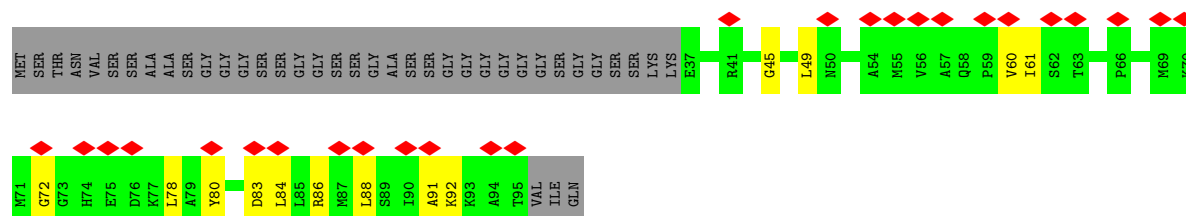
• Molecule 3: Small capsomere-interacting protein



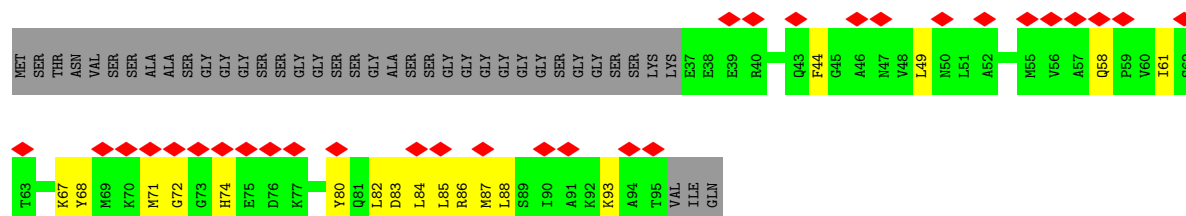
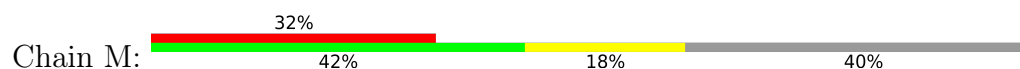
• Molecule 3: Small capsomere-interacting protein



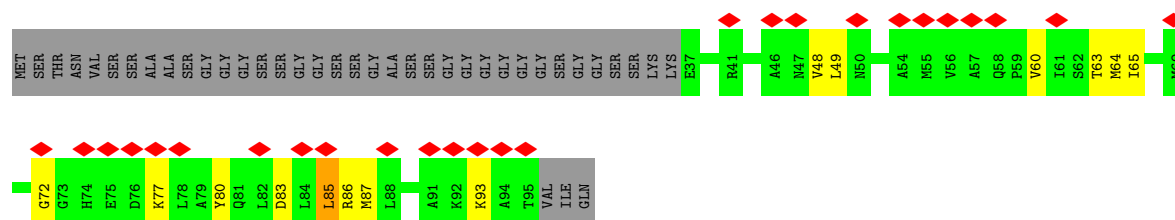
• Molecule 3: Small capsomere-interacting protein



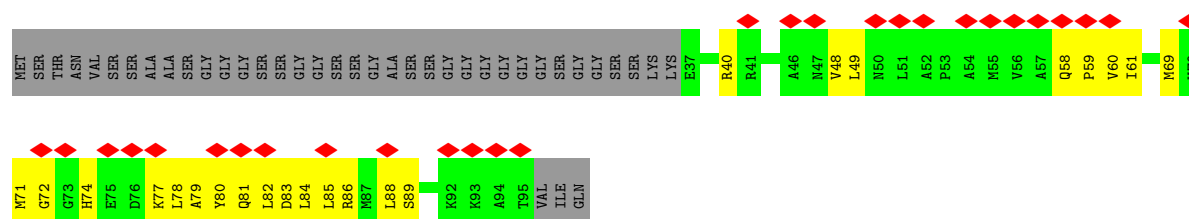
• Molecule 3: Small capsomere-interacting protein



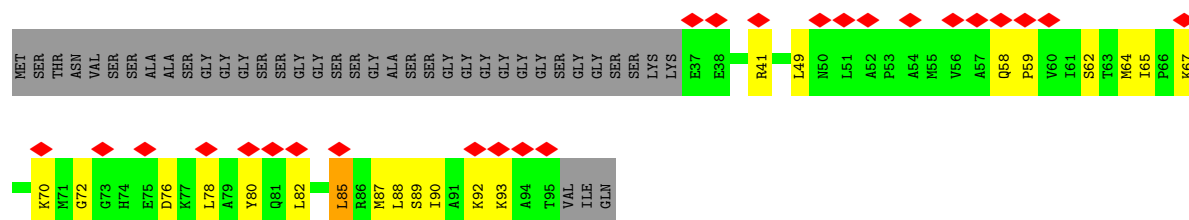
- Molecule 3: Small capsomere-interacting protein



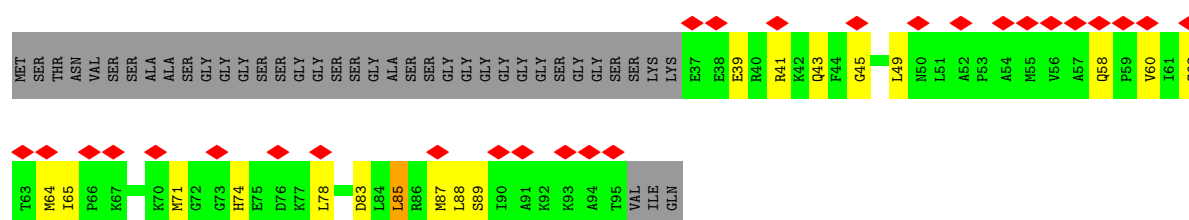
- Molecule 3: Small capsomere-interacting protein



- Molecule 3: Small capsomere-interacting protein

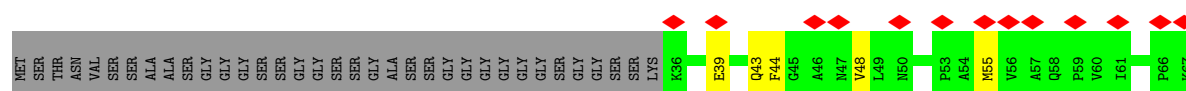


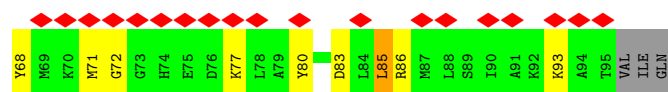
- Molecule 3: Small capsomere-interacting protein



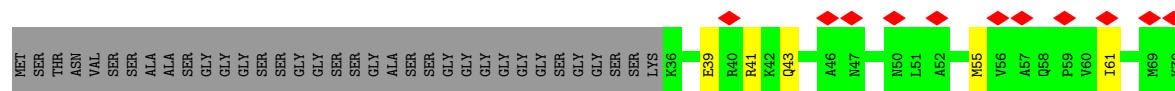
- Molecule 3: Small capsomere-interacting protein



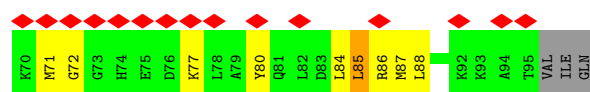
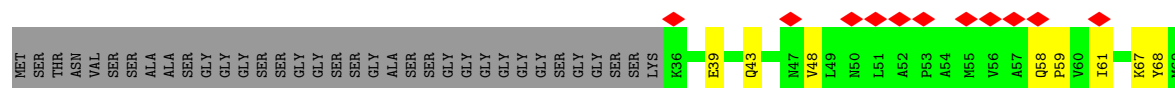
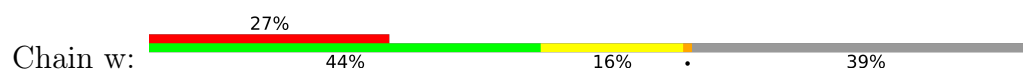




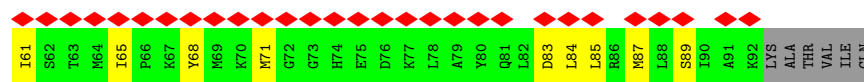
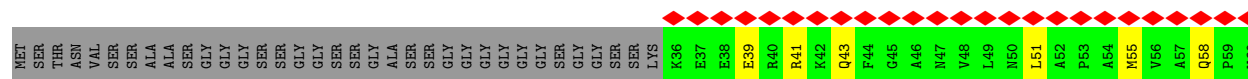
• Molecule 3: Small capsomere-interacting protein



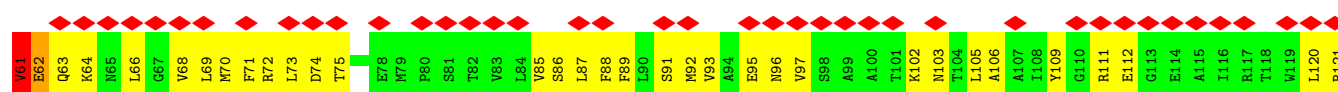
• Molecule 3: Small capsomere-interacting protein

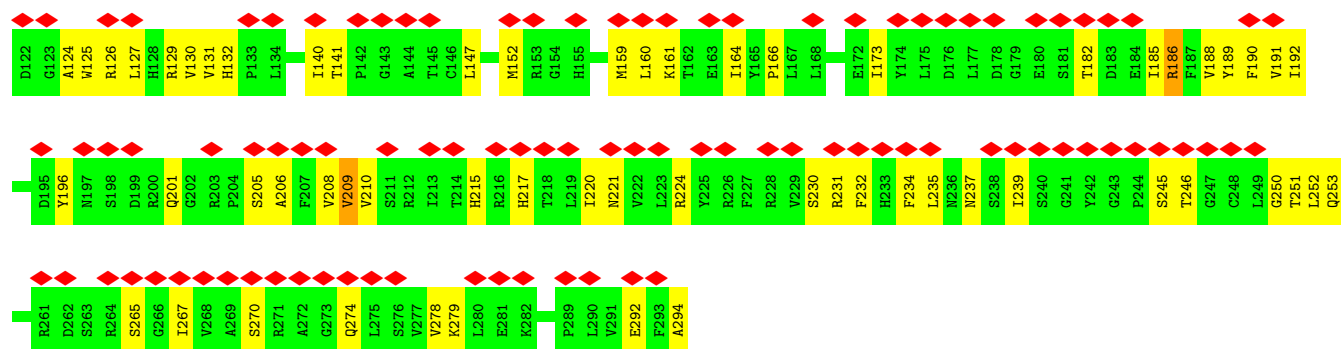


• Molecule 3: Small capsomere-interacting protein

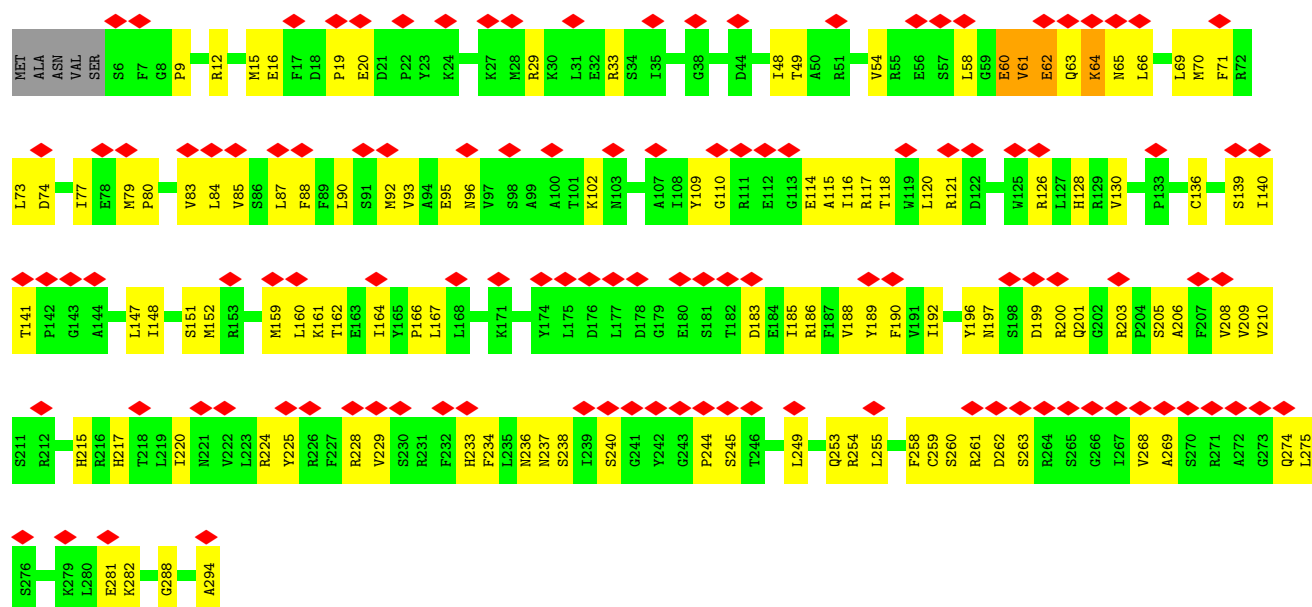
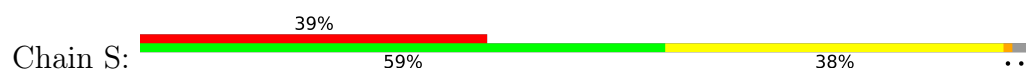


• Molecule 4: Minor capsid protein

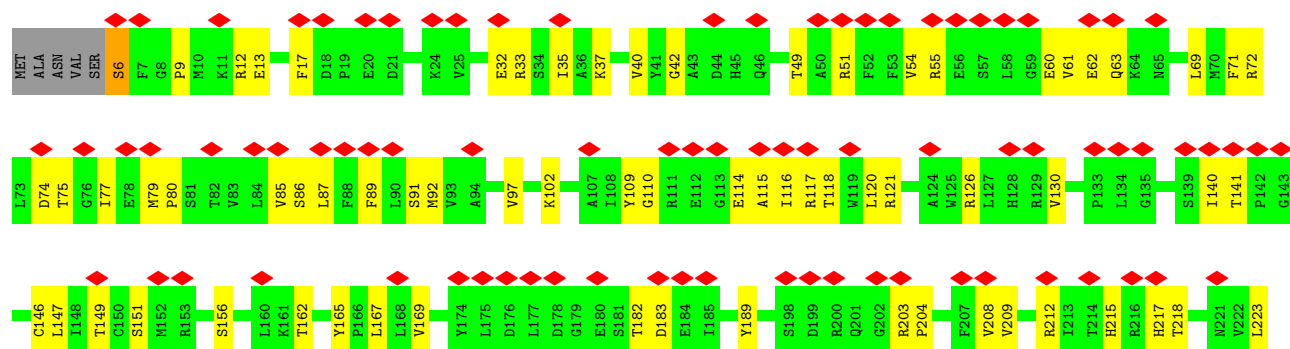
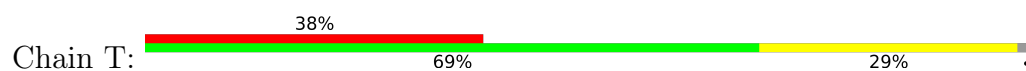




• Molecule 4: Minor capsid protein

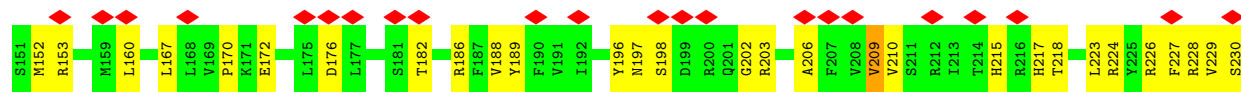
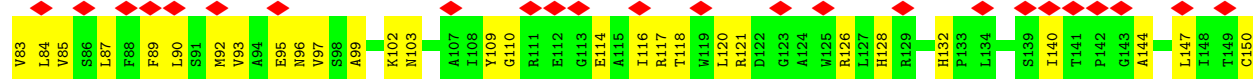


• Molecule 4: Minor capsid protein

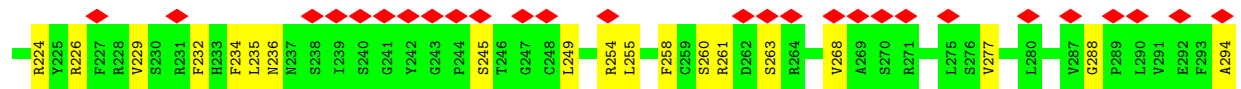
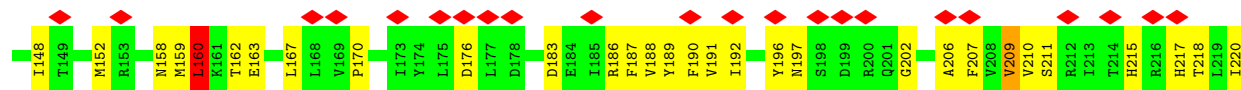




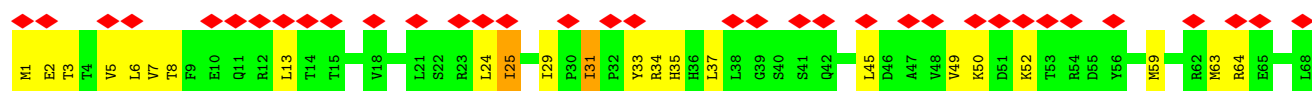
• Molecule 4: Minor capsid protein

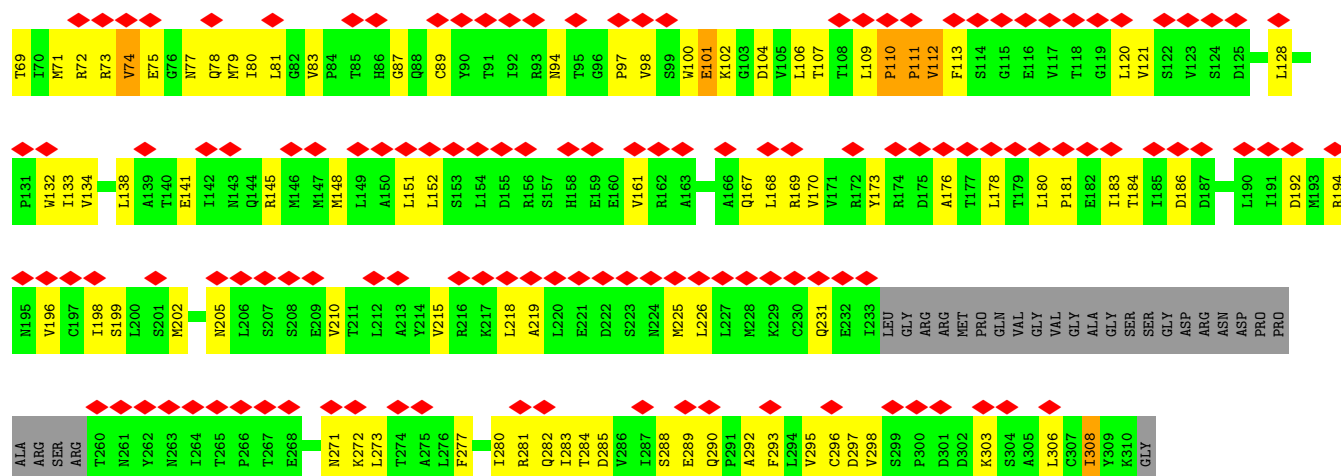


• Molecule 4: Minor capsid protein

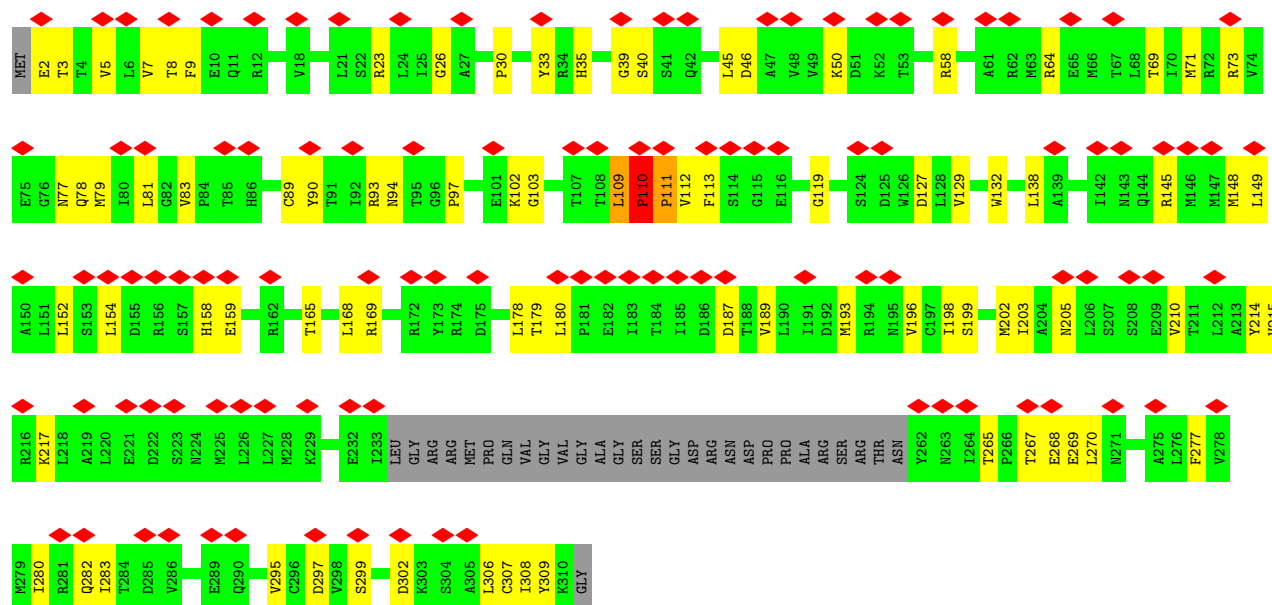


• Molecule 5: Triplex capsid protein 2

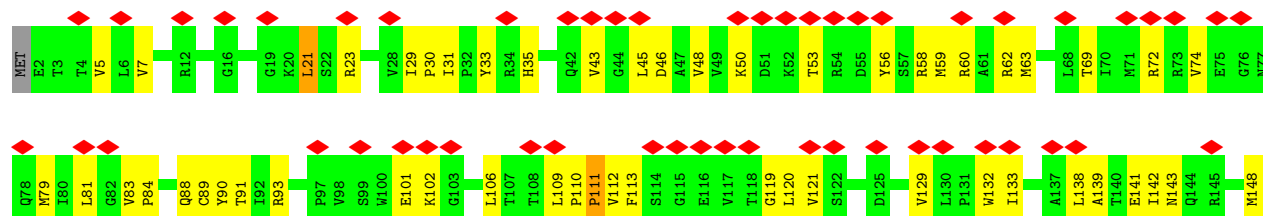


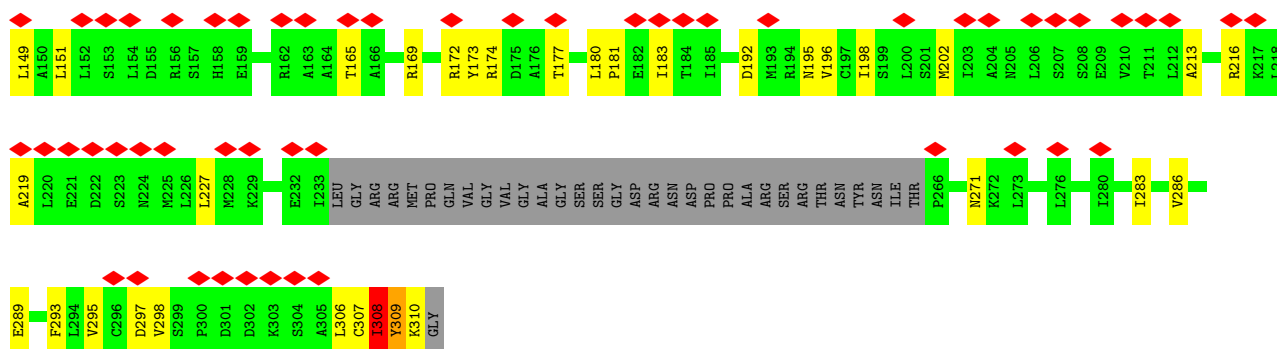


• Molecule 5: Triplex capsid protein 2

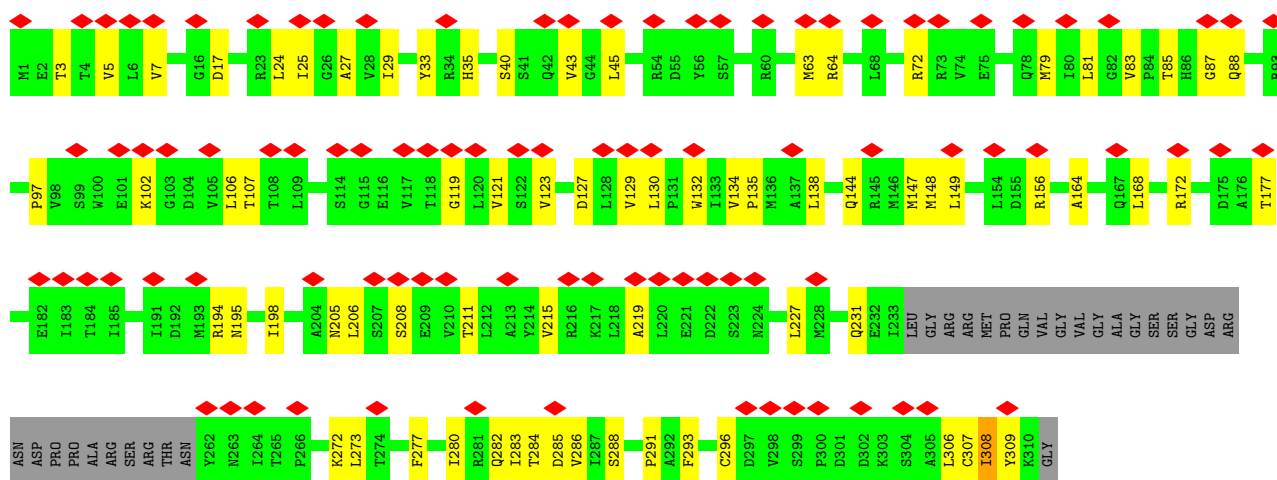


• Molecule 5: Triplex capsid protein 2

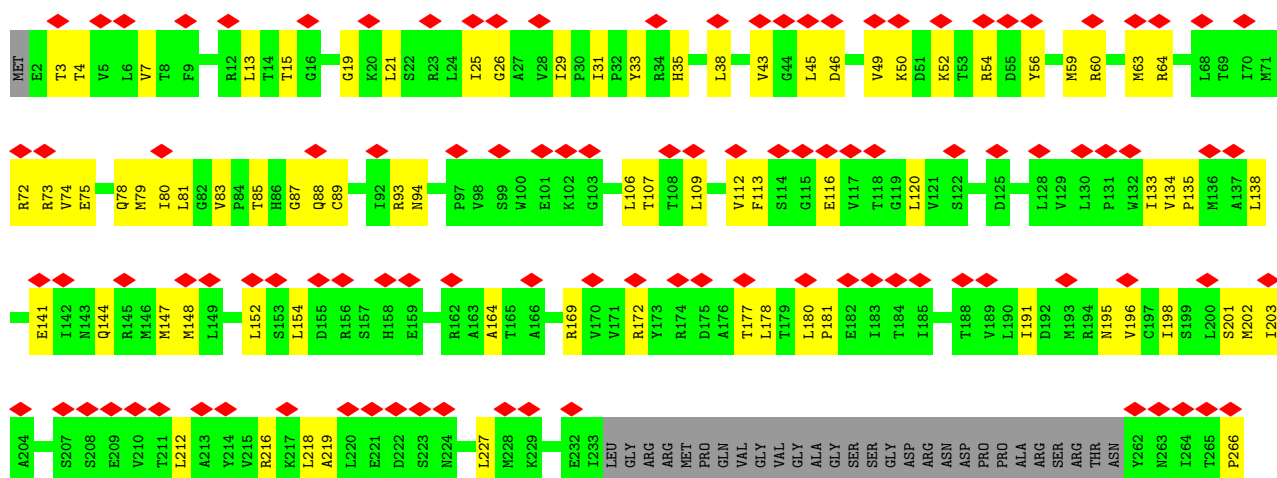
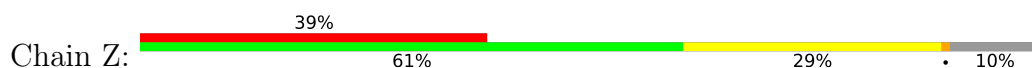




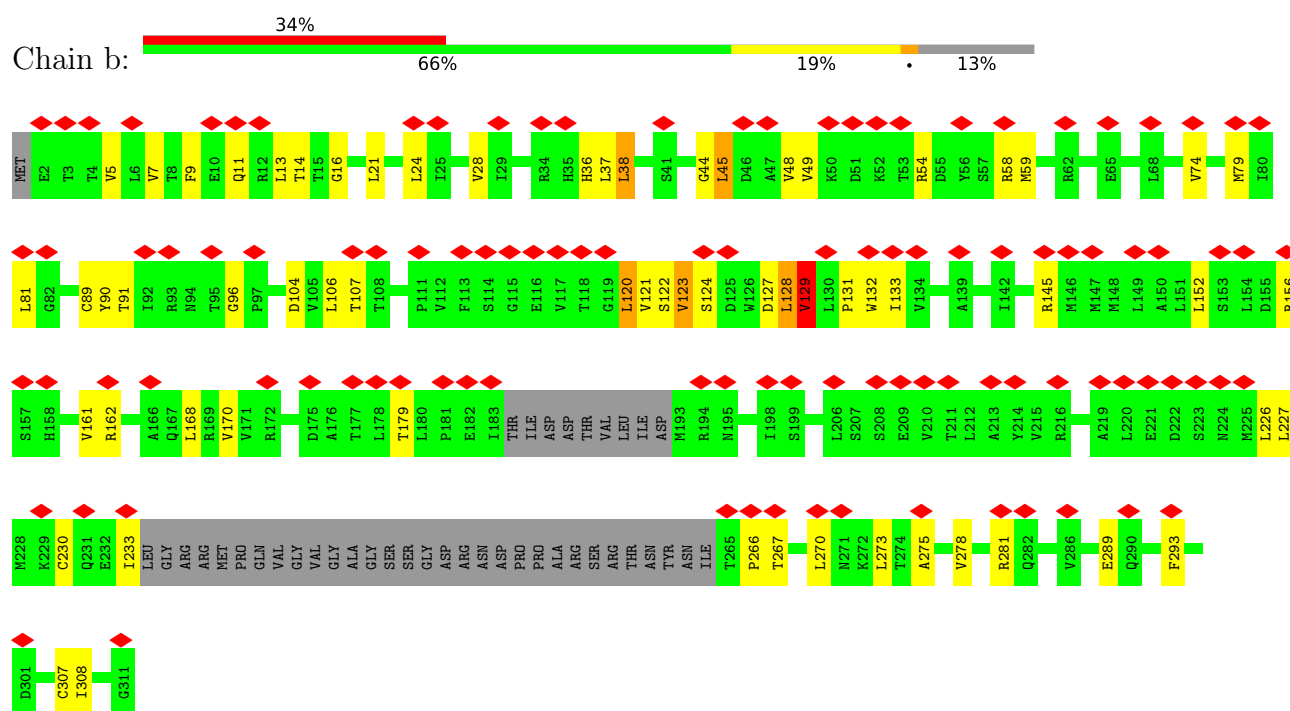
• Molecule 5: Triplex capsid protein 2



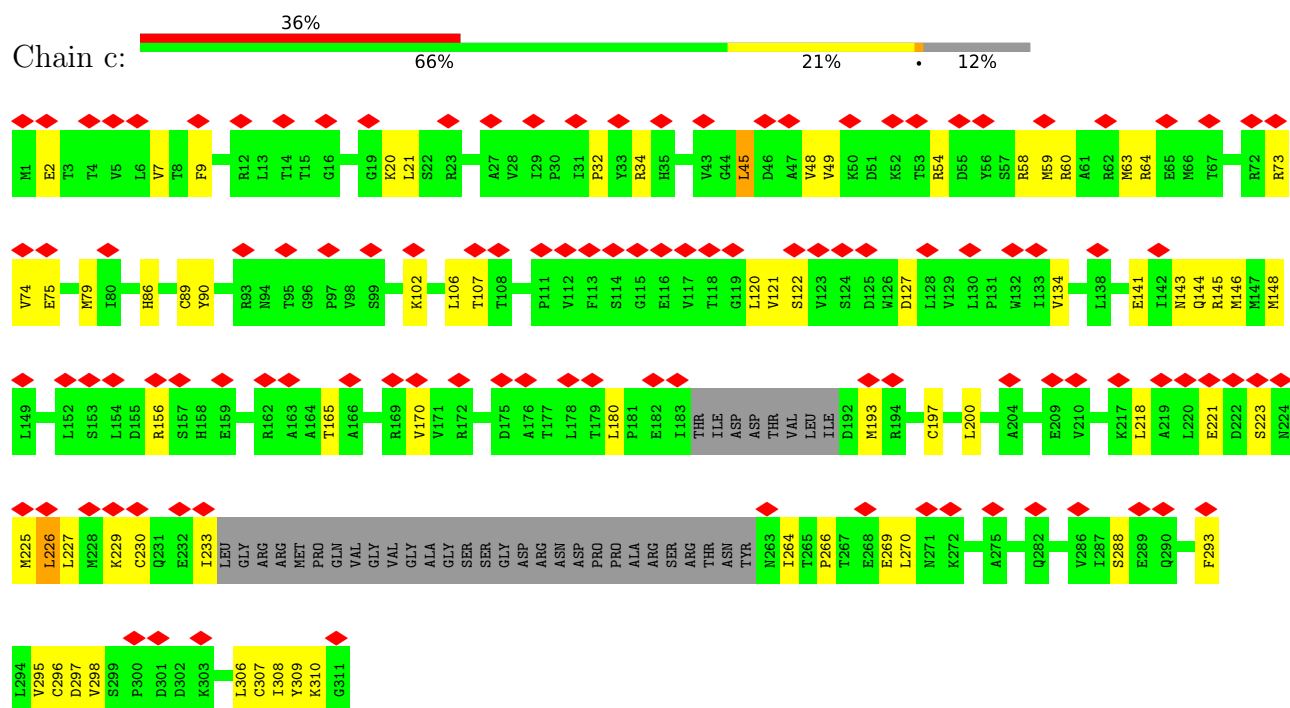
• Molecule 5: Triplex capsid protein 2



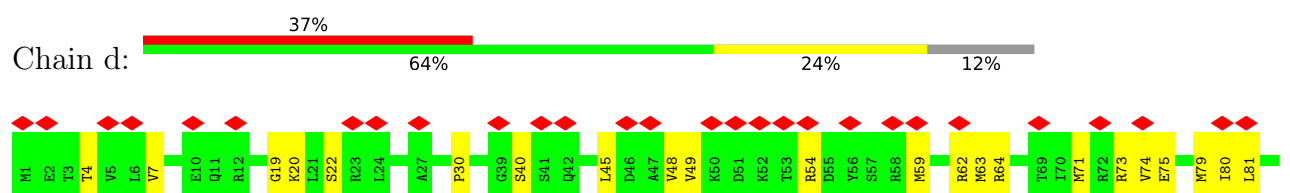


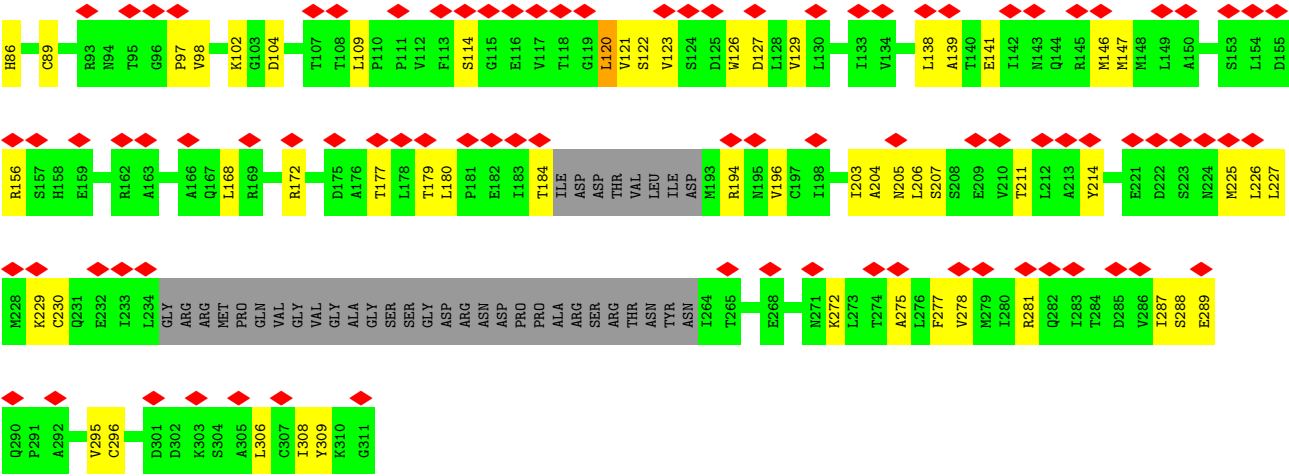


• Molecule 5: Triplex capsid protein 2



• Molecule 5: Triplex capsid protein 2





## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|-----------------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, I                                | Depositor |
| Number of particles used             | 47982                                   | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF                       | Depositor |
| CTF correction method                | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope                           | FEI TITAN KRIOS                         | Depositor |
| Voltage (kV)                         | 300                                     | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 25                                      | Depositor |
| Minimum defocus (nm)                 | 1000                                    | Depositor |
| Maximum defocus (nm)                 | 3000                                    | Depositor |
| Magnification                        | 47000                                   | Depositor |
| Image detector                       | AGFA SCIENTA FILM                       | Depositor |
| Maximum map value                    | 13.184                                  | Depositor |
| Minimum map value                    | -7.318                                  | Depositor |
| Average map value                    | 0.000                                   | Depositor |
| Map value standard deviation         | 1.000                                   | Depositor |
| Recommended contour level            | 4                                       | Depositor |
| Map size (Å)                         | 1729.2799, 1729.2799, 1729.2799         | wwPDB     |
| Map dimensions                       | 1280, 1280, 1280                        | wwPDB     |
| Map angles (°)                       | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing (Å)                    | 1.351, 1.351, 1.351                     | 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   | A     | 0.34         | 0/10779       | 0.63        | 1/14662 (0.0%) |
| 1   | B     | 0.36         | 0/10591       | 0.65        | 2/14408 (0.0%) |
| 1   | C     | 0.41         | 0/10590       | 0.66        | 0/14407        |
| 1   | D     | 0.41         | 0/10615       | 0.67        | 1/14442 (0.0%) |
| 1   | E     | 0.29         | 0/10735       | 0.61        | 2/14602 (0.0%) |
| 1   | F     | 0.35         | 0/10648       | 0.63        | 4/14488 (0.0%) |
| 1   | G     | 0.43         | 0/10823       | 0.69        | 0/14724        |
| 1   | H     | 0.35         | 0/10823       | 0.65        | 4/14724 (0.0%) |
| 1   | I     | 0.32         | 0/10662       | 0.62        | 0/14506        |
| 1   | k     | 0.35         | 0/10445       | 0.67        | 6/14213 (0.0%) |
| 1   | l     | 0.35         | 0/10790       | 0.67        | 6/14677 (0.0%) |
| 1   | m     | 0.36         | 0/10604       | 0.69        | 7/14426 (0.0%) |
| 1   | n     | 0.31         | 0/10779       | 0.67        | 4/14662 (0.0%) |
| 1   | o     | 0.33         | 0/10607       | 0.67        | 4/14430 (0.0%) |
| 1   | p     | 0.33         | 0/10485       | 0.68        | 2/14261 (0.0%) |
| 1   | q     | 0.28         | 0/9837        | 0.66        | 8/13377 (0.1%) |
| 2   | 2     | 0.57         | 1/1493 (0.1%) | 0.81        | 5/2016 (0.2%)  |
| 2   | 3     | 0.34         | 1/1696 (0.1%) | 0.75        | 7/2294 (0.3%)  |
| 2   | e     | 0.57         | 1/1493 (0.1%) | 0.81        | 5/2016 (0.2%)  |
| 2   | f     | 0.57         | 1/1493 (0.1%) | 0.81        | 5/2016 (0.2%)  |
| 2   | g     | 0.57         | 1/1493 (0.1%) | 0.81        | 5/2016 (0.2%)  |
| 2   | h     | 0.34         | 1/1696 (0.1%) | 0.75        | 7/2294 (0.3%)  |
| 2   | i     | 0.34         | 1/1696 (0.1%) | 0.75        | 7/2294 (0.3%)  |
| 2   | j     | 0.34         | 1/1696 (0.1%) | 0.75        | 7/2294 (0.3%)  |
| 3   | J     | 0.26         | 0/477         | 0.58        | 0/637          |
| 3   | K     | 0.27         | 0/468         | 0.60        | 0/626          |
| 3   | L     | 0.26         | 0/468         | 0.54        | 0/626          |
| 3   | M     | 0.38         | 0/468         | 0.60        | 0/626          |
| 3   | N     | 0.27         | 0/468         | 0.57        | 0/626          |
| 3   | O     | 0.28         | 0/468         | 0.58        | 0/626          |
| 3   | P     | 0.30         | 0/468         | 0.59        | 0/626          |
| 3   | Q     | 0.28         | 0/468         | 0.54        | 0/626          |
| 3   | R     | 0.29         | 0/468         | 0.58        | 0/626          |
| 3   | r     | 0.30         | 0/477         | 0.75        | 0/637          |

| Mol | Chain | Bond lengths |                 | Bond angles |                   |
|-----|-------|--------------|-----------------|-------------|-------------------|
|     |       | RMSZ         | # Z  >5         | RMSZ        | # Z  >5           |
| 3   | s     | 0.27         | 0/468           | 0.65        | 0/626             |
| 3   | t     | 0.30         | 0/468           | 0.64        | 0/626             |
| 3   | u     | 0.28         | 0/477           | 0.66        | 0/637             |
| 3   | v     | 0.26         | 0/477           | 0.65        | 0/637             |
| 3   | w     | 0.31         | 0/477           | 0.69        | 0/637             |
| 3   | x     | 0.32         | 0/456           | 0.78        | 1/609 (0.2%)      |
| 4   | S     | 0.34         | 0/2357          | 0.66        | 0/3185            |
| 4   | T     | 0.33         | 1/2357 (0.0%)   | 0.74        | 3/3185 (0.1%)     |
| 4   | U     | 0.32         | 0/2357          | 0.70        | 1/3185 (0.0%)     |
| 4   | V     | 0.30         | 0/2357          | 0.68        | 1/3185 (0.0%)     |
| 4   | y     | 0.37         | 0/2020          | 0.78        | 2/2735 (0.1%)     |
| 5   | 1     | 0.29         | 0/2037          | 0.66        | 0/2761            |
| 5   | W     | 0.28         | 0/2232          | 0.69        | 2/3031 (0.1%)     |
| 5   | X     | 0.25         | 0/2196          | 0.63        | 1/2980 (0.0%)     |
| 5   | Y     | 0.30         | 0/2240          | 0.68        | 0/3041            |
| 5   | Z     | 0.27         | 0/2232          | 0.63        | 0/3031            |
| 5   | a     | 0.31         | 0/2113          | 0.64        | 0/2862            |
| 5   | b     | 0.26         | 0/2138          | 0.59        | 0/2897            |
| 5   | c     | 0.30         | 0/2170          | 0.63        | 0/2940            |
| 5   | d     | 0.31         | 0/2169          | 0.62        | 0/2939            |
| 5   | z     | 0.30         | 0/2255          | 0.70        | 1/3062 (0.0%)     |
| All | All   | 0.35         | 9/223320 (0.0%) | 0.67        | 111/303322 (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 |
|-----|-------|---------------------|---------------------|
| 4   | T     | 0                   | 2                   |

All (9) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 2   | e     | 209 | SER  | C-N   | 18.71 | 1.56        | 1.33     |
| 2   | 2     | 209 | SER  | C-N   | 18.68 | 1.56        | 1.33     |
| 2   | g     | 209 | SER  | C-N   | 18.68 | 1.56        | 1.33     |
| 2   | f     | 209 | SER  | C-N   | 18.66 | 1.56        | 1.33     |
| 2   | 3     | 96  | THR  | C-N   | -6.52 | 1.24        | 1.33     |
| 2   | h     | 96  | THR  | C-N   | -6.50 | 1.24        | 1.33     |
| 2   | j     | 96  | THR  | C-N   | -6.50 | 1.24        | 1.33     |
| 2   | i     | 96  | THR  | C-N   | -6.50 | 1.24        | 1.33     |

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| Mol | Chain | Res | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 4   | T     | 6   | SER  | C-N   | 6.50 | 1.44        | 1.33     |

All (111) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms  | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|--------|-------------|----------|
| 2   | e     | 209  | SER  | O-C-N  | -15.29 | 104.33      | 122.22   |
| 2   | f     | 209  | SER  | O-C-N  | -15.28 | 104.34      | 122.22   |
| 2   | 2     | 209  | SER  | O-C-N  | -15.28 | 104.35      | 122.22   |
| 2   | g     | 209  | SER  | O-C-N  | -15.26 | 104.36      | 122.22   |
| 4   | T     | 6    | SER  | CA-C-N | -12.09 | 103.24      | 122.23   |
| 4   | T     | 6    | SER  | C-N-CA | -12.09 | 103.24      | 122.23   |
| 5   | W     | 210  | VAL  | N-CA-C | -8.95  | 104.55      | 111.62   |
| 1   | m     | 310  | LYS  | N-CA-C | -8.73  | 101.45      | 110.97   |
| 2   | 2     | 255  | ARG  | CA-C-N | -8.34  | 109.42      | 119.84   |
| 2   | 2     | 255  | ARG  | C-N-CA | -8.34  | 109.42      | 119.84   |
| 2   | g     | 255  | ARG  | CA-C-N | -8.32  | 109.44      | 119.84   |
| 2   | g     | 255  | ARG  | C-N-CA | -8.32  | 109.44      | 119.84   |
| 2   | e     | 255  | ARG  | CA-C-N | -8.32  | 109.44      | 119.84   |
| 2   | e     | 255  | ARG  | C-N-CA | -8.32  | 109.44      | 119.84   |
| 2   | f     | 255  | ARG  | CA-C-N | -8.31  | 109.45      | 119.84   |
| 2   | f     | 255  | ARG  | C-N-CA | -8.31  | 109.45      | 119.84   |
| 1   | l     | 956  | GLY  | N-CA-C | -7.43  | 95.58       | 113.18   |
| 5   | X     | 308  | ILE  | N-CA-C | 7.20   | 117.27      | 108.06   |
| 1   | l     | 957  | PHE  | N-CA-C | 7.13   | 119.15      | 109.24   |
| 1   | q     | 1186 | VAL  | CA-C-N | 6.90   | 129.72      | 123.10   |
| 1   | q     | 1186 | VAL  | C-N-CA | 6.90   | 129.72      | 123.10   |
| 2   | f     | 254  | ASP  | N-CA-C | 6.77   | 119.61      | 109.25   |
| 2   | e     | 254  | ASP  | N-CA-C | 6.77   | 119.60      | 109.25   |
| 2   | g     | 254  | ASP  | N-CA-C | 6.76   | 119.60      | 109.25   |
| 2   | h     | 134  | ASP  | N-CA-C | -6.75  | 103.84      | 111.07   |
| 2   | 2     | 254  | ASP  | N-CA-C | 6.75   | 119.58      | 109.25   |
| 2   | i     | 134  | ASP  | N-CA-C | -6.75  | 103.85      | 111.07   |
| 2   | 3     | 134  | ASP  | N-CA-C | -6.74  | 103.85      | 111.07   |
| 2   | j     | 134  | ASP  | N-CA-C | -6.74  | 103.86      | 111.07   |
| 4   | U     | 61   | VAL  | N-CA-C | 6.42   | 117.94      | 110.62   |
| 2   | 3     | 275  | THR  | N-CA-C | 6.34   | 117.98      | 111.14   |
| 2   | h     | 275  | THR  | N-CA-C | 6.34   | 117.98      | 111.14   |
| 2   | j     | 275  | THR  | N-CA-C | 6.32   | 117.97      | 111.14   |
| 2   | i     | 275  | THR  | N-CA-C | 6.29   | 117.93      | 111.14   |
| 2   | h     | 96   | THR  | O-C-N  | -6.24  | 114.92      | 122.22   |
| 2   | i     | 96   | THR  | O-C-N  | -6.22  | 114.94      | 122.22   |
| 5   | z     | 110  | PRO  | O-C-N  | 6.22   | 124.17      | 121.31   |

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| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 2   | j     | 96   | THR  | O-C-N  | -6.20 | 114.96      | 122.22   |
| 2   | 3     | 96   | THR  | O-C-N  | -6.16 | 115.02      | 122.22   |
| 1   | E     | 487  | ARG  | CA-C-N | 6.12  | 133.23      | 121.54   |
| 1   | E     | 487  | ARG  | C-N-CA | 6.12  | 133.23      | 121.54   |
| 1   | q     | 45   | GLU  | CA-C-N | 6.11  | 133.20      | 121.54   |
| 1   | q     | 45   | GLU  | C-N-CA | 6.11  | 133.20      | 121.54   |
| 1   | m     | 1174 | ASN  | CA-C-N | 5.98  | 129.92      | 121.61   |
| 1   | m     | 1174 | ASN  | C-N-CA | 5.98  | 129.92      | 121.61   |
| 2   | 2     | 202  | ASP  | N-CA-C | 5.95  | 122.97      | 109.81   |
| 2   | e     | 202  | ASP  | N-CA-C | 5.95  | 122.97      | 109.81   |
| 2   | g     | 202  | ASP  | N-CA-C | 5.94  | 122.94      | 109.81   |
| 2   | f     | 202  | ASP  | N-CA-C | 5.93  | 122.91      | 109.81   |
| 1   | n     | 837  | PRO  | CA-C-N | 5.82  | 132.65      | 121.54   |
| 1   | n     | 837  | PRO  | C-N-CA | 5.82  | 132.65      | 121.54   |
| 4   | V     | 160  | LEU  | N-CA-C | -5.81 | 104.86      | 113.40   |
| 1   | q     | 649  | PHE  | CA-C-N | 5.79  | 132.61      | 121.54   |
| 1   | q     | 649  | PHE  | C-N-CA | 5.79  | 132.61      | 121.54   |
| 1   | m     | 1330 | ASP  | CA-C-N | 5.78  | 130.57      | 121.56   |
| 1   | m     | 1330 | ASP  | C-N-CA | 5.78  | 130.57      | 121.56   |
| 2   | i     | 96   | THR  | CA-C-N | 5.66  | 131.93      | 121.52   |
| 2   | i     | 96   | THR  | C-N-CA | 5.66  | 131.93      | 121.52   |
| 3   | x     | 55   | MET  | N-CA-C | 5.64  | 117.88      | 111.11   |
| 2   | h     | 96   | THR  | CA-C-N | 5.63  | 131.89      | 121.52   |
| 2   | h     | 96   | THR  | C-N-CA | 5.63  | 131.89      | 121.52   |
| 2   | j     | 96   | THR  | CA-C-N | 5.63  | 131.88      | 121.52   |
| 2   | j     | 96   | THR  | C-N-CA | 5.63  | 131.88      | 121.52   |
| 2   | 3     | 96   | THR  | CA-C-N | 5.62  | 131.86      | 121.52   |
| 2   | 3     | 96   | THR  | C-N-CA | 5.62  | 131.86      | 121.52   |
| 1   | B     | 591  | GLY  | CA-C-N | 5.61  | 129.23      | 120.82   |
| 1   | B     | 591  | GLY  | C-N-CA | 5.61  | 129.23      | 120.82   |
| 5   | W     | 110  | PRO  | C-N-CD | -5.51 | 102.42      | 125.00   |
| 1   | p     | 302  | SER  | CA-C-N | 5.47  | 132.00      | 121.54   |
| 1   | p     | 302  | SER  | C-N-CA | 5.47  | 132.00      | 121.54   |
| 1   | o     | 609  | PRO  | CA-C-N | 5.43  | 131.91      | 121.54   |
| 1   | o     | 609  | PRO  | C-N-CA | 5.43  | 131.91      | 121.54   |
| 1   | A     | 960  | SER  | N-CA-C | 5.39  | 121.73      | 109.81   |
| 1   | F     | 691  | GLU  | CA-C-N | 5.38  | 131.81      | 121.54   |
| 1   | F     | 691  | GLU  | C-N-CA | 5.38  | 131.81      | 121.54   |
| 1   | H     | 958  | PRO  | CA-C-N | 5.35  | 131.75      | 121.54   |
| 1   | H     | 958  | PRO  | C-N-CA | 5.35  | 131.75      | 121.54   |
| 1   | l     | 749  | ASN  | C-N-CD | -5.32 | 103.21      | 125.00   |
| 1   | H     | 1208 | THR  | CA-C-N | 5.30  | 131.66      | 121.54   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 1   | H     | 1208 | THR  | C-N-CA   | 5.30  | 131.66      | 121.54   |
| 1   | F     | 972  | ARG  | CA-C-N   | 5.29  | 127.57      | 120.58   |
| 1   | F     | 972  | ARG  | C-N-CA   | 5.29  | 127.57      | 120.58   |
| 1   | o     | 588  | ALA  | N-CA-C   | 5.25  | 121.42      | 109.81   |
| 1   | k     | 1155 | THR  | N-CA-C   | 5.25  | 116.49      | 108.52   |
| 1   | k     | 691  | GLU  | N-CA-C   | -5.22 | 105.65      | 112.23   |
| 4   | T     | 6    | SER  | O-C-N    | 5.20  | 131.32      | 123.00   |
| 1   | k     | 956  | GLY  | N-CA-C   | -5.19 | 100.89      | 113.18   |
| 4   | y     | 61   | VAL  | N-CA-C   | -5.16 | 98.61       | 109.34   |
| 1   | o     | 715  | ARG  | N-CA-C   | -5.10 | 108.08      | 114.56   |
| 1   | m     | 1261 | THR  | CA-C-N   | 5.07  | 131.22      | 121.54   |
| 1   | m     | 1261 | THR  | C-N-CA   | 5.07  | 131.22      | 121.54   |
| 1   | n     | 84   | LEU  | CA-C-N   | 5.06  | 127.31      | 120.38   |
| 1   | n     | 84   | LEU  | C-N-CA   | 5.06  | 127.31      | 120.38   |
| 1   | D     | 691  | GLU  | N-CA-C   | -5.05 | 100.05      | 110.80   |
| 1   | q     | 1305 | ALA  | CA-C-N   | 5.04  | 130.69      | 121.97   |
| 1   | q     | 1305 | ALA  | C-N-CA   | 5.04  | 130.69      | 121.97   |
| 2   | h     | 199  | ASP  | CA-C-N   | 5.04  | 127.44      | 120.49   |
| 2   | h     | 199  | ASP  | C-N-CA   | 5.04  | 127.44      | 120.49   |
| 4   | y     | 186  | ARG  | CB-CG-CD | -5.03 | 99.73       | 111.30   |
| 1   | k     | 1263 | PHE  | N-CA-C   | -5.03 | 105.49      | 110.97   |
| 1   | l     | 1260 | LYS  | CA-C-N   | 5.03  | 131.14      | 121.54   |
| 1   | l     | 1260 | LYS  | C-N-CA   | 5.03  | 131.14      | 121.54   |
| 1   | k     | 818  | PHE  | CA-C-N   | 5.02  | 131.13      | 121.54   |
| 1   | k     | 818  | PHE  | C-N-CA   | 5.02  | 131.13      | 121.54   |
| 1   | l     | 958  | PRO  | N-CA-C   | -5.01 | 102.14      | 112.47   |
| 2   | 3     | 199  | ASP  | CA-C-N   | 5.01  | 127.41      | 120.49   |
| 2   | 3     | 199  | ASP  | C-N-CA   | 5.01  | 127.41      | 120.49   |
| 2   | j     | 199  | ASP  | CA-C-N   | 5.01  | 127.40      | 120.49   |
| 2   | j     | 199  | ASP  | C-N-CA   | 5.01  | 127.40      | 120.49   |
| 2   | i     | 199  | ASP  | CA-C-N   | 5.00  | 127.39      | 120.49   |
| 2   | i     | 199  | ASP  | C-N-CA   | 5.00  | 127.39      | 120.49   |

There are no chirality outliers.

All (2) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 4   | T     | 203 | ARG  | Peptide |
| 4   | T     | 248 | CYS  | Peptide |

## 5.2 Too-close contacts ⓘ

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 10537 | 0        | 10392    | 346     | 0            |
| 1   | B     | 10351 | 0        | 10195    | 286     | 0            |
| 1   | C     | 10350 | 0        | 10200    | 286     | 0            |
| 1   | D     | 10375 | 0        | 10228    | 434     | 0            |
| 1   | E     | 10495 | 0        | 10355    | 423     | 0            |
| 1   | F     | 10407 | 0        | 10250    | 454     | 0            |
| 1   | G     | 10580 | 0        | 10431    | 524     | 0            |
| 1   | H     | 10580 | 0        | 10436    | 352     | 0            |
| 1   | I     | 10421 | 0        | 10266    | 276     | 0            |
| 1   | k     | 10209 | 0        | 10068    | 465     | 0            |
| 1   | l     | 10548 | 0        | 10408    | 523     | 0            |
| 1   | m     | 10364 | 0        | 10209    | 672     | 0            |
| 1   | n     | 10538 | 0        | 10394    | 379     | 0            |
| 1   | o     | 10368 | 0        | 10219    | 338     | 0            |
| 1   | p     | 10252 | 0        | 10114    | 386     | 0            |
| 1   | q     | 9621  | 0        | 9467     | 280     | 0            |
| 2   | 2     | 1469  | 0        | 1492     | 149     | 0            |
| 2   | 3     | 1665  | 0        | 1672     | 199     | 0            |
| 2   | e     | 1469  | 0        | 1492     | 181     | 0            |
| 2   | f     | 1469  | 0        | 1493     | 134     | 0            |
| 2   | g     | 1469  | 0        | 1493     | 122     | 0            |
| 2   | h     | 1665  | 0        | 1672     | 207     | 0            |
| 2   | i     | 1665  | 0        | 1672     | 184     | 0            |
| 2   | j     | 1665  | 0        | 1672     | 169     | 0            |
| 3   | J     | 471   | 0        | 502      | 33      | 0            |
| 3   | K     | 462   | 0        | 489      | 11      | 0            |
| 3   | L     | 462   | 0        | 489      | 13      | 0            |
| 3   | M     | 462   | 0        | 489      | 67      | 0            |
| 3   | N     | 462   | 0        | 489      | 17      | 0            |
| 3   | O     | 462   | 0        | 489      | 34      | 0            |
| 3   | P     | 462   | 0        | 489      | 57      | 0            |
| 3   | Q     | 462   | 0        | 489      | 15      | 0            |
| 3   | R     | 462   | 0        | 489      | 46      | 0            |
| 3   | r     | 471   | 0        | 502      | 71      | 0            |
| 3   | s     | 462   | 0        | 489      | 21      | 0            |
| 3   | t     | 462   | 0        | 489      | 74      | 0            |
| 3   | u     | 471   | 0        | 502      | 17      | 0            |

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| Mol | Chain | Non-H  | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 3   | v     | 471    | 0        | 502      | 16      | 0            |
| 3   | w     | 471    | 0        | 502      | 17      | 0            |
| 3   | x     | 450    | 0        | 477      | 18      | 0            |
| 4   | S     | 2305   | 0        | 2306     | 137     | 0            |
| 4   | T     | 2305   | 0        | 2306     | 89      | 0            |
| 4   | U     | 2305   | 0        | 2306     | 98      | 0            |
| 4   | V     | 2305   | 0        | 2306     | 84      | 0            |
| 4   | y     | 1977   | 0        | 1983     | 113     | 0            |
| 5   | l     | 2009   | 0        | 2086     | 57      | 0            |
| 5   | W     | 2201   | 0        | 2278     | 92      | 0            |
| 5   | X     | 2166   | 0        | 2246     | 90      | 0            |
| 5   | Y     | 2209   | 0        | 2290     | 64      | 0            |
| 5   | Z     | 2201   | 0        | 2278     | 72      | 0            |
| 5   | a     | 2085   | 0        | 2165     | 69      | 0            |
| 5   | b     | 2109   | 0        | 2186     | 46      | 0            |
| 5   | c     | 2141   | 0        | 2219     | 71      | 0            |
| 5   | d     | 2140   | 0        | 2227     | 54      | 0            |
| 5   | z     | 2224   | 0        | 2303     | 99      | 0            |
| All | All   | 218639 | 0        | 217652   | 7576    | 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 17.

All (7576) 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) |
|------------------|-------------------|--------------------------|-------------------|
| 2:3:258:PHE:CE1  | 3:r:90:ILE:HG22   | 1.25                     | 1.65              |
| 1:D:429:VAL:HG12 | 1:D:431:PHE:CE2   | 1.32                     | 1.64              |
| 1:G:431:PHE:CZ   | 1:G:1310:THR:HG23 | 1.15                     | 1.64              |
| 2:i:111:ALA:HB2  | 4:U:232:PHE:CE2   | 1.16                     | 1.62              |
| 1:D:431:PHE:CE1  | 1:D:1310:THR:HA   | 1.29                     | 1.62              |
| 1:q:1098:PHE:CZ  | 1:q:1119:THR:HG21 | 1.33                     | 1.62              |
| 1:G:431:PHE:CE1  | 1:G:1310:THR:HA   | 1.12                     | 1.61              |
| 1:k:818:PHE:CZ   | 3:r:58:GLN:HB3    | 1.26                     | 1.61              |
| 2:e:208:PRO:HG3  | 2:h:95:LEU:CD1    | 1.13                     | 1.60              |
| 1:G:431:PHE:HE1  | 1:G:1310:THR:CA   | 1.05                     | 1.58              |
| 1:D:692:LEU:HD12 | 1:D:695:LEU:CG    | 1.30                     | 1.58              |
| 2:f:208:PRO:HG3  | 2:i:95:LEU:CD1    | 1.13                     | 1.56              |
| 1:q:1098:PHE:CE2 | 1:q:1119:THR:CG2  | 1.84                     | 1.56              |
| 2:2:208:PRO:HG3  | 2:3:95:LEU:CD1    | 1.13                     | 1.56              |
| 2:3:91:HIS:HD2   | 2:3:195:TYR:CE1   | 1.22                     | 1.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:i:91:HIS:HD2    | 2:i:195:TYR:CE1   | 1.22                     | 1.55              |
| 2:g:208:PRO:CG    | 2:j:95:LEU:HD11   | 1.35                     | 1.55              |
| 5:Y:205:ASN:HD22  | 5:c:233:ILE:CG2   | 1.16                     | 1.55              |
| 1:D:692:LEU:HD12  | 1:D:695:LEU:CD1   | 1.19                     | 1.54              |
| 2:g:208:PRO:HG3   | 2:j:95:LEU:CD1    | 1.13                     | 1.54              |
| 1:H:1019:THR:HG23 | 1:H:1160:LEU:CD1  | 1.32                     | 1.53              |
| 2:g:208:PRO:CG    | 2:j:95:LEU:CD1    | 1.85                     | 1.52              |
| 2:e:208:PRO:CG    | 2:h:95:LEU:HD11   | 1.35                     | 1.52              |
| 2:h:91:HIS:HD2    | 2:h:195:TYR:CE1   | 1.23                     | 1.52              |
| 1:D:429:VAL:CG1   | 1:D:431:PHE:CE2   | 1.89                     | 1.52              |
| 2:j:91:HIS:HD2    | 2:j:195:TYR:CE1   | 1.22                     | 1.52              |
| 1:D:692:LEU:CD1   | 1:D:695:LEU:CD1   | 1.83                     | 1.52              |
| 1:m:431:PHE:CZ    | 1:m:1310:THR:HG23 | 1.43                     | 1.50              |
| 2:e:258:PHE:HZ    | 3:t:87:MET:CG     | 1.19                     | 1.50              |
| 1:D:431:PHE:CZ    | 1:D:1310:THR:HG23 | 1.41                     | 1.50              |
| 1:D:431:PHE:HE1   | 1:D:1310:THR:CA   | 1.22                     | 1.49              |
| 1:D:813:PHE:CZ    | 3:M:85:LEU:HB3    | 1.46                     | 1.49              |
| 1:H:1019:THR:CG2  | 1:H:1160:LEU:HD11 | 1.36                     | 1.49              |
| 2:2:208:PRO:CG    | 2:3:95:LEU:HD11   | 1.35                     | 1.49              |
| 1:A:788:CYS:SG    | 1:A:992:LEU:HB3   | 1.52                     | 1.48              |
| 2:f:208:PRO:CG    | 2:i:95:LEU:HD11   | 1.35                     | 1.48              |
| 1:D:813:PHE:CD1   | 3:M:85:LEU:HG     | 1.48                     | 1.47              |
| 2:i:91:HIS:CD2    | 2:i:195:TYR:CD1   | 2.03                     | 1.47              |
| 2:h:91:HIS:CD2    | 2:h:195:TYR:CD1   | 2.03                     | 1.47              |
| 2:3:91:HIS:CD2    | 2:3:195:TYR:CD1   | 2.03                     | 1.46              |
| 2:j:91:HIS:CD2    | 2:j:195:TYR:CD1   | 2.03                     | 1.46              |
| 2:f:208:PRO:CG    | 2:i:95:LEU:CD1    | 1.85                     | 1.46              |
| 2:e:258:PHE:CZ    | 3:t:87:MET:SD     | 2.09                     | 1.45              |
| 2:e:258:PHE:CZ    | 3:t:87:MET:HG3    | 1.53                     | 1.44              |
| 2:3:91:HIS:CD2    | 2:3:195:TYR:CE1   | 2.06                     | 1.43              |
| 2:e:258:PHE:CE1   | 3:t:60:VAL:HG23   | 1.49                     | 1.43              |
| 1:G:429:VAL:CG1   | 1:G:431:PHE:HE2   | 1.28                     | 1.43              |
| 1:m:1160:LEU:HD23 | 1:m:1214:ASN:ND2  | 1.33                     | 1.43              |
| 2:3:91:HIS:HD2    | 2:3:195:TYR:CD1   | 1.36                     | 1.43              |
| 2:i:91:HIS:HD2    | 2:i:195:TYR:CD1   | 1.36                     | 1.42              |
| 1:k:813:PHE:CE1   | 3:r:85:LEU:HD22   | 1.51                     | 1.42              |
| 2:e:208:PRO:CG    | 2:h:95:LEU:CD1    | 1.85                     | 1.42              |
| 2:j:91:HIS:HD2    | 2:j:195:TYR:CD1   | 1.36                     | 1.42              |
| 1:D:813:PHE:CE1   | 3:M:85:LEU:HG     | 1.54                     | 1.42              |
| 2:h:91:HIS:CD2    | 2:h:195:TYR:CE1   | 2.06                     | 1.42              |
| 2:i:91:HIS:CD2    | 2:i:195:TYR:CE1   | 2.06                     | 1.41              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 5:W:110:PRO:HB2  | 5:W:111:PRO:CD    | 1.39                     | 1.41              |
| 5:Y:205:ASN:ND2  | 5:c:233:ILE:HG22  | 1.24                     | 1.41              |
| 2:2:208:PRO:CG   | 2:3:95:LEU:CD1    | 1.85                     | 1.41              |
| 2:e:262:TYR:OH   | 3:t:87:MET:CB     | 1.67                     | 1.41              |
| 1:G:429:VAL:CG1  | 1:G:431:PHE:CE2   | 2.01                     | 1.41              |
| 2:j:91:HIS:CD2   | 2:j:195:TYR:CE1   | 2.06                     | 1.40              |
| 1:G:750:PRO:CD   | 2:h:269:ARG:NH2   | 1.85                     | 1.40              |
| 2:f:200:VAL:HG21 | 2:f:215:ARG:CG    | 1.52                     | 1.40              |
| 2:2:262:TYR:OH   | 3:x:87:MET:CE     | 1.68                     | 1.40              |
| 2:e:200:VAL:HG21 | 2:e:215:ARG:CG    | 1.52                     | 1.40              |
| 2:2:200:VAL:HG21 | 2:2:215:ARG:CG    | 1.52                     | 1.39              |
| 2:h:91:HIS:HD2   | 2:h:195:TYR:CD1   | 1.36                     | 1.39              |
| 2:f:66:ARG:NE    | 2:f:68:THR:HG22   | 1.30                     | 1.39              |
| 1:m:138:THR:HG21 | 5:W:73:ARG:NH1    | 1.28                     | 1.39              |
| 2:i:111:ALA:HB2  | 4:U:232:PHE:CD2   | 1.58                     | 1.38              |
| 1:F:817:PHE:CE2  | 1:F:819:LEU:O     | 1.77                     | 1.38              |
| 1:k:1019:THR:CB  | 1:k:1160:LEU:HD11 | 1.53                     | 1.38              |
| 1:D:819:LEU:HG   | 3:M:58:GLN:NE2    | 1.08                     | 1.37              |
| 1:G:83:ASP:CG    | 1:m:147:THR:HG22  | 1.50                     | 1.36              |
| 2:3:258:PHE:CE1  | 3:r:90:ILE:CG2    | 2.06                     | 1.36              |
| 2:g:200:VAL:HG21 | 2:g:215:ARG:CG    | 1.52                     | 1.36              |
| 2:e:285:GLU:HG3  | 3:t:67:LYS:CE     | 1.55                     | 1.36              |
| 2:e:206:GLU:CB   | 2:h:132:TYR:HD2   | 1.39                     | 1.35              |
| 2:i:111:ALA:CB   | 4:U:232:PHE:CE2   | 2.07                     | 1.35              |
| 2:g:206:GLU:CB   | 2:j:132:TYR:HD2   | 1.39                     | 1.35              |
| 2:e:200:VAL:CG2  | 2:e:215:ARG:HG2   | 1.57                     | 1.35              |
| 1:G:431:PHE:CZ   | 1:G:1310:THR:CG2  | 2.08                     | 1.35              |
| 1:G:750:PRO:HD2  | 2:h:269:ARG:NH2   | 1.02                     | 1.35              |
| 1:m:429:VAL:HG12 | 1:m:431:PHE:CE2   | 1.60                     | 1.34              |
| 2:e:258:PHE:CZ   | 3:t:60:VAL:HG23   | 1.62                     | 1.34              |
| 2:f:206:GLU:CB   | 2:i:132:TYR:HD2   | 1.39                     | 1.34              |
| 1:m:431:PHE:CE1  | 1:m:1310:THR:HA   | 1.61                     | 1.34              |
| 1:A:788:CYS:SG   | 1:A:992:LEU:CB    | 2.15                     | 1.34              |
| 2:f:66:ARG:HE    | 2:f:68:THR:CG2    | 1.40                     | 1.34              |
| 2:f:200:VAL:CG2  | 2:f:215:ARG:HG2   | 1.57                     | 1.33              |
| 2:2:206:GLU:CB   | 2:3:132:TYR:HD2   | 1.39                     | 1.33              |
| 1:G:748:ARG:HD2  | 2:h:269:ARG:NH1   | 1.43                     | 1.32              |
| 2:g:200:VAL:CG2  | 2:g:215:ARG:HG2   | 1.57                     | 1.32              |
| 2:e:258:PHE:CE1  | 3:t:60:VAL:CG2    | 2.12                     | 1.32              |
| 1:G:429:VAL:HG12 | 1:G:431:PHE:CE2   | 1.60                     | 1.31              |
| 2:2:200:VAL:CG2  | 2:2:215:ARG:HG2   | 1.57                     | 1.31              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:E:740:LEU:CD1  | 1:E:767:LEU:HD21  | 1.58                     | 1.31              |
| 2:e:258:PHE:CE2  | 3:t:87:MET:SD     | 2.23                     | 1.31              |
| 2:h:92:LEU:O     | 2:h:96:THR:HG23   | 1.25                     | 1.31              |
| 1:D:429:VAL:CG1  | 1:D:431:PHE:CZ    | 2.13                     | 1.31              |
| 1:F:332:ARG:NH2  | 1:l:12:PRO:HB2    | 1.44                     | 1.30              |
| 4:V:79:MET:HB3   | 4:V:80:PRO:CD     | 1.49                     | 1.30              |
| 1:k:135:ALA:HB2  | 4:y:161:LYS:O     | 1.13                     | 1.30              |
| 2:h:258:PHE:HE1  | 3:P:90:ILE:CG2    | 1.43                     | 1.30              |
| 4:y:73:LEU:HD21  | 4:y:131:VAL:CG1   | 1.63                     | 1.29              |
| 1:G:431:PHE:HZ   | 1:G:1310:THR:CG2  | 1.41                     | 1.29              |
| 2:e:258:PHE:CZ   | 3:t:87:MET:CG     | 2.06                     | 1.29              |
| 1:G:1072:LEU:HB2 | 1:m:19:ASP:O      | 1.33                     | 1.28              |
| 2:i:92:LEU:O     | 2:i:96:THR:HG23   | 1.25                     | 1.28              |
| 1:G:83:ASP:OD1   | 1:m:147:THR:CG2   | 1.82                     | 1.28              |
| 2:2:200:VAL:O    | 2:3:86:ALA:HB1    | 1.31                     | 1.28              |
| 2:h:258:PHE:CE1  | 3:P:90:ILE:CG2    | 2.17                     | 1.28              |
| 5:X:88:GLN:C     | 5:X:308:ILE:HG23  | 1.59                     | 1.28              |
| 2:f:200:VAL:O    | 2:i:86:ALA:HB1    | 1.31                     | 1.27              |
| 2:3:92:LEU:O     | 2:3:96:THR:HG23   | 1.25                     | 1.27              |
| 1:I:813:PHE:CZ   | 3:R:85:LEU:HB3    | 1.68                     | 1.27              |
| 1:D:813:PHE:CE1  | 3:M:85:LEU:CG     | 2.19                     | 1.26              |
| 1:F:1019:THR:OG1 | 1:F:1160:LEU:HD11 | 1.25                     | 1.26              |
| 1:m:432:TYR:OH   | 1:m:1321:LEU:HD12 | 1.11                     | 1.25              |
| 2:2:262:TYR:OH   | 3:x:87:MET:HE2    | 1.19                     | 1.25              |
| 4:S:217:HIS:HE1  | 5:W:64:ARG:NH1    | 1.33                     | 1.25              |
| 4:y:73:LEU:HG    | 4:y:130:VAL:O     | 1.37                     | 1.25              |
| 5:X:88:GLN:O     | 5:X:308:ILE:HG23  | 1.22                     | 1.25              |
| 2:i:94:LEU:HD21  | 2:i:222:LEU:CD2   | 1.67                     | 1.25              |
| 2:g:200:VAL:O    | 2:j:86:ALA:HB1    | 1.31                     | 1.25              |
| 1:G:748:ARG:CD   | 2:h:269:ARG:NH1   | 1.99                     | 1.24              |
| 2:3:94:LEU:HD21  | 2:3:222:LEU:CD2   | 1.67                     | 1.24              |
| 2:e:200:VAL:O    | 2:h:86:ALA:CB     | 1.84                     | 1.24              |
| 2:g:200:VAL:O    | 2:j:86:ALA:CB     | 1.84                     | 1.24              |
| 1:m:161:VAL:HG13 | 4:S:16:GLU:OE2    | 1.34                     | 1.24              |
| 2:e:200:VAL:O    | 2:h:86:ALA:HB1    | 1.31                     | 1.24              |
| 2:f:200:VAL:O    | 2:i:86:ALA:CB     | 1.84                     | 1.24              |
| 2:h:208:PRO:HB3  | 5:a:229:LYS:NZ    | 1.52                     | 1.24              |
| 2:h:258:PHE:CE1  | 3:P:90:ILE:HG22   | 1.69                     | 1.24              |
| 2:j:94:LEU:HD21  | 2:j:222:LEU:CD2   | 1.67                     | 1.24              |
| 1:m:863:HIS:CE1  | 3:t:92:LYS:O      | 1.90                     | 1.23              |
| 2:2:200:VAL:O    | 2:3:86:ALA:CB     | 1.84                     | 1.23              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:j:92:LEU:O     | 2:j:96:THR:HG23   | 1.25                     | 1.23              |
| 4:y:72:ARG:C     | 4:y:73:LEU:HD12   | 1.61                     | 1.23              |
| 1:k:818:PHE:CZ   | 3:r:58:GLN:CB     | 2.19                     | 1.23              |
| 1:k:950:TYR:CD1  | 1:k:956:GLY:O     | 1.92                     | 1.23              |
| 1:D:819:LEU:CG   | 3:M:58:GLN:NE2    | 2.00                     | 1.23              |
| 1:D:431:PHE:HE1  | 1:D:1310:THR:CB   | 1.51                     | 1.22              |
| 2:h:94:LEU:HD21  | 2:h:222:LEU:CD2   | 1.67                     | 1.22              |
| 1:G:116:MET:O    | 1:m:37:ARG:N      | 1.72                     | 1.22              |
| 1:D:819:LEU:CD1  | 3:M:58:GLN:HG3    | 1.70                     | 1.22              |
| 2:3:262:TYR:CE1  | 3:r:87:MET:HE1    | 1.75                     | 1.22              |
| 1:D:819:LEU:HD12 | 3:M:58:GLN:HG3    | 1.22                     | 1.21              |
| 1:I:754:ASP:N    | 3:R:83:ASP:OD1    | 1.72                     | 1.21              |
| 2:h:208:PRO:CB   | 5:a:229:LYS:NZ    | 2.01                     | 1.21              |
| 2:e:206:GLU:CG   | 2:h:132:TYR:HD2   | 1.53                     | 1.21              |
| 2:i:111:ALA:CB   | 4:U:232:PHE:CD2   | 2.22                     | 1.21              |
| 1:o:765:GLU:HB3  | 1:o:766:PRO:CD    | 1.71                     | 1.20              |
| 2:e:262:TYR:CZ   | 3:t:87:MET:HB2    | 1.75                     | 1.20              |
| 2:i:66:ARG:NH1   | 2:i:69:GLN:HE21   | 1.36                     | 1.20              |
| 2:g:206:GLU:CG   | 2:j:132:TYR:HD2   | 1.53                     | 1.20              |
| 1:k:1019:THR:OG1 | 1:k:1160:LEU:HD11 | 1.03                     | 1.20              |
| 1:m:1160:LEU:CD2 | 1:m:1214:ASN:ND2  | 2.05                     | 1.20              |
| 1:G:431:PHE:HE1  | 1:G:1310:THR:CB   | 1.54                     | 1.19              |
| 2:e:206:GLU:CB   | 2:h:132:TYR:CD2   | 2.24                     | 1.19              |
| 1:G:431:PHE:CE1  | 1:G:1310:THR:CA   | 1.91                     | 1.19              |
| 1:G:431:PHE:CD1  | 1:G:1310:THR:HA   | 1.76                     | 1.19              |
| 2:2:206:GLU:CG   | 2:3:132:TYR:HD2   | 1.53                     | 1.19              |
| 2:f:206:GLU:CB   | 2:i:132:TYR:CD2   | 2.24                     | 1.19              |
| 2:i:111:ALA:HB2  | 4:U:232:PHE:CZ    | 1.78                     | 1.19              |
| 1:F:82:HIS:HB2   | 1:l:147:THR:CG2   | 1.71                     | 1.19              |
| 1:F:817:PHE:HE2  | 1:F:819:LEU:O     | 0.86                     | 1.19              |
| 1:m:51:PHE:HB3   | 1:n:87:MET:SD     | 1.82                     | 1.19              |
| 1:q:1115:VAL:O   | 1:q:1119:THR:N    | 1.75                     | 1.19              |
| 2:2:206:GLU:CB   | 2:3:132:TYR:CD2   | 2.24                     | 1.19              |
| 2:g:206:GLU:CB   | 2:j:132:TYR:CD2   | 2.24                     | 1.19              |
| 1:D:692:LEU:CD1  | 1:D:695:LEU:HG    | 1.73                     | 1.18              |
| 1:l:950:TYR:CE1  | 1:l:956:GLY:O     | 1.95                     | 1.18              |
| 2:f:206:GLU:CG   | 2:i:132:TYR:HD2   | 1.53                     | 1.18              |
| 1:D:692:LEU:HD12 | 1:D:695:LEU:HG    | 1.20                     | 1.18              |
| 1:D:813:PHE:CZ   | 3:M:85:LEU:CB     | 2.25                     | 1.18              |
| 1:k:1019:THR:OG1 | 1:k:1160:LEU:CD1  | 1.90                     | 1.18              |
| 5:X:112:VAL:O    | 5:X:113:PHE:CG    | 1.97                     | 1.18              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:o:488:GLU:OE1   | 1:o:490:MET:HE2   | 1.43                     | 1.18              |
| 1:q:1098:PHE:CZ   | 1:q:1119:THR:CG2  | 2.09                     | 1.18              |
| 1:F:1160:LEU:HD23 | 1:F:1214:ASN:ND2  | 1.59                     | 1.18              |
| 1:m:51:PHE:CD1    | 1:n:87:MET:HB3    | 1.78                     | 1.18              |
| 2:g:206:GLU:CG    | 2:j:132:TYR:CD2   | 2.28                     | 1.17              |
| 1:H:838:LEU:O     | 1:H:842:LEU:HD23  | 1.45                     | 1.17              |
| 1:q:1115:VAL:HG12 | 1:q:1119:THR:OG1  | 1.42                     | 1.17              |
| 1:F:83:ASP:OD1    | 1:l:147:THR:OG1   | 1.63                     | 1.16              |
| 5:W:110:PRO:CB    | 5:W:111:PRO:HD2   | 1.76                     | 1.16              |
| 4:V:79:MET:CB     | 4:V:80:PRO:CD     | 2.24                     | 1.15              |
| 1:k:748:ARG:NH1   | 2:3:272:ASP:OD2   | 1.77                     | 1.15              |
| 2:2:206:GLU:CG    | 2:3:132:TYR:CD2   | 2.28                     | 1.15              |
| 2:e:206:GLU:CG    | 2:h:132:TYR:CD2   | 2.28                     | 1.15              |
| 2:f:206:GLU:CG    | 2:i:132:TYR:CD2   | 2.28                     | 1.15              |
| 2:i:238:LEU:HD22  | 2:i:271:VAL:HG11  | 1.28                     | 1.15              |
| 1:G:750:PRO:CD    | 2:h:269:ARG:HH22  | 1.47                     | 1.15              |
| 1:F:314:VAL:CG2   | 1:m:333:ILE:HD11  | 1.75                     | 1.15              |
| 1:F:332:ARG:CD    | 1:l:12:PRO:HG2    | 1.76                     | 1.15              |
| 1:G:1263:PHE:CD1  | 1:m:30:GLU:C      | 2.25                     | 1.15              |
| 1:l:1136:THR:HB   | 4:T:116:ILE:CD1   | 1.75                     | 1.15              |
| 1:k:1207:GLN:NE2  | 1:p:437:ILE:HG21  | 1.60                     | 1.15              |
| 2:e:105:LEU:HD11  | 2:e:212:VAL:CG1   | 1.77                     | 1.15              |
| 2:e:206:GLU:HG3   | 2:h:132:TYR:CD2   | 1.82                     | 1.15              |
| 1:D:692:LEU:CD1   | 1:D:695:LEU:HD12  | 1.57                     | 1.14              |
| 1:D:431:PHE:CD1   | 1:D:1310:THR:HA   | 1.82                     | 1.14              |
| 1:G:135:ALA:HB2   | 4:S:161:LYS:O     | 1.44                     | 1.14              |
| 2:2:105:LEU:HD11  | 2:2:212:VAL:CG1   | 1.77                     | 1.14              |
| 2:f:206:GLU:HG3   | 2:i:132:TYR:CD2   | 1.82                     | 1.14              |
| 2:2:104:LYS:CD    | 2:3:92:LEU:HD12   | 1.78                     | 1.14              |
| 2:e:258:PHE:HZ    | 3:t:87:MET:SD     | 1.58                     | 1.14              |
| 2:g:105:LEU:HD11  | 2:g:212:VAL:CG1   | 1.77                     | 1.14              |
| 2:g:206:GLU:HG3   | 2:j:132:TYR:CD2   | 1.82                     | 1.14              |
| 2:g:104:LYS:CD    | 2:j:92:LEU:HD12   | 1.78                     | 1.13              |
| 1:D:692:LEU:CG    | 1:D:695:LEU:HD12  | 1.76                     | 1.13              |
| 1:E:33:PHE:CE2    | 1:m:118:SER:O     | 2.01                     | 1.13              |
| 1:I:813:PHE:CE2   | 3:R:85:LEU:CB     | 2.31                     | 1.13              |
| 1:m:432:TYR:CZ    | 1:m:1321:LEU:HD12 | 1.83                     | 1.13              |
| 2:e:104:LYS:CD    | 2:h:92:LEU:HD12   | 1.78                     | 1.13              |
| 2:f:104:LYS:CD    | 2:i:92:LEU:HD12   | 1.77                     | 1.13              |
| 1:F:82:HIS:HB2    | 1:l:147:THR:HG21  | 1.14                     | 1.13              |
| 1:m:429:VAL:CG1   | 1:m:431:PHE:CE2   | 2.32                     | 1.13              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:D:692:LEU:HB2   | 1:D:705:LEU:CD2   | 1.79                     | 1.12              |
| 1:G:1263:PHE:HD1  | 1:m:30:GLU:O      | 1.31                     | 1.12              |
| 1:H:1019:THR:HG23 | 1:H:1160:LEU:HD12 | 1.30                     | 1.12              |
| 2:f:105:LEU:HD11  | 2:f:212:VAL:CG1   | 1.77                     | 1.12              |
| 5:Z:88:GLN:O      | 5:Z:308:ILE:HG23  | 1.49                     | 1.12              |
| 1:F:344:SER:CB    | 1:l:14:LEU:HD11   | 1.79                     | 1.12              |
| 1:m:863:HIS:HE1   | 3:t:92:LYS:O      | 1.20                     | 1.12              |
| 2:2:206:GLU:HG3   | 2:3:132:TYR:CD2   | 1.82                     | 1.12              |
| 1:D:429:VAL:HG13  | 1:D:431:PHE:CZ    | 1.84                     | 1.12              |
| 1:m:147:THR:O     | 1:m:149:LEU:N     | 1.81                     | 1.12              |
| 1:m:514:ALA:HA    | 1:m:517:ASP:OD2   | 1.47                     | 1.12              |
| 2:h:93:PRO:CG     | 2:h:195:TYR:OH    | 1.98                     | 1.12              |
| 2:i:93:PRO:CG     | 2:i:195:TYR:OH    | 1.98                     | 1.12              |
| 2:j:93:PRO:CG     | 2:j:195:TYR:OH    | 1.98                     | 1.12              |
| 1:G:863:HIS:CE1   | 3:P:93:LYS:HA     | 1.85                     | 1.11              |
| 1:o:1159:ILE:O    | 1:o:1160:LEU:HD23 | 1.47                     | 1.11              |
| 2:e:285:GLU:HG3   | 3:t:67:LYS:HE2    | 1.30                     | 1.11              |
| 2:f:206:GLU:O     | 2:i:132:TYR:CB    | 1.98                     | 1.11              |
| 2:e:206:GLU:O     | 2:h:132:TYR:CB    | 1.99                     | 1.11              |
| 4:V:79:MET:HB3    | 4:V:80:PRO:HD2    | 1.12                     | 1.11              |
| 1:k:758:MET:CB    | 3:r:79:ALA:HB1    | 1.80                     | 1.10              |
| 1:m:1153:ARG:HG3  | 1:m:1283:LEU:HD12 | 1.31                     | 1.10              |
| 2:3:93:PRO:CG     | 2:3:195:TYR:OH    | 1.98                     | 1.10              |
| 1:m:748:ARG:HH11  | 2:e:269:ARG:NH1   | 1.47                     | 1.10              |
| 2:3:258:PHE:CD1   | 3:r:91:ALA:HA     | 1.84                     | 1.10              |
| 1:F:819:LEU:HD12  | 3:O:58:GLN:HG2    | 1.29                     | 1.10              |
| 1:k:596:LEU:HD12  | 1:k:985:THR:O     | 1.50                     | 1.10              |
| 1:l:950:TYR:CD1   | 1:l:956:GLY:O     | 2.04                     | 1.10              |
| 2:2:206:GLU:O     | 2:3:132:TYR:CB    | 1.99                     | 1.10              |
| 2:i:107:GLY:O     | 4:U:232:PHE:CE1   | 2.03                     | 1.10              |
| 2:g:206:GLU:O     | 2:j:132:TYR:CB    | 1.99                     | 1.10              |
| 2:j:285:GLU:OE2   | 3:M:67:LYS:HE3    | 1.50                     | 1.10              |
| 1:F:344:SER:HB2   | 1:l:14:LEU:CD1    | 1.81                     | 1.10              |
| 1:p:692:LEU:HD23  | 1:p:1010:MET:HE2  | 1.31                     | 1.10              |
| 1:q:1115:VAL:O    | 1:q:1119:THR:OG1  | 1.68                     | 1.10              |
| 1:E:740:LEU:HD11  | 1:E:767:LEU:HD21  | 1.32                     | 1.09              |
| 1:q:974:PRO:O     | 1:q:978:TYR:HD2   | 1.31                     | 1.09              |
| 2:f:104:LYS:HD2   | 2:i:92:LEU:HD12   | 1.33                     | 1.09              |
| 1:A:813:PHE:CZ    | 3:J:85:LEU:HG     | 1.87                     | 1.09              |
| 1:D:431:PHE:CE1   | 1:D:1310:THR:HG23 | 1.86                     | 1.09              |
| 1:k:744:HIS:N     | 2:2:173:MET:O     | 1.85                     | 1.09              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:3:66:ARG:HG2    | 2:3:69:GLN:HG3    | 1.32                     | 1.09              |
| 2:j:238:LEU:HD22  | 2:j:271:VAL:HG11  | 1.28                     | 1.09              |
| 1:D:431:PHE:CZ    | 1:D:1310:THR:CG2  | 2.36                     | 1.09              |
| 1:D:431:PHE:CE1   | 1:D:1310:THR:CA   | 2.06                     | 1.09              |
| 1:G:813:PHE:CZ    | 3:P:85:LEU:HD12   | 1.87                     | 1.09              |
| 1:q:1115:VAL:CG1  | 1:q:1119:THR:OG1  | 1.99                     | 1.09              |
| 2:i:66:ARG:NH1    | 2:i:69:GLN:NE2    | 2.01                     | 1.09              |
| 1:G:813:PHE:CD2   | 3:P:85:LEU:HG     | 1.88                     | 1.08              |
| 2:3:238:LEU:HD22  | 2:3:271:VAL:HG11  | 1.28                     | 1.08              |
| 1:p:1019:THR:HG23 | 1:p:1160:LEU:CD1  | 1.83                     | 1.08              |
| 2:e:104:LYS:CD    | 2:h:92:LEU:CD1    | 2.31                     | 1.08              |
| 1:E:666:GLY:H     | 1:F:643:GLN:NE2   | 1.51                     | 1.08              |
| 2:g:104:LYS:CD    | 2:j:92:LEU:CD1    | 2.31                     | 1.08              |
| 2:2:104:LYS:HD2   | 2:3:92:LEU:HD12   | 1.33                     | 1.08              |
| 2:3:94:LEU:CD2    | 2:3:222:LEU:HD23  | 1.83                     | 1.08              |
| 2:i:94:LEU:CD2    | 2:i:222:LEU:HD23  | 1.83                     | 1.08              |
| 4:V:79:MET:CG     | 4:V:80:PRO:HD3    | 1.84                     | 1.08              |
| 1:D:431:PHE:CE1   | 1:D:1310:THR:CB   | 2.35                     | 1.08              |
| 1:m:1153:ARG:HD2  | 1:m:1283:LEU:HD13 | 1.28                     | 1.08              |
| 1:o:710:ALA:O     | 1:o:713:ASP:OD1   | 1.72                     | 1.08              |
| 1:q:1098:PHE:CE2  | 1:q:1119:THR:HG23 | 1.69                     | 1.08              |
| 2:e:262:TYR:OH    | 3:t:87:MET:HB2    | 0.90                     | 1.08              |
| 1:k:1019:THR:N    | 1:k:1160:LEU:HD12 | 1.69                     | 1.07              |
| 1:k:1160:LEU:HD23 | 1:k:1214:ASN:ND2  | 1.69                     | 1.07              |
| 2:f:104:LYS:CD    | 2:i:92:LEU:CD1    | 2.31                     | 1.07              |
| 2:j:94:LEU:CD2    | 2:j:222:LEU:HD23  | 1.83                     | 1.07              |
| 4:y:73:LEU:HD21   | 4:y:131:VAL:HG12  | 1.28                     | 1.07              |
| 1:D:692:LEU:CD1   | 1:D:695:LEU:HD11  | 1.81                     | 1.07              |
| 1:G:83:ASP:OD1    | 1:m:147:THR:HG22  | 1.46                     | 1.07              |
| 1:G:431:PHE:CE1   | 1:G:1310:THR:HG23 | 1.88                     | 1.07              |
| 1:m:432:TYR:OH    | 1:m:1321:LEU:CD1  | 2.01                     | 1.07              |
| 2:i:66:ARG:HD2    | 2:i:69:GLN:HG3    | 1.36                     | 1.07              |
| 1:F:341:LEU:HB2   | 1:l:14:LEU:HG     | 1.36                     | 1.07              |
| 1:G:1017:ALA:C    | 1:G:1018:LEU:HD12 | 1.80                     | 1.07              |
| 2:2:104:LYS:CD    | 2:3:92:LEU:CD1    | 2.31                     | 1.07              |
| 1:E:30:GLU:HB3    | 1:m:1263:PHE:HE2  | 1.14                     | 1.07              |
| 1:E:740:LEU:HD13  | 1:E:767:LEU:CD2   | 1.84                     | 1.07              |
| 2:3:66:ARG:CG     | 2:3:69:GLN:HG3    | 1.85                     | 1.07              |
| 2:e:284:GLU:HB2   | 3:t:67:LYS:HZ3    | 1.16                     | 1.07              |
| 2:e:285:GLU:HG3   | 3:t:67:LYS:HE3    | 1.23                     | 1.07              |
| 2:f:206:GLU:O     | 2:i:132:TYR:HB3   | 1.54                     | 1.07              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:726:ARG:NH1  | 1:B:945:ASN:OD1   | 1.88                     | 1.07              |
| 1:A:813:PHE:CE2  | 3:J:85:LEU:HB3    | 1.89                     | 1.07              |
| 1:F:314:VAL:HG22 | 1:m:333:ILE:HD11  | 1.11                     | 1.07              |
| 1:G:748:ARG:NE   | 2:h:269:ARG:HH11  | 1.51                     | 1.07              |
| 1:k:784:VAL:O    | 1:k:788:CYS:HB2   | 1.54                     | 1.07              |
| 1:m:431:PHE:HE1  | 1:m:1310:THR:CA   | 1.66                     | 1.06              |
| 1:q:1293:SER:O   | 1:q:1297:LYS:HA   | 1.55                     | 1.06              |
| 1:G:863:HIS:HE1  | 3:P:93:LYS:HA     | 1.02                     | 1.06              |
| 1:k:758:MET:HB3  | 3:r:79:ALA:HB1    | 1.36                     | 1.06              |
| 1:l:950:TYR:O    | 1:l:957:PHE:CE2   | 2.08                     | 1.06              |
| 5:W:110:PRO:CB   | 5:W:111:PRO:CD    | 2.22                     | 1.06              |
| 1:G:430:TYR:O    | 1:G:431:PHE:CG    | 2.09                     | 1.06              |
| 1:m:748:ARG:NE   | 2:e:269:ARG:NH2   | 2.01                     | 1.06              |
| 2:h:94:LEU:CD2   | 2:h:222:LEU:HD23  | 1.83                     | 1.06              |
| 1:m:748:ARG:NH1  | 2:e:269:ARG:HH12  | 1.54                     | 1.06              |
| 1:o:740:LEU:HD13 | 1:o:767:LEU:HD21  | 1.33                     | 1.06              |
| 1:p:1019:THR:OG1 | 1:p:1160:LEU:CD1  | 2.03                     | 1.06              |
| 2:h:238:LEU:HD22 | 2:h:271:VAL:HG11  | 1.28                     | 1.06              |
| 2:j:285:GLU:OE2  | 3:M:67:LYS:CE     | 2.03                     | 1.06              |
| 1:k:744:HIS:CE1  | 2:2:174:ARG:O     | 2.08                     | 1.05              |
| 2:e:206:GLU:O    | 2:h:132:TYR:HB3   | 1.54                     | 1.05              |
| 2:f:208:PRO:CG   | 2:i:95:LEU:HD13   | 1.86                     | 1.05              |
| 1:l:1136:THR:CB  | 4:T:116:ILE:HD11  | 1.86                     | 1.05              |
| 2:e:174:ARG:HD3  | 2:h:274:THR:HG22  | 1.38                     | 1.05              |
| 1:F:111:ARG:HG3  | 1:l:40:TYR:HB3    | 1.36                     | 1.05              |
| 1:G:431:PHE:CE1  | 1:G:1310:THR:CB   | 2.31                     | 1.05              |
| 5:X:112:VAL:O    | 5:X:113:PHE:CD1   | 2.09                     | 1.05              |
| 4:S:217:HIS:CE1  | 5:W:64:ARG:NH1    | 2.23                     | 1.05              |
| 1:F:819:LEU:HD12 | 3:O:58:GLN:CG     | 1.85                     | 1.05              |
| 2:2:174:ARG:HD3  | 2:3:274:THR:HG22  | 1.38                     | 1.05              |
| 4:y:73:LEU:CG    | 4:y:130:VAL:O     | 2.03                     | 1.05              |
| 2:2:208:PRO:CG   | 2:3:95:LEU:HD13   | 1.86                     | 1.04              |
| 2:g:206:GLU:O    | 2:j:132:TYR:HB3   | 1.54                     | 1.04              |
| 1:k:135:ALA:CB   | 4:y:161:LYS:O     | 2.05                     | 1.04              |
| 1:m:431:PHE:CZ   | 1:m:1310:THR:CG2  | 2.39                     | 1.04              |
| 1:q:1098:PHE:CE2 | 1:q:1119:THR:HG21 | 1.69                     | 1.04              |
| 2:g:174:ARG:HD3  | 2:j:274:THR:HG22  | 1.38                     | 1.04              |
| 2:g:206:GLU:C    | 2:j:132:TYR:HB3   | 1.83                     | 1.04              |
| 4:V:79:MET:CB    | 4:V:80:PRO:HD3    | 1.87                     | 1.04              |
| 1:E:29:GLY:CA    | 1:m:207:MET:HG3   | 1.87                     | 1.04              |
| 1:m:1153:ARG:HG3 | 1:m:1283:LEU:CD1  | 1.86                     | 1.04              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:o:1160:LEU:HD22 | 1:o:1214:ASN:ND2  | 1.72                     | 1.04              |
| 1:o:765:GLU:CB    | 1:o:766:PRO:CD    | 2.29                     | 1.04              |
| 2:2:206:GLU:C     | 2:3:132:TYR:HB3   | 1.83                     | 1.04              |
| 2:e:208:PRO:CG    | 2:h:95:LEU:HD13   | 1.86                     | 1.04              |
| 1:E:30:GLU:HB3    | 1:m:1263:PHE:CE2  | 1.92                     | 1.04              |
| 1:m:431:PHE:HZ    | 1:m:1310:THR:CG2  | 1.69                     | 1.04              |
| 2:e:258:PHE:CD1   | 3:t:60:VAL:HG23   | 1.92                     | 1.04              |
| 2:g:104:LYS:HD2   | 2:j:92:LEU:HD12   | 1.33                     | 1.04              |
| 1:E:740:LEU:HD13  | 1:E:767:LEU:HD21  | 1.33                     | 1.03              |
| 1:q:1115:VAL:C    | 1:q:1119:THR:OG1  | 2.01                     | 1.03              |
| 1:E:33:PHE:CZ     | 1:m:118:SER:O     | 2.11                     | 1.03              |
| 1:H:1019:THR:CG2  | 1:H:1160:LEU:CD1  | 2.09                     | 1.03              |
| 1:m:138:THR:CG2   | 5:W:73:ARG:NH1    | 2.21                     | 1.03              |
| 1:m:748:ARG:CZ    | 2:e:269:ARG:HH22  | 1.69                     | 1.03              |
| 1:p:1019:THR:CG2  | 1:p:1160:LEU:CD1  | 2.36                     | 1.03              |
| 2:e:104:LYS:HD2   | 2:h:92:LEU:HD12   | 1.33                     | 1.03              |
| 1:I:813:PHE:CZ    | 3:R:85:LEU:CB     | 2.42                     | 1.03              |
| 1:l:1048:VAL:HG21 | 4:T:37:LYS:HG2    | 1.39                     | 1.03              |
| 1:o:765:GLU:HB3   | 1:o:766:PRO:HD3   | 1.03                     | 1.03              |
| 1:D:813:PHE:CE1   | 3:M:85:LEU:CD1    | 2.42                     | 1.03              |
| 1:H:1019:THR:HG21 | 1:H:1160:LEU:HD11 | 1.38                     | 1.03              |
| 2:e:206:GLU:C     | 2:h:132:TYR:HB3   | 1.83                     | 1.03              |
| 1:m:431:PHE:CE1   | 1:m:1310:THR:CA   | 2.41                     | 1.02              |
| 2:h:208:PRO:HB3   | 5:a:229:LYS:HZ1   | 1.00                     | 1.02              |
| 1:G:1019:THR:HG23 | 1:G:1160:LEU:CG   | 1.90                     | 1.02              |
| 2:2:104:LYS:HD2   | 2:3:92:LEU:CD1    | 1.90                     | 1.02              |
| 2:g:208:PRO:CG    | 2:j:95:LEU:HD13   | 1.86                     | 1.02              |
| 1:D:813:PHE:HE1   | 3:M:85:LEU:HD12   | 1.23                     | 1.02              |
| 1:F:332:ARG:HD3   | 1:l:12:PRO:CG     | 1.88                     | 1.02              |
| 2:f:206:GLU:C     | 2:i:132:TYR:HB3   | 1.83                     | 1.02              |
| 1:D:813:PHE:CE1   | 3:M:85:LEU:HD12   | 1.94                     | 1.02              |
| 2:f:174:ARG:HD3   | 2:i:274:THR:HG22  | 1.38                     | 1.02              |
| 1:m:51:PHE:CE1    | 1:n:87:MET:HB3    | 1.93                     | 1.02              |
| 1:m:1153:ARG:CG   | 1:m:1283:LEU:CD1  | 2.38                     | 1.02              |
| 2:e:258:PHE:CE1   | 3:t:87:MET:HG3    | 1.95                     | 1.02              |
| 5:Y:205:ASN:ND2   | 5:c:233:ILE:CG2   | 1.94                     | 1.02              |
| 2:2:206:GLU:O     | 2:3:132:TYR:HB3   | 1.54                     | 1.01              |
| 2:f:66:ARG:NH1    | 2:f:294:LEU:HD13  | 1.75                     | 1.01              |
| 2:g:202:ASP:HB2   | 2:j:86:ALA:HA     | 1.42                     | 1.01              |
| 2:g:104:LYS:HD2   | 2:j:92:LEU:CD1    | 1.90                     | 1.01              |
| 1:D:819:LEU:HD12  | 3:M:58:GLN:CG     | 1.91                     | 1.01              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:F:332:ARG:HD3   | 1:l:12:PRO:HG2    | 1.05                     | 1.01              |
| 1:G:116:MET:N     | 1:m:37:ARG:O      | 1.94                     | 1.01              |
| 2:2:206:GLU:HB3   | 2:3:132:TYR:CB    | 1.91                     | 1.01              |
| 2:f:104:LYS:HD2   | 2:i:92:LEU:CD1    | 1.90                     | 1.01              |
| 1:D:692:LEU:HB2   | 1:D:705:LEU:HD22  | 1.36                     | 1.00              |
| 1:o:765:GLU:CB    | 1:o:766:PRO:HD3   | 1.90                     | 1.00              |
| 1:q:1098:PHE:CE2  | 1:q:1119:THR:HG22 | 1.94                     | 1.00              |
| 2:e:206:GLU:HB3   | 2:h:132:TYR:CB    | 1.91                     | 1.00              |
| 1:F:341:LEU:HB2   | 1:l:14:LEU:CG     | 1.90                     | 1.00              |
| 1:F:1019:THR:CB   | 1:F:1160:LEU:HD11 | 1.90                     | 1.00              |
| 1:I:813:PHE:CE2   | 3:R:85:LEU:HB3    | 1.92                     | 1.00              |
| 1:m:691:GLU:OE2   | 1:n:953:CYS:HB2   | 1.61                     | 1.00              |
| 1:m:752:THR:O     | 3:t:86:ARG:HD3    | 1.62                     | 1.00              |
| 2:2:202:ASP:HB2   | 2:3:86:ALA:HA     | 1.42                     | 1.00              |
| 1:m:514:ALA:HA    | 1:m:517:ASP:CG    | 1.76                     | 1.00              |
| 2:f:206:GLU:HB3   | 2:i:132:TYR:CB    | 1.91                     | 1.00              |
| 2:f:105:LEU:HD21  | 2:f:212:VAL:HG11  | 1.44                     | 1.00              |
| 1:G:1019:THR:HG23 | 1:G:1160:LEU:HG   | 1.41                     | 1.00              |
| 1:l:1130:GLU:HG2  | 4:T:77:ILE:HG23   | 1.03                     | 1.00              |
| 2:2:206:GLU:HA    | 2:3:132:TYR:CD2   | 1.97                     | 1.00              |
| 1:F:1160:LEU:HD23 | 1:F:1214:ASN:HD22 | 1.19                     | 1.00              |
| 2:e:206:GLU:CA    | 2:h:132:TYR:CD2   | 2.45                     | 1.00              |
| 2:g:206:GLU:CA    | 2:j:132:TYR:CD2   | 2.45                     | 1.00              |
| 2:f:206:GLU:HA    | 2:i:132:TYR:CD2   | 1.97                     | 0.99              |
| 1:m:748:ARG:NE    | 2:e:269:ARG:HH22  | 1.58                     | 0.99              |
| 1:D:692:LEU:HD12  | 1:D:695:LEU:HD12  | 1.15                     | 0.99              |
| 2:h:208:PRO:CB    | 5:a:229:LYS:HZ1   | 1.68                     | 0.99              |
| 1:D:431:PHE:CE1   | 1:D:1310:THR:CG2  | 2.45                     | 0.99              |
| 1:D:692:LEU:HD11  | 1:D:695:LEU:HD11  | 1.41                     | 0.99              |
| 2:g:208:PRO:HG3   | 2:j:95:LEU:HD13   | 1.42                     | 0.99              |
| 1:G:431:PHE:CE1   | 1:G:1310:THR:CG2  | 2.43                     | 0.99              |
| 2:f:206:GLU:CA    | 2:i:132:TYR:CD2   | 2.45                     | 0.99              |
| 2:g:206:GLU:HB3   | 2:j:132:TYR:CB    | 1.91                     | 0.99              |
| 1:A:128:ILE:HG22  | 1:B:102:ALA:HB3   | 1.42                     | 0.99              |
| 1:F:341:LEU:HB2   | 1:l:14:LEU:CD2    | 1.93                     | 0.99              |
| 2:2:206:GLU:CA    | 2:3:132:TYR:CD2   | 2.45                     | 0.99              |
| 2:e:284:GLU:CB    | 3:t:67:LYS:HZ3    | 1.76                     | 0.99              |
| 2:g:206:GLU:HA    | 2:j:132:TYR:CD2   | 1.97                     | 0.99              |
| 1:F:819:LEU:HD11  | 3:O:59:PRO:CD     | 1.92                     | 0.98              |
| 1:D:501:TYR:OH    | 1:D:959:LEU:O     | 1.80                     | 0.98              |
| 1:I:813:PHE:CE2   | 3:R:85:LEU:HB2    | 1.97                     | 0.98              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:I:813:PHE:CD1   | 3:R:85:LEU:HG     | 1.97                     | 0.98              |
| 1:p:1019:THR:CG2  | 1:p:1160:LEU:HD11 | 1.93                     | 0.98              |
| 2:e:104:LYS:HD2   | 2:h:92:LEU:CD1    | 1.90                     | 0.98              |
| 1:m:1160:LEU:HD22 | 1:m:1214:ASN:HB2  | 1.39                     | 0.98              |
| 2:i:66:ARG:HH11   | 2:i:69:GLN:HE21   | 1.11                     | 0.98              |
| 1:G:429:VAL:HG13  | 1:G:431:PHE:CE2   | 1.97                     | 0.98              |
| 2:e:202:ASP:HB2   | 2:h:86:ALA:HA     | 1.42                     | 0.98              |
| 1:k:1019:THR:CB   | 1:k:1160:LEU:CD1  | 2.37                     | 0.98              |
| 1:q:431:PHE:O     | 1:q:438:PRO:HA    | 1.63                     | 0.98              |
| 2:h:238:LEU:CD2   | 2:h:271:VAL:HG11  | 1.93                     | 0.98              |
| 1:A:437:ILE:HD13  | 1:B:1207:GLN:HE21 | 1.24                     | 0.98              |
| 1:m:432:TYR:CZ    | 1:m:1321:LEU:CD1  | 2.46                     | 0.98              |
| 2:3:238:LEU:CD2   | 2:3:271:VAL:HG11  | 1.93                     | 0.98              |
| 1:m:748:ARG:HE    | 2:e:269:ARG:NH2   | 1.57                     | 0.98              |
| 1:k:744:HIS:HE1   | 2:2:178:VAL:HG23  | 1.28                     | 0.98              |
| 1:m:51:PHE:CD1    | 1:n:87:MET:C      | 2.42                     | 0.98              |
| 1:m:1153:ARG:HD2  | 1:m:1283:LEU:CD1  | 1.93                     | 0.98              |
| 2:f:202:ASP:HB2   | 2:i:86:ALA:HA     | 1.42                     | 0.98              |
| 2:j:238:LEU:CD2   | 2:j:271:VAL:HG11  | 1.93                     | 0.98              |
| 1:F:255:ILE:HG23  | 1:l:16:VAL:HG21   | 1.45                     | 0.97              |
| 2:e:285:GLU:OE2   | 3:t:67:LYS:HG3    | 1.62                     | 0.97              |
| 1:F:83:ASP:CG     | 1:l:147:THR:OG1   | 2.07                     | 0.97              |
| 1:G:813:PHE:CE2   | 3:P:85:LEU:HG     | 1.98                     | 0.97              |
| 1:I:725:PRO:HA    | 1:I:774:THR:OG1   | 1.62                     | 0.97              |
| 1:m:1153:ARG:CG   | 1:m:1283:LEU:HD12 | 1.93                     | 0.97              |
| 2:2:206:GLU:HB3   | 2:3:132:TYR:HB3   | 1.46                     | 0.97              |
| 2:3:93:PRO:HG2    | 2:3:195:TYR:OH    | 1.64                     | 0.97              |
| 5:X:88:GLN:O      | 5:X:308:ILE:CG2   | 2.12                     | 0.97              |
| 2:f:206:GLU:HB3   | 2:i:132:TYR:HB3   | 1.45                     | 0.97              |
| 1:G:1072:LEU:CB   | 1:m:19:ASP:O      | 2.11                     | 0.97              |
| 1:H:1160:LEU:HD23 | 1:H:1214:ASN:CG   | 1.89                     | 0.97              |
| 1:E:42:ASP:OD2    | 1:m:112:GLN:NE2   | 1.97                     | 0.97              |
| 1:k:200:HIS:CG    | 1:p:1085:ARG:HE   | 1.81                     | 0.97              |
| 1:k:813:PHE:CE1   | 3:r:85:LEU:CD2    | 2.48                     | 0.97              |
| 2:e:206:GLU:HA    | 2:h:132:TYR:CD2   | 1.97                     | 0.97              |
| 1:l:104:GLY:O     | 5:z:37:LEU:HD23   | 1.65                     | 0.97              |
| 2:2:105:LEU:HD21  | 2:2:212:VAL:HG11  | 1.44                     | 0.97              |
| 1:m:161:VAL:HG13  | 4:S:16:GLU:CD     | 1.90                     | 0.97              |
| 1:A:813:PHE:CE1   | 3:J:85:LEU:HG     | 2.00                     | 0.97              |
| 2:e:258:PHE:CZ    | 3:t:60:VAL:CG2    | 2.40                     | 0.97              |
| 1:p:1019:THR:OG1  | 1:p:1160:LEU:HD11 | 1.65                     | 0.96              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:2:208:PRO:HG3   | 2:3:95:LEU:HD13   | 1.43                     | 0.96              |
| 1:k:203:ILE:HG21  | 1:p:383:GLN:HE22  | 1.27                     | 0.96              |
| 1:p:692:LEU:HD22  | 1:p:1010:MET:HG3  | 1.45                     | 0.96              |
| 5:X:88:GLN:C      | 5:X:308:ILE:CG2   | 2.37                     | 0.96              |
| 1:G:319:HIS:CD2   | 1:n:319:HIS:CG    | 2.53                     | 0.96              |
| 2:i:238:LEU:CD2   | 2:i:271:VAL:HG11  | 1.93                     | 0.96              |
| 1:o:1160:LEU:CD2  | 1:o:1214:ASN:ND2  | 2.29                     | 0.96              |
| 2:i:93:PRO:HG2    | 2:i:195:TYR:OH    | 1.64                     | 0.96              |
| 1:G:748:ARG:HD2   | 2:h:269:ARG:HH12  | 1.20                     | 0.96              |
| 1:E:740:LEU:CD1   | 1:E:767:LEU:CD2   | 2.42                     | 0.96              |
| 2:f:200:VAL:O     | 2:i:86:ALA:CA     | 2.14                     | 0.96              |
| 2:2:202:ASP:OD1   | 2:2:211:LEU:HD22  | 1.66                     | 0.96              |
| 2:e:105:LEU:HD21  | 2:e:212:VAL:HG11  | 1.44                     | 0.96              |
| 2:e:206:GLU:HB3   | 2:h:132:TYR:HB3   | 1.46                     | 0.96              |
| 2:g:105:LEU:HD21  | 2:g:212:VAL:HG11  | 1.44                     | 0.96              |
| 2:g:200:VAL:O     | 2:j:86:ALA:CA     | 2.14                     | 0.96              |
| 1:A:788:CYS:SG    | 1:A:992:LEU:HB2   | 2.02                     | 0.96              |
| 2:g:202:ASP:OD1   | 2:g:211:LEU:HD22  | 1.66                     | 0.96              |
| 2:3:258:PHE:HD1   | 3:r:91:ALA:HA     | 1.22                     | 0.95              |
| 5:W:110:PRO:HB2   | 5:W:111:PRO:HD3   | 1.44                     | 0.95              |
| 1:k:744:HIS:HE1   | 2:2:178:VAL:CG2   | 1.79                     | 0.95              |
| 1:l:1130:GLU:CG   | 4:T:77:ILE:HG23   | 1.94                     | 0.95              |
| 2:3:79:ARG:NH1    | 2:3:277:TYR:HE1   | 1.64                     | 0.95              |
| 2:j:79:ARG:NH1    | 2:j:277:TYR:HE1   | 1.64                     | 0.95              |
| 1:k:950:TYR:CE1   | 1:k:956:GLY:O     | 2.17                     | 0.95              |
| 1:m:1160:LEU:HD22 | 1:m:1214:ASN:CB   | 1.95                     | 0.95              |
| 2:h:208:PRO:CB    | 5:a:229:LYS:HZ2   | 1.70                     | 0.95              |
| 1:E:959:LEU:O     | 1:E:960:SER:O     | 1.84                     | 0.95              |
| 1:G:429:VAL:HG12  | 1:G:431:PHE:HE2   | 0.81                     | 0.95              |
| 1:G:117:VAL:HB    | 1:m:33:PHE:CE2    | 2.02                     | 0.95              |
| 2:2:200:VAL:O     | 2:3:86:ALA:CA     | 2.14                     | 0.95              |
| 2:3:258:PHE:HE1   | 3:r:90:ILE:HG22   | 1.12                     | 0.95              |
| 2:e:104:LYS:HD3   | 2:h:92:LEU:CD1    | 1.97                     | 0.95              |
| 2:h:79:ARG:NH1    | 2:h:277:TYR:HE1   | 1.64                     | 0.95              |
| 1:G:1016:PHE:CD2  | 1:G:1018:LEU:HD11 | 2.01                     | 0.95              |
| 1:o:1031:LEU:HG   | 1:o:1079:CYS:HB3  | 1.49                     | 0.95              |
| 1:E:25:LYS:NZ     | 1:m:205:ARG:HE    | 1.65                     | 0.95              |
| 2:2:206:GLU:CA    | 2:3:132:TYR:HD2   | 1.80                     | 0.95              |
| 2:e:202:ASP:OD1   | 2:e:211:LEU:HD22  | 1.66                     | 0.95              |
| 2:f:104:LYS:HD3   | 2:i:92:LEU:CD1    | 1.97                     | 0.95              |
| 2:j:93:PRO:HG2    | 2:j:195:TYR:OH    | 1.64                     | 0.95              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:y:73:LEU:HD21   | 4:y:131:VAL:HG13  | 1.49                     | 0.95              |
| 1:A:813:PHE:CE2   | 3:J:85:LEU:CB     | 2.50                     | 0.94              |
| 1:G:319:HIS:NE2   | 1:n:319:HIS:CD2   | 2.35                     | 0.94              |
| 2:e:200:VAL:O     | 2:h:86:ALA:CA     | 2.14                     | 0.94              |
| 2:e:258:PHE:CE1   | 3:t:60:VAL:HG21   | 2.02                     | 0.94              |
| 1:F:314:VAL:CG2   | 1:m:333:ILE:CD1   | 2.45                     | 0.94              |
| 1:m:1160:LEU:CD2  | 1:m:1214:ASN:HD22 | 1.72                     | 0.94              |
| 1:q:974:PRO:O     | 1:q:978:TYR:CD2   | 2.20                     | 0.94              |
| 5:b:120:LEU:HG    | 5:b:129:VAL:HA    | 1.48                     | 0.94              |
| 1:k:758:MET:HG3   | 3:r:83:ASP:HB2    | 1.47                     | 0.94              |
| 2:h:91:HIS:HD2    | 2:h:195:TYR:CZ    | 1.86                     | 0.94              |
| 1:k:1188:PRO:HB3  | 1:k:1260:LYS:O    | 1.67                     | 0.94              |
| 2:e:206:GLU:HB3   | 2:h:132:TYR:CD2   | 2.03                     | 0.94              |
| 2:e:284:GLU:H     | 3:t:67:LYS:NZ     | 1.65                     | 0.94              |
| 2:f:208:PRO:HG3   | 2:i:95:LEU:HD13   | 1.42                     | 0.94              |
| 2:g:206:GLU:HB3   | 2:j:132:TYR:HB3   | 1.46                     | 0.94              |
| 1:I:813:PHE:CE1   | 3:R:85:LEU:HG     | 2.02                     | 0.94              |
| 1:E:25:LYS:HZ3    | 1:m:205:ARG:HE    | 1.08                     | 0.94              |
| 1:m:51:PHE:CB     | 1:n:87:MET:SD     | 2.56                     | 0.94              |
| 2:f:202:ASP:OD1   | 2:f:211:LEU:HD22  | 1.66                     | 0.94              |
| 2:i:79:ARG:NH1    | 2:i:277:TYR:HE1   | 1.64                     | 0.94              |
| 1:k:744:HIS:ND1   | 2:2:174:ARG:C     | 2.26                     | 0.93              |
| 1:k:1160:LEU:HD23 | 1:k:1214:ASN:CG   | 1.93                     | 0.93              |
| 1:m:431:PHE:CE1   | 1:m:1310:THR:HG23 | 2.03                     | 0.93              |
| 2:3:111:ALA:HB1   | 4:y:232:PHE:CE1   | 2.03                     | 0.93              |
| 2:2:206:GLU:HB3   | 2:3:132:TYR:CD2   | 2.03                     | 0.93              |
| 2:e:284:GLU:N     | 3:t:67:LYS:NZ     | 2.16                     | 0.93              |
| 2:3:258:PHE:CD1   | 3:r:90:ILE:HG22   | 2.03                     | 0.93              |
| 1:G:120:TYR:HE2   | 1:m:35:ASN:CB     | 1.79                     | 0.93              |
| 1:m:51:PHE:HD1    | 1:n:88:THR:N      | 1.66                     | 0.93              |
| 2:h:208:PRO:HD3   | 4:S:236:ASN:ND2   | 1.83                     | 0.93              |
| 2:f:66:ARG:HE     | 2:f:68:THR:HG22   | 0.85                     | 0.93              |
| 1:E:26:LEU:HD13   | 1:m:206:ARG:O     | 1.68                     | 0.93              |
| 1:m:51:PHE:CD1    | 1:n:87:MET:CB     | 2.50                     | 0.93              |
| 2:i:91:HIS:HD2    | 2:i:195:TYR:CZ    | 1.86                     | 0.93              |
| 2:g:208:PRO:HG2   | 2:j:95:LEU:CD1    | 1.99                     | 0.93              |
| 2:j:91:HIS:HD2    | 2:j:195:TYR:CZ    | 1.86                     | 0.93              |
| 1:D:819:LEU:HG    | 3:M:58:GLN:CD     | 1.94                     | 0.93              |
| 2:2:104:LYS:HD3   | 2:3:92:LEU:CD1    | 1.97                     | 0.93              |
| 1:F:332:ARG:HH21  | 1:l:12:PRO:HB2    | 1.22                     | 0.93              |
| 1:k:744:HIS:HD1   | 2:2:175:ALA:HA    | 1.32                     | 0.93              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:3:91:HIS:HD2   | 2:3:195:TYR:CZ   | 1.86                     | 0.93              |
| 2:g:206:GLU:HB3  | 2:j:132:TYR:CD2  | 2.03                     | 0.93              |
| 1:G:750:PRO:HD2  | 2:h:269:ARG:HH21 | 1.32                     | 0.93              |
| 2:e:258:PHE:HE2  | 3:t:87:MET:SD    | 1.87                     | 0.93              |
| 1:F:311:GLU:HG2  | 1:m:326:PHE:HE1  | 1.33                     | 0.92              |
| 1:D:813:PHE:CD1  | 3:M:85:LEU:CG    | 2.44                     | 0.92              |
| 1:E:746:GLU:HG2  | 1:E:767:LEU:HD11 | 1.49                     | 0.92              |
| 1:H:1018:LEU:HB3 | 1:H:1157:GLU:OE2 | 1.69                     | 0.92              |
| 1:m:1201:HIS:HD1 | 1:m:1212:THR:HG1 | 1.18                     | 0.92              |
| 4:V:79:MET:HB3   | 4:V:80:PRO:HD3   | 1.46                     | 0.92              |
| 1:E:813:PHE:CD2  | 3:N:85:LEU:HG    | 2.05                     | 0.92              |
| 1:m:138:THR:CG2  | 5:W:73:ARG:HH12  | 1.77                     | 0.92              |
| 1:G:202:THR:HA   | 1:m:22:THR:HB    | 1.48                     | 0.92              |
| 1:G:253:GLU:O    | 1:m:19:ASP:OD2   | 1.85                     | 0.92              |
| 2:2:208:PRO:HG2  | 2:3:95:LEU:CD1   | 1.99                     | 0.92              |
| 2:3:79:ARG:HH11  | 2:3:277:TYR:HE1  | 1.17                     | 0.92              |
| 2:h:110:ALA:HB3  | 5:a:225:MET:HG2  | 1.50                     | 0.92              |
| 1:F:819:LEU:HD11 | 3:O:59:PRO:HD2   | 1.50                     | 0.92              |
| 1:k:758:MET:HB3  | 3:r:79:ALA:CB    | 1.98                     | 0.92              |
| 1:m:431:PHE:HE1  | 1:m:1310:THR:CB  | 1.83                     | 0.92              |
| 2:h:93:PRO:HG2   | 2:h:195:TYR:OH   | 1.64                     | 0.92              |
| 2:f:206:GLU:HB3  | 2:i:132:TYR:CD2  | 2.03                     | 0.92              |
| 2:g:206:GLU:CA   | 2:j:132:TYR:HD2  | 1.80                     | 0.92              |
| 1:F:204:ALA:HB3  | 1:l:26:LEU:HD22  | 1.51                     | 0.92              |
| 1:E:753:SER:HB2  | 3:N:83:ASP:OD1   | 1.69                     | 0.92              |
| 1:G:744:HIS:HB2  | 2:e:175:ALA:N    | 1.84                     | 0.92              |
| 2:f:206:GLU:HG3  | 2:i:132:TYR:CE2  | 2.05                     | 0.92              |
| 2:f:206:GLU:CA   | 2:i:132:TYR:HD2  | 1.80                     | 0.91              |
| 2:j:79:ARG:HH11  | 2:j:277:TYR:HE1  | 1.17                     | 0.91              |
| 1:G:1263:PHE:HD1 | 1:m:30:GLU:C     | 1.66                     | 0.91              |
| 2:h:275:THR:O    | 2:h:279:LEU:HG   | 1.71                     | 0.91              |
| 1:A:813:PHE:CE2  | 3:J:85:LEU:HG    | 2.04                     | 0.91              |
| 1:l:749:ASN:HD22 | 1:l:757:ARG:CB   | 1.83                     | 0.91              |
| 2:h:258:PHE:CE1  | 3:P:90:ILE:HG21  | 2.06                     | 0.91              |
| 2:g:104:LYS:HD3  | 2:j:92:LEU:CD1   | 1.97                     | 0.91              |
| 4:V:61:VAL:HG11  | 4:V:88:PHE:HD2   | 1.35                     | 0.91              |
| 2:2:206:GLU:HG3  | 2:3:132:TYR:CE2  | 2.05                     | 0.91              |
| 2:e:206:GLU:HG3  | 2:h:132:TYR:CE2  | 2.05                     | 0.91              |
| 2:j:84:LEU:HG    | 2:j:230:TRP:HH2  | 1.34                     | 0.91              |
| 4:y:70:MET:HA    | 4:y:85:VAL:O     | 1.70                     | 0.91              |
| 1:k:68:LEU:CD1   | 1:k:301:ALA:O    | 2.19                     | 0.91              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:q:1098:PHE:CE1  | 1:q:1119:THR:HG21 | 2.05                     | 0.91              |
| 2:h:84:LEU:HG     | 2:h:230:TRP:HH2   | 1.34                     | 0.91              |
| 1:B:1201:HIS:HD1  | 1:B:1212:THR:HG1  | 1.16                     | 0.91              |
| 2:i:84:LEU:HG     | 2:i:230:TRP:HH2   | 1.34                     | 0.91              |
| 2:i:66:ARG:HH11   | 2:i:69:GLN:NE2    | 1.63                     | 0.91              |
| 1:F:332:ARG:NH2   | 1:l:12:PRO:CB     | 2.34                     | 0.91              |
| 1:G:86:LYS:HZ1    | 1:m:149:LEU:HD22  | 1.36                     | 0.91              |
| 2:e:208:PRO:HG2   | 2:h:95:LEU:CD1    | 1.99                     | 0.91              |
| 4:S:217:HIS:HE1   | 5:W:64:ARG:HH12   | 1.12                     | 0.91              |
| 1:k:1019:THR:CG2  | 1:k:1160:LEU:HD11 | 2.01                     | 0.91              |
| 2:h:258:PHE:HE1   | 3:P:90:ILE:HG22   | 1.13                     | 0.91              |
| 2:h:285:GLU:HG2   | 3:P:67:LYS:HE2    | 1.50                     | 0.91              |
| 1:G:341:LEU:CD1   | 1:m:12:PRO:HB2    | 2.00                     | 0.90              |
| 1:D:429:VAL:HG11  | 1:D:431:PHE:CZ    | 2.06                     | 0.90              |
| 2:f:66:ARG:HH12   | 2:f:294:LEU:HB3   | 1.35                     | 0.90              |
| 2:f:208:PRO:HG2   | 2:i:95:LEU:CD1    | 1.99                     | 0.90              |
| 2:e:206:GLU:CA    | 2:h:132:TYR:HD2   | 1.80                     | 0.90              |
| 1:A:810:VAL:HG21  | 3:J:78:LEU:HD22   | 1.52                     | 0.90              |
| 1:D:429:VAL:HG11  | 1:D:431:PHE:CE2   | 2.05                     | 0.90              |
| 1:l:749:ASN:HD22  | 1:l:757:ARG:HB2   | 1.37                     | 0.90              |
| 2:j:275:THR:O     | 2:j:279:LEU:HG    | 1.71                     | 0.90              |
| 1:H:504:ARG:NH1   | 2:h:135:ASP:OD1   | 2.04                     | 0.90              |
| 1:k:813:PHE:CD1   | 3:r:85:LEU:HD22   | 2.06                     | 0.90              |
| 1:k:1019:THR:HG23 | 1:k:1160:LEU:HD13 | 1.54                     | 0.90              |
| 2:i:275:THR:O     | 2:i:279:LEU:HG    | 1.71                     | 0.90              |
| 1:l:944:LEU:HD21  | 1:l:957:PHE:CZ    | 2.07                     | 0.90              |
| 2:g:206:GLU:HG3   | 2:j:132:TYR:CE2   | 2.05                     | 0.90              |
| 1:F:311:GLU:HG2   | 1:m:326:PHE:CE1   | 2.07                     | 0.90              |
| 2:h:79:ARG:HH11   | 2:h:277:TYR:HE1   | 1.17                     | 0.90              |
| 4:U:235:LEU:HD22  | 5:c:233:ILE:HD11  | 1.53                     | 0.90              |
| 1:A:380:THR:HG22  | 1:B:99:PRO:HB2    | 1.53                     | 0.90              |
| 1:F:344:SER:HB2   | 1:l:14:LEU:HD11   | 0.92                     | 0.90              |
| 1:k:784:VAL:O     | 1:k:788:CYS:CB    | 2.20                     | 0.90              |
| 1:m:431:PHE:HE1   | 1:m:1310:THR:HA   | 1.11                     | 0.90              |
| 2:i:113:PRO:HB3   | 4:U:233:HIS:CE1   | 2.07                     | 0.90              |
| 2:3:84:LEU:HG     | 2:3:230:TRP:HH2   | 1.34                     | 0.89              |
| 2:e:284:GLU:N     | 3:t:67:LYS:HZ1    | 1.69                     | 0.89              |
| 1:H:1156:CYS:HB2  | 1:H:1245:PRO:HD2  | 1.51                     | 0.89              |
| 1:l:950:TYR:O     | 1:l:957:PHE:HE2   | 1.49                     | 0.89              |
| 1:m:51:PHE:CE1    | 1:n:87:MET:C      | 2.50                     | 0.89              |
| 2:3:275:THR:O     | 2:3:279:LEU:HG    | 1.71                     | 0.89              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:D:692:LEU:HG   | 1:D:695:LEU:HD12  | 1.54                     | 0.89              |
| 1:k:596:LEU:CD1  | 1:k:985:THR:O     | 2.20                     | 0.89              |
| 1:G:117:VAL:HG12 | 1:m:36:PHE:HB2    | 1.55                     | 0.89              |
| 1:k:930:PRO:HG3  | 1:k:957:PHE:HE1   | 1.37                     | 0.89              |
| 1:q:221:LYS:O    | 1:q:225:LEU:HB2   | 1.72                     | 0.89              |
| 1:k:788:CYS:O    | 1:k:989:VAL:HG13  | 1.72                     | 0.89              |
| 1:m:748:ARG:HH11 | 2:e:269:ARG:HH12  | 0.90                     | 0.89              |
| 1:p:1003:SER:O   | 1:p:1007:LEU:HB2  | 1.73                     | 0.89              |
| 1:q:805:LEU:O    | 1:q:809:LEU:HB2   | 1.73                     | 0.89              |
| 2:f:66:ARG:HH12  | 2:f:294:LEU:CB    | 1.86                     | 0.89              |
| 2:g:174:ARG:HD3  | 2:j:274:THR:CG2   | 2.03                     | 0.89              |
| 2:e:174:ARG:HD3  | 2:h:274:THR:CG2   | 2.03                     | 0.89              |
| 1:k:758:MET:HB2  | 3:r:79:ALA:HB1    | 1.54                     | 0.89              |
| 2:3:258:PHE:CZ   | 3:r:90:ILE:CG2    | 2.54                     | 0.89              |
| 2:e:104:LYS:HD3  | 2:h:92:LEU:HD12   | 1.54                     | 0.89              |
| 2:3:238:LEU:HD22 | 2:3:271:VAL:CG1   | 2.03                     | 0.89              |
| 2:h:94:LEU:HD21  | 2:h:222:LEU:HD23  | 0.90                     | 0.89              |
| 1:m:759:ILE:HG22 | 3:t:76:ASP:OD2    | 1.73                     | 0.88              |
| 2:j:238:LEU:HD22 | 2:j:271:VAL:CG1   | 2.03                     | 0.88              |
| 1:k:1168:GLU:HA  | 1:p:438:PRO:HG2   | 1.55                     | 0.88              |
| 1:m:51:PHE:CD1   | 1:n:88:THR:N      | 2.41                     | 0.88              |
| 1:p:692:LEU:HD23 | 1:p:1010:MET:CE   | 2.03                     | 0.88              |
| 1:q:1098:PHE:HE2 | 1:q:1119:THR:HG23 | 1.34                     | 0.88              |
| 5:W:110:PRO:HB2  | 5:W:111:PRO:HD2   | 0.89                     | 0.88              |
| 1:F:1019:THR:OG1 | 1:F:1160:LEU:CD1  | 2.18                     | 0.88              |
| 1:k:744:HIS:CE1  | 2:2:178:VAL:CG2   | 2.56                     | 0.88              |
| 1:m:51:PHE:CD1   | 1:n:87:MET:CA     | 2.57                     | 0.88              |
| 1:k:200:HIS:NE2  | 1:p:1085:ARG:HG3  | 1.88                     | 0.88              |
| 2:3:94:LEU:CD2   | 2:3:222:LEU:CD2   | 2.47                     | 0.88              |
| 1:H:184:LEU:HB3  | 1:H:1032:LEU:HD21 | 1.54                     | 0.88              |
| 1:m:429:VAL:HG12 | 1:m:431:PHE:HE2   | 1.10                     | 0.88              |
| 2:h:208:PRO:HB2  | 5:a:229:LYS:NZ    | 1.88                     | 0.88              |
| 1:H:1018:LEU:CB  | 1:H:1157:GLU:OE2  | 2.21                     | 0.88              |
| 1:k:1207:GLN:HG2 | 1:p:1150:HIS:NE2  | 1.87                     | 0.88              |
| 2:f:174:ARG:HD3  | 2:i:274:THR:CG2   | 2.03                     | 0.88              |
| 2:3:92:LEU:O     | 2:3:96:THR:CG2    | 2.20                     | 0.88              |
| 2:i:107:GLY:O    | 4:U:232:PHE:HE1   | 1.56                     | 0.88              |
| 2:j:94:LEU:HD21  | 2:j:222:LEU:HD23  | 0.89                     | 0.88              |
| 1:D:429:VAL:CG1  | 1:D:431:PHE:HE2   | 1.48                     | 0.88              |
| 1:n:710:ALA:O    | 1:n:713:ASP:OD1   | 1.91                     | 0.88              |
| 2:2:104:LYS:HD3  | 2:3:92:LEU:HD12   | 1.54                     | 0.88              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:y:72:ARG:C      | 4:y:73:LEU:CD1    | 2.46                     | 0.88              |
| 1:G:1263:PHE:CD1  | 1:m:30:GLU:O      | 2.22                     | 0.87              |
| 1:m:1153:ARG:CD   | 1:m:1283:LEU:HD13 | 2.03                     | 0.87              |
| 1:m:1153:ARG:CD   | 1:m:1283:LEU:CD1  | 2.53                     | 0.87              |
| 2:3:88:ARG:HD3    | 2:3:132:TYR:CZ    | 2.09                     | 0.87              |
| 1:F:86:LYS:NZ     | 1:l:144:PHE:HZ    | 1.71                     | 0.87              |
| 2:2:174:ARG:HD3   | 2:3:274:THR:CG2   | 2.03                     | 0.87              |
| 2:h:238:LEU:HD22  | 2:h:271:VAL:CG1   | 2.02                     | 0.87              |
| 2:i:79:ARG:HH11   | 2:i:277:TYR:HE1   | 1.17                     | 0.87              |
| 1:G:429:VAL:HG13  | 1:G:431:PHE:CZ    | 2.08                     | 0.87              |
| 2:h:285:GLU:CD    | 3:P:67:LYS:NZ     | 2.32                     | 0.87              |
| 2:f:66:ARG:NE     | 2:f:68:THR:CG2    | 2.13                     | 0.87              |
| 1:p:1160:LEU:HD23 | 1:p:1214:ASN:CG   | 2.00                     | 0.87              |
| 2:j:285:GLU:CD    | 3:M:67:LYS:HE3    | 1.99                     | 0.87              |
| 4:y:73:LEU:CD2    | 4:y:131:VAL:HG12  | 2.04                     | 0.87              |
| 1:F:819:LEU:HD12  | 3:O:58:GLN:CB     | 2.04                     | 0.87              |
| 1:m:1053:ARG:HG2  | 5:W:306:LEU:HD22  | 1.54                     | 0.87              |
| 1:G:319:HIS:NE2   | 1:n:319:HIS:CG    | 2.42                     | 0.87              |
| 1:q:79:ILE:O      | 1:q:1042:ILE:HA   | 1.75                     | 0.87              |
| 2:h:88:ARG:HD3    | 2:h:132:TYR:CZ    | 2.09                     | 0.87              |
| 2:i:94:LEU:CD2    | 2:i:222:LEU:CD2   | 2.47                     | 0.87              |
| 1:k:203:ILE:CG2   | 1:p:383:GLN:HE22  | 1.87                     | 0.87              |
| 5:X:307:CYS:C     | 5:X:308:ILE:HG13  | 1.99                     | 0.87              |
| 1:D:430:TYR:O     | 1:D:431:PHE:CG    | 2.27                     | 0.87              |
| 2:e:208:PRO:HG3   | 2:h:95:LEU:HD13   | 1.43                     | 0.87              |
| 1:G:114:THR:N     | 1:m:39:TYR:O      | 2.08                     | 0.86              |
| 2:h:92:LEU:O      | 2:h:96:THR:CG2    | 2.20                     | 0.86              |
| 2:j:88:ARG:HD3    | 2:j:132:TYR:CZ    | 2.09                     | 0.86              |
| 2:h:258:PHE:CD1   | 3:P:90:ILE:HG22   | 2.10                     | 0.86              |
| 2:i:238:LEU:HD22  | 2:i:271:VAL:CG1   | 2.03                     | 0.86              |
| 2:j:94:LEU:CD2    | 2:j:222:LEU:CD2   | 2.47                     | 0.86              |
| 1:n:1031:LEU:HG   | 1:n:1079:CYS:HB3  | 1.57                     | 0.86              |
| 2:h:258:PHE:HE1   | 3:P:90:ILE:CB     | 1.87                     | 0.86              |
| 2:i:88:ARG:HD3    | 2:i:132:TYR:CZ    | 2.09                     | 0.86              |
| 1:G:1019:THR:OG1  | 1:G:1158:VAL:HB   | 1.74                     | 0.86              |
| 1:G:429:VAL:CG1   | 1:G:431:PHE:CZ    | 2.59                     | 0.86              |
| 1:I:753:SER:HB2   | 3:R:83:ASP:OD2    | 1.75                     | 0.86              |
| 1:p:1160:LEU:HD23 | 1:p:1214:ASN:ND2  | 1.89                     | 0.86              |
| 2:h:94:LEU:CD2    | 2:h:222:LEU:CD2   | 2.47                     | 0.86              |
| 1:G:330:ALA:HA    | 1:n:314:VAL:HG21  | 1.56                     | 0.86              |
| 1:m:141:LYS:HD3   | 4:S:20:GLU:H      | 1.40                     | 0.86              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:Y:205:ASN:HD22  | 5:c:233:ILE:HG23  | 1.41                     | 0.86              |
| 1:k:1207:GLN:HE22 | 1:p:437:ILE:HG21  | 1.36                     | 0.86              |
| 1:E:691:GLU:OE1   | 1:F:952:ARG:HG3   | 1.75                     | 0.85              |
| 1:m:1031:LEU:HG   | 1:m:1079:CYS:HB3  | 1.59                     | 0.85              |
| 1:p:1019:THR:CB   | 1:p:1160:LEU:CD1  | 2.53                     | 0.85              |
| 1:E:40:TYR:HB3    | 1:m:111:ARG:HG3   | 1.56                     | 0.85              |
| 1:G:813:PHE:CZ    | 3:P:85:LEU:CD1    | 2.58                     | 0.85              |
| 1:m:1234:GLU:OE2  | 5:a:51:ASP:OD1    | 1.93                     | 0.85              |
| 4:y:72:ARG:O      | 4:y:73:LEU:HG     | 1.76                     | 0.85              |
| 1:F:86:LYS:HZ1    | 1:l:144:PHE:HZ    | 0.87                     | 0.85              |
| 2:i:93:PRO:CD     | 2:i:195:TYR:OH    | 2.24                     | 0.85              |
| 4:y:73:LEU:CD2    | 4:y:131:VAL:CG1   | 2.54                     | 0.85              |
| 1:D:692:LEU:HD11  | 1:D:695:LEU:CD1   | 1.95                     | 0.85              |
| 2:2:206:GLU:HB3   | 2:3:132:TYR:C     | 2.01                     | 0.85              |
| 1:A:1153:ARG:HH12 | 1:B:1209:PHE:HZ   | 1.23                     | 0.85              |
| 1:F:813:PHE:CD1   | 3:O:85:LEU:HG     | 2.11                     | 0.85              |
| 1:o:740:LEU:CD1   | 1:o:767:LEU:HD21  | 2.07                     | 0.85              |
| 1:l:1130:GLU:HG2  | 4:T:77:ILE:CG2    | 1.99                     | 0.85              |
| 2:h:285:GLU:OE2   | 3:P:67:LYS:NZ     | 2.09                     | 0.85              |
| 1:E:29:GLY:HA3    | 1:m:207:MET:HG3   | 1.56                     | 0.85              |
| 1:G:1016:PHE:HD2  | 1:G:1018:LEU:HD11 | 1.39                     | 0.85              |
| 1:k:1019:THR:HG23 | 1:k:1160:LEU:CD1  | 2.06                     | 0.85              |
| 2:e:258:PHE:CD1   | 3:t:60:VAL:CG2    | 2.55                     | 0.85              |
| 2:h:93:PRO:CD     | 2:h:195:TYR:OH    | 2.24                     | 0.85              |
| 2:i:92:LEU:O      | 2:i:96:THR:CG2    | 2.19                     | 0.85              |
| 1:D:813:PHE:CE2   | 3:M:85:LEU:HB3    | 2.12                     | 0.84              |
| 1:k:813:PHE:CZ    | 3:r:85:LEU:HD22   | 2.11                     | 0.84              |
| 1:q:1115:VAL:O    | 1:q:1119:THR:CB   | 2.24                     | 0.84              |
| 2:3:93:PRO:CD     | 2:3:195:TYR:OH    | 2.24                     | 0.84              |
| 2:3:258:PHE:HE1   | 3:r:90:ILE:CB     | 1.89                     | 0.84              |
| 2:e:206:GLU:HB3   | 2:h:132:TYR:C     | 2.01                     | 0.84              |
| 2:3:258:PHE:CE1   | 3:r:90:ILE:CB     | 2.60                     | 0.84              |
| 2:i:276:ALA:O     | 2:i:280:LEU:HG    | 1.77                     | 0.84              |
| 1:D:819:LEU:CD1   | 3:M:58:GLN:CG     | 2.50                     | 0.84              |
| 1:F:1019:THR:N    | 1:F:1160:LEU:CD1  | 2.40                     | 0.84              |
| 1:l:1048:VAL:O    | 4:T:40:VAL:O      | 1.95                     | 0.84              |
| 5:X:112:VAL:O     | 5:X:113:PHE:CD2   | 2.29                     | 0.84              |
| 2:2:105:LEU:HD11  | 2:2:212:VAL:HG12  | 1.59                     | 0.84              |
| 2:e:258:PHE:CE2   | 3:t:60:VAL:HG23   | 2.10                     | 0.84              |
| 2:f:206:GLU:HB3   | 2:i:132:TYR:C     | 2.01                     | 0.84              |
| 2:g:208:PRO:HG2   | 2:j:95:LEU:HD13   | 1.58                     | 0.84              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:t:85:LEU:HD13  | 3:t:88:LEU:HD12   | 1.56                     | 0.84              |
| 5:X:307:CYS:O    | 5:X:308:ILE:HG13  | 1.76                     | 0.84              |
| 1:D:819:LEU:HD11 | 3:M:58:GLN:HG3    | 1.60                     | 0.84              |
| 1:k:1019:THR:CG2 | 1:k:1160:LEU:CD1  | 2.55                     | 0.84              |
| 2:3:258:PHE:CD1  | 3:r:91:ALA:CA     | 2.60                     | 0.84              |
| 2:e:105:LEU:HD11 | 2:e:212:VAL:HG12  | 1.59                     | 0.84              |
| 2:j:91:HIS:CD2   | 2:j:195:TYR:CG    | 2.66                     | 0.84              |
| 1:m:752:THR:O    | 3:t:86:ARG:CD     | 2.25                     | 0.84              |
| 2:e:208:PRO:HG2  | 2:h:95:LEU:HD13   | 1.58                     | 0.84              |
| 2:h:276:ALA:O    | 2:h:280:LEU:HG    | 1.77                     | 0.84              |
| 2:g:206:GLU:HB3  | 2:j:132:TYR:C     | 2.01                     | 0.84              |
| 2:2:208:PRO:HG2  | 2:3:95:LEU:HD13   | 1.58                     | 0.84              |
| 2:3:94:LEU:HD21  | 2:3:222:LEU:HD23  | 0.89                     | 0.84              |
| 2:g:104:LYS:HD3  | 2:j:92:LEU:HD12   | 1.54                     | 0.84              |
| 4:V:79:MET:HG3   | 4:V:80:PRO:HD3    | 1.58                     | 0.84              |
| 1:D:813:PHE:CE1  | 3:M:85:LEU:HB3    | 2.13                     | 0.84              |
| 1:E:30:GLU:O     | 1:m:1263:PHE:HD2  | 1.58                     | 0.84              |
| 2:3:272:ASP:HB3  | 2:3:275:THR:OG1   | 1.78                     | 0.84              |
| 1:G:115:VAL:HG22 | 1:m:38:LEU:CD1    | 2.08                     | 0.84              |
| 2:h:208:PRO:HB2  | 5:a:229:LYS:HZ2   | 1.41                     | 0.84              |
| 2:i:94:LEU:HD21  | 2:i:222:LEU:HD23  | 0.90                     | 0.84              |
| 2:j:93:PRO:CD    | 2:j:195:TYR:OH    | 2.24                     | 0.84              |
| 2:j:276:ALA:O    | 2:j:280:LEU:HG    | 1.77                     | 0.84              |
| 1:D:813:PHE:CE2  | 3:M:85:LEU:CB     | 2.61                     | 0.84              |
| 1:G:450:LEU:HD21 | 1:G:1018:LEU:HD21 | 1.59                     | 0.84              |
| 2:3:66:ARG:HG2   | 2:3:69:GLN:CG     | 2.07                     | 0.84              |
| 2:j:272:ASP:HB3  | 2:j:275:THR:OG1   | 1.78                     | 0.84              |
| 1:D:431:PHE:HZ   | 1:D:1310:THR:CG2  | 1.80                     | 0.83              |
| 1:l:431:PHE:O    | 1:l:438:PRO:HA    | 1.78                     | 0.83              |
| 2:h:272:ASP:HB3  | 2:h:275:THR:OG1   | 1.78                     | 0.83              |
| 2:f:206:GLU:O    | 2:i:132:TYR:HB2   | 1.78                     | 0.83              |
| 1:E:25:LYS:HD3   | 1:m:205:ARG:CZ    | 2.08                     | 0.83              |
| 1:k:113:THR:HG23 | 1:p:167:ASN:HD22  | 1.40                     | 0.83              |
| 2:2:202:ASP:HB2  | 2:3:86:ALA:CA     | 2.07                     | 0.83              |
| 2:3:91:HIS:CD2   | 2:3:195:TYR:CG    | 2.66                     | 0.83              |
| 2:f:208:PRO:HG2  | 2:i:95:LEU:HD13   | 1.58                     | 0.83              |
| 2:i:272:ASP:HB3  | 2:i:275:THR:OG1   | 1.78                     | 0.83              |
| 1:k:1207:GLN:NE2 | 1:p:437:ILE:CG2   | 2.41                     | 0.83              |
| 2:3:276:ALA:O    | 2:3:280:LEU:HG    | 1.77                     | 0.83              |
| 1:D:813:PHE:CE1  | 3:M:85:LEU:CB     | 2.57                     | 0.83              |
| 1:D:819:LEU:HG   | 3:M:58:GLN:HE21   | 1.01                     | 0.83              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:G:430:TYR:O     | 1:G:431:PHE:CD2   | 2.31                     | 0.83              |
| 4:S:61:VAL:HG11   | 4:S:88:PHE:HD2    | 1.42                     | 0.83              |
| 1:E:19:ASP:HB2    | 1:m:252:THR:HB    | 1.60                     | 0.83              |
| 1:p:692:LEU:CD2   | 1:p:1010:MET:HE2  | 2.08                     | 0.83              |
| 2:g:105:LEU:HD11  | 2:g:212:VAL:HG12  | 1.59                     | 0.83              |
| 4:S:224:ARG:HH21  | 5:W:282:GLN:HE21  | 1.21                     | 0.83              |
| 1:I:957:PHE:HB2   | 1:I:959:LEU:HD11  | 1.60                     | 0.83              |
| 1:k:950:TYR:HD1   | 1:k:956:GLY:O     | 1.57                     | 0.83              |
| 2:g:104:LYS:CD    | 2:j:92:LEU:HD13   | 2.08                     | 0.83              |
| 4:S:217:HIS:CE1   | 5:W:64:ARG:HH12   | 1.90                     | 0.83              |
| 1:G:86:LYS:NZ     | 1:m:149:LEU:HD22  | 1.93                     | 0.83              |
| 2:h:84:LEU:HG     | 2:h:230:TRP:CH2   | 2.14                     | 0.83              |
| 2:e:104:LYS:CD    | 2:h:92:LEU:HD13   | 2.08                     | 0.83              |
| 2:i:91:HIS:CD2    | 2:i:195:TYR:CG    | 2.66                     | 0.83              |
| 2:g:202:ASP:HB2   | 2:j:86:ALA:CA     | 2.07                     | 0.83              |
| 4:y:72:ARG:O      | 4:y:73:LEU:HD12   | 1.78                     | 0.83              |
| 1:k:1160:LEU:CD2  | 1:k:1214:ASN:ND2  | 2.42                     | 0.83              |
| 1:l:1136:THR:HB   | 4:T:116:ILE:HD11  | 0.89                     | 0.83              |
| 1:m:1048:VAL:HB   | 4:S:15:MET:HG3    | 1.59                     | 0.83              |
| 2:h:285:GLU:OE2   | 3:P:67:LYS:CE     | 2.27                     | 0.83              |
| 1:G:120:TYR:HE2   | 1:m:35:ASN:HB2    | 1.43                     | 0.82              |
| 2:2:104:LYS:CD    | 2:3:92:LEU:HD13   | 2.08                     | 0.82              |
| 2:h:91:HIS:CD2    | 2:h:195:TYR:CG    | 2.66                     | 0.82              |
| 2:f:66:ARG:HG2    | 2:f:69:GLN:HG3    | 1.60                     | 0.82              |
| 4:y:72:ARG:O      | 4:y:73:LEU:CD1    | 2.26                     | 0.82              |
| 1:G:83:ASP:OD2    | 1:m:147:THR:HG22  | 1.79                     | 0.82              |
| 1:A:653:TYR:HB2   | 1:A:786:TYR:CE2   | 2.13                     | 0.82              |
| 1:l:950:TYR:HB3   | 1:l:957:PHE:CE2   | 2.14                     | 0.82              |
| 1:q:1098:PHE:CD2  | 1:q:1119:THR:CG2  | 2.60                     | 0.82              |
| 1:A:813:PHE:CE2   | 3:J:85:LEU:CG     | 2.63                     | 0.82              |
| 2:f:104:LYS:HD3   | 2:i:92:LEU:HD12   | 1.54                     | 0.82              |
| 2:j:92:LEU:O      | 2:j:96:THR:CG2    | 2.20                     | 0.82              |
| 1:m:431:PHE:CE1   | 1:m:1310:THR:CB   | 2.62                     | 0.82              |
| 2:3:84:LEU:HG     | 2:3:230:TRP:CH2   | 2.14                     | 0.82              |
| 2:e:206:GLU:O     | 2:h:132:TYR:HB2   | 1.78                     | 0.82              |
| 2:f:104:LYS:CD    | 2:i:92:LEU:HD13   | 2.08                     | 0.82              |
| 3:t:83:ASP:O      | 3:t:86:ARG:HG2    | 1.79                     | 0.82              |
| 1:B:664:GLY:HA3   | 1:C:644:ARG:HH21  | 1.45                     | 0.82              |
| 1:F:1019:THR:HG23 | 1:F:1160:LEU:HD13 | 1.62                     | 0.82              |
| 2:f:105:LEU:HD11  | 2:f:212:VAL:HG12  | 1.59                     | 0.82              |
| 2:j:84:LEU:HG     | 2:j:230:TRP:CH2   | 2.14                     | 0.82              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:F:1019:THR:N    | 1:F:1160:LEU:HD12 | 1.95                     | 0.82              |
| 1:k:744:HIS:HD1   | 2:2:175:ALA:CA    | 1.91                     | 0.82              |
| 2:g:206:GLU:O     | 2:j:132:TYR:HB2   | 1.78                     | 0.82              |
| 4:y:72:ARG:O      | 4:y:73:LEU:CG     | 2.28                     | 0.82              |
| 1:E:11:LEU:CD1    | 1:m:323:MET:HE1   | 2.10                     | 0.82              |
| 1:F:819:LEU:HD11  | 3:O:59:PRO:HD3    | 1.62                     | 0.82              |
| 5:z:112:VAL:O     | 5:z:113:PHE:CG    | 2.33                     | 0.82              |
| 1:F:86:LYS:NZ     | 1:l:144:PHE:CZ    | 2.48                     | 0.81              |
| 1:G:83:ASP:OD1    | 1:m:147:THR:CB    | 2.27                     | 0.81              |
| 1:m:1160:LEU:CD2  | 1:m:1214:ASN:CG   | 2.52                     | 0.81              |
| 1:o:740:LEU:HD13  | 1:o:767:LEU:CD2   | 2.07                     | 0.81              |
| 2:2:206:GLU:O     | 2:3:132:TYR:HB2   | 1.78                     | 0.81              |
| 2:i:84:LEU:HG     | 2:i:230:TRP:CH2   | 2.14                     | 0.81              |
| 4:S:217:HIS:HE1   | 5:W:64:ARG:HH11   | 1.24                     | 0.81              |
| 1:E:20:LEU:HD12   | 1:l:379:ASN:OD1   | 1.81                     | 0.81              |
| 1:k:205:ARG:HB3   | 1:p:381:ASP:HB3   | 1.61                     | 0.81              |
| 1:l:813:PHE:HZ    | 3:s:82:LEU:HD12   | 1.45                     | 0.81              |
| 1:o:765:GLU:CB    | 1:o:766:PRO:HD2   | 2.10                     | 0.81              |
| 2:e:284:GLU:HB2   | 3:t:67:LYS:NZ     | 1.94                     | 0.81              |
| 1:A:104:GLY:O     | 5:b:37:LEU:HD13   | 1.81                     | 0.81              |
| 1:F:819:LEU:CD1   | 3:O:58:GLN:HG2    | 2.08                     | 0.81              |
| 1:H:1017:ALA:O    | 1:H:1160:LEU:N    | 2.14                     | 0.81              |
| 1:m:429:VAL:CG1   | 1:m:431:PHE:HE2   | 1.82                     | 0.81              |
| 1:q:1098:PHE:CD2  | 1:q:1119:THR:HG22 | 2.15                     | 0.81              |
| 1:D:818:PHE:C     | 3:M:58:GLN:HE22   | 1.89                     | 0.81              |
| 1:m:429:VAL:CG1   | 1:m:431:PHE:CZ    | 2.63                     | 0.81              |
| 2:f:202:ASP:HB2   | 2:i:86:ALA:CA     | 2.07                     | 0.81              |
| 5:Y:206:LEU:O     | 5:Y:272:LYS:HE2   | 1.80                     | 0.81              |
| 1:E:20:LEU:HD12   | 1:l:379:ASN:CG    | 2.06                     | 0.81              |
| 4:S:228:ARG:HG2   | 5:a:224:ASN:O     | 1.81                     | 0.81              |
| 1:F:201:GLY:C     | 1:l:22:THR:HB     | 2.05                     | 0.81              |
| 1:k:521:LYS:HD2   | 1:p:440:ARG:NH2   | 1.95                     | 0.81              |
| 1:k:1168:GLU:HA   | 1:p:438:PRO:CG    | 2.10                     | 0.81              |
| 2:e:206:GLU:CB    | 2:h:132:TYR:HB3   | 2.11                     | 0.81              |
| 2:e:284:GLU:CA    | 3:t:67:LYS:HZ3    | 1.92                     | 0.81              |
| 1:p:1019:THR:HG23 | 1:p:1160:LEU:HD13 | 1.61                     | 0.81              |
| 5:X:89:CYS:HA     | 5:X:308:ILE:CG1   | 2.10                     | 0.81              |
| 5:X:112:VAL:HG21  | 5:X:132:TRP:CE3   | 2.15                     | 0.81              |
| 1:q:394:PHE:O     | 1:q:1021:VAL:HA   | 1.81                     | 0.81              |
| 2:f:206:GLU:CB    | 2:i:132:TYR:HB3   | 2.11                     | 0.81              |
| 1:m:51:PHE:CG     | 1:n:87:MET:HB3    | 2.16                     | 0.80              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:F:82:HIS:CB     | 1:l:147:THR:CG2   | 2.58                     | 0.80              |
| 1:p:659:ILE:O     | 1:p:663:LEU:HB2   | 1.80                     | 0.80              |
| 1:A:1031:LEU:CG   | 1:A:1079:CYS:HB3  | 2.11                     | 0.80              |
| 1:k:203:ILE:HG23  | 1:p:383:GLN:OE1   | 1.82                     | 0.80              |
| 1:k:744:HIS:CE1   | 2:2:178:VAL:HG23  | 2.16                     | 0.80              |
| 2:3:66:ARG:HD3    | 2:3:68:THR:CG2    | 2.11                     | 0.80              |
| 2:3:262:TYR:CE1   | 3:r:87:MET:CE     | 2.63                     | 0.80              |
| 1:E:25:LYS:HZ3    | 1:m:205:ARG:NE    | 1.80                     | 0.80              |
| 1:k:930:PRO:HG3   | 1:k:957:PHE:CE1   | 2.16                     | 0.80              |
| 1:m:1280:GLU:OE2  | 1:n:206:ARG:NE    | 2.15                     | 0.80              |
| 2:3:262:TYR:CD1   | 3:r:87:MET:HE1    | 2.16                     | 0.80              |
| 1:k:1019:THR:N    | 1:k:1160:LEU:CD1  | 2.44                     | 0.80              |
| 2:h:93:PRO:HG2    | 2:h:195:TYR:CZ    | 2.17                     | 0.80              |
| 2:f:66:ARG:CZ     | 2:f:68:THR:HG22   | 2.11                     | 0.80              |
| 2:i:79:ARG:NH1    | 2:i:277:TYR:CE1   | 2.50                     | 0.80              |
| 1:G:750:PRO:CG    | 2:h:269:ARG:HH21  | 1.95                     | 0.80              |
| 2:2:206:GLU:CB    | 2:3:132:TYR:HB3   | 2.11                     | 0.80              |
| 2:3:91:HIS:CD2    | 2:3:195:TYR:CZ    | 2.66                     | 0.80              |
| 2:i:93:PRO:HG2    | 2:i:195:TYR:CZ    | 2.17                     | 0.80              |
| 4:y:73:LEU:CD2    | 4:y:130:VAL:O     | 2.30                     | 0.80              |
| 5:W:265:THR:HG21  | 5:W:268:GLU:OE1   | 1.82                     | 0.80              |
| 1:D:430:TYR:O     | 1:D:431:PHE:CD1   | 2.34                     | 0.80              |
| 1:D:692:LEU:CD1   | 1:D:695:LEU:CG    | 2.17                     | 0.80              |
| 1:G:750:PRO:CD    | 2:h:269:ARG:HH21  | 1.85                     | 0.80              |
| 5:z:110:PRO:O     | 5:z:111:PRO:O     | 1.99                     | 0.80              |
| 1:m:141:LYS:HD2   | 4:S:20:GLU:HA     | 1.64                     | 0.79              |
| 2:j:91:HIS:NE2    | 2:j:195:TYR:CD1   | 2.51                     | 0.79              |
| 1:G:1017:ALA:O    | 1:G:1018:LEU:HD12 | 1.81                     | 0.79              |
| 1:k:1161:THR:HG22 | 1:k:1216:TRP:CZ3  | 2.16                     | 0.79              |
| 1:l:511:ALA:O     | 1:l:515:LYS:HB2   | 1.82                     | 0.79              |
| 2:h:91:HIS:NE2    | 2:h:195:TYR:CD1   | 2.51                     | 0.79              |
| 1:F:314:VAL:HG23  | 1:m:333:ILE:CD1   | 2.12                     | 0.79              |
| 1:p:1019:THR:OG1  | 1:p:1160:LEU:HD12 | 1.80                     | 0.79              |
| 1:q:393:THR:HA    | 1:q:1022:ARG:O    | 1.82                     | 0.79              |
| 2:h:79:ARG:NH1    | 2:h:277:TYR:CE1   | 2.50                     | 0.79              |
| 2:h:91:HIS:CD2    | 2:h:195:TYR:CZ    | 2.66                     | 0.79              |
| 2:g:206:GLU:CB    | 2:j:132:TYR:HB3   | 2.11                     | 0.79              |
| 2:j:79:ARG:NH1    | 2:j:277:TYR:CE1   | 2.50                     | 0.79              |
| 1:E:34:ASN:HB2    | 1:m:1264:LYS:CE   | 2.12                     | 0.79              |
| 2:3:79:ARG:NH1    | 2:3:277:TYR:CE1   | 2.50                     | 0.79              |
| 2:3:258:PHE:HE1   | 3:r:90:ILE:C      | 1.91                     | 0.79              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:i:91:HIS:CD2    | 2:i:195:TYR:CZ    | 2.66                     | 0.79              |
| 1:m:1160:LEU:HD23 | 1:m:1214:ASN:HD22 | 1.28                     | 0.79              |
| 2:2:200:VAL:O     | 2:3:86:ALA:HA     | 1.83                     | 0.79              |
| 1:F:1160:LEU:CD2  | 1:F:1214:ASN:ND2  | 2.44                     | 0.79              |
| 1:G:319:HIS:CD2   | 1:n:319:HIS:CD2   | 2.70                     | 0.79              |
| 1:m:138:THR:HG21  | 5:W:73:ARG:HH12   | 0.97                     | 0.79              |
| 1:p:1019:THR:CB   | 1:p:1160:LEU:HD11 | 2.13                     | 0.79              |
| 2:e:285:GLU:CG    | 3:t:67:LYS:HE2    | 2.12                     | 0.79              |
| 2:i:93:PRO:HD2    | 2:i:195:TYR:OH    | 1.83                     | 0.79              |
| 1:k:688:ARG:O     | 1:k:691:GLU:HG3   | 1.82                     | 0.79              |
| 1:k:744:HIS:CE1   | 2:2:178:VAL:HG21  | 2.18                     | 0.79              |
| 1:n:697:GLY:H     | 1:o:509:ARG:HH22  | 1.29                     | 0.79              |
| 2:j:93:PRO:HG2    | 2:j:195:TYR:CZ    | 2.17                     | 0.79              |
| 1:I:813:PHE:CG    | 3:R:85:LEU:HG     | 2.17                     | 0.79              |
| 5:1:7:VAL:O       | 5:1:78:GLN:HA     | 1.82                     | 0.79              |
| 2:f:200:VAL:O     | 2:i:86:ALA:HA     | 1.83                     | 0.78              |
| 2:h:93:PRO:HD2    | 2:h:195:TYR:OH    | 1.83                     | 0.78              |
| 2:g:208:PRO:CB    | 2:j:95:LEU:HD11   | 2.12                     | 0.78              |
| 1:k:744:HIS:ND1   | 2:2:174:ARG:O     | 2.15                     | 0.78              |
| 2:2:208:PRO:CB    | 2:3:95:LEU:HD11   | 2.12                     | 0.78              |
| 2:2:262:TYR:OH    | 3:x:87:MET:HE1    | 1.80                     | 0.78              |
| 2:3:91:HIS:NE2    | 2:3:195:TYR:CD1   | 2.51                     | 0.78              |
| 2:3:93:PRO:HG2    | 2:3:195:TYR:CZ    | 2.17                     | 0.78              |
| 2:f:66:ARG:NH1    | 2:f:294:LEU:CD1   | 2.45                     | 0.78              |
| 1:F:1053:ARG:HD3  | 5:X:306:LEU:HD22  | 1.64                     | 0.78              |
| 1:G:117:VAL:HA    | 1:m:36:PHE:HA     | 1.65                     | 0.78              |
| 1:G:819:LEU:CD1   | 3:P:59:PRO:HD2    | 2.13                     | 0.78              |
| 1:m:51:PHE:HD1    | 1:n:88:THR:H      | 1.32                     | 0.78              |
| 2:3:66:ARG:HD3    | 2:3:68:THR:HG22   | 1.66                     | 0.78              |
| 2:g:200:VAL:O     | 2:j:86:ALA:HA     | 1.83                     | 0.78              |
| 1:F:333:ILE:HD11  | 1:m:314:VAL:HG23  | 1.63                     | 0.78              |
| 1:o:814:TYR:OH    | 3:v:81:GLN:HG3    | 1.82                     | 0.78              |
| 1:q:978:TYR:O     | 1:q:982:CYS:HB3   | 1.84                     | 0.78              |
| 2:f:208:PRO:CB    | 2:i:95:LEU:HD11   | 2.12                     | 0.78              |
| 2:i:91:HIS:NE2    | 2:i:195:TYR:CD1   | 2.51                     | 0.78              |
| 2:j:93:PRO:HD2    | 2:j:195:TYR:OH    | 1.83                     | 0.78              |
| 1:F:1017:ALA:HB3  | 1:F:1160:LEU:O    | 1.84                     | 0.78              |
| 1:l:1139:ARG:HH11 | 4:T:80:PRO:HD3    | 1.49                     | 0.78              |
| 1:m:432:TYR:HH    | 1:m:1321:LEU:HD12 | 0.97                     | 0.78              |
| 1:k:818:PHE:HZ    | 3:r:58:GLN:HB3    | 0.98                     | 0.78              |
| 1:q:246:MET:O     | 1:q:250:CYS:HB2   | 1.84                     | 0.78              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:q:614:LEU:O     | 1:q:618:LEU:HB2   | 1.84                     | 0.78              |
| 1:q:1188:PRO:HG3  | 1:q:1263:PHE:HD2  | 1.49                     | 0.78              |
| 5:z:109:LEU:HB3   | 5:z:132:TRP:O     | 1.84                     | 0.78              |
| 1:F:1263:PHE:CD2  | 1:l:30:GLU:HG2    | 2.18                     | 0.77              |
| 1:G:120:TYR:CE2   | 1:m:35:ASN:CB     | 2.66                     | 0.77              |
| 2:2:101:ASP:HA    | 2:2:104:LYS:HG2   | 1.66                     | 0.77              |
| 2:2:199:ASP:OD2   | 2:3:83:LYS:HE3    | 1.83                     | 0.77              |
| 2:3:258:PHE:HE1   | 3:r:90:ILE:CG2    | 1.71                     | 0.77              |
| 1:A:785:TYR:HE2   | 1:A:786:TYR:CE1   | 2.02                     | 0.77              |
| 1:G:317:ILE:HD11  | 1:m:148:LEU:HD11  | 1.64                     | 0.77              |
| 1:k:817:PHE:HB2   | 3:r:58:GLN:NE2    | 1.98                     | 0.77              |
| 5:X:89:CYS:HA     | 5:X:308:ILE:HG12  | 1.66                     | 0.77              |
| 5:Y:205:ASN:ND2   | 5:c:233:ILE:HG23  | 1.97                     | 0.77              |
| 1:A:1324:THR:HG23 | 1:B:1326:LYS:NZ   | 1.99                     | 0.77              |
| 1:H:1031:LEU:HD23 | 1:H:1081:ALA:HB2  | 1.64                     | 0.77              |
| 1:D:429:VAL:CG1   | 1:D:431:PHE:HZ    | 1.95                     | 0.77              |
| 1:F:1264:LYS:HG3  | 1:l:31:GLU:OE1    | 1.84                     | 0.77              |
| 1:k:203:ILE:CG2   | 1:p:383:GLN:NE2   | 2.46                     | 0.77              |
| 2:f:199:ASP:OD2   | 2:i:83:LYS:HE3    | 1.83                     | 0.77              |
| 2:g:199:ASP:OD2   | 2:j:83:LYS:HE3    | 1.83                     | 0.77              |
| 1:F:1018:LEU:C    | 1:F:1160:LEU:HD12 | 2.10                     | 0.77              |
| 1:p:1019:THR:CB   | 1:p:1160:LEU:HD12 | 2.14                     | 0.77              |
| 2:3:93:PRO:HD2    | 2:3:195:TYR:OH    | 1.83                     | 0.77              |
| 2:e:208:PRO:CB    | 2:h:95:LEU:HD11   | 2.12                     | 0.77              |
| 1:m:84:LEU:O      | 5:a:77:ASN:ND2    | 2.17                     | 0.77              |
| 1:n:1322:LYS:HG2  | 1:o:1329:LEU:HD12 | 1.67                     | 0.77              |
| 1:o:745:ILE:HG23  | 1:o:765:GLU:O     | 1.84                     | 0.77              |
| 2:e:208:PRO:CB    | 2:h:95:LEU:CD1    | 2.62                     | 0.77              |
| 2:f:208:PRO:CB    | 2:i:95:LEU:CD1    | 2.62                     | 0.77              |
| 1:D:819:LEU:CG    | 3:M:58:GLN:CD     | 2.55                     | 0.77              |
| 1:G:748:ARG:NH2   | 2:h:269:ARG:HD3   | 1.99                     | 0.77              |
| 1:l:950:TYR:CB    | 1:l:957:PHE:CZ    | 2.67                     | 0.77              |
| 2:2:208:PRO:CB    | 2:3:95:LEU:CD1    | 2.62                     | 0.77              |
| 2:2:262:TYR:OH    | 3:x:87:MET:SD     | 2.43                     | 0.77              |
| 2:e:101:ASP:HA    | 2:e:104:LYS:HG2   | 1.66                     | 0.77              |
| 2:j:91:HIS:CD2    | 2:j:195:TYR:CZ    | 2.66                     | 0.77              |
| 1:B:1031:LEU:HG   | 1:B:1079:CYS:HB3  | 1.66                     | 0.77              |
| 1:F:332:ARG:HH21  | 1:l:12:PRO:CB     | 1.96                     | 0.77              |
| 1:G:430:TYR:O     | 1:G:431:PHE:CD1   | 2.37                     | 0.77              |
| 1:k:1018:LEU:C    | 1:k:1160:LEU:HD12 | 2.10                     | 0.77              |
| 1:q:126:ILE:O     | 1:q:1062:SER:HA   | 1.85                     | 0.77              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:k:818:PHE:CE2   | 3:r:58:GLN:HB3    | 2.14                     | 0.77              |
| 1:A:585:LYS:NZ    | 1:B:571:ASP:OD1   | 2.17                     | 0.77              |
| 2:e:199:ASP:OD2   | 2:h:83:LYS:HE3    | 1.83                     | 0.77              |
| 2:e:200:VAL:O     | 2:h:86:ALA:HA     | 1.83                     | 0.77              |
| 1:E:26:LEU:CD1    | 1:m:206:ARG:O     | 2.32                     | 0.76              |
| 1:F:82:HIS:HB2    | 1:l:147:THR:HG23  | 1.65                     | 0.76              |
| 1:G:748:ARG:CZ    | 2:h:269:ARG:HD3   | 2.15                     | 0.76              |
| 1:m:1053:ARG:HG2  | 5:W:306:LEU:CD2   | 2.14                     | 0.76              |
| 2:e:202:ASP:HB2   | 2:h:86:ALA:CA     | 2.07                     | 0.76              |
| 1:H:1318:GLU:O    | 1:H:1322:LYS:HB2  | 1.84                     | 0.76              |
| 2:2:105:LEU:CD1   | 2:2:212:VAL:CG1   | 2.61                     | 0.76              |
| 1:H:1160:LEU:HD23 | 1:H:1214:ASN:CB   | 2.16                     | 0.76              |
| 2:e:206:GLU:HB3   | 2:h:132:TYR:CG    | 2.20                     | 0.76              |
| 1:G:431:PHE:HD1   | 1:G:1309:HIS:O    | 1.67                     | 0.76              |
| 2:2:207:ASP:OD1   | 2:2:208:PRO:HD2   | 1.86                     | 0.76              |
| 2:3:258:PHE:CE1   | 3:r:91:ALA:N      | 2.54                     | 0.76              |
| 2:g:207:ASP:OD1   | 2:g:208:PRO:HD2   | 1.86                     | 0.76              |
| 1:G:813:PHE:CG    | 3:P:85:LEU:HG     | 2.20                     | 0.76              |
| 1:G:818:PHE:CG    | 3:P:88:LEU:HD13   | 2.20                     | 0.76              |
| 1:H:1019:THR:HG23 | 1:H:1160:LEU:HD11 | 0.90                     | 0.76              |
| 2:g:198:LEU:O     | 2:g:199:ASP:C     | 2.28                     | 0.76              |
| 2:g:206:GLU:HB3   | 2:j:132:TYR:CG    | 2.21                     | 0.76              |
| 2:g:208:PRO:CB    | 2:j:95:LEU:CD1    | 2.62                     | 0.76              |
| 4:y:61:VAL:HG11   | 4:y:88:PHE:CD2    | 2.21                     | 0.76              |
| 1:l:688:ARG:HA    | 1:l:691:GLU:HG2   | 1.65                     | 0.76              |
| 2:i:93:PRO:HG2    | 2:i:195:TYR:CE2   | 2.21                     | 0.76              |
| 1:D:688:ARG:NH1   | 1:E:953:CYS:SG    | 2.59                     | 0.76              |
| 1:G:116:MET:SD    | 1:m:37:ARG:NH2    | 2.59                     | 0.76              |
| 1:G:117:VAL:HG12  | 1:m:36:PHE:CB     | 2.16                     | 0.76              |
| 1:A:148:LEU:HD21  | 1:B:333:ILE:HG22  | 1.65                     | 0.76              |
| 1:E:9:GLU:HB3     | 1:m:116:MET:SD    | 2.26                     | 0.76              |
| 1:E:52:GLU:HG2    | 1:F:91:LYS:HZ3    | 1.49                     | 0.76              |
| 1:m:235:ARG:HH11  | 1:m:239:GLN:HG3   | 1.49                     | 0.76              |
| 2:f:206:GLU:HB3   | 2:i:132:TYR:CG    | 2.20                     | 0.76              |
| 1:A:128:ILE:HG22  | 1:B:102:ALA:CB    | 2.16                     | 0.76              |
| 1:A:1031:LEU:HG   | 1:A:1079:CYS:HB3  | 1.65                     | 0.76              |
| 1:k:203:ILE:HG21  | 1:p:383:GLN:NE2   | 2.01                     | 0.76              |
| 1:D:818:PHE:CB    | 3:M:88:LEU:HD13   | 2.15                     | 0.76              |
| 1:E:255:ILE:HG23  | 1:G:16:VAL:HG21   | 1.67                     | 0.76              |
| 1:G:1147:ALA:HA   | 1:H:1206:PRO:HG3  | 1.65                     | 0.76              |
| 2:2:198:LEU:O     | 2:2:199:ASP:C     | 2.28                     | 0.76              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:h:285:GLU:CD   | 3:P:67:LYS:HZ3   | 1.92                     | 0.76              |
| 2:f:105:LEU:CD1  | 2:f:212:VAL:CG1  | 2.61                     | 0.76              |
| 2:j:93:PRO:HG2   | 2:j:195:TYR:CE2  | 2.21                     | 0.76              |
| 1:E:23:HIS:CD2   | 1:m:205:ARG:HA   | 2.20                     | 0.75              |
| 1:E:1130:GLU:HG2 | 4:S:77:ILE:HG23  | 1.66                     | 0.75              |
| 1:m:1003:SER:O   | 1:m:1007:LEU:HB2 | 1.86                     | 0.75              |
| 2:2:206:GLU:HB3  | 2:3:132:TYR:CG   | 2.20                     | 0.75              |
| 2:e:105:LEU:CD1  | 2:e:212:VAL:CG1  | 2.61                     | 0.75              |
| 1:B:748:ARG:HD2  | 1:B:750:PRO:HD3  | 1.68                     | 0.75              |
| 2:f:101:ASP:HA   | 2:f:104:LYS:HG2  | 1.66                     | 0.75              |
| 2:g:101:ASP:HA   | 2:g:104:LYS:HG2  | 1.66                     | 0.75              |
| 1:D:744:HIS:N    | 2:g:173:MET:O    | 2.19                     | 0.75              |
| 1:E:22:THR:HB    | 1:m:201:GLY:O    | 1.85                     | 0.75              |
| 1:G:83:ASP:CG    | 1:m:147:THR:CG2  | 2.36                     | 0.75              |
| 1:m:91:LYS:HA    | 1:m:119:LYS:O    | 1.87                     | 0.75              |
| 2:3:93:PRO:HG2   | 2:3:195:TYR:CE2  | 2.21                     | 0.75              |
| 1:C:1297:LYS:HG2 | 1:C:1299:CYS:H   | 1.50                     | 0.75              |
| 1:E:433:ASN:HD21 | 1:E:439:GLN:HE21 | 1.34                     | 0.75              |
| 1:E:667:ALA:HA   | 1:F:644:ARG:HH22 | 1.51                     | 0.75              |
| 5:Z:88:GLN:C     | 5:Z:308:ILE:HG23 | 2.10                     | 0.75              |
| 2:i:111:ALA:HB1  | 4:U:232:PHE:CD2  | 2.19                     | 0.75              |
| 1:E:25:LYS:NZ    | 1:m:205:ARG:NE   | 2.34                     | 0.75              |
| 1:G:748:ARG:NE   | 2:h:269:ARG:NH1  | 2.21                     | 0.75              |
| 1:q:433:ASN:HD21 | 1:q:439:GLN:HB2  | 1.50                     | 0.75              |
| 2:e:198:LEU:O    | 2:e:199:ASP:C    | 2.28                     | 0.75              |
| 1:A:1318:GLU:O   | 1:A:1322:LYS:HB2 | 1.87                     | 0.75              |
| 1:F:198:MET:HE1  | 1:l:21:LEU:HD12  | 1.69                     | 0.75              |
| 1:G:429:VAL:HG11 | 1:G:431:PHE:HE2  | 1.49                     | 0.75              |
| 1:k:758:MET:HG3  | 3:r:79:ALA:O     | 1.86                     | 0.75              |
| 1:l:813:PHE:CZ   | 3:s:82:LEU:HD12  | 2.21                     | 0.75              |
| 2:e:207:ASP:OD1  | 2:e:208:PRO:HD2  | 1.86                     | 0.75              |
| 1:B:156:ASP:OD1  | 1:C:338:GLN:NE2  | 2.19                     | 0.75              |
| 1:F:818:PHE:O    | 1:F:819:LEU:HG   | 1.87                     | 0.75              |
| 1:k:688:ARG:O    | 1:k:691:GLU:CG   | 2.35                     | 0.75              |
| 2:f:207:ASP:OD1  | 2:f:208:PRO:HD2  | 1.86                     | 0.75              |
| 1:k:1017:ALA:HB3 | 1:k:1160:LEU:O   | 1.87                     | 0.74              |
| 1:p:784:VAL:O    | 1:p:788:CYS:HB3  | 1.87                     | 0.74              |
| 2:2:105:LEU:HD11 | 2:2:212:VAL:HG11 | 1.69                     | 0.74              |
| 1:E:666:GLY:N    | 1:F:643:GLN:NE2  | 2.31                     | 0.74              |
| 1:G:83:ASP:OD1   | 1:m:147:THR:HG21 | 1.82                     | 0.74              |
| 1:l:950:TYR:HB3  | 1:l:957:PHE:CD2  | 2.21                     | 0.74              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:i:66:ARG:HH12   | 2:i:69:GLN:HE21   | 1.29                     | 0.74              |
| 4:y:61:VAL:HG11   | 4:y:88:PHE:HD2    | 1.51                     | 0.74              |
| 1:l:1048:VAL:CG2  | 4:T:37:LYS:HG2    | 2.16                     | 0.74              |
| 2:e:284:GLU:H     | 3:t:67:LYS:HZ1    | 1.28                     | 0.74              |
| 2:h:93:PRO:HG2    | 2:h:195:TYR:CE2   | 2.21                     | 0.74              |
| 1:k:1207:GLN:HE22 | 1:p:437:ILE:CG2   | 1.99                     | 0.74              |
| 5:b:45:LEU:CD2    | 5:b:48:VAL:HB     | 2.17                     | 0.74              |
| 1:n:1031:LEU:CG   | 1:n:1079:CYS:HB3  | 2.16                     | 0.74              |
| 2:f:105:LEU:HD11  | 2:f:212:VAL:HG11  | 1.69                     | 0.74              |
| 1:D:692:LEU:CB    | 1:D:705:LEU:CD2   | 2.62                     | 0.74              |
| 1:E:20:LEU:CD1    | 1:l:379:ASN:OD1   | 2.34                     | 0.74              |
| 1:H:813:PHE:CD2   | 3:Q:85:LEU:HG     | 2.23                     | 0.74              |
| 1:l:944:LEU:HD21  | 1:l:957:PHE:CE1   | 2.21                     | 0.74              |
| 1:m:430:TYR:O     | 1:m:431:PHE:CG    | 2.40                     | 0.74              |
| 1:m:1160:LEU:HD22 | 1:m:1214:ASN:CG   | 2.12                     | 0.74              |
| 2:2:105:LEU:CD1   | 2:2:216:LEU:CD1   | 2.66                     | 0.74              |
| 2:h:285:GLU:CG    | 3:P:67:LYS:HE2    | 2.17                     | 0.74              |
| 1:A:783:LYS:O     | 1:A:787:LEU:HB3   | 1.88                     | 0.74              |
| 1:A:1019:THR:OG1  | 1:A:1160:LEU:HD11 | 1.87                     | 0.74              |
| 1:E:20:LEU:HD12   | 1:l:379:ASN:ND2   | 2.03                     | 0.74              |
| 1:m:51:PHE:CE1    | 1:n:87:MET:CB     | 2.71                     | 0.74              |
| 1:p:1160:LEU:CD2  | 1:p:1214:ASN:ND2  | 2.51                     | 0.74              |
| 2:h:208:PRO:HD3   | 4:S:236:ASN:HD21  | 1.51                     | 0.74              |
| 2:f:105:LEU:CD1   | 2:f:216:LEU:CD1   | 2.66                     | 0.74              |
| 2:g:105:LEU:CD1   | 2:g:216:LEU:CD1   | 2.66                     | 0.74              |
| 1:F:314:VAL:HG22  | 1:m:333:ILE:CD1   | 2.02                     | 0.74              |
| 1:G:341:LEU:HD12  | 1:m:12:PRO:HB2    | 1.68                     | 0.74              |
| 1:k:200:HIS:CD2   | 1:p:1085:ARG:HE   | 2.06                     | 0.74              |
| 1:l:127:THR:HA    | 1:l:1061:VAL:O    | 1.88                     | 0.74              |
| 1:p:788:CYS:O     | 1:p:989:VAL:HG13  | 1.87                     | 0.74              |
| 1:B:1009:ARG:NH1  | 1:C:527:ASP:OD2   | 2.20                     | 0.73              |
| 3:t:69:MET:CE     | 3:t:70:LYS:HE2    | 2.18                     | 0.73              |
| 1:I:813:PHE:CE1   | 3:R:85:LEU:HD12   | 2.23                     | 0.73              |
| 1:l:749:ASN:N     | 1:l:750:PRO:HD3   | 2.03                     | 0.73              |
| 2:g:105:LEU:CD1   | 2:g:212:VAL:CG1   | 2.61                     | 0.73              |
| 1:F:255:ILE:HG23  | 1:l:16:VAL:CG2    | 2.16                     | 0.73              |
| 1:p:1297:LYS:HG2  | 1:p:1299:CYS:H    | 1.52                     | 0.73              |
| 1:D:818:PHE:HZ    | 3:M:61:ILE:HG21   | 1.51                     | 0.73              |
| 1:H:1018:LEU:N    | 1:H:1018:LEU:HD12 | 2.03                     | 0.73              |
| 1:k:817:PHE:HB2   | 3:r:58:GLN:HE22   | 1.54                     | 0.73              |
| 2:g:208:PRO:CG    | 2:j:95:LEU:HD12   | 2.15                     | 0.73              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:y:73:LEU:HD23   | 4:y:130:VAL:C     | 2.13                     | 0.73              |
| 1:F:1053:ARG:CZ   | 5:X:306:LEU:HD11  | 2.19                     | 0.73              |
| 1:k:431:PHE:O     | 1:k:438:PRO:HA    | 1.87                     | 0.73              |
| 1:m:1017:ALA:O    | 1:m:1160:LEU:O    | 2.05                     | 0.73              |
| 2:e:105:LEU:HD11  | 2:e:212:VAL:HG11  | 1.69                     | 0.73              |
| 4:S:217:HIS:CE1   | 5:W:64:ARG:HH11   | 1.99                     | 0.73              |
| 1:F:326:PHE:CE1   | 1:m:311:GLU:HG2   | 2.23                     | 0.73              |
| 1:F:1160:LEU:CD2  | 1:F:1214:ASN:HD22 | 1.98                     | 0.73              |
| 1:G:813:PHE:CE2   | 3:P:85:LEU:CG     | 2.71                     | 0.73              |
| 1:k:818:PHE:CE1   | 3:r:58:GLN:HB3    | 2.15                     | 0.73              |
| 5:Y:205:ASN:HD21  | 5:c:233:ILE:C     | 1.96                     | 0.73              |
| 1:q:1186:VAL:HA   | 1:q:1188:PRO:HD3  | 1.69                     | 0.73              |
| 1:E:1133:SER:HA   | 4:S:116:ILE:HD13  | 1.69                     | 0.73              |
| 1:o:1031:LEU:CG   | 1:o:1079:CYS:HB3  | 2.18                     | 0.73              |
| 2:h:272:ASP:CB    | 2:h:275:THR:OG1   | 2.37                     | 0.73              |
| 4:y:245:SER:HB2   | 5:z:272:LYS:HG3   | 1.71                     | 0.73              |
| 1:l:1132:ILE:HG22 | 4:T:116:ILE:HG12  | 1.71                     | 0.73              |
| 1:q:397:PRO:HA    | 1:q:1018:LEU:O    | 1.89                     | 0.73              |
| 2:e:105:LEU:CD1   | 2:e:216:LEU:CD1   | 2.66                     | 0.73              |
| 1:E:23:HIS:NE2    | 1:m:205:ARG:HG3   | 2.03                     | 0.72              |
| 5:Y:205:ASN:HD22  | 5:c:233:ILE:HG22  | 0.56                     | 0.72              |
| 1:C:1028:THR:HG21 | 1:C:1080:THR:HG23 | 1.71                     | 0.72              |
| 1:G:1019:THR:HG23 | 1:G:1160:LEU:CD2  | 2.19                     | 0.72              |
| 2:3:272:ASP:CB    | 2:3:275:THR:OG1   | 2.37                     | 0.72              |
| 2:i:208:PRO:HB2   | 5:c:229:LYS:NZ    | 2.04                     | 0.72              |
| 5:z:112:VAL:O     | 5:z:113:PHE:CD2   | 2.42                     | 0.72              |
| 1:F:252:THR:HB    | 1:l:19:ASP:HB2    | 1.71                     | 0.72              |
| 1:G:1019:THR:CG2  | 1:G:1160:LEU:HD21 | 2.20                     | 0.72              |
| 1:l:749:ASN:HD22  | 1:l:757:ARG:CG    | 2.02                     | 0.72              |
| 2:j:272:ASP:CB    | 2:j:275:THR:OG1   | 2.37                     | 0.72              |
| 5:W:7:VAL:HB      | 5:W:79:MET:HB2    | 1.72                     | 0.72              |
| 1:F:93:LEU:HD23   | 1:l:8:THR:OG1     | 1.88                     | 0.72              |
| 1:H:433:ASN:HD21  | 1:H:439:GLN:HE21  | 1.38                     | 0.72              |
| 1:m:431:PHE:CE1   | 1:m:1310:THR:CG2  | 2.70                     | 0.72              |
| 1:o:1019:THR:HG23 | 1:o:1160:LEU:HD12 | 1.70                     | 0.72              |
| 1:D:483:ARG:HG3   | 1:D:484:GLU:HG2   | 1.72                     | 0.72              |
| 1:G:750:PRO:CG    | 2:h:269:ARG:NH2   | 2.51                     | 0.72              |
| 1:I:813:PHE:CE1   | 3:R:85:LEU:CG     | 2.72                     | 0.72              |
| 1:m:1048:VAL:CB   | 4:S:15:MET:HG3    | 2.19                     | 0.72              |
| 2:e:285:GLU:CG    | 3:t:67:LYS:CE     | 2.51                     | 0.72              |
| 1:F:1072:LEU:O    | 1:l:33:PHE:CZ     | 2.43                     | 0.72              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:G:333:ILE:HD12  | 1:n:314:VAL:HG22 | 1.72                     | 0.72              |
| 4:y:73:LEU:CD2    | 4:y:130:VAL:C    | 2.63                     | 0.72              |
| 1:F:111:ARG:CG    | 1:l:40:TYR:HB3   | 2.16                     | 0.72              |
| 1:I:813:PHE:CZ    | 3:R:85:LEU:CG    | 2.73                     | 0.72              |
| 1:k:53:ALA:HA     | 1:l:322:ILE:HB   | 1.72                     | 0.72              |
| 1:o:810:VAL:HG13  | 3:v:81:GLN:HE22  | 1.55                     | 0.72              |
| 2:f:198:LEU:O     | 2:f:199:ASP:C    | 2.28                     | 0.72              |
| 1:A:1160:LEU:HD23 | 1:A:1214:ASN:ND2 | 2.04                     | 0.72              |
| 1:D:813:PHE:HE2   | 3:M:82:LEU:HA    | 1.55                     | 0.72              |
| 1:E:813:PHE:CE2   | 3:N:85:LEU:HG    | 2.25                     | 0.72              |
| 1:n:1297:LYS:HG2  | 1:n:1299:CYS:H   | 1.54                     | 0.72              |
| 1:o:488:GLU:OE1   | 1:o:490:MET:CE   | 2.33                     | 0.72              |
| 1:A:653:TYR:CB    | 1:A:786:TYR:CE2  | 2.72                     | 0.72              |
| 1:G:118:SER:CB    | 1:m:3:GLU:HG3    | 2.19                     | 0.72              |
| 1:I:810:VAL:HG21  | 3:R:78:LEU:HD22  | 1.71                     | 0.71              |
| 1:m:752:THR:C     | 3:t:86:ARG:HD3   | 2.15                     | 0.71              |
| 1:o:765:GLU:HB2   | 1:o:766:PRO:HD2  | 1.70                     | 0.71              |
| 2:2:262:TYR:CZ    | 3:x:87:MET:CE    | 2.72                     | 0.71              |
| 1:G:326:PHE:HZ    | 1:n:315:THR:HA   | 1.55                     | 0.71              |
| 1:H:1159:ILE:O    | 1:H:1214:ASN:ND2 | 2.19                     | 0.71              |
| 2:i:272:ASP:CB    | 2:i:275:THR:OG1  | 2.37                     | 0.71              |
| 1:A:380:THR:O     | 1:B:205:ARG:HD2  | 1.90                     | 0.71              |
| 1:G:319:HIS:CD2   | 1:n:319:HIS:ND1  | 2.59                     | 0.71              |
| 1:k:787:LEU:HD23  | 1:k:787:LEU:O    | 1.90                     | 0.71              |
| 1:A:653:TYR:CB    | 1:A:786:TYR:HE2  | 2.03                     | 0.71              |
| 1:G:1074:TYR:CE2  | 1:m:32:MET:SD    | 2.84                     | 0.71              |
| 1:m:94:PHE:HB2    | 1:m:117:VAL:HG23 | 1.70                     | 0.71              |
| 1:q:1293:SER:O    | 1:q:1297:LYS:CA  | 2.35                     | 0.71              |
| 1:G:83:ASP:OD1    | 1:m:147:THR:HB   | 1.91                     | 0.71              |
| 1:A:1153:ARG:NH2  | 1:B:1209:PHE:CZ  | 2.59                     | 0.71              |
| 1:E:30:GLU:CB     | 1:m:1263:PHE:CE2 | 2.73                     | 0.71              |
| 1:F:326:PHE:HE1   | 1:m:311:GLU:HG2  | 1.54                     | 0.71              |
| 1:G:430:TYR:C     | 1:G:431:PHE:CG   | 2.69                     | 0.71              |
| 1:G:1072:LEU:HD23 | 1:m:19:ASP:H     | 1.53                     | 0.71              |
| 4:T:72:ARG:HH12   | 5:b:104:ASP:HB2  | 1.55                     | 0.71              |
| 1:G:53:ALA:HA     | 1:H:322:ILE:HB   | 1.73                     | 0.71              |
| 1:G:323:MET:HE1   | 1:m:7:ALA:HB1    | 1.71                     | 0.71              |
| 1:H:1274:GLN:HE21 | 1:H:1291:THR:H   | 1.39                     | 0.71              |
| 1:I:813:PHE:CZ    | 3:R:85:LEU:HG    | 2.24                     | 0.71              |
| 1:k:127:THR:HG23  | 1:k:1061:VAL:O   | 1.91                     | 0.71              |
| 1:l:1057:THR:HG21 | 4:T:33:ARG:CZ    | 2.20                     | 0.71              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:n:1318:GLU:O    | 1:n:1322:LYS:HB2  | 1.90                     | 0.71              |
| 1:q:734:VAL:HG23  | 1:q:876:GLU:HG3   | 1.72                     | 0.71              |
| 2:h:285:GLU:OE2   | 3:P:67:LYS:HD3    | 1.89                     | 0.71              |
| 5:W:111:PRO:O     | 5:W:113:PHE:CD2   | 2.43                     | 0.71              |
| 5:X:89:CYS:CB     | 5:X:308:ILE:HG12  | 2.21                     | 0.71              |
| 1:F:198:MET:HE1   | 1:l:21:LEU:CD1    | 2.20                     | 0.71              |
| 3:r:79:ALA:O      | 3:r:83:ASP:HB2    | 1.91                     | 0.71              |
| 1:A:785:TYR:HD2   | 1:A:786:TYR:CD2   | 2.08                     | 0.71              |
| 1:G:311:GLU:OE2   | 1:n:311:GLU:OE2   | 2.09                     | 0.71              |
| 1:G:877:ILE:HB    | 1:G:898:GLN:HB2   | 1.72                     | 0.71              |
| 2:2:174:ARG:CD    | 2:3:274:THR:HG22  | 2.20                     | 0.71              |
| 2:3:261:VAL:HG11  | 3:r:93:LYS:HE2    | 1.73                     | 0.71              |
| 1:G:314:VAL:HB    | 1:n:326:PHE:CZ    | 2.26                     | 0.70              |
| 1:n:813:PHE:CZ    | 3:u:85:LEU:HG     | 2.26                     | 0.70              |
| 2:g:174:ARG:CD    | 2:j:274:THR:HG22  | 2.20                     | 0.70              |
| 1:E:14:LEU:CD2    | 1:m:344:SER:HB2   | 2.20                     | 0.70              |
| 1:E:877:ILE:HB    | 1:E:898:GLN:HB2   | 1.73                     | 0.70              |
| 1:F:1045:THR:HB   | 1:l:145:GLU:HG2   | 1.73                     | 0.70              |
| 1:H:810:VAL:HG21  | 3:Q:78:LEU:HD22   | 1.73                     | 0.70              |
| 1:k:1161:THR:HG22 | 1:k:1216:TRP:CE3  | 2.26                     | 0.70              |
| 1:l:1137:PHE:CG   | 4:T:55:ARG:NH2    | 2.58                     | 0.70              |
| 1:m:1149:LEU:HD13 | 1:n:1207:GLN:HB2  | 1.74                     | 0.70              |
| 1:q:1115:VAL:O    | 1:q:1119:THR:CA   | 2.39                     | 0.70              |
| 2:i:66:ARG:HG2    | 2:i:67:GLU:H      | 1.54                     | 0.70              |
| 1:A:1298:PRO:HB3  | 1:A:1302:LEU:HB2  | 1.73                     | 0.70              |
| 1:F:341:LEU:O     | 1:l:14:LEU:CD2    | 2.38                     | 0.70              |
| 1:l:1049:THR:HA   | 4:T:40:VAL:O      | 1.91                     | 0.70              |
| 1:E:497:LEU:HD21  | 1:E:922:PRO:HD2   | 1.72                     | 0.70              |
| 1:G:813:PHE:CE1   | 3:P:85:LEU:CD1    | 2.73                     | 0.70              |
| 1:k:813:PHE:CE2   | 3:r:85:LEU:HB3    | 2.27                     | 0.70              |
| 1:l:749:ASN:ND2   | 1:l:757:ARG:HB2   | 2.07                     | 0.70              |
| 2:e:285:GLU:CG    | 3:t:67:LYS:HE3    | 2.10                     | 0.70              |
| 1:l:950:TYR:HB3   | 1:l:957:PHE:CZ    | 2.26                     | 0.70              |
| 1:m:1051:GLU:HG2  | 5:a:34:ARG:NH2    | 2.06                     | 0.70              |
| 2:e:261:VAL:HG11  | 3:t:90:ILE:HG22   | 1.73                     | 0.70              |
| 1:H:1046:PRO:HG3  | 1:H:1063:GLN:HE21 | 1.56                     | 0.70              |
| 1:o:52:GLU:O      | 1:p:89:THR:O      | 2.09                     | 0.70              |
| 5:X:112:VAL:HG21  | 5:X:132:TRP:CD2   | 2.27                     | 0.70              |
| 1:A:437:ILE:HD13  | 1:B:1207:GLN:NE2  | 2.01                     | 0.70              |
| 1:A:813:PHE:CD1   | 3:J:85:LEU:HG     | 2.27                     | 0.70              |
| 1:E:30:GLU:O      | 1:m:1263:PHE:CD2  | 2.44                     | 0.70              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:o:603:LEU:HB3   | 1:o:794:LEU:HD21  | 1.74                     | 0.70              |
| 1:n:1099:GLN:HE22 | 1:n:1142:ASP:HB2  | 1.56                     | 0.70              |
| 2:g:105:LEU:HD11  | 2:g:212:VAL:HG11  | 1.69                     | 0.70              |
| 2:g:105:LEU:CD2   | 2:g:212:VAL:HG11  | 2.22                     | 0.70              |
| 1:A:785:TYR:CE2   | 1:A:786:TYR:CE1   | 2.80                     | 0.70              |
| 1:D:1054:ASP:CG   | 4:V:46:GLN:HB2    | 2.17                     | 0.70              |
| 1:l:1133:SER:HA   | 4:T:116:ILE:HD13  | 1.74                     | 0.70              |
| 1:q:816:LYS:HG2   | 3:x:51:LEU:HB2    | 1.74                     | 0.70              |
| 4:U:117:ARG:HE    | 4:U:120:LEU:HD12  | 1.55                     | 0.70              |
| 1:G:450:LEU:HD21  | 1:G:1018:LEU:CD2  | 2.22                     | 0.69              |
| 1:I:148:LEU:O     | 1:I:148:LEU:HD23  | 1.92                     | 0.69              |
| 1:k:744:HIS:HD1   | 2:2:175:ALA:N     | 1.90                     | 0.69              |
| 1:o:688:ARG:NH1   | 1:p:953:CYS:SG    | 2.65                     | 0.69              |
| 2:e:105:LEU:CD1   | 2:e:212:VAL:HG12  | 2.22                     | 0.69              |
| 1:A:1031:LEU:CD2  | 1:A:1079:CYS:HB3  | 2.21                     | 0.69              |
| 1:G:1018:LEU:CD2  | 1:G:1159:ILE:CD1  | 2.70                     | 0.69              |
| 1:H:91:LYS:HA     | 1:H:119:LYS:O     | 1.92                     | 0.69              |
| 1:m:748:ARG:NH1   | 2:e:269:ARG:HH22  | 1.90                     | 0.69              |
| 1:F:333:ILE:HD11  | 1:m:314:VAL:CG2   | 2.22                     | 0.69              |
| 1:m:51:PHE:CZ     | 1:n:87:MET:HB3    | 2.27                     | 0.69              |
| 2:e:105:LEU:CD2   | 2:e:212:VAL:HG11  | 2.22                     | 0.69              |
| 1:A:1160:LEU:HD23 | 1:A:1214:ASN:CG   | 2.16                     | 0.69              |
| 1:I:725:PRO:CA    | 1:I:774:THR:OG1   | 2.40                     | 0.69              |
| 1:p:1019:THR:N    | 1:p:1160:LEU:HD12 | 2.07                     | 0.69              |
| 2:2:262:TYR:CZ    | 3:x:87:MET:HE2    | 2.23                     | 0.69              |
| 1:G:429:VAL:HG11  | 1:G:431:PHE:CE2   | 2.22                     | 0.69              |
| 2:2:105:LEU:CD1   | 2:2:212:VAL:HG12  | 2.22                     | 0.69              |
| 1:B:724:LEU:HB3   | 1:B:772:ARG:HB2   | 1.73                     | 0.69              |
| 1:D:692:LEU:HD13  | 1:D:695:LEU:HG    | 1.73                     | 0.69              |
| 1:E:8:THR:OG1     | 1:m:93:LEU:HD22   | 1.93                     | 0.69              |
| 1:F:201:GLY:O     | 1:l:22:THR:HB     | 1.92                     | 0.69              |
| 1:H:1160:LEU:HD23 | 1:H:1214:ASN:HB2  | 1.73                     | 0.69              |
| 1:m:748:ARG:HH11  | 2:e:269:ARG:CZ    | 2.05                     | 0.69              |
| 2:i:113:PRO:HB3   | 4:U:233:HIS:HE1   | 1.57                     | 0.69              |
| 2:i:208:PRO:HG3   | 4:U:236:ASN:ND2   | 2.07                     | 0.69              |
| 1:E:31:GLU:OE1    | 1:m:1261:THR:HG21 | 1.92                     | 0.69              |
| 1:F:341:LEU:CB    | 1:l:14:LEU:HG     | 2.19                     | 0.69              |
| 1:o:767:LEU:HD12  | 1:o:767:LEU:O     | 1.91                     | 0.69              |
| 5:z:13:LEU:C      | 5:z:13:LEU:HD12   | 2.17                     | 0.69              |
| 1:A:1053:ARG:NH2  | 5:c:297:ASP:OD2   | 2.22                     | 0.69              |
| 1:G:319:HIS:CD2   | 1:n:319:HIS:CE1   | 2.80                     | 0.69              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:G:1297:LYS:HG2  | 1:G:1299:CYS:H    | 1.58                     | 0.69              |
| 1:H:141:LYS:HD3   | 4:V:29:ARG:HG2    | 1.74                     | 0.69              |
| 1:I:773:ARG:H     | 1:I:773:ARG:HD3   | 1.58                     | 0.69              |
| 1:l:538:PHE:O     | 1:l:557:ARG:HB2   | 1.92                     | 0.69              |
| 1:l:950:TYR:HB2   | 1:l:957:PHE:CZ    | 2.28                     | 0.69              |
| 1:l:1137:PHE:HE2  | 4:T:117:ARG:NH2   | 1.90                     | 0.69              |
| 1:m:141:LYS:HD3   | 4:S:20:GLU:N      | 2.07                     | 0.69              |
| 1:o:756:ALA:HA    | 1:o:759:ILE:HG12  | 1.75                     | 0.69              |
| 1:p:223:LYS:O     | 1:p:227:THR:HB    | 1.93                     | 0.69              |
| 2:2:202:ASP:OD1   | 2:2:211:LEU:CD2   | 2.41                     | 0.69              |
| 2:f:174:ARG:CD    | 2:i:274:THR:HG22  | 2.20                     | 0.69              |
| 2:g:202:ASP:OD1   | 2:g:211:LEU:CD2   | 2.41                     | 0.69              |
| 1:A:688:ARG:NH1   | 1:B:953:CYS:SG    | 2.65                     | 0.69              |
| 1:D:30:GLU:HG3    | 1:H:1262:LEU:HB3  | 1.74                     | 0.69              |
| 1:G:333:ILE:HD12  | 1:n:314:VAL:CG2   | 2.23                     | 0.69              |
| 1:m:147:THR:O     | 1:m:148:LEU:C     | 2.35                     | 0.69              |
| 1:o:490:MET:HE3   | 1:o:876:GLU:HB2   | 1.75                     | 0.69              |
| 2:2:66:ARG:O      | 2:2:67:GLU:HG2    | 1.93                     | 0.69              |
| 2:2:208:PRO:CG    | 2:3:95:LEU:HD12   | 2.15                     | 0.69              |
| 2:f:202:ASP:OD1   | 2:f:211:LEU:CD2   | 2.41                     | 0.69              |
| 2:g:176:GLU:O     | 2:g:179:ASN:N     | 2.26                     | 0.69              |
| 2:j:272:ASP:OD2   | 2:j:275:THR:HG21  | 1.93                     | 0.69              |
| 5:X:7:VAL:HB      | 5:X:79:MET:HB2    | 1.75                     | 0.69              |
| 1:A:148:LEU:HD21  | 1:B:333:ILE:CG2   | 2.23                     | 0.69              |
| 1:A:978:TYR:O     | 1:A:982:CYS:HB3   | 1.93                     | 0.69              |
| 1:C:810:VAL:HG21  | 3:L:78:LEU:HD22   | 1.73                     | 0.69              |
| 1:F:1019:THR:HG23 | 1:F:1160:LEU:CD1  | 2.23                     | 0.69              |
| 1:G:1188:PRO:HB3  | 1:G:1261:THR:H    | 1.57                     | 0.69              |
| 2:h:272:ASP:OD2   | 2:h:275:THR:HG21  | 1.93                     | 0.69              |
| 2:f:105:LEU:HD12  | 2:f:216:LEU:CD1   | 2.23                     | 0.69              |
| 1:A:79:ILE:HB     | 1:A:1042:ILE:HG22 | 1.75                     | 0.68              |
| 1:I:965:HIS:HB3   | 1:I:968:HIS:HB2   | 1.75                     | 0.68              |
| 1:m:1159:ILE:O    | 1:m:1160:LEU:HD23 | 1.93                     | 0.68              |
| 2:2:176:GLU:O     | 2:2:179:ASN:N     | 2.26                     | 0.68              |
| 2:e:176:GLU:O     | 2:e:179:ASN:N     | 2.26                     | 0.68              |
| 1:B:4:ASN:ND2     | 1:C:318:ALA:O     | 2.26                     | 0.68              |
| 1:D:813:PHE:CG    | 3:M:85:LEU:HG     | 2.21                     | 0.68              |
| 1:G:94:PHE:HB2    | 1:G:117:VAL:HG23  | 1.75                     | 0.68              |
| 1:G:118:SER:HB2   | 1:m:3:GLU:HG3     | 1.75                     | 0.68              |
| 1:l:749:ASN:ND2   | 1:l:757:ARG:CB    | 2.54                     | 0.68              |
| 2:e:262:TYR:OH    | 3:t:87:MET:HB3    | 1.85                     | 0.68              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:i:66:ARG:HD3    | 2:i:68:THR:CG2    | 2.23                     | 0.68              |
| 2:i:272:ASP:OD2   | 2:i:275:THR:HG21  | 1.93                     | 0.68              |
| 1:A:813:PHE:CZ    | 3:J:85:LEU:CG     | 2.72                     | 0.68              |
| 1:I:1318:GLU:O    | 1:I:1322:LYS:HB2  | 1.94                     | 0.68              |
| 1:n:713:ASP:OD2   | 1:n:715:ARG:HB2   | 1.94                     | 0.68              |
| 1:o:1318:GLU:O    | 1:o:1322:LYS:HB2  | 1.93                     | 0.68              |
| 2:e:174:ARG:CD    | 2:h:274:THR:HG22  | 2.20                     | 0.68              |
| 2:f:176:GLU:O     | 2:f:179:ASN:N     | 2.26                     | 0.68              |
| 2:g:105:LEU:HD12  | 2:g:216:LEU:CD1   | 2.23                     | 0.68              |
| 4:U:152:MET:HE3   | 5:c:296:CYS:HB2   | 1.75                     | 0.68              |
| 1:D:54:ILE:HG23   | 1:E:93:LEU:HD13   | 1.75                     | 0.68              |
| 1:I:754:ASP:N     | 3:R:83:ASP:CG     | 2.50                     | 0.68              |
| 1:o:777:GLU:HG3   | 1:p:951:GLN:HE21  | 1.57                     | 0.68              |
| 2:g:66:ARG:O      | 2:g:70:LEU:HD23   | 1.94                     | 0.68              |
| 1:A:813:PHE:CD2   | 3:J:85:LEU:HD23   | 2.28                     | 0.68              |
| 1:A:1132:ILE:HG22 | 4:U:116:ILE:HG23  | 1.75                     | 0.68              |
| 1:F:310:LYS:O     | 1:m:333:ILE:HD12  | 1.94                     | 0.68              |
| 1:k:953:CYS:HA    | 1:p:688:ARG:NH2   | 2.07                     | 0.68              |
| 1:n:111:ARG:NH2   | 5:W:299:SER:OG    | 2.26                     | 0.68              |
| 2:i:208:PRO:HB2   | 5:c:229:LYS:HZ1   | 1.56                     | 0.68              |
| 1:C:1322:LYS:HG2  | 1:D:1329:LEU:HD22 | 1.76                     | 0.68              |
| 1:m:138:THR:HG21  | 5:W:73:ARG:HH11   | 1.50                     | 0.68              |
| 1:m:161:VAL:CG1   | 4:S:16:GLU:CD     | 2.64                     | 0.68              |
| 1:m:1019:THR:CG2  | 1:m:1160:LEU:HD12 | 2.23                     | 0.68              |
| 2:f:208:PRO:CG    | 2:i:95:LEU:HD12   | 2.15                     | 0.68              |
| 3:P:85:LEU:HD22   | 3:P:88:LEU:HD12   | 1.74                     | 0.68              |
| 1:F:1160:LEU:HD23 | 1:F:1214:ASN:CG   | 2.19                     | 0.68              |
| 1:H:842:LEU:HD12  | 1:H:842:LEU:O     | 1.94                     | 0.68              |
| 1:I:978:TYR:O     | 1:I:982:CYS:HB3   | 1.94                     | 0.68              |
| 1:p:431:PHE:HB2   | 1:p:439:GLN:HB3   | 1.76                     | 0.68              |
| 2:e:105:LEU:HD12  | 2:e:216:LEU:CD1   | 2.23                     | 0.68              |
| 2:h:238:LEU:HD22  | 2:h:271:VAL:HG21  | 1.76                     | 0.68              |
| 2:h:258:PHE:HE1   | 3:P:90:ILE:HB     | 1.58                     | 0.68              |
| 1:D:152:LEU:HD21  | 1:G:10:LEU:HB3    | 1.76                     | 0.68              |
| 1:H:1093:ARG:C    | 1:H:1155:THR:HG21 | 2.19                     | 0.68              |
| 1:I:534:GLU:OE2   | 1:I:557:ARG:NH1   | 2.27                     | 0.68              |
| 2:3:258:PHE:CE1   | 3:r:90:ILE:C      | 2.71                     | 0.68              |
| 1:A:664:GLY:HA3   | 1:B:644:ARG:HH11  | 1.59                     | 0.68              |
| 1:F:1219:GLN:HB2  | 1:F:1222:SER:HB3  | 1.76                     | 0.68              |
| 1:k:1161:THR:HG22 | 1:k:1216:TRP:CH2  | 2.28                     | 0.68              |
| 1:m:1297:LYS:HG2  | 1:m:1299:CYS:H    | 1.59                     | 0.68              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:f:66:ARG:HG3    | 2:f:69:GLN:H      | 1.59                     | 0.68              |
| 4:S:126:ARG:HG2   | 4:S:128:HIS:H     | 1.59                     | 0.68              |
| 1:A:1031:LEU:HD21 | 1:A:1079:CYS:HB3  | 1.76                     | 0.68              |
| 1:H:838:LEU:O     | 1:H:842:LEU:CD2   | 2.34                     | 0.68              |
| 1:k:243:TYR:HH    | 1:k:1079:CYS:HG   | 1.39                     | 0.68              |
| 1:l:391:GLU:O     | 1:l:1297:LYS:HB3  | 1.94                     | 0.68              |
| 1:m:141:LYS:CD    | 4:S:20:GLU:HA     | 2.24                     | 0.68              |
| 1:o:422:GLU:HA    | 1:o:579:GLN:HE21  | 1.58                     | 0.68              |
| 1:o:567:LEU:HD22  | 1:o:1161:THR:HG21 | 1.75                     | 0.68              |
| 2:3:272:ASP:OD2   | 2:3:275:THR:HG21  | 1.93                     | 0.68              |
| 2:g:105:LEU:CD1   | 2:g:212:VAL:HG12  | 2.22                     | 0.68              |
| 1:l:79:ILE:HB     | 1:l:1042:ILE:HG22 | 1.75                     | 0.67              |
| 1:m:509:ARG:HD2   | 1:m:513:GLU:HB2   | 1.75                     | 0.67              |
| 1:m:748:ARG:CZ    | 2:e:269:ARG:NH2   | 2.46                     | 0.67              |
| 1:q:757:ARG:NH1   | 1:q:868:VAL:O     | 2.27                     | 0.67              |
| 2:f:66:ARG:HH21   | 2:f:68:THR:HG21   | 1.58                     | 0.67              |
| 2:f:105:LEU:CD1   | 2:f:212:VAL:HG12  | 2.22                     | 0.67              |
| 3:P:41:ARG:HH22   | 3:P:62:SER:HA     | 1.58                     | 0.67              |
| 4:U:243:GLY:HA2   | 5:Y:272:LYS:HD2   | 1.76                     | 0.67              |
| 1:F:205:ARG:HH11  | 1:l:23:HIS:CE1    | 2.11                     | 0.67              |
| 1:H:688:ARG:NH1   | 1:I:953:CYS:SG    | 2.68                     | 0.67              |
| 1:I:877:ILE:HB    | 1:I:898:GLN:HB2   | 1.77                     | 0.67              |
| 1:k:818:PHE:HZ    | 3:r:58:GLN:CB     | 1.83                     | 0.67              |
| 1:o:71:ALA:HB3    | 1:o:371:GLU:HB2   | 1.75                     | 0.67              |
| 2:e:208:PRO:CG    | 2:h:95:LEU:HD12   | 2.15                     | 0.67              |
| 2:i:238:LEU:HD22  | 2:i:271:VAL:HG21  | 1.76                     | 0.67              |
| 1:F:82:HIS:CB     | 1:l:147:THR:HG23  | 2.24                     | 0.67              |
| 1:F:1055:ILE:HG21 | 5:X:91:THR:HG22   | 1.75                     | 0.67              |
| 1:k:644:ARG:NH2   | 1:p:669:VAL:O     | 2.25                     | 0.67              |
| 1:o:1031:LEU:HD23 | 1:o:1081:ALA:HB2  | 1.76                     | 0.67              |
| 5:Y:7:VAL:HB      | 5:Y:79:MET:HB2    | 1.75                     | 0.67              |
| 1:B:688:ARG:NH1   | 1:C:953:CYS:SG    | 2.67                     | 0.67              |
| 1:C:278:HIS:O     | 1:C:282:GLN:NE2   | 2.27                     | 0.67              |
| 1:D:813:PHE:CE2   | 3:M:85:LEU:HB2    | 2.29                     | 0.67              |
| 1:m:531:LEU:O     | 1:m:1219:GLN:NE2  | 2.28                     | 0.67              |
| 1:p:441:ILE:HD13  | 1:p:1092:SER:HB3  | 1.77                     | 0.67              |
| 1:q:887:HIS:HE1   | 1:q:1108:ASN:H    | 1.42                     | 0.67              |
| 2:g:105:LEU:CD1   | 2:g:216:LEU:HD12  | 2.25                     | 0.67              |
| 5:X:89:CYS:CA     | 5:X:308:ILE:HG12  | 2.24                     | 0.67              |
| 5:a:106:LEU:HB2   | 5:a:293:PHE:HB2   | 1.77                     | 0.67              |
| 1:F:71:ALA:HB3    | 1:F:371:GLU:HB2   | 1.77                     | 0.67              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:F:294:ARG:HD2   | 1:F:357:GLN:HB3   | 1.76                     | 0.67              |
| 1:l:435:ASP:OD1   | 1:l:435:ASP:N     | 2.27                     | 0.67              |
| 4:y:93:VAL:HG21   | 4:y:121:ARG:HE    | 1.57                     | 0.67              |
| 5:X:59:MET:SD     | 5:X:111:PRO:HG2   | 2.35                     | 0.67              |
| 1:E:667:ALA:HB2   | 1:F:643:GLN:HA    | 1.75                     | 0.67              |
| 2:i:66:ARG:HG2    | 2:i:67:GLU:N      | 2.10                     | 0.67              |
| 5:z:13:LEU:HD12   | 5:z:13:LEU:O      | 1.94                     | 0.67              |
| 5:Z:106:LEU:HD12  | 5:Z:135:PRO:HA    | 1.77                     | 0.67              |
| 1:E:11:LEU:HD12   | 1:m:323:MET:HE1   | 1.77                     | 0.67              |
| 1:m:1093:ARG:NH1  | 1:m:1283:LEU:HD21 | 2.10                     | 0.67              |
| 2:3:92:LEU:N      | 2:3:93:PRO:HD2    | 2.10                     | 0.67              |
| 2:h:92:LEU:N      | 2:h:93:PRO:HD2    | 2.10                     | 0.67              |
| 1:B:726:ARG:HD3   | 1:C:941:ARG:NH2   | 2.10                     | 0.67              |
| 1:E:34:ASN:HB2    | 1:m:1264:LYS:HE3  | 1.77                     | 0.67              |
| 1:H:819:LEU:HD12  | 3:Q:58:GLN:HB3    | 1.76                     | 0.67              |
| 1:A:813:PHE:CD2   | 3:J:85:LEU:HG     | 2.30                     | 0.67              |
| 1:G:319:HIS:CE1   | 1:n:319:HIS:HB3   | 2.30                     | 0.67              |
| 1:I:618:LEU:HD21  | 1:I:864:LEU:HB3   | 1.77                     | 0.67              |
| 1:l:877:ILE:HB    | 1:l:898:GLN:HB2   | 1.76                     | 0.67              |
| 1:n:1313:THR:HG23 | 1:n:1316:LEU:H    | 1.60                     | 0.67              |
| 2:f:105:LEU:CD2   | 2:f:212:VAL:HG11  | 2.22                     | 0.67              |
| 5:W:109:LEU:HG    | 5:W:110:PRO:HD2   | 1.76                     | 0.67              |
| 1:G:744:HIS:HB2   | 2:e:175:ALA:H     | 1.59                     | 0.67              |
| 1:l:634:THR:HB    | 1:l:668:VAL:HG11  | 1.77                     | 0.67              |
| 1:l:1130:GLU:HG3  | 4:T:77:ILE:HD12   | 1.76                     | 0.67              |
| 1:m:141:LYS:HG2   | 4:S:20:GLU:HG3    | 1.77                     | 0.67              |
| 1:q:1019:THR:O    | 1:q:1158:VAL:HB   | 1.95                     | 0.67              |
| 2:2:105:LEU:HD12  | 2:2:216:LEU:CD1   | 2.23                     | 0.67              |
| 2:j:92:LEU:N      | 2:j:93:PRO:HD2    | 2.10                     | 0.67              |
| 2:j:238:LEU:HD22  | 2:j:271:VAL:HG21  | 1.76                     | 0.67              |
| 4:y:61:VAL:O      | 4:y:64:LYS:N      | 2.27                     | 0.67              |
| 4:y:231:ARG:HA    | 4:y:234:PHE:HB3   | 1.76                     | 0.67              |
| 4:S:93:VAL:HG21   | 4:S:121:ARG:HE    | 1.60                     | 0.67              |
| 1:D:1097:LEU:HA   | 1:D:1100:VAL:HB   | 1.76                     | 0.66              |
| 1:D:1228:TYR:HB2  | 1:D:1250:PHE:HD2  | 1.59                     | 0.66              |
| 1:G:430:TYR:C     | 1:G:431:PHE:CD2   | 2.72                     | 0.66              |
| 1:G:1019:THR:HG1  | 1:G:1158:VAL:HB   | 1.59                     | 0.66              |
| 1:l:779:MET:HG2   | 1:l:783:LYS:HE2   | 1.76                     | 0.66              |
| 1:m:1031:LEU:CG   | 1:m:1079:CYS:HB3  | 2.23                     | 0.66              |
| 2:2:105:LEU:CD1   | 2:2:216:LEU:HD12  | 2.25                     | 0.66              |
| 2:3:78:LEU:O      | 2:3:82:GLU:HG2    | 1.95                     | 0.66              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:e:105:LEU:CD1   | 2:e:216:LEU:HD12  | 2.25                     | 0.66              |
| 2:e:202:ASP:OD1   | 2:e:211:LEU:CD2   | 2.41                     | 0.66              |
| 4:S:225:TYR:O     | 4:S:228:ARG:NH2   | 2.28                     | 0.66              |
| 5:X:112:VAL:C     | 5:X:113:PHE:CG    | 2.70                     | 0.66              |
| 5:Y:156:ARG:HH21  | 5:c:266:PRO:HD3   | 1.59                     | 0.66              |
| 1:o:660:ALA:O     | 1:p:606:HIS:NE2   | 2.27                     | 0.66              |
| 1:p:497:LEU:HD21  | 1:p:922:PRO:HD2   | 1.76                     | 0.66              |
| 2:i:78:LEU:O      | 2:i:82:GLU:HG2    | 1.95                     | 0.66              |
| 5:X:308:ILE:O     | 5:X:309:TYR:CD2   | 2.48                     | 0.66              |
| 1:A:753:SER:HA    | 3:J:86:ARG:HD3    | 1.77                     | 0.66              |
| 1:A:754:ASP:N     | 3:J:83:ASP:OD1    | 2.28                     | 0.66              |
| 1:A:813:PHE:CD2   | 3:J:85:LEU:CG     | 2.79                     | 0.66              |
| 1:F:1263:PHE:HB2  | 1:l:30:GLU:O      | 1.95                     | 0.66              |
| 1:G:726:ARG:NH1   | 1:H:945:ASN:OD1   | 2.28                     | 0.66              |
| 1:I:1177:ARG:HH21 | 1:I:1181:SER:HB3  | 1.60                     | 0.66              |
| 1:l:1144:GLY:HA2  | 1:l:1282:ASP:HB2  | 1.75                     | 0.66              |
| 1:n:813:PHE:CE1   | 3:u:85:LEU:HG     | 2.30                     | 0.66              |
| 1:o:436:ARG:HH22  | 1:o:1327:LEU:HD11 | 1.60                     | 0.66              |
| 1:q:429:VAL:HG13  | 1:q:1311:GLY:H    | 1.59                     | 0.66              |
| 1:B:1318:GLU:OE1  | 1:C:1330:ASP:OD2  | 2.13                     | 0.66              |
| 1:D:482:ARG:HH22  | 1:D:961:PRO:HB3   | 1.60                     | 0.66              |
| 1:E:14:LEU:HD13   | 1:l:58:TYR:CE1    | 2.30                     | 0.66              |
| 1:F:1019:THR:N    | 1:F:1160:LEU:HD11 | 2.10                     | 0.66              |
| 1:G:757:ARG:NH2   | 1:G:868:VAL:O     | 2.29                     | 0.66              |
| 1:G:1149:LEU:HB2  | 1:H:1207:GLN:HB2  | 1.76                     | 0.66              |
| 1:H:603:LEU:HB3   | 1:H:794:LEU:HD21  | 1.77                     | 0.66              |
| 2:i:113:PRO:HG2   | 4:U:233:HIS:NE2   | 2.10                     | 0.66              |
| 4:V:126:ARG:HG2   | 4:V:128:HIS:H     | 1.59                     | 0.66              |
| 5:X:110:PRO:HB2   | 5:X:111:PRO:HD2   | 1.77                     | 0.66              |
| 5:Z:198:ILE:HG12  | 5:d:226:LEU:HD11  | 1.77                     | 0.66              |
| 1:B:795:ASN:ND2   | 1:B:982:CYS:SG    | 2.69                     | 0.66              |
| 1:l:174:ARG:HH22  | 1:m:99:PRO:CA     | 2.07                     | 0.66              |
| 1:q:1115:VAL:HG13 | 1:q:1119:THR:OG1  | 1.94                     | 0.66              |
| 2:i:92:LEU:N      | 2:i:93:PRO:HD2    | 2.10                     | 0.66              |
| 4:U:121:ARG:HH11  | 4:U:126:ARG:HH11  | 1.41                     | 0.66              |
| 5:X:112:VAL:HG21  | 5:X:132:TRP:CZ3   | 2.29                     | 0.66              |
| 1:E:34:ASN:HB2    | 1:m:1264:LYS:HE2  | 1.78                     | 0.66              |
| 1:H:677:ARG:NH2   | 1:I:601:ALA:O     | 2.28                     | 0.66              |
| 1:H:1018:LEU:HB2  | 1:H:1157:GLU:OE2  | 1.95                     | 0.66              |
| 1:k:126:ILE:HD11  | 1:k:1063:GLN:HE21 | 1.60                     | 0.66              |
| 1:n:1031:LEU:HD23 | 1:n:1081:ALA:CB   | 2.25                     | 0.66              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:3:130:ALA:C     | 2:3:132:TYR:H     | 2.04                     | 0.66              |
| 3:M:85:LEU:HD22   | 3:M:88:LEU:HD12   | 1.77                     | 0.66              |
| 1:l:512:ASN:HD22  | 1:l:966:GLU:HG2   | 1.61                     | 0.66              |
| 2:3:238:LEU:HD22  | 2:3:271:VAL:HG21  | 1.76                     | 0.66              |
| 1:D:1297:LYS:HG2  | 1:D:1299:CYS:H    | 1.58                     | 0.66              |
| 1:E:31:GLU:CD     | 1:m:1261:THR:HG21 | 2.21                     | 0.66              |
| 1:q:1115:VAL:C    | 1:q:1119:THR:HG1  | 1.96                     | 0.66              |
| 2:e:261:VAL:HG11  | 3:t:90:ILE:CG2    | 2.25                     | 0.66              |
| 2:h:78:LEU:O      | 2:h:82:GLU:HG2    | 1.96                     | 0.66              |
| 1:D:446:ALA:HA    | 1:D:1094:MET:HG3  | 1.77                     | 0.66              |
| 1:F:330:ALA:O     | 1:m:310:LYS:HB3   | 1.95                     | 0.66              |
| 1:G:118:SER:CB    | 1:m:3:GLU:CG      | 2.74                     | 0.66              |
| 1:o:621:GLY:HA3   | 1:o:654:ASP:HB3   | 1.76                     | 0.66              |
| 2:j:88:ARG:HD3    | 2:j:132:TYR:OH    | 1.96                     | 0.66              |
| 4:y:55:ARG:HG2    | 4:y:57:SER:H      | 1.61                     | 0.66              |
| 4:T:121:ARG:HH11  | 4:T:126:ARG:HH11  | 1.42                     | 0.66              |
| 5:X:308:ILE:O     | 5:X:309:TYR:HD2   | 1.79                     | 0.66              |
| 1:D:744:HIS:CD2   | 2:g:173:MET:HG2   | 2.31                     | 0.66              |
| 1:G:576:ARG:HH11  | 1:G:1014:PRO:HA   | 1.60                     | 0.66              |
| 1:q:562:ASN:ND2   | 1:q:970:TRP:O     | 2.29                     | 0.66              |
| 3:Q:41:ARG:HH22   | 3:Q:62:SER:HA     | 1.61                     | 0.66              |
| 1:A:483:ARG:NH2   | 1:A:508:PRO:O     | 2.30                     | 0.65              |
| 2:f:105:LEU:CD1   | 2:f:216:LEU:HD12  | 2.25                     | 0.65              |
| 5:X:110:PRO:O     | 5:X:111:PRO:O     | 2.14                     | 0.65              |
| 1:D:560:VAL:HA    | 1:D:999:MET:HE3   | 1.79                     | 0.65              |
| 1:D:1177:ARG:HH21 | 1:D:1181:SER:HB3  | 1.61                     | 0.65              |
| 1:G:185:LEU:HB3   | 1:G:388:ARG:HH22  | 1.61                     | 0.65              |
| 1:k:125:PRO:HG3   | 5:z:8:THR:OG1     | 1.96                     | 0.65              |
| 1:k:726:ARG:NH1   | 1:l:945:ASN:OD1   | 2.30                     | 0.65              |
| 1:l:752:THR:O     | 3:s:86:ARG:NH2    | 2.30                     | 0.65              |
| 1:o:620:HIS:HE1   | 1:o:903:ASN:HA    | 1.62                     | 0.65              |
| 2:h:88:ARG:HD3    | 2:h:132:TYR:OH    | 1.96                     | 0.65              |
| 1:F:1019:THR:CB   | 1:F:1160:LEU:CD1  | 2.73                     | 0.65              |
| 1:G:431:PHE:O     | 1:G:439:GLN:N     | 2.22                     | 0.65              |
| 1:G:1298:PRO:HB3  | 1:G:1302:LEU:HB2  | 1.78                     | 0.65              |
| 1:n:967:TYR:O     | 1:n:972:ARG:NH2   | 2.29                     | 0.65              |
| 1:o:1031:LEU:HD23 | 1:o:1081:ALA:CB   | 2.27                     | 0.65              |
| 1:q:883:PRO:HA    | 1:q:886:ARG:HG2   | 1.78                     | 0.65              |
| 2:j:78:LEU:O      | 2:j:82:GLU:HG2    | 1.95                     | 0.65              |
| 1:H:53:ALA:HA     | 1:I:322:ILE:HB    | 1.76                     | 0.65              |
| 1:k:257:ASP:O     | 1:q:46:ARG:NH2    | 2.30                     | 0.65              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:3:88:ARG:HD3    | 2:3:132:TYR:OH    | 1.96                     | 0.65              |
| 1:E:29:GLY:C      | 1:m:207:MET:HG3   | 2.20                     | 0.65              |
| 1:H:1159:ILE:HG13 | 1:H:1223:LEU:HD12 | 1.77                     | 0.65              |
| 1:k:750:PRO:HD2   | 2:3:269:ARG:NH2   | 2.11                     | 0.65              |
| 1:m:57:THR:HA     | 1:n:93:LEU:O      | 1.97                     | 0.65              |
| 1:B:128:ILE:HG22  | 1:C:102:ALA:HB3   | 1.77                     | 0.65              |
| 1:l:717:TRP:HE1   | 1:l:731:VAL:HG11  | 1.62                     | 0.65              |
| 1:p:87:MET:SD     | 1:p:1066:ASN:ND2  | 2.70                     | 0.65              |
| 1:q:428:THR:HA    | 1:q:441:ILE:O     | 1.96                     | 0.65              |
| 2:2:206:GLU:CA    | 2:3:132:TYR:HB3   | 2.27                     | 0.65              |
| 5:z:169:ARG:HB2   | 5:z:180:LEU:HB2   | 1.76                     | 0.65              |
| 1:A:1310:THR:HB   | 1:A:1339:ILE:HB   | 1.79                     | 0.65              |
| 1:E:21:LEU:HD11   | 1:m:194:LEU:HD11  | 1.77                     | 0.65              |
| 1:H:802:GLY:HA3   | 1:H:872:ALA:HB2   | 1.77                     | 0.65              |
| 1:l:509:ARG:HD2   | 1:l:513:GLU:HB2   | 1.77                     | 0.65              |
| 1:l:1133:SER:HB2  | 4:T:80:PRO:HG2    | 1.78                     | 0.65              |
| 2:i:66:ARG:CG     | 2:i:67:GLU:H      | 2.09                     | 0.65              |
| 5:X:112:VAL:CG2   | 5:X:132:TRP:CE3   | 2.79                     | 0.65              |
| 1:G:382:VAL:HB    | 1:H:101:VAL:HG13  | 1.77                     | 0.65              |
| 1:I:962:ILE:O     | 1:I:963:PHE:CG    | 2.50                     | 0.65              |
| 1:n:424:GLN:HB3   | 1:n:575:LEU:HD21  | 1.79                     | 0.65              |
| 1:p:393:THR:HA    | 1:p:1023:THR:HA   | 1.78                     | 0.65              |
| 2:i:88:ARG:HD3    | 2:i:132:TYR:OH    | 1.96                     | 0.65              |
| 5:a:21:LEU:HB3    | 5:a:74:VAL:HG21   | 1.77                     | 0.65              |
| 1:A:813:PHE:CG    | 3:J:85:LEU:HD23   | 2.32                     | 0.65              |
| 1:B:838:LEU:O     | 1:B:842:LEU:HD23  | 1.97                     | 0.65              |
| 1:E:14:LEU:HD22   | 1:m:344:SER:HB2   | 1.78                     | 0.65              |
| 1:F:116:MET:HE3   | 1:l:5:TRP:HB3     | 1.77                     | 0.65              |
| 1:k:794:LEU:O     | 1:k:797:HIS:ND1   | 2.30                     | 0.65              |
| 1:l:749:ASN:N     | 1:l:750:PRO:CD    | 2.60                     | 0.65              |
| 1:l:1048:VAL:HG21 | 4:T:37:LYS:CG     | 2.23                     | 0.65              |
| 1:m:1156:CYS:HB2  | 1:m:1245:PRO:HD2  | 1.79                     | 0.65              |
| 1:q:1187:ASP:N    | 1:q:1188:PRO:CD   | 2.59                     | 0.65              |
| 2:e:206:GLU:CA    | 2:h:132:TYR:HB3   | 2.27                     | 0.65              |
| 2:i:113:PRO:CB    | 4:U:233:HIS:CE1   | 2.79                     | 0.65              |
| 4:V:160:LEU:HB3   | 4:V:162:THR:OG1   | 1.96                     | 0.65              |
| 1:A:647:LEU:HD11  | 1:A:672:ALA:HB1   | 1.79                     | 0.65              |
| 1:B:585:LYS:HG3   | 1:C:983:ALA:HB2   | 1.79                     | 0.65              |
| 1:k:134:ALA:HB3   | 4:y:161:LYS:HG3   | 1.79                     | 0.65              |
| 1:k:688:ARG:NH1   | 1:l:953:CYS:SG    | 2.70                     | 0.65              |
| 1:l:688:ARG:NH1   | 1:m:953:CYS:SG    | 2.70                     | 0.65              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:m:161:VAL:CG1   | 4:S:16:GLU:OE2    | 2.28                     | 0.65              |
| 1:E:691:GLU:CD    | 1:F:952:ARG:HG3   | 2.20                     | 0.64              |
| 1:G:750:PRO:HG2   | 2:h:269:ARG:HH21  | 1.62                     | 0.64              |
| 1:I:1171:ARG:HH12 | 1:I:1332:THR:HG22 | 1.62                     | 0.64              |
| 1:m:1046:PRO:HA   | 1:m:1062:SER:O    | 1.97                     | 0.64              |
| 1:n:389:ASP:HA    | 1:n:1027:GLU:HA   | 1.79                     | 0.64              |
| 1:o:804:ASN:O     | 1:o:808:LEU:HB2   | 1.97                     | 0.64              |
| 1:B:300:PRO:HB3   | 1:B:351:LEU:HD13  | 1.79                     | 0.64              |
| 1:E:1156:CYS:HB2  | 1:E:1245:PRO:HD2  | 1.79                     | 0.64              |
| 1:G:71:ALA:HB3    | 1:G:371:GLU:HB2   | 1.78                     | 0.64              |
| 1:k:744:HIS:HD1   | 2:2:174:ARG:C     | 2.00                     | 0.64              |
| 1:k:1160:LEU:HD23 | 1:k:1214:ASN:CB   | 2.27                     | 0.64              |
| 5:z:13:LEU:HD23   | 5:z:77:ASN:OD1    | 1.97                     | 0.64              |
| 1:B:664:GLY:HA3   | 1:C:644:ARG:NH2   | 2.12                     | 0.64              |
| 1:B:1029:ASP:HB2  | 1:B:1082:HIS:HB3  | 1.79                     | 0.64              |
| 1:F:1029:ASP:HB2  | 1:F:1082:HIS:HB3  | 1.79                     | 0.64              |
| 1:k:777:GLU:HG3   | 1:l:951:GLN:HE21  | 1.61                     | 0.64              |
| 1:m:1053:ARG:CG   | 5:W:306:LEU:HD22  | 2.27                     | 0.64              |
| 1:E:21:LEU:HD11   | 1:m:194:LEU:CD1   | 2.26                     | 0.64              |
| 1:G:52:GLU:H      | 1:H:321:ALA:HA    | 1.61                     | 0.64              |
| 1:H:1160:LEU:CD2  | 1:H:1214:ASN:HB2  | 2.27                     | 0.64              |
| 1:I:813:PHE:CE1   | 3:R:85:LEU:CD1    | 2.80                     | 0.64              |
| 1:k:663:LEU:HD21  | 1:k:669:VAL:H     | 1.63                     | 0.64              |
| 1:l:162:LEU:O     | 1:l:166:LYS:HB2   | 1.97                     | 0.64              |
| 1:o:664:GLY:HA2   | 1:p:644:ARG:HH11  | 1.61                     | 0.64              |
| 1:p:1177:ARG:HH21 | 1:p:1181:SER:HB3  | 1.62                     | 0.64              |
| 1:q:635:ARG:HB3   | 1:q:849:ASP:HB2   | 1.79                     | 0.64              |
| 2:2:105:LEU:HD12  | 2:2:216:LEU:HD11  | 1.80                     | 0.64              |
| 5:c:146:MET:HB3   | 5:c:193:MET:HE2   | 1.80                     | 0.64              |
| 1:B:1167:LEU:HD23 | 1:B:1171:ARG:HG3  | 1.78                     | 0.64              |
| 1:E:959:LEU:C     | 1:E:960:SER:O     | 2.41                     | 0.64              |
| 1:G:862:PHE:CD2   | 3:P:92:LYS:HE3    | 2.32                     | 0.64              |
| 1:l:585:LYS:HG3   | 1:m:983:ALA:HB2   | 1.78                     | 0.64              |
| 1:q:1186:VAL:C    | 1:q:1188:PRO:HD3  | 2.23                     | 0.64              |
| 2:h:285:GLU:OE2   | 3:P:67:LYS:CD     | 2.45                     | 0.64              |
| 1:B:1046:PRO:HG3  | 1:B:1063:GLN:HE21 | 1.63                     | 0.64              |
| 1:E:26:LEU:HD22   | 1:m:204:ALA:O     | 1.97                     | 0.64              |
| 1:H:184:LEU:CB    | 1:H:1032:LEU:HD21 | 2.27                     | 0.64              |
| 1:l:1219:GLN:HB2  | 1:l:1222:SER:HB3  | 1.80                     | 0.64              |
| 1:m:235:ARG:HH12  | 1:m:243:TYR:HB2   | 1.62                     | 0.64              |
| 1:m:1160:LEU:HD23 | 1:m:1214:ASN:CG   | 2.12                     | 0.64              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:o:557:ARG:HA    | 1:o:972:ARG:HH12 | 1.63                     | 0.64              |
| 2:h:130:ALA:C     | 2:h:132:TYR:H    | 2.04                     | 0.64              |
| 3:t:60:VAL:O      | 3:t:87:MET:CE    | 2.46                     | 0.64              |
| 4:y:48:ILE:HG23   | 4:y:152:MET:HB2  | 1.80                     | 0.64              |
| 5:z:64:ARG:HH21   | 5:z:289:GLU:HG2  | 1.61                     | 0.64              |
| 5:z:219:ALA:HB1   | 5:z:231:GLN:HE21 | 1.62                     | 0.64              |
| 1:E:1031:LEU:HG   | 1:E:1079:CYS:HB3 | 1.79                     | 0.64              |
| 1:G:86:LYS:HZ1    | 1:m:149:LEU:CD2  | 2.09                     | 0.64              |
| 1:G:127:THR:H     | 1:H:103:THR:HA   | 1.62                     | 0.64              |
| 1:l:1130:GLU:CG   | 4:T:77:ILE:HD12  | 2.27                     | 0.64              |
| 1:m:1051:GLU:HG2  | 5:a:34:ARG:HH21  | 1.63                     | 0.64              |
| 2:3:261:VAL:CG1   | 3:r:93:LYS:HE2   | 2.28                     | 0.64              |
| 2:i:113:PRO:CG    | 4:U:233:HIS:NE2  | 2.61                     | 0.64              |
| 2:g:206:GLU:CA    | 2:j:132:TYR:HB3  | 2.27                     | 0.64              |
| 1:A:877:ILE:HB    | 1:A:898:GLN:HB2  | 1.79                     | 0.64              |
| 1:A:967:TYR:O     | 1:A:972:ARG:NH2  | 2.30                     | 0.64              |
| 1:E:14:LEU:HD13   | 1:l:58:TYR:HE1   | 1.62                     | 0.64              |
| 1:l:760:ALA:HA    | 1:l:763:GLN:HB3  | 1.80                     | 0.64              |
| 2:f:105:LEU:HD12  | 2:f:216:LEU:HD11 | 1.80                     | 0.64              |
| 2:j:130:ALA:C     | 2:j:132:TYR:H    | 2.04                     | 0.64              |
| 4:V:96:ASN:ND2    | 4:V:206:ALA:O    | 2.31                     | 0.64              |
| 5:z:110:PRO:CB    | 5:z:111:PRO:HD2  | 2.28                     | 0.64              |
| 5:X:102:LYS:HB3   | 5:X:298:VAL:H    | 1.63                     | 0.64              |
| 1:A:1021:VAL:HG22 | 1:A:1156:CYS:HB3 | 1.80                     | 0.64              |
| 1:E:745:ILE:HG22  | 1:E:767:LEU:HD23 | 1.80                     | 0.64              |
| 1:k:79:ILE:O      | 1:k:1042:ILE:HA  | 1.97                     | 0.64              |
| 1:k:819:LEU:HD21  | 3:r:92:LYS:HB2   | 1.80                     | 0.64              |
| 1:o:483:ARG:NH2   | 1:o:508:PRO:O    | 2.31                     | 0.64              |
| 1:q:794:LEU:HB3   | 1:q:797:HIS:H    | 1.61                     | 0.64              |
| 1:q:1188:PRO:HG3  | 1:q:1263:PHE:CD2 | 2.31                     | 0.64              |
| 5:a:224:ASN:HB2   | 5:a:226:LEU:HD22 | 1.80                     | 0.64              |
| 1:F:341:LEU:O     | 1:l:14:LEU:HD21  | 1.98                     | 0.64              |
| 1:m:1032:LEU:HG   | 1:m:1032:LEU:O   | 1.98                     | 0.64              |
| 2:2:105:LEU:CD2   | 2:2:212:VAL:HG11 | 2.22                     | 0.64              |
| 2:i:130:ALA:C     | 2:i:132:TYR:H    | 2.04                     | 0.64              |
| 2:i:208:PRO:HG3   | 4:U:236:ASN:CG   | 2.23                     | 0.64              |
| 2:j:260:ARG:HG2   | 2:j:289:LEU:HD11 | 1.80                     | 0.64              |
| 4:U:70:MET:HB3    | 4:U:84:LEU:HD11  | 1.80                     | 0.64              |
| 4:V:224:ARG:HH21  | 5:Z:282:GLN:HE21 | 1.44                     | 0.64              |
| 1:l:6:THR:HG23    | 1:l:46:ARG:HA    | 1.81                     | 0.63              |
| 5:z:110:PRO:O     | 5:z:111:PRO:C    | 2.40                     | 0.63              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 5:1:111:PRO:HD3  | 5:1:131:PRO:HA    | 1.79                     | 0.63              |
| 1:D:278:HIS:O    | 1:D:282:GLN:NE2   | 2.31                     | 0.63              |
| 1:E:965:HIS:HB3  | 1:E:968:HIS:HB2   | 1.80                     | 0.63              |
| 1:G:432:TYR:CE2  | 1:G:1321:LEU:HD13 | 2.33                     | 0.63              |
| 1:k:784:VAL:C    | 1:k:788:CYS:HB2   | 2.22                     | 0.63              |
| 1:l:1137:PHE:HB3 | 4:T:55:ARG:NH2    | 2.13                     | 0.63              |
| 5:Y:273:LEU:HD22 | 5:c:148:MET:HG3   | 1.81                     | 0.63              |
| 1:B:79:ILE:HB    | 1:B:1042:ILE:HG22 | 1.77                     | 0.63              |
| 1:C:490:MET:HE3  | 1:C:876:GLU:HB2   | 1.80                     | 0.63              |
| 1:C:929:ASP:HB3  | 1:C:932:LEU:HB3   | 1.81                     | 0.63              |
| 1:G:191:CYS:HG   | 1:G:243:TYR:HH    | 1.42                     | 0.63              |
| 1:k:744:HIS:CD2  | 2:2:173:MET:O     | 2.51                     | 0.63              |
| 1:n:813:PHE:CE2  | 3:u:85:LEU:HG     | 2.33                     | 0.63              |
| 1:o:66:THR:HG23  | 1:o:69:GLY:H      | 1.62                     | 0.63              |
| 3:t:69:MET:HE3   | 3:t:70:LYS:HE2    | 1.81                     | 0.63              |
| 5:W:109:LEU:HB3  | 5:W:132:TRP:HB2   | 1.79                     | 0.63              |
| 1:D:431:PHE:HD1  | 1:D:1309:HIS:O    | 1.81                     | 0.63              |
| 1:D:667:ALA:HB2  | 1:E:643:GLN:HG2   | 1.81                     | 0.63              |
| 1:G:114:THR:O    | 1:m:39:TYR:N      | 2.30                     | 0.63              |
| 1:G:197:LEU:O    | 1:m:22:THR:HG22   | 1.98                     | 0.63              |
| 1:G:647:LEU:HD11 | 1:G:672:ALA:HB1   | 1.79                     | 0.63              |
| 1:I:755:VAL:HG11 | 3:R:80:TYR:CZ     | 2.33                     | 0.63              |
| 1:o:344:SER:H    | 1:o:347:LEU:HD12  | 1.63                     | 0.63              |
| 1:q:718:PRO:HB2  | 1:q:786:TYR:HB2   | 1.80                     | 0.63              |
| 4:S:69:LEU:HD11  | 4:S:255:LEU:HD21  | 1.81                     | 0.63              |
| 1:E:1072:LEU:HG  | 1:G:18:ILE:HD12   | 1.79                     | 0.63              |
| 1:F:79:ILE:HB    | 1:F:1042:ILE:HG22 | 1.81                     | 0.63              |
| 1:G:326:PHE:HE1  | 1:n:318:ALA:CB    | 2.11                     | 0.63              |
| 1:G:534:GLU:OE2  | 1:G:557:ARG:NH1   | 2.32                     | 0.63              |
| 1:q:423:ASN:ND2  | 1:q:1334:TYR:O    | 2.32                     | 0.63              |
| 5:X:141:GLU:OE1  | 5:b:281:ARG:NH1   | 2.31                     | 0.63              |
| 5:1:156:ARG:HH21 | 5:1:162:ARG:HG3   | 1.63                     | 0.63              |
| 1:E:434:LYS:NZ   | 1:F:215:ASN:OD1   | 2.31                     | 0.63              |
| 1:l:950:TYR:HB2  | 1:l:957:PHE:CE1   | 2.34                     | 0.63              |
| 1:l:1027:GLU:OE1 | 1:l:1085:ARG:NH2  | 2.32                     | 0.63              |
| 1:m:1054:ASP:OD2 | 5:W:89:CYS:O      | 2.16                     | 0.63              |
| 1:o:185:LEU:HB3  | 1:o:388:ARG:HH22  | 1.64                     | 0.63              |
| 1:p:589:PRO:HB2  | 1:p:592:HIS:HB3   | 1.81                     | 0.63              |
| 2:e:105:LEU:HD21 | 2:e:212:VAL:CG1   | 2.25                     | 0.63              |
| 5:W:280:ILE:HA   | 5:W:283:ILE:HG22  | 1.80                     | 0.63              |
| 1:E:19:ASP:CB    | 1:m:252:THR:HB    | 2.28                     | 0.63              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:G:713:ASP:O    | 1:G:783:LYS:NZ    | 2.31                     | 0.63              |
| 1:m:51:PHE:CG    | 1:n:87:MET:SD     | 2.91                     | 0.63              |
| 2:3:260:ARG:HG2  | 2:3:289:LEU:HD11  | 1.80                     | 0.63              |
| 5:c:73:ARG:NH2   | 5:c:75:GLU:OE2    | 2.31                     | 0.63              |
| 1:B:877:ILE:HB   | 1:B:898:GLN:HB2   | 1.81                     | 0.63              |
| 1:D:819:LEU:HG   | 3:M:58:GLN:HE22   | 1.48                     | 0.63              |
| 1:G:1016:PHE:CE2 | 1:G:1018:LEU:HD11 | 2.34                     | 0.63              |
| 1:l:1230:THR:H   | 1:l:1251:THR:HG22 | 1.64                     | 0.63              |
| 1:q:1187:ASP:N   | 1:q:1188:PRO:HD3  | 2.13                     | 0.63              |
| 2:f:206:GLU:CA   | 2:i:132:TYR:HB3   | 2.27                     | 0.63              |
| 3:t:60:VAL:O     | 3:t:87:MET:HE3    | 1.99                     | 0.63              |
| 4:S:70:MET:HB3   | 4:S:84:LEU:HD11   | 1.79                     | 0.63              |
| 4:U:188:VAL:HG22 | 4:U:210:VAL:HG12  | 1.80                     | 0.63              |
| 1:A:785:TYR:CE2  | 1:A:786:TYR:CZ    | 2.86                     | 0.63              |
| 1:A:1297:LYS:HG2 | 1:A:1299:CYS:H    | 1.64                     | 0.63              |
| 1:C:481:CYS:SG   | 1:C:482:ARG:N     | 2.71                     | 0.63              |
| 1:F:341:LEU:HB2  | 1:l:14:LEU:HD21   | 1.79                     | 0.63              |
| 1:I:819:LEU:HD11 | 3:R:59:PRO:HD2    | 1.81                     | 0.63              |
| 1:k:495:ARG:NH2  | 1:k:804:ASN:OD1   | 2.32                     | 0.63              |
| 1:q:515:LYS:NZ   | 1:q:534:GLU:OE2   | 2.32                     | 0.63              |
| 1:D:819:LEU:CD1  | 3:M:58:GLN:CD     | 2.72                     | 0.62              |
| 1:F:1230:THR:HA  | 1:F:1233:ARG:HB3  | 1.79                     | 0.62              |
| 1:I:513:GLU:HA   | 1:I:973:THR:HG21  | 1.81                     | 0.62              |
| 1:k:744:HIS:N    | 2:2:174:ARG:HA    | 2.14                     | 0.62              |
| 1:n:88:THR:HG22  | 1:n:89:THR:HG23   | 1.80                     | 0.62              |
| 1:o:231:LEU:HG   | 1:o:235:ARG:HH12  | 1.63                     | 0.62              |
| 1:o:710:ALA:HA   | 1:o:713:ASP:CG    | 2.24                     | 0.62              |
| 2:h:260:ARG:HG2  | 2:h:289:LEU:HD11  | 1.80                     | 0.62              |
| 2:f:208:PRO:HD3  | 2:i:131:VAL:HG22  | 1.81                     | 0.62              |
| 4:y:66:LEU:HD11  | 4:y:140:ILE:HB    | 1.80                     | 0.62              |
| 1:A:783:LYS:O    | 1:A:787:LEU:CB    | 2.47                     | 0.62              |
| 1:D:965:HIS:HB3  | 1:D:968:HIS:HB2   | 1.80                     | 0.62              |
| 1:E:223:LYS:O    | 1:E:227:THR:HB    | 1.99                     | 0.62              |
| 1:F:333:ILE:CD1  | 1:m:314:VAL:HG23  | 2.29                     | 0.62              |
| 1:G:323:MET:HE1  | 1:m:7:ALA:CB      | 2.28                     | 0.62              |
| 1:G:1228:TYR:HB2 | 1:G:1250:PHE:HD2  | 1.64                     | 0.62              |
| 1:H:441:ILE:HD13 | 1:H:1092:SER:HB3  | 1.81                     | 0.62              |
| 1:k:950:TYR:HD1  | 1:k:956:GLY:C     | 2.07                     | 0.62              |
| 1:k:1326:LYS:HZ2 | 1:p:1324:THR:H    | 1.47                     | 0.62              |
| 1:m:663:LEU:HD23 | 1:n:644:ARG:HH12  | 1.64                     | 0.62              |
| 1:o:812:LEU:O    | 1:o:836:ASN:ND2   | 2.32                     | 0.62              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:o:1160:LEU:HD23 | 1:o:1214:ASN:ND2  | 2.12                     | 0.62              |
| 2:i:260:ARG:HG2   | 2:i:289:LEU:HD11  | 1.80                     | 0.62              |
| 5:1:60:ARG:NH1    | 5:1:143:ASN:OD1   | 2.32                     | 0.62              |
| 5:a:7:VAL:HB      | 5:a:79:MET:HB3    | 1.80                     | 0.62              |
| 1:A:1009:ARG:NH1  | 1:A:1118:ALA:O    | 2.32                     | 0.62              |
| 1:H:1157:GLU:HG3  | 1:H:1158:VAL:N    | 2.14                     | 0.62              |
| 1:k:757:ARG:HA    | 1:k:768:PHE:HE2   | 1.63                     | 0.62              |
| 1:m:965:HIS:HB3   | 1:m:968:HIS:HB2   | 1.80                     | 0.62              |
| 1:p:1093:ARG:HH11 | 1:p:1153:ARG:HD2  | 1.63                     | 0.62              |
| 1:q:1186:VAL:CA   | 1:q:1188:PRO:HD3  | 2.29                     | 0.62              |
| 2:e:282:ARG:NH1   | 3:t:71:MET:SD     | 2.72                     | 0.62              |
| 1:A:433:ASN:HD21  | 1:A:439:GLN:HE21  | 1.48                     | 0.62              |
| 1:A:1206:PRO:HG3  | 1:F:1147:ALA:HB1  | 1.81                     | 0.62              |
| 1:k:818:PHE:CE1   | 3:r:58:GLN:CB     | 2.77                     | 0.62              |
| 1:k:1330:ASP:HB2  | 1:p:1318:GLU:OE1  | 1.98                     | 0.62              |
| 1:m:372:HIS:HD2   | 1:m:375:LYS:HG3   | 1.65                     | 0.62              |
| 2:2:208:PRO:HD3   | 2:3:131:VAL:HG22  | 1.81                     | 0.62              |
| 5:1:149:LEU:O     | 5:1:153:SER:HB2   | 1.99                     | 0.62              |
| 1:F:1097:LEU:HA   | 1:F:1100:VAL:HB   | 1.82                     | 0.62              |
| 1:G:201:GLY:O     | 1:m:26:LEU:CD2    | 2.47                     | 0.62              |
| 2:3:66:ARG:CD     | 2:3:69:GLN:HG3    | 2.27                     | 0.62              |
| 2:g:105:LEU:HD12  | 2:g:216:LEU:HD11  | 1.80                     | 0.62              |
| 2:g:208:PRO:HD3   | 2:j:131:VAL:HG22  | 1.81                     | 0.62              |
| 5:z:273:LEU:HD22  | 5:1:148:MET:HG3   | 1.80                     | 0.62              |
| 1:C:726:ARG:NH1   | 1:D:945:ASN:OD1   | 2.33                     | 0.62              |
| 1:D:1156:CYS:HB2  | 1:D:1245:PRO:HD2  | 1.80                     | 0.62              |
| 1:G:688:ARG:NH1   | 1:H:953:CYS:SG    | 2.72                     | 0.62              |
| 1:H:119:LYS:NZ    | 1:H:1071:GLY:O    | 2.32                     | 0.62              |
| 1:H:1159:ILE:CG1  | 1:H:1223:LEU:HD12 | 2.29                     | 0.62              |
| 1:k:1160:LEU:HD23 | 1:k:1214:ASN:HD22 | 1.61                     | 0.62              |
| 1:m:1146:PRO:N    | 1:n:210:ARG:HH22  | 1.97                     | 0.62              |
| 1:n:664:GLY:HA2   | 1:o:644:ARG:HH11  | 1.64                     | 0.62              |
| 2:e:105:LEU:HD12  | 2:e:216:LEU:HD11  | 1.80                     | 0.62              |
| 4:S:61:VAL:HG11   | 4:S:88:PHE:CD2    | 2.31                     | 0.62              |
| 1:C:590:GLU:HG2   | 1:D:597:GLN:HE22  | 1.65                     | 0.62              |
| 1:D:429:VAL:HG12  | 1:D:431:PHE:HE2   | 0.81                     | 0.62              |
| 1:F:560:VAL:HA    | 1:F:999:MET:HE3   | 1.82                     | 0.62              |
| 1:k:97:GLN:HE21   | 1:p:167:ASN:HB2   | 1.65                     | 0.62              |
| 1:k:953:CYS:HB2   | 1:p:691:GLU:OE2   | 1.98                     | 0.62              |
| 1:l:486:VAL:O     | 1:l:965:HIS:NE2   | 2.31                     | 0.62              |
| 1:m:165:VAL:HG13  | 4:S:12:ARG:HB2    | 1.80                     | 0.62              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:m:656:VAL:HG23 | 1:m:676:TYR:HD1   | 1.65                     | 0.62              |
| 2:e:208:PRO:HD3  | 2:h:131:VAL:HG22  | 1.81                     | 0.62              |
| 1:A:965:HIS:HB3  | 1:A:968:HIS:HB2   | 1.82                     | 0.62              |
| 1:G:862:PHE:HD2  | 3:P:92:LYS:HE3    | 1.65                     | 0.62              |
| 1:o:664:GLY:HA2  | 1:p:644:ARG:NH1   | 2.15                     | 0.62              |
| 1:p:1230:THR:O   | 1:p:1234:GLU:HB2  | 2.00                     | 0.62              |
| 4:U:79:MET:HG3   | 4:U:80:PRO:HD3    | 1.82                     | 0.62              |
| 4:U:126:ARG:HG2  | 4:U:128:HIS:H     | 1.63                     | 0.62              |
| 5:z:59:MET:HG3   | 5:z:111:PRO:HG2   | 1.81                     | 0.62              |
| 5:z:72:ARG:HB2   | 5:z:80:ILE:O      | 1.99                     | 0.62              |
| 5:b:45:LEU:HD23  | 5:b:48:VAL:HB     | 1.82                     | 0.62              |
| 1:F:1344:PRO:HB2 | 1:F:1347:GLN:HB2  | 1.82                     | 0.62              |
| 1:l:497:LEU:HD21 | 1:l:922:PRO:HD2   | 1.79                     | 0.62              |
| 1:l:950:TYR:CB   | 1:l:957:PHE:CE1   | 2.83                     | 0.62              |
| 1:n:131:GLU:OE1  | 1:o:112:GLN:NE2   | 2.32                     | 0.62              |
| 1:n:159:ASN:ND2  | 1:o:338:GLN:HB2   | 2.14                     | 0.62              |
| 1:o:810:VAL:HG21 | 3:v:78:LEU:HD11   | 1.81                     | 0.62              |
| 1:p:219:GLY:O    | 1:p:223:LYS:HB2   | 1.99                     | 0.62              |
| 5:W:265:THR:HG21 | 5:W:268:GLU:CD    | 2.25                     | 0.62              |
| 5:d:7:VAL:HB     | 5:d:79:MET:HB3    | 1.82                     | 0.62              |
| 1:A:4:ASN:ND2    | 1:B:318:ALA:O     | 2.30                     | 0.62              |
| 1:B:183:VAL:HG21 | 1:B:1067:THR:HG21 | 1.82                     | 0.62              |
| 1:B:1009:ARG:NH1 | 1:B:1118:ALA:O    | 2.32                     | 0.62              |
| 1:B:1297:LYS:HG2 | 1:B:1299:CYS:H    | 1.64                     | 0.62              |
| 1:C:79:ILE:HB    | 1:C:1042:ILE:HG22 | 1.82                     | 0.62              |
| 1:C:248:THR:O    | 1:C:366:ARG:NH2   | 2.30                     | 0.62              |
| 1:D:458:ALA:HB3  | 1:D:890:PRO:HG2   | 1.80                     | 0.62              |
| 1:F:813:PHE:CE1  | 3:O:85:LEU:HG     | 2.35                     | 0.62              |
| 1:F:915:GLN:NE2  | 1:F:936:ALA:O     | 2.33                     | 0.62              |
| 1:G:116:MET:O    | 1:m:37:ARG:CA     | 2.48                     | 0.62              |
| 1:G:722:GLN:NE2  | 1:G:904:GLY:O     | 2.32                     | 0.62              |
| 1:G:1073:GLY:HA3 | 1:m:21:LEU:HD23   | 1.81                     | 0.62              |
| 1:q:453:PRO:HB2  | 1:q:1104:HIS:HB3  | 1.79                     | 0.62              |
| 4:U:51:ARG:HD3   | 4:U:147:LEU:HD21  | 1.82                     | 0.62              |
| 5:z:5:VAL:HB     | 5:z:81:LEU:HB2    | 1.82                     | 0.62              |
| 5:W:169:ARG:HA   | 5:W:180:LEU:HD23  | 1.81                     | 0.62              |
| 1:A:393:THR:HA   | 1:A:1023:THR:HA   | 1.80                     | 0.61              |
| 1:A:813:PHE:CG   | 3:J:85:LEU:CD2    | 2.83                     | 0.61              |
| 1:E:11:LEU:HD13  | 1:m:323:MET:SD    | 2.40                     | 0.61              |
| 1:E:191:CYS:HG   | 1:E:243:TYR:HH    | 1.48                     | 0.61              |
| 1:E:959:LEU:O    | 1:E:960:SER:C     | 2.43                     | 0.61              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:G:925:ARG:NH2   | 1:G:966:GLU:OE2   | 2.33                     | 0.61              |
| 1:H:1003:SER:O    | 1:H:1007:LEU:HB2  | 1.99                     | 0.61              |
| 1:H:1016:PHE:HE1  | 1:H:1018:LEU:HD21 | 1.65                     | 0.61              |
| 1:k:1055:ILE:HD11 | 4:y:164:ILE:HG12  | 1.81                     | 0.61              |
| 1:o:1300:ARG:H    | 1:o:1303:GLN:HE21 | 1.48                     | 0.61              |
| 2:3:258:PHE:CE1   | 3:r:90:ILE:HB     | 2.33                     | 0.61              |
| 4:T:167:LEU:HB3   | 4:T:280:LEU:HB2   | 1.81                     | 0.61              |
| 4:V:215:HIS:HD2   | 4:V:218:THR:H     | 1.46                     | 0.61              |
| 1:A:663:LEU:HD21  | 1:A:669:VAL:H     | 1.64                     | 0.61              |
| 1:D:430:TYR:C     | 1:D:431:PHE:CG    | 2.76                     | 0.61              |
| 1:D:819:LEU:HD12  | 3:M:58:GLN:CD     | 2.24                     | 0.61              |
| 1:F:725:PRO:HG2   | 1:F:728:ALA:HB2   | 1.82                     | 0.61              |
| 1:G:118:SER:N     | 1:m:5:TRP:HH2     | 1.98                     | 0.61              |
| 1:k:978:TYR:O     | 1:k:982:CYS:HB3   | 2.00                     | 0.61              |
| 1:l:104:GLY:O     | 5:z:37:LEU:CD2    | 2.47                     | 0.61              |
| 1:l:458:ALA:HB1   | 1:l:461:CYS:HB3   | 1.81                     | 0.61              |
| 1:l:908:THR:HG22  | 1:l:909:THR:HG23  | 1.82                     | 0.61              |
| 1:l:944:LEU:HD21  | 1:l:957:PHE:HZ    | 1.60                     | 0.61              |
| 1:n:489:HIS:O     | 1:n:496:ARG:NH1   | 2.32                     | 0.61              |
| 1:n:497:LEU:HD21  | 1:n:922:PRO:HD2   | 1.81                     | 0.61              |
| 1:n:611:LEU:HD11  | 1:n:861:LEU:HD21  | 1.82                     | 0.61              |
| 1:o:1184:LEU:HD21 | 1:o:1265:THR:HG21 | 1.82                     | 0.61              |
| 5:a:48:VAL:HG22   | 5:a:62:ARG:HE     | 1.63                     | 0.61              |
| 1:B:52:GLU:OE2    | 1:C:91:LYS:NZ     | 2.19                     | 0.61              |
| 1:D:1320:GLN:HB3  | 1:D:1327:LEU:HA   | 1.81                     | 0.61              |
| 1:E:610:GLU:HG3   | 1:E:911:PRO:HB3   | 1.81                     | 0.61              |
| 1:H:1228:TYR:HB2  | 1:H:1250:PHE:HD2  | 1.63                     | 0.61              |
| 1:k:134:ALA:CB    | 4:y:161:LYS:HG3   | 2.30                     | 0.61              |
| 1:m:431:PHE:HE1   | 1:m:1310:THR:OG1  | 1.83                     | 0.61              |
| 1:m:492:HIS:HD2   | 1:m:495:ARG:HB2   | 1.64                     | 0.61              |
| 1:o:420:THR:HG22  | 1:o:422:GLU:H     | 1.65                     | 0.61              |
| 1:o:1316:LEU:HD22 | 1:o:1331:GLU:HB3  | 1.82                     | 0.61              |
| 1:p:148:LEU:HD13  | 1:q:32:MET:HG2    | 1.82                     | 0.61              |
| 1:q:558:ILE:HA    | 1:q:885:GLN:HE22  | 1.64                     | 0.61              |
| 1:q:565:GLU:N     | 1:q:978:TYR:OH    | 2.32                     | 0.61              |
| 2:h:258:PHE:CE1   | 3:P:90:ILE:HB     | 2.35                     | 0.61              |
| 4:U:189:TYR:HB2   | 4:U:209:VAL:HG13  | 1.83                     | 0.61              |
| 1:D:431:PHE:CE1   | 1:D:1310:THR:OG1  | 2.53                     | 0.61              |
| 1:E:252:THR:HB    | 1:G:19:ASP:HB2    | 1.81                     | 0.61              |
| 1:E:863:HIS:CE1   | 3:N:93:LYS:HA     | 2.35                     | 0.61              |
| 1:H:159:ASN:HD22  | 1:I:338:GLN:HB2   | 1.65                     | 0.61              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:l:988:SER:HA    | 1:l:991:THR:HG22  | 1.83                     | 0.61              |
| 1:o:1160:LEU:HD22 | 1:o:1214:ASN:HD22 | 1.62                     | 0.61              |
| 2:3:91:HIS:O      | 2:3:95:LEU:HG     | 2.00                     | 0.61              |
| 2:h:91:HIS:O      | 2:h:95:LEU:HG     | 2.01                     | 0.61              |
| 4:S:92:MET:HA     | 4:S:102:LYS:HG3   | 1.81                     | 0.61              |
| 1:B:1041:VAL:HG12 | 1:B:1067:THR:HG22 | 1.83                     | 0.61              |
| 1:C:1297:LYS:HD3  | 1:C:1299:CYS:HB2  | 1.83                     | 0.61              |
| 1:C:1298:PRO:O    | 1:C:1302:LEU:N    | 2.30                     | 0.61              |
| 1:I:813:PHE:CD2   | 3:R:85:LEU:HG     | 2.35                     | 0.61              |
| 1:k:925:ARG:NH2   | 1:k:966:GLU:OE2   | 2.33                     | 0.61              |
| 1:q:546:GLU:H     | 1:q:549:GLN:HB2   | 1.66                     | 0.61              |
| 1:q:566:ALA:H     | 1:q:569:PRO:HG3   | 1.63                     | 0.61              |
| 5:Y:45:LEU:HD21   | 5:Y:63:MET:HE2    | 1.81                     | 0.61              |
| 1:E:713:ASP:O     | 1:E:783:LYS:NZ    | 2.33                     | 0.61              |
| 1:H:191:CYS:HG    | 1:H:243:TYR:HH    | 1.47                     | 0.61              |
| 1:H:1230:THR:HA   | 1:H:1233:ARG:HB3  | 1.81                     | 0.61              |
| 1:l:1276:CYS:SG   | 1:l:1277:ILE:N    | 2.73                     | 0.61              |
| 1:m:434:LYS:HE3   | 1:n:218:GLN:HG2   | 1.82                     | 0.61              |
| 1:m:1019:THR:HG21 | 1:m:1160:LEU:HD12 | 1.82                     | 0.61              |
| 1:p:1201:HIS:HD1  | 1:p:1212:THR:HG1  | 1.47                     | 0.61              |
| 1:q:651:ASN:ND2   | 1:q:906:CYS:SG    | 2.71                     | 0.61              |
| 4:y:72:ARG:CA     | 4:y:73:LEU:HD12   | 2.28                     | 0.61              |
| 4:U:215:HIS:HD2   | 4:U:218:THR:H     | 1.47                     | 0.61              |
| 1:C:1097:LEU:HA   | 1:C:1100:VAL:HB   | 1.82                     | 0.61              |
| 1:F:967:TYR:O     | 1:F:972:ARG:NH2   | 2.34                     | 0.61              |
| 1:H:481:CYS:SG    | 1:H:482:ARG:N     | 2.71                     | 0.61              |
| 1:k:66:THR:HG23   | 1:k:69:GLY:H      | 1.65                     | 0.61              |
| 1:k:1184:LEU:HD21 | 1:k:1265:THR:HG21 | 1.83                     | 0.61              |
| 1:m:761:MET:HE1   | 1:m:768:PHE:H     | 1.64                     | 0.61              |
| 1:o:433:ASN:HD21  | 1:o:439:GLN:HE21  | 1.49                     | 0.61              |
| 1:q:639:ASN:HB2   | 1:q:849:ASP:HB3   | 1.83                     | 0.61              |
| 2:h:285:GLU:CD    | 3:P:67:LYS:CE     | 2.73                     | 0.61              |
| 2:f:104:LYS:HD3   | 2:i:92:LEU:HD13   | 1.78                     | 0.61              |
| 2:j:91:HIS:O      | 2:j:95:LEU:HG     | 2.01                     | 0.61              |
| 4:y:73:LEU:HD23   | 4:y:130:VAL:O     | 2.01                     | 0.61              |
| 1:A:1018:LEU:HD23 | 1:A:1157:GLU:OE1  | 2.00                     | 0.61              |
| 1:G:278:HIS:O     | 1:G:282:GLN:NE2   | 2.33                     | 0.61              |
| 1:G:806:LYS:HA    | 3:P:82:LEU:HD22   | 1.82                     | 0.61              |
| 1:G:1133:SER:OG   | 1:G:1139:ARG:NH1  | 2.34                     | 0.61              |
| 1:H:734:VAL:HG12  | 1:H:739:PRO:HA    | 1.83                     | 0.61              |
| 1:l:688:ARG:HH12  | 1:m:797:HIS:HE1   | 1.46                     | 0.61              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:o:726:ARG:NH2   | 1:o:776:ASP:OD2   | 2.34                     | 0.61              |
| 2:f:66:ARG:HH11   | 2:f:294:LEU:HD13  | 1.62                     | 0.61              |
| 1:C:257:ASP:HB2   | 1:C:269:ARG:HH12  | 1.66                     | 0.61              |
| 1:D:713:ASP:O     | 1:D:783:LYS:NZ    | 2.33                     | 0.61              |
| 1:D:1156:CYS:SG   | 1:D:1157:GLU:N    | 2.73                     | 0.61              |
| 1:E:717:TRP:HE1   | 1:E:731:VAL:HG11  | 1.65                     | 0.61              |
| 1:G:483:ARG:NH2   | 1:G:508:PRO:O     | 2.33                     | 0.61              |
| 1:n:59:CYS:HA     | 1:o:95:TYR:HB3    | 1.82                     | 0.61              |
| 1:o:810:VAL:HG13  | 3:v:81:GLN:NE2    | 2.14                     | 0.61              |
| 1:o:1233:ARG:O    | 1:o:1238:HIS:ND1  | 2.33                     | 0.61              |
| 2:f:105:LEU:HD21  | 2:f:212:VAL:CG1   | 2.25                     | 0.61              |
| 2:i:91:HIS:O      | 2:i:95:LEU:HG     | 2.00                     | 0.61              |
| 5:X:110:PRO:O     | 5:X:111:PRO:C     | 2.44                     | 0.61              |
| 5:a:122:SER:HB2   | 5:a:127:ASP:HB3   | 1.81                     | 0.61              |
| 1:E:1228:TYR:HB2  | 1:E:1250:PHE:HD2  | 1.65                     | 0.61              |
| 1:G:329:HIS:ND1   | 1:m:12:PRO:HD2    | 2.16                     | 0.61              |
| 1:I:771:ALA:O     | 1:I:773:ARG:HD3   | 2.00                     | 0.61              |
| 1:k:750:PRO:HG2   | 2:3:269:ARG:NH2   | 2.15                     | 0.61              |
| 1:l:141:LYS:HG2   | 4:T:32:GLU:OE1    | 2.01                     | 0.61              |
| 1:l:950:TYR:HE1   | 1:l:956:GLY:O     | 1.75                     | 0.61              |
| 1:m:1274:GLN:HE21 | 1:m:1290:GLY:HA3  | 1.64                     | 0.61              |
| 1:o:523:PHE:HZ    | 1:o:534:GLU:HG3   | 1.66                     | 0.61              |
| 1:p:1041:VAL:HG12 | 1:p:1067:THR:HG22 | 1.82                     | 0.61              |
| 3:K:85:LEU:HD22   | 3:K:88:LEU:HD12   | 1.81                     | 0.61              |
| 4:U:51:ARG:HB3    | 4:U:147:LEU:HD11  | 1.83                     | 0.61              |
| 1:B:1031:LEU:CG   | 1:B:1079:CYS:HB3  | 2.29                     | 0.60              |
| 1:B:1298:PRO:HA   | 1:B:1301:PHE:HB3  | 1.81                     | 0.60              |
| 1:D:534:GLU:OE2   | 1:D:557:ARG:NH1   | 2.34                     | 0.60              |
| 1:F:589:PRO:HB2   | 1:F:592:HIS:HB3   | 1.83                     | 0.60              |
| 1:H:696:ASN:HA    | 1:I:952:ARG:HH22  | 1.66                     | 0.60              |
| 1:I:717:TRP:HE1   | 1:I:731:VAL:HG11  | 1.65                     | 0.60              |
| 1:k:200:HIS:HB2   | 1:k:216:ILE:HD11  | 1.82                     | 0.60              |
| 1:m:431:PHE:HD1   | 1:m:1309:HIS:O    | 1.84                     | 0.60              |
| 1:m:748:ARG:NH1   | 2:e:269:ARG:NH1   | 2.25                     | 0.60              |
| 1:n:606:HIS:HA    | 1:n:909:THR:HG21  | 1.83                     | 0.60              |
| 1:o:392:LEU:HA    | 1:o:1297:LYS:HB3  | 1.83                     | 0.60              |
| 5:z:25:ILE:HA     | 5:z:71:MET:HB3    | 1.81                     | 0.60              |
| 5:Y:119:GLY:HA3   | 5:Y:129:VAL:HA    | 1.83                     | 0.60              |
| 5:Z:46:ASP:OD2    | 5:Z:50:LYS:NZ     | 2.34                     | 0.60              |
| 1:A:651:ASN:O     | 1:A:786:TYR:HE1   | 1.83                     | 0.60              |
| 1:A:1156:CYS:HB2  | 1:A:1245:PRO:HD2  | 1.83                     | 0.60              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:734:VAL:HG11  | 1:C:878:ARG:HH11  | 1.66                     | 0.60              |
| 1:D:750:PRO:HA    | 3:M:86:ARG:HH22   | 1.66                     | 0.60              |
| 1:D:818:PHE:CD2   | 3:M:58:GLN:NE2    | 2.69                     | 0.60              |
| 1:D:1219:GLN:HB2  | 1:D:1222:SER:HB3  | 1.81                     | 0.60              |
| 1:F:264:VAL:HB    | 1:F:268:GLU:HB2   | 1.83                     | 0.60              |
| 1:F:813:PHE:HE2   | 3:O:82:LEU:HA     | 1.65                     | 0.60              |
| 1:G:319:HIS:CE1   | 1:n:319:HIS:CB    | 2.85                     | 0.60              |
| 1:G:664:GLY:O     | 1:H:644:ARG:NH2   | 2.34                     | 0.60              |
| 1:G:1073:GLY:HA3  | 1:m:21:LEU:CD2    | 2.31                     | 0.60              |
| 1:G:1322:LYS:HG2  | 1:H:1329:LEU:HD22 | 1.82                     | 0.60              |
| 1:H:560:VAL:HA    | 1:H:999:MET:HE3   | 1.82                     | 0.60              |
| 1:k:930:PRO:HD3   | 1:k:957:PHE:CZ    | 2.35                     | 0.60              |
| 1:l:849:ASP:HB3   | 1:l:852:VAL:H     | 1.65                     | 0.60              |
| 1:l:959:LEU:HB3   | 1:l:963:PHE:HE2   | 1.65                     | 0.60              |
| 1:n:128:ILE:HD11  | 1:n:168:THR:HG23  | 1.82                     | 0.60              |
| 1:o:724:LEU:HB3   | 1:o:772:ARG:HB2   | 1.81                     | 0.60              |
| 1:p:206:ARG:NH2   | 1:p:209:THR:OG1   | 2.34                     | 0.60              |
| 2:2:105:LEU:CD1   | 2:2:216:LEU:HD11  | 2.31                     | 0.60              |
| 5:z:59:MET:CG     | 5:z:111:PRO:HG2   | 2.31                     | 0.60              |
| 1:A:99:PRO:HG3    | 1:F:62:ILE:HD11   | 1.84                     | 0.60              |
| 1:D:431:PHE:HZ    | 1:D:1310:THR:HG23 | 0.87                     | 0.60              |
| 1:D:1195:LEU:HD22 | 1:D:1220:ARG:HH12 | 1.66                     | 0.60              |
| 1:G:275:VAL:HG12  | 1:G:371:GLU:HB3   | 1.83                     | 0.60              |
| 1:G:595:THR:OG1   | 1:G:678:ASN:ND2   | 2.35                     | 0.60              |
| 1:H:656:VAL:HG23  | 1:H:676:TYR:HD1   | 1.65                     | 0.60              |
| 1:I:809:LEU:HG    | 1:I:812:LEU:HD12  | 1.83                     | 0.60              |
| 1:m:432:TYR:CE2   | 1:m:1321:LEU:CD1  | 2.83                     | 0.60              |
| 1:n:618:LEU:HD22  | 1:n:864:LEU:HG    | 1.82                     | 0.60              |
| 1:o:380:THR:HG22  | 1:p:99:PRO:HB2    | 1.82                     | 0.60              |
| 1:p:79:ILE:HB     | 1:p:1042:ILE:HG22 | 1.82                     | 0.60              |
| 1:p:725:PRO:HA    | 1:p:774:THR:H     | 1.66                     | 0.60              |
| 2:i:88:ARG:CD     | 2:i:132:TYR:OH    | 2.49                     | 0.60              |
| 2:g:105:LEU:HD21  | 2:g:212:VAL:CG1   | 2.25                     | 0.60              |
| 4:T:51:ARG:HB3    | 4:T:147:LEU:HD11  | 1.83                     | 0.60              |
| 4:T:110:GLY:HA2   | 4:T:114:GLU:HB3   | 1.82                     | 0.60              |
| 4:T:182:THR:HG21  | 4:T:212:ARG:HD3   | 1.83                     | 0.60              |
| 5:W:265:THR:O     | 5:W:269:GLU:HG2   | 2.01                     | 0.60              |
| 5:Y:156:ARG:NH2   | 5:c:264:ILE:O     | 2.34                     | 0.60              |
| 5:Y:296:CYS:SG    | 5:c:34:ARG:NH2    | 2.74                     | 0.60              |
| 5:Z:307:CYS:C     | 5:Z:308:ILE:HG13  | 2.27                     | 0.60              |
| 1:A:1028:THR:HG21 | 1:A:1080:THR:HG23 | 1.83                     | 0.60              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:1022:ARG:NH2 | 1:C:1308:GLN:OE1 | 2.34                     | 0.60              |
| 1:F:1298:PRO:HB3 | 1:F:1302:LEU:HB2 | 1.83                     | 0.60              |
| 1:G:115:VAL:HG22 | 1:m:38:LEU:HD13  | 1.82                     | 0.60              |
| 1:H:54:ILE:HD11  | 1:I:323:MET:HG3  | 1.81                     | 0.60              |
| 1:H:413:ASN:O    | 1:I:413:ASN:ND2  | 2.33                     | 0.60              |
| 1:H:534:GLU:OE2  | 1:H:557:ARG:NH1  | 2.33                     | 0.60              |
| 1:k:703:PRO:HG3  | 1:l:948:PRO:HB2  | 1.83                     | 0.60              |
| 1:k:950:TYR:CD1  | 1:k:956:GLY:C    | 2.77                     | 0.60              |
| 1:m:760:ALA:HB1  | 1:m:766:PRO:HG2  | 1.82                     | 0.60              |
| 1:n:52:GLU:OE2   | 1:o:91:LYS:NZ    | 2.35                     | 0.60              |
| 2:i:66:ARG:HD3   | 2:i:68:THR:HG23  | 1.83                     | 0.60              |
| 5:b:156:ARG:HH21 | 5:b:162:ARG:HG3  | 1.66                     | 0.60              |
| 1:C:275:VAL:HG22 | 1:C:1032:LEU:HB3 | 1.84                     | 0.60              |
| 1:F:200:HIS:O    | 1:F:212:GLN:NE2  | 2.35                     | 0.60              |
| 1:F:483:ARG:NH2  | 1:F:508:PRO:O    | 2.34                     | 0.60              |
| 1:F:486:VAL:O    | 1:F:965:HIS:NE2  | 2.31                     | 0.60              |
| 1:G:1116:ARG:HD3 | 1:G:1123:ARG:HG2 | 1.83                     | 0.60              |
| 1:k:606:HIS:HA   | 1:k:909:THR:HG21 | 1.83                     | 0.60              |
| 1:m:667:ALA:HA   | 1:n:644:ARG:NH1  | 2.16                     | 0.60              |
| 1:q:431:PHE:HB2  | 1:q:439:GLN:HB3  | 1.83                     | 0.60              |
| 2:h:113:PRO:HG3  | 4:S:229:VAL:HG13 | 1.82                     | 0.60              |
| 1:A:754:ASP:HB2  | 3:J:86:ARG:NH1   | 2.16                     | 0.60              |
| 1:C:696:ASN:HA   | 1:D:952:ARG:HH22 | 1.65                     | 0.60              |
| 1:E:381:ASP:HA   | 1:F:205:ARG:HD2  | 1.82                     | 0.60              |
| 1:F:1053:ARG:CZ  | 5:X:306:LEU:CD1  | 2.79                     | 0.60              |
| 1:G:117:VAL:HB   | 1:m:33:PHE:CD2   | 2.35                     | 0.60              |
| 1:G:860:GLU:HA   | 1:G:863:HIS:HD2  | 1.65                     | 0.60              |
| 1:G:862:PHE:O    | 3:P:89:SER:HB3   | 2.00                     | 0.60              |
| 1:H:606:HIS:HA   | 1:H:909:THR:HG21 | 1.84                     | 0.60              |
| 1:I:753:SER:C    | 3:R:83:ASP:OD1   | 2.43                     | 0.60              |
| 1:k:203:ILE:CG2  | 1:p:383:GLN:OE1  | 2.50                     | 0.60              |
| 1:m:920:VAL:HG12 | 1:m:937:ASN:HD22 | 1.67                     | 0.60              |
| 1:o:1085:ARG:HG2 | 1:p:200:HIS:HD1  | 1.65                     | 0.60              |
| 2:3:88:ARG:CD    | 2:3:132:TYR:OH   | 2.49                     | 0.60              |
| 2:j:285:GLU:OE2  | 3:M:67:LYS:CD    | 2.50                     | 0.60              |
| 1:A:653:TYR:HB3  | 1:A:786:TYR:HE2  | 1.64                     | 0.60              |
| 1:l:534:GLU:OE2  | 1:l:557:ARG:NH1  | 2.35                     | 0.60              |
| 1:p:692:LEU:HB3  | 1:p:1010:MET:HE2 | 1.84                     | 0.60              |
| 1:q:540:ASP:HB3  | 1:q:555:THR:HB   | 1.84                     | 0.60              |
| 1:q:639:ASN:HD22 | 1:q:642:ARG:HD3  | 1.66                     | 0.60              |
| 2:i:113:PRO:CB   | 4:U:233:HIS:NE2  | 2.65                     | 0.60              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:j:88:ARG:CD     | 2:j:132:TYR:OH    | 2.49                     | 0.60              |
| 2:j:285:GLU:OE2   | 3:M:67:LYS:NZ     | 2.34                     | 0.60              |
| 4:y:73:LEU:CD2    | 4:y:131:VAL:HG13  | 2.26                     | 0.60              |
| 4:S:196:TYR:HB3   | 4:S:237:ASN:HD22  | 1.67                     | 0.60              |
| 1:D:643:GLN:O     | 1:D:644:ARG:NH2   | 2.35                     | 0.60              |
| 1:F:325:ASP:HB3   | 1:F:328:GLN:HB3   | 1.83                     | 0.60              |
| 1:k:818:PHE:CE1   | 3:r:58:GLN:OE1    | 2.54                     | 0.60              |
| 1:l:950:TYR:CB    | 1:l:957:PHE:CE2   | 2.85                     | 0.60              |
| 1:o:278:HIS:O     | 1:o:282:GLN:NE2   | 2.34                     | 0.60              |
| 2:e:105:LEU:CD1   | 2:e:216:LEU:HD11  | 2.31                     | 0.60              |
| 5:X:112:VAL:CG2   | 5:X:132:TRP:CD2   | 2.84                     | 0.60              |
| 1:E:590:GLU:HG2   | 1:F:597:GLN:OE1   | 2.02                     | 0.60              |
| 1:G:431:PHE:CD1   | 1:G:1309:HIS:O    | 2.54                     | 0.60              |
| 1:G:813:PHE:CE2   | 3:P:85:LEU:HB3    | 2.37                     | 0.60              |
| 1:H:62:ILE:HD11   | 1:I:99:PRO:HG3    | 1.83                     | 0.60              |
| 1:I:713:ASP:O     | 1:I:783:LYS:NZ    | 2.34                     | 0.60              |
| 1:q:430:TYR:H     | 1:q:1311:GLY:HA3  | 1.65                     | 0.60              |
| 4:y:73:LEU:HD23   | 4:y:130:VAL:HG23  | 1.83                     | 0.60              |
| 5:Y:296:CYS:HB2   | 5:Y:308:ILE:HD11  | 1.83                     | 0.60              |
| 5:c:7:VAL:HB      | 5:c:79:MET:HB3    | 1.83                     | 0.60              |
| 1:B:701:ASP:OD2   | 1:B:1108:ASN:ND2  | 2.35                     | 0.60              |
| 1:C:138:THR:HG22  | 1:C:142:GLU:HB2   | 1.84                     | 0.60              |
| 1:C:860:GLU:HA    | 1:C:863:HIS:HD2   | 1.65                     | 0.60              |
| 1:D:818:PHE:HZ    | 3:M:61:ILE:CG2    | 2.14                     | 0.60              |
| 1:E:31:GLU:OE1    | 1:m:1261:THR:CB   | 2.50                     | 0.60              |
| 1:G:1149:LEU:HD21 | 1:H:1182:SER:HB3  | 1.84                     | 0.60              |
| 1:k:1019:THR:CA   | 1:k:1160:LEU:CD1  | 2.80                     | 0.60              |
| 1:l:232:ASP:OD1   | 1:l:1352:ASN:ND2  | 2.35                     | 0.60              |
| 1:l:602:SER:HA    | 1:l:646:LEU:HD13  | 1.84                     | 0.60              |
| 1:m:257:ASP:HB2   | 1:m:269:ARG:HH12  | 1.66                     | 0.60              |
| 1:p:1019:THR:HG21 | 1:p:1160:LEU:HD11 | 1.81                     | 0.60              |
| 2:2:105:LEU:HD21  | 2:2:212:VAL:CG1   | 2.25                     | 0.60              |
| 4:U:196:TYR:HB3   | 4:U:237:ASN:HD22  | 1.67                     | 0.60              |
| 1:B:434:LYS:NZ    | 1:C:215:ASN:OD1   | 2.34                     | 0.59              |
| 1:B:1147:ALA:HB1  | 1:C:1206:PRO:HG3  | 1.84                     | 0.59              |
| 1:C:6:THR:HG23    | 1:C:46:ARG:HA     | 1.84                     | 0.59              |
| 1:E:148:LEU:HD12  | 1:E:151:LYS:HD3   | 1.84                     | 0.59              |
| 1:E:1007:LEU:HD22 | 1:E:1012:LEU:HD23 | 1.83                     | 0.59              |
| 1:F:116:MET:CE    | 1:l:5:TRP:HB3     | 2.31                     | 0.59              |
| 1:G:77:HIS:NE2    | 1:G:349:GLN:OE1   | 2.34                     | 0.59              |
| 1:G:206:ARG:NH1   | 1:G:209:THR:OG1   | 2.33                     | 0.59              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:G:1156:CYS:SG   | 1:G:1157:GLU:N    | 2.73                     | 0.59              |
| 1:k:564:PRO:HD2   | 1:k:567:LEU:HD12  | 1.83                     | 0.59              |
| 1:k:819:LEU:CD2   | 3:r:92:LYS:HB2    | 2.32                     | 0.59              |
| 1:k:832:ALA:HB3   | 1:k:855:ASN:HD21  | 1.67                     | 0.59              |
| 1:o:965:HIS:HB3   | 1:o:968:HIS:HB2   | 1.84                     | 0.59              |
| 1:p:600:ARG:HH11  | 1:p:794:LEU:HD23  | 1.67                     | 0.59              |
| 1:q:877:ILE:HG13  | 1:q:898:GLN:HG3   | 1.83                     | 0.59              |
| 2:h:88:ARG:CD     | 2:h:132:TYR:OH    | 2.49                     | 0.59              |
| 2:g:105:LEU:CD1   | 2:g:216:LEU:HD11  | 2.31                     | 0.59              |
| 4:y:191:VAL:HA    | 4:y:251:THR:O     | 2.02                     | 0.59              |
| 1:B:817:PHE:HB2   | 3:K:58:GLN:HE22   | 1.68                     | 0.59              |
| 1:E:929:ASP:HB3   | 1:E:932:LEU:HB3   | 1.84                     | 0.59              |
| 1:F:233:ARG:O     | 1:F:235:ARG:NH2   | 2.34                     | 0.59              |
| 1:I:1219:GLN:HB2  | 1:I:1222:SER:HB3  | 1.84                     | 0.59              |
| 1:m:877:ILE:HB    | 1:m:898:GLN:HB2   | 1.84                     | 0.59              |
| 1:o:129:PRO:O     | 1:p:100:ARG:NH1   | 2.35                     | 0.59              |
| 1:o:1159:ILE:O    | 1:o:1160:LEU:CD2  | 2.38                     | 0.59              |
| 1:q:643:GLN:NE2   | 1:q:849:ASP:OD1   | 2.34                     | 0.59              |
| 2:g:197:VAL:O     | 2:g:197:VAL:HG12  | 2.01                     | 0.59              |
| 4:V:69:LEU:HB2    | 4:V:87:LEU:HB2    | 1.83                     | 0.59              |
| 1:A:1053:ARG:HG2  | 5:c:306:LEU:HD22  | 1.83                     | 0.59              |
| 1:C:925:ARG:NH2   | 1:C:971:HIS:O     | 2.32                     | 0.59              |
| 1:F:1228:TYR:HB2  | 1:F:1250:PHE:HD2  | 1.66                     | 0.59              |
| 1:G:813:PHE:CZ    | 3:P:85:LEU:HG     | 2.37                     | 0.59              |
| 1:I:278:HIS:O     | 1:I:282:GLN:NE2   | 2.35                     | 0.59              |
| 1:I:708:VAL:HG22  | 1:I:1003:SER:HA   | 1.83                     | 0.59              |
| 1:l:504:ARG:NH2   | 1:l:942:VAL:O     | 2.34                     | 0.59              |
| 1:B:534:GLU:OE2   | 1:B:557:ARG:NH1   | 2.33                     | 0.59              |
| 1:D:248:THR:O     | 1:D:366:ARG:NH2   | 2.34                     | 0.59              |
| 1:D:653:TYR:HA    | 1:D:656:VAL:HG12  | 1.84                     | 0.59              |
| 1:F:292:ILE:HG12  | 1:F:361:LEU:HB3   | 1.84                     | 0.59              |
| 1:k:758:MET:HB3   | 3:r:79:ALA:CA     | 2.32                     | 0.59              |
| 1:l:177:ILE:HG21  | 1:l:376:VAL:HG21  | 1.84                     | 0.59              |
| 1:l:630:ILE:HD13  | 1:l:662:ARG:HE    | 1.67                     | 0.59              |
| 1:m:1048:VAL:HG11 | 4:S:15:MET:HB3    | 1.84                     | 0.59              |
| 1:o:415:ILE:HD12  | 1:o:1315:ALA:HB1  | 1.82                     | 0.59              |
| 1:o:1297:LYS:HG2  | 1:o:1299:CYS:H    | 1.67                     | 0.59              |
| 1:q:715:ARG:O     | 1:q:898:GLN:NE2   | 2.35                     | 0.59              |
| 4:U:69:LEU:HB2    | 4:U:87:LEU:HB2    | 1.82                     | 0.59              |
| 5:X:198:ILE:HG12  | 5:b:226:LEU:HD11  | 1.83                     | 0.59              |
| 1:A:1321:LEU:HD12 | 1:A:1327:LEU:HD11 | 1.84                     | 0.59              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:D:46:ARG:NH2    | 1:G:136:CYS:SG    | 2.75                     | 0.59              |
| 1:F:100:ARG:NH1   | 1:F:110:SER:O     | 2.34                     | 0.59              |
| 1:F:819:LEU:HD12  | 3:O:58:GLN:HB3    | 1.82                     | 0.59              |
| 1:H:1160:LEU:HD23 | 1:H:1214:ASN:ND2  | 2.18                     | 0.59              |
| 1:I:492:HIS:HD2   | 1:I:495:ARG:HB2   | 1.67                     | 0.59              |
| 1:k:750:PRO:O     | 2:3:269:ARG:NH2   | 2.36                     | 0.59              |
| 1:k:817:PHE:CB    | 3:r:58:GLN:HE22   | 2.15                     | 0.59              |
| 1:l:53:ALA:HA     | 1:m:322:ILE:HB    | 1.83                     | 0.59              |
| 1:m:1048:VAL:CG2  | 4:S:15:MET:HG3    | 2.32                     | 0.59              |
| 1:n:589:PRO:HB2   | 1:n:592:HIS:HB3   | 1.83                     | 0.59              |
| 1:n:616:GLU:HB2   | 1:n:655:MET:HG3   | 1.84                     | 0.59              |
| 1:o:719:PRO:HD2   | 1:o:786:TYR:HB3   | 1.82                     | 0.59              |
| 1:p:184:LEU:HD13  | 1:p:1039:THR:HG21 | 1.84                     | 0.59              |
| 3:x:65:ILE:HA     | 3:x:68:TYR:HB2    | 1.83                     | 0.59              |
| 4:T:235:LEU:HD11  | 5:b:233:ILE:HD11  | 1.84                     | 0.59              |
| 4:V:61:VAL:O      | 4:V:64:LYS:N      | 2.33                     | 0.59              |
| 5:Z:203:ILE:HG22  | 5:d:204:ALA:HB2   | 1.84                     | 0.59              |
| 1:A:141:LYS:HD3   | 4:U:29:ARG:HG2    | 1.85                     | 0.59              |
| 1:B:1156:CYS:HB2  | 1:B:1245:PRO:HD2  | 1.84                     | 0.59              |
| 1:D:1054:ASP:OD1  | 4:V:46:GLN:HB2    | 2.02                     | 0.59              |
| 1:E:30:GLU:CG     | 1:m:1262:LEU:HB3  | 2.32                     | 0.59              |
| 1:F:388:ARG:HD3   | 1:F:1295:VAL:H    | 1.67                     | 0.59              |
| 1:G:86:LYS:NZ     | 1:m:149:LEU:HB2   | 2.17                     | 0.59              |
| 1:H:128:ILE:HD11  | 1:H:168:THR:HG23  | 1.83                     | 0.59              |
| 1:I:635:ARG:NH2   | 1:I:849:ASP:OD2   | 2.35                     | 0.59              |
| 1:k:749:ASN:HB3   | 1:k:757:ARG:HD3   | 1.84                     | 0.59              |
| 1:l:131:GLU:O     | 1:m:112:GLN:NE2   | 2.36                     | 0.59              |
| 1:l:783:LYS:O     | 1:l:787:LEU:HB2   | 2.02                     | 0.59              |
| 1:m:1048:VAL:HG11 | 4:S:15:MET:CB     | 2.33                     | 0.59              |
| 1:o:863:HIS:HE1   | 3:v:93:LYS:HA     | 1.67                     | 0.59              |
| 2:3:66:ARG:CD     | 2:3:68:THR:CG2    | 2.81                     | 0.59              |
| 2:f:174:ARG:HH11  | 2:i:274:THR:HG22  | 1.68                     | 0.59              |
| 2:i:94:LEU:CD2    | 2:i:222:LEU:HD21  | 2.33                     | 0.59              |
| 1:A:1156:CYS:SG   | 1:A:1246:CYS:N    | 2.75                     | 0.59              |
| 1:E:25:LYS:CD     | 1:m:205:ARG:CZ    | 2.80                     | 0.59              |
| 1:E:29:GLY:HA3    | 1:m:207:MET:CG    | 2.29                     | 0.59              |
| 1:E:42:ASP:N      | 1:l:131:GLU:OE2   | 2.30                     | 0.59              |
| 1:E:616:GLU:HB2   | 1:E:655:MET:HG3   | 1.83                     | 0.59              |
| 1:F:753:SER:HB2   | 3:O:83:ASP:OD2    | 2.02                     | 0.59              |
| 1:F:1053:ARG:HD3  | 5:X:306:LEU:CD2   | 2.33                     | 0.59              |
| 1:G:813:PHE:CE1   | 3:P:85:LEU:HD12   | 2.34                     | 0.59              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:H:146:ASP:HB2   | 1:H:151:LYS:HG3   | 1.85                     | 0.59              |
| 1:H:1310:THR:HB   | 1:H:1339:ILE:HB   | 1.84                     | 0.59              |
| 1:l:389:ASP:HB3   | 1:l:1027:GLU:HG2  | 1.83                     | 0.59              |
| 1:m:1313:THR:HG23 | 1:m:1316:LEU:H    | 1.68                     | 0.59              |
| 1:p:1230:THR:HA   | 1:p:1233:ARG:HB3  | 1.84                     | 0.59              |
| 2:f:197:VAL:O     | 2:f:197:VAL:HG12  | 2.01                     | 0.59              |
| 4:T:249:LEU:H     | 4:T:294:ALA:HA    | 1.68                     | 0.59              |
| 5:d:146:MET:HE3   | 5:d:180:LEU:HG    | 1.84                     | 0.59              |
| 1:A:512:ASN:HD22  | 1:A:966:GLU:HG2   | 1.66                     | 0.59              |
| 1:C:66:THR:HG23   | 1:C:69:GLY:H      | 1.67                     | 0.59              |
| 1:C:497:LEU:HD21  | 1:C:922:PRO:HD2   | 1.85                     | 0.59              |
| 1:E:603:LEU:HD23  | 1:E:794:LEU:HD11  | 1.85                     | 0.59              |
| 1:H:534:GLU:O     | 1:H:1219:GLN:NE2  | 2.36                     | 0.59              |
| 1:k:200:HIS:CE1   | 1:p:1085:ARG:HE   | 2.21                     | 0.59              |
| 1:k:818:PHE:CE1   | 3:r:58:GLN:CD     | 2.81                     | 0.59              |
| 1:l:726:ARG:NH1   | 1:m:945:ASN:OD1   | 2.35                     | 0.59              |
| 1:m:483:ARG:NH2   | 1:m:508:PRO:O     | 2.36                     | 0.59              |
| 1:n:420:THR:HG22  | 1:n:422:GLU:H     | 1.68                     | 0.59              |
| 2:2:197:VAL:O     | 2:2:197:VAL:HG12  | 2.01                     | 0.59              |
| 2:f:66:ARG:O      | 2:f:70:LEU:HD23   | 2.03                     | 0.59              |
| 2:f:260:ARG:HD3   | 2:f:289:LEU:HD21  | 1.85                     | 0.59              |
| 5:W:203:ILE:HG21  | 5:a:203:ILE:HG22  | 1.84                     | 0.59              |
| 1:B:758:MET:HG3   | 3:K:83:ASP:HB2    | 1.85                     | 0.59              |
| 1:G:117:VAL:HB    | 1:m:33:PHE:CZ     | 2.38                     | 0.59              |
| 1:G:253:GLU:O     | 1:m:19:ASP:CG     | 2.45                     | 0.59              |
| 1:o:1160:LEU:HD22 | 1:o:1214:ASN:CG   | 2.27                     | 0.59              |
| 1:p:462:LEU:HD22  | 1:p:890:PRO:HG3   | 1.85                     | 0.59              |
| 1:q:255:ILE:HD11  | 1:q:1072:LEU:HD23 | 1.83                     | 0.59              |
| 1:q:713:ASP:OD1   | 1:q:783:LYS:NZ    | 2.36                     | 0.59              |
| 5:b:7:VAL:HB      | 5:b:79:MET:HB3    | 1.83                     | 0.59              |
| 5:b:21:LEU:HB3    | 5:b:74:VAL:HG21   | 1.84                     | 0.59              |
| 1:A:483:ARG:HG3   | 1:A:484:GLU:HG2   | 1.85                     | 0.59              |
| 1:A:813:PHE:HZ    | 1:A:865:VAL:HG11  | 1.68                     | 0.59              |
| 1:F:123:LYS:HE2   | 5:b:9:PHE:O       | 2.03                     | 0.59              |
| 1:G:120:TYR:CE2   | 1:m:35:ASN:HB3    | 2.38                     | 0.59              |
| 1:I:431:PHE:HB2   | 1:I:439:GLN:HB3   | 1.85                     | 0.59              |
| 1:I:500:PHE:HB2   | 1:I:961:PRO:HG3   | 1.84                     | 0.59              |
| 1:I:975:PHE:HE1   | 1:I:995:MET:HB3   | 1.68                     | 0.59              |
| 1:k:436:ARG:HH22  | 1:k:1350:LEU:HB2  | 1.68                     | 0.59              |
| 1:k:584:THR:HG21  | 1:k:689:THR:HG22  | 1.85                     | 0.59              |
| 1:k:985:THR:OG1   | 1:k:986:LEU:N     | 2.36                     | 0.59              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:m:223:LYS:O     | 1:m:227:THR:HB    | 2.03                     | 0.59              |
| 1:m:534:GLU:OE2   | 1:m:557:ARG:NH1   | 2.36                     | 0.59              |
| 1:q:654:ASP:OD1   | 1:q:773:ARG:NH2   | 2.36                     | 0.59              |
| 1:q:1041:VAL:HG12 | 1:q:1067:THR:HG22 | 1.84                     | 0.59              |
| 2:e:258:PHE:CG    | 3:t:60:VAL:HG23   | 2.36                     | 0.59              |
| 4:y:61:VAL:HG21   | 4:y:109:TYR:HE2   | 1.67                     | 0.59              |
| 5:Y:29:ILE:HD12   | 5:Y:81:LEU:HD21   | 1.83                     | 0.59              |
| 1:A:393:THR:OG1   | 1:A:1248:GLN:NE2  | 2.36                     | 0.58              |
| 1:F:341:LEU:CB    | 1:l:14:LEU:CD2    | 2.75                     | 0.58              |
| 1:F:483:ARG:HG3   | 1:F:484:GLU:HG2   | 1.84                     | 0.58              |
| 1:G:906:CYS:SG    | 1:G:907:MET:N     | 2.76                     | 0.58              |
| 1:G:1073:GLY:HA2  | 1:m:32:MET:HG3    | 1.85                     | 0.58              |
| 1:k:1179:ARG:NH1  | 1:k:1211:SER:O    | 2.36                     | 0.58              |
| 1:n:264:VAL:HB    | 1:n:268:GLU:HB2   | 1.83                     | 0.58              |
| 1:p:1156:CYS:HB2  | 1:p:1245:PRO:HD2  | 1.85                     | 0.58              |
| 3:K:61:ILE:HG13   | 3:K:84:LEU:HD11   | 1.84                     | 0.58              |
| 3:Q:39:GLU:OE2    | 3:Q:43:GLN:NE2    | 2.35                     | 0.58              |
| 4:y:189:TYR:HB2   | 4:y:209:VAL:HG13  | 1.83                     | 0.58              |
| 5:z:152:LEU:HD13  | 5:l:270:LEU:HG    | 1.85                     | 0.58              |
| 5:Y:45:LEU:HD11   | 5:Y:63:MET:HG2    | 1.85                     | 0.58              |
| 1:A:102:ALA:HB3   | 1:F:128:ILE:HG22  | 1.84                     | 0.58              |
| 1:C:1276:CYS:SG   | 1:C:1277:ILE:N    | 2.75                     | 0.58              |
| 1:D:703:PRO:HG3   | 1:E:948:PRO:HB2   | 1.83                     | 0.58              |
| 1:D:708:VAL:HG22  | 1:D:1003:SER:HA   | 1.85                     | 0.58              |
| 1:E:128:ILE:HD11  | 1:E:168:THR:HG23  | 1.85                     | 0.58              |
| 1:l:156:ASP:OD1   | 1:m:338:GLN:NE2   | 2.37                     | 0.58              |
| 2:2:197:VAL:C     | 2:2:199:ASP:H     | 2.12                     | 0.58              |
| 2:2:260:ARG:HD3   | 2:2:289:LEU:HD21  | 1.85                     | 0.58              |
| 4:y:61:VAL:O      | 4:y:62:GLU:C      | 2.45                     | 0.58              |
| 4:V:232:PHE:HE1   | 5:d:225:MET:O     | 1.84                     | 0.58              |
| 5:z:7:VAL:HB      | 5:z:79:MET:HB2    | 1.84                     | 0.58              |
| 1:E:31:GLU:OE1    | 1:m:1261:THR:OG1  | 2.19                     | 0.58              |
| 1:F:323:MET:HB2   | 1:F:326:PHE:HD2   | 1.69                     | 0.58              |
| 1:G:202:THR:HA    | 1:m:22:THR:CB     | 2.27                     | 0.58              |
| 1:I:701:ASP:OD2   | 1:I:1108:ASN:ND2  | 2.35                     | 0.58              |
| 1:I:1297:LYS:HG2  | 1:I:1299:CYS:H    | 1.68                     | 0.58              |
| 1:k:607:GLN:NE2   | 1:p:665:ASP:OD1   | 2.35                     | 0.58              |
| 1:k:1230:THR:HA   | 1:k:1233:ARG:HB3  | 1.83                     | 0.58              |
| 1:o:294:ARG:HD2   | 1:o:357:GLN:HB3   | 1.85                     | 0.58              |
| 2:2:66:ARG:O      | 2:2:67:GLU:CG     | 2.51                     | 0.58              |
| 2:i:133:GLY:O     | 2:i:136:TYR:HB3   | 2.04                     | 0.58              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:y:59:GLY:O      | 4:y:63:GLN:HB2    | 2.03                     | 0.58              |
| 4:V:188:VAL:HG22  | 4:V:210:VAL:HG12  | 1.85                     | 0.58              |
| 1:A:722:GLN:NE2   | 1:A:904:GLY:O     | 2.36                     | 0.58              |
| 1:B:440:ARG:HH12  | 1:C:521:LYS:HB3   | 1.68                     | 0.58              |
| 1:B:1031:LEU:HD23 | 1:B:1081:ALA:HB2  | 1.84                     | 0.58              |
| 1:C:207:MET:N     | 1:C:207:MET:SD    | 2.76                     | 0.58              |
| 1:D:119:LYS:NZ    | 1:D:1072:LEU:O    | 2.36                     | 0.58              |
| 1:D:419:ASP:OD1   | 1:D:424:GLN:NE2   | 2.36                     | 0.58              |
| 1:D:818:PHE:CZ    | 3:M:61:ILE:CG2    | 2.87                     | 0.58              |
| 1:E:30:GLU:C      | 1:m:1263:PHE:HD2  | 2.10                     | 0.58              |
| 1:E:1139:ARG:NH1  | 4:S:79:MET:HB3    | 2.18                     | 0.58              |
| 1:F:734:VAL:HG11  | 1:F:878:ARG:HH11  | 1.68                     | 0.58              |
| 1:I:509:ARG:HB2   | 1:I:513:GLU:HB2   | 1.86                     | 0.58              |
| 1:I:725:PRO:HG2   | 1:I:728:ALA:HB2   | 1.86                     | 0.58              |
| 1:I:1048:VAL:HG22 | 1:I:1061:VAL:HG12 | 1.86                     | 0.58              |
| 1:I:1228:TYR:HB2  | 1:I:1250:PHE:HD2  | 1.68                     | 0.58              |
| 1:m:104:GLY:HA3   | 1:m:107:ILE:HD12  | 1.85                     | 0.58              |
| 1:m:165:VAL:CG1   | 4:S:9:PRO:HA      | 2.34                     | 0.58              |
| 1:o:53:ALA:HB3    | 1:p:89:THR:O      | 2.03                     | 0.58              |
| 1:p:500:PHE:HE2   | 1:p:958:PRO:HB2   | 1.67                     | 0.58              |
| 2:2:174:ARG:HH11  | 2:3:274:THR:HG22  | 1.68                     | 0.58              |
| 2:3:133:GLY:O     | 2:3:136:TYR:HB3   | 2.04                     | 0.58              |
| 2:f:66:ARG:NH1    | 2:f:294:LEU:HB3   | 2.14                     | 0.58              |
| 2:j:133:GLY:O     | 2:j:136:TYR:HB3   | 2.04                     | 0.58              |
| 4:S:228:ARG:HG2   | 5:a:224:ASN:HB3   | 1.85                     | 0.58              |
| 1:A:785:TYR:CD2   | 1:A:786:TYR:CE2   | 2.91                     | 0.58              |
| 1:B:727:ASN:ND2   | 1:B:776:ASP:OD1   | 2.37                     | 0.58              |
| 1:B:1276:CYS:SG   | 1:B:1277:ILE:N    | 2.75                     | 0.58              |
| 1:E:534:GLU:OE2   | 1:E:557:ARG:NH1   | 2.36                     | 0.58              |
| 1:F:113:THR:HG23  | 1:l:38:LEU:HD11   | 1.84                     | 0.58              |
| 1:F:332:ARG:HD2   | 1:l:12:PRO:HG2    | 1.82                     | 0.58              |
| 1:F:757:ARG:HH22  | 1:F:869:PRO:HA    | 1.68                     | 0.58              |
| 1:H:507:PRO:HD2   | 1:H:958:PRO:HB3   | 1.86                     | 0.58              |
| 1:I:77:HIS:HB3    | 1:I:1040:ALA:HA   | 1.86                     | 0.58              |
| 1:I:79:ILE:HB     | 1:I:1042:ILE:HG22 | 1.85                     | 0.58              |
| 1:k:208:ALA:HB3   | 1:k:213:ARG:HE    | 1.68                     | 0.58              |
| 1:o:534:GLU:OE2   | 1:o:557:ARG:NH1   | 2.36                     | 0.58              |
| 1:p:722:GLN:NE2   | 1:p:904:GLY:O     | 2.36                     | 0.58              |
| 5:z:101:GLU:O     | 5:z:104:ASP:OD1   | 2.21                     | 0.58              |
| 5:d:48:VAL:HG22   | 5:d:62:ARG:HE     | 1.67                     | 0.58              |
| 1:D:606:HIS:HA    | 1:D:909:THR:HG21  | 1.85                     | 0.58              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:D:662:ARG:HH21  | 1:D:663:LEU:HD13  | 1.68                     | 0.58              |
| 1:E:1139:ARG:HH11 | 4:S:80:PRO:HD3    | 1.68                     | 0.58              |
| 1:F:603:LEU:HB3   | 1:F:794:LEU:HD21  | 1.86                     | 0.58              |
| 1:l:1166:ASP:HA   | 1:l:1170:PHE:HD2  | 1.69                     | 0.58              |
| 1:m:517:ASP:OD1   | 1:m:517:ASP:N     | 2.36                     | 0.58              |
| 1:m:688:ARG:HH12  | 1:n:797:HIS:CE1   | 2.21                     | 0.58              |
| 1:n:119:LYS:HB3   | 1:n:1069:GLU:HB3  | 1.86                     | 0.58              |
| 1:o:1276:CYS:SG   | 1:o:1277:ILE:N    | 2.75                     | 0.58              |
| 2:e:207:ASP:OD2   | 2:e:209:SER:HB3   | 2.04                     | 0.58              |
| 2:g:197:VAL:C     | 2:g:199:ASP:H     | 2.12                     | 0.58              |
| 4:y:96:ASN:ND2    | 4:y:206:ALA:O     | 2.32                     | 0.58              |
| 4:S:96:ASN:ND2    | 4:S:206:ALA:O     | 2.37                     | 0.58              |
| 4:T:69:LEU:HD12   | 4:T:87:LEU:HD22   | 1.86                     | 0.58              |
| 5:X:297:ASP:HB2   | 5:X:306:LEU:HD12  | 1.85                     | 0.58              |
| 5:Y:102:LYS:NZ    | 5:c:32:PRO:O      | 2.37                     | 0.58              |
| 5:1:168:LEU:O     | 5:1:170:VAL:N     | 2.36                     | 0.58              |
| 1:A:813:PHE:HE2   | 3:J:85:LEU:HB3    | 1.63                     | 0.58              |
| 1:A:1019:THR:CG2  | 1:A:1160:LEU:HD11 | 2.33                     | 0.58              |
| 1:D:441:ILE:HD13  | 1:D:1092:SER:HB3  | 1.84                     | 0.58              |
| 1:D:692:LEU:HB2   | 1:D:705:LEU:HD21  | 1.76                     | 0.58              |
| 1:E:490:MET:HE3   | 1:E:876:GLU:HB2   | 1.85                     | 0.58              |
| 1:E:1099:GLN:O    | 1:E:1239:ASN:ND2  | 2.37                     | 0.58              |
| 1:G:277:THR:HG21  | 1:G:387:GLU:HG3   | 1.84                     | 0.58              |
| 1:G:1018:LEU:CD2  | 1:G:1159:ILE:HD13 | 2.33                     | 0.58              |
| 1:H:345:GLN:O     | 1:H:349:GLN:NE2   | 2.37                     | 0.58              |
| 1:H:482:ARG:HH22  | 1:H:961:PRO:HB3   | 1.69                     | 0.58              |
| 1:o:562:ASN:HD22  | 1:o:972:ARG:HB2   | 1.67                     | 0.58              |
| 1:q:214:ALA:HB1   | 1:q:1183:MET:HG2  | 1.86                     | 0.58              |
| 5:W:214:TYR:HB3   | 5:a:201:SER:HB2   | 1.86                     | 0.58              |
| 5:1:7:VAL:HB      | 5:1:79:MET:HB3    | 1.85                     | 0.58              |
| 1:A:1276:CYS:SG   | 1:A:1277:ILE:N    | 2.74                     | 0.58              |
| 1:B:724:LEU:HB2   | 1:B:769:VAL:HG21  | 1.86                     | 0.58              |
| 1:C:717:TRP:HE1   | 1:C:731:VAL:HG11  | 1.69                     | 0.58              |
| 1:E:1262:LEU:HB3  | 1:G:30:GLU:HG3    | 1.85                     | 0.58              |
| 1:F:1321:LEU:HD12 | 1:F:1327:LEU:HD21 | 1.84                     | 0.58              |
| 1:G:1018:LEU:HD21 | 1:G:1159:ILE:CD1  | 2.33                     | 0.58              |
| 1:G:1179:ARG:NH1  | 1:G:1211:SER:O    | 2.37                     | 0.58              |
| 1:I:1201:HIS:ND1  | 1:I:1212:THR:OG1  | 2.36                     | 0.58              |
| 1:l:677:ARG:NH2   | 1:m:601:ALA:O     | 2.36                     | 0.58              |
| 1:m:172:MET:HE3   | 4:S:12:ARG:HH21   | 1.69                     | 0.58              |
| 1:q:755:VAL:HG21  | 3:x:71:MET:HE2    | 1.85                     | 0.58              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:3:94:LEU:CD2    | 2:3:222:LEU:HD21  | 2.33                     | 0.58              |
| 2:h:91:HIS:HD2    | 2:h:195:TYR:CG    | 2.08                     | 0.58              |
| 2:h:133:GLY:O     | 2:h:136:TYR:HB3   | 2.04                     | 0.58              |
| 2:j:66:ARG:O      | 2:j:290:PHE:CZ    | 2.57                     | 0.58              |
| 4:T:215:HIS:HD2   | 4:T:218:THR:H     | 1.50                     | 0.58              |
| 1:C:196:THR:HG23  | 1:C:200:HIS:HD2   | 1.69                     | 0.58              |
| 1:C:795:ASN:ND2   | 1:C:982:CYS:SG    | 2.76                     | 0.58              |
| 1:D:1167:LEU:HD23 | 1:D:1171:ARG:HE   | 1.68                     | 0.58              |
| 1:G:921:ILE:HG22  | 1:G:923:PHE:HB3   | 1.85                     | 0.58              |
| 1:G:1177:ARG:NH1  | 1:G:1198:LEU:O    | 2.36                     | 0.58              |
| 1:I:1156:CYS:HB2  | 1:I:1245:PRO:HD2  | 1.85                     | 0.58              |
| 1:k:744:HIS:ND1   | 2:2:175:ALA:HA    | 2.12                     | 0.58              |
| 1:k:750:PRO:HD2   | 2:3:269:ARG:HH22  | 1.67                     | 0.58              |
| 1:m:141:LYS:HB3   | 4:S:20:GLU:HG2    | 1.84                     | 0.58              |
| 1:m:1159:ILE:O    | 1:m:1214:ASN:ND2  | 2.37                     | 0.58              |
| 1:p:127:THR:HA    | 1:p:1061:VAL:O    | 2.04                     | 0.58              |
| 2:f:197:VAL:C     | 2:f:199:ASP:H     | 2.12                     | 0.58              |
| 2:g:174:ARG:HH11  | 2:j:274:THR:HG22  | 1.68                     | 0.58              |
| 4:V:61:VAL:CG1    | 4:V:88:PHE:HD2    | 2.14                     | 0.58              |
| 5:X:151:LEU:HD13  | 5:b:273:LEU:HD13  | 1.84                     | 0.58              |
| 5:c:45:LEU:HD23   | 5:c:45:LEU:O      | 2.04                     | 0.58              |
| 1:A:232:ASP:OD1   | 1:A:1082:HIS:ND1  | 2.37                     | 0.58              |
| 1:A:1019:THR:HG23 | 1:A:1160:LEU:HD11 | 1.85                     | 0.58              |
| 1:A:1021:VAL:HG23 | 1:A:1245:PRO:HB2  | 1.86                     | 0.58              |
| 1:D:726:ARG:NH2   | 1:D:776:ASP:OD2   | 2.37                     | 0.58              |
| 1:D:818:PHE:CG    | 3:M:88:LEU:HD13   | 2.38                     | 0.58              |
| 1:E:20:LEU:CD1    | 1:l:379:ASN:CG    | 2.75                     | 0.58              |
| 1:F:492:HIS:HD2   | 1:F:495:ARG:HB2   | 1.68                     | 0.58              |
| 1:G:724:LEU:HB3   | 1:G:772:ARG:HB2   | 1.86                     | 0.58              |
| 1:H:379:ASN:HA    | 1:I:205:ARG:HH22  | 1.69                     | 0.58              |
| 1:I:958:PRO:O     | 1:I:959:LEU:C     | 2.47                     | 0.58              |
| 2:3:66:ARG:CD     | 2:3:68:THR:HG23   | 2.34                     | 0.58              |
| 2:f:105:LEU:CD1   | 2:f:216:LEU:HD11  | 2.31                     | 0.58              |
| 2:i:208:PRO:CB    | 5:c:229:LYS:NZ    | 2.67                     | 0.58              |
| 4:S:200:ARG:HH22  | 4:S:244:PRO:HB3   | 1.68                     | 0.58              |
| 4:S:249:LEU:HB3   | 4:S:294:ALA:HA    | 1.86                     | 0.58              |
| 4:U:217:HIS:HE1   | 5:Y:286:VAL:HG22  | 1.69                     | 0.58              |
| 1:C:653:TYR:HA    | 1:C:656:VAL:HG12  | 1.86                     | 0.57              |
| 1:D:325:ASP:HB3   | 1:D:328:GLN:HB3   | 1.86                     | 0.57              |
| 1:E:758:MET:HG3   | 3:N:83:ASP:HB2    | 1.85                     | 0.57              |
| 1:F:116:MET:SD    | 1:l:9:GLU:HB3     | 2.44                     | 0.57              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:F:1262:LEU:HB3  | 1:l:30:GLU:HG3    | 1.86                     | 0.57              |
| 1:G:118:SER:N     | 1:m:33:PHE:HE2    | 2.02                     | 0.57              |
| 1:G:806:LYS:NZ    | 3:P:76:ASP:OD2    | 2.35                     | 0.57              |
| 1:l:576:ARG:HH11  | 1:l:1007:LEU:HD21 | 1.69                     | 0.57              |
| 1:m:1298:PRO:O    | 1:m:1302:LEU:N    | 2.28                     | 0.57              |
| 1:n:1171:ARG:HH12 | 1:n:1332:THR:HG22 | 1.68                     | 0.57              |
| 1:q:482:ARG:NH2   | 1:q:485:PHE:O     | 2.36                     | 0.57              |
| 2:e:197:VAL:O     | 2:e:197:VAL:HG12  | 2.01                     | 0.57              |
| 2:f:207:ASP:OD2   | 2:f:209:SER:HB3   | 2.04                     | 0.57              |
| 4:y:235:LEU:HD21  | 5:z:198:ILE:HG23  | 1.85                     | 0.57              |
| 4:S:66:LEU:HD21   | 4:S:139:SER:H     | 1.69                     | 0.57              |
| 5:z:151:LEU:HD13  | 5:1:273:LEU:HD13  | 1.86                     | 0.57              |
| 5:z:184:THR:HG22  | 5:z:186:ASP:HB2   | 1.86                     | 0.57              |
| 5:z:210:VAL:HG11  | 5:1:152:LEU:HD23  | 1.86                     | 0.57              |
| 1:F:849:ASP:HB3   | 1:F:852:VAL:H     | 1.68                     | 0.57              |
| 1:F:1297:LYS:HG2  | 1:F:1299:CYS:H    | 1.69                     | 0.57              |
| 1:H:925:ARG:NH2   | 1:H:971:HIS:O     | 2.35                     | 0.57              |
| 1:k:135:ALA:N     | 4:y:161:LYS:HB3   | 2.18                     | 0.57              |
| 1:n:866:ALA:O     | 3:u:86:ARG:NH2    | 2.37                     | 0.57              |
| 1:p:231:LEU:HA    | 1:p:235:ARG:HD2   | 1.86                     | 0.57              |
| 1:p:232:ASP:OD1   | 1:p:1352:ASN:ND2  | 2.36                     | 0.57              |
| 1:p:602:SER:HA    | 1:p:646:LEU:HD13  | 1.85                     | 0.57              |
| 1:p:688:ARG:HA    | 1:p:691:GLU:OE2   | 2.03                     | 0.57              |
| 2:2:207:ASP:OD2   | 2:2:209:SER:HB3   | 2.04                     | 0.57              |
| 2:e:174:ARG:HH11  | 2:h:274:THR:HG22  | 1.68                     | 0.57              |
| 2:j:66:ARG:C      | 2:j:68:THR:H      | 2.12                     | 0.57              |
| 4:S:234:PHE:HB2   | 4:S:249:LEU:HD13  | 1.86                     | 0.57              |
| 1:A:434:LYS:NZ    | 1:B:215:ASN:OD1   | 2.37                     | 0.57              |
| 1:C:393:THR:HA    | 1:C:1023:THR:HA   | 1.86                     | 0.57              |
| 1:C:442:SER:OG    | 1:D:521:LYS:NZ    | 2.34                     | 0.57              |
| 1:D:433:ASN:HD21  | 1:D:439:GLN:HE21  | 1.53                     | 0.57              |
| 1:E:53:ALA:HA     | 1:F:322:ILE:HB    | 1.86                     | 0.57              |
| 1:F:1156:CYS:HB2  | 1:F:1245:PRO:HD2  | 1.86                     | 0.57              |
| 1:G:495:ARG:NH2   | 1:G:762:ASP:OD2   | 2.37                     | 0.57              |
| 1:k:601:ALA:O     | 1:p:677:ARG:NH2   | 2.37                     | 0.57              |
| 1:k:1160:LEU:CD2  | 1:k:1214:ASN:HD22 | 2.14                     | 0.57              |
| 1:l:689:THR:O     | 1:l:692:LEU:HD22  | 2.04                     | 0.57              |
| 1:l:1333:HIS:HB2  | 1:l:1336:ASN:HB3  | 1.86                     | 0.57              |
| 1:m:52:GLU:O      | 1:n:89:THR:O      | 2.21                     | 0.57              |
| 1:m:141:LYS:HG2   | 4:S:19:PRO:HB2    | 1.84                     | 0.57              |
| 1:o:610:GLU:HA    | 1:o:613:TYR:HD2   | 1.68                     | 0.57              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:o:703:PRO:HG3   | 1:p:948:PRO:HB2   | 1.85                     | 0.57              |
| 1:q:243:TYR:OH    | 1:q:1079:CYS:SG   | 2.57                     | 0.57              |
| 2:h:94:LEU:CD2    | 2:h:222:LEU:HD21  | 2.33                     | 0.57              |
| 2:g:104:LYS:HD3   | 2:j:92:LEU:HD13   | 1.77                     | 0.57              |
| 2:g:260:ARG:HD3   | 2:g:289:LEU:HD21  | 1.85                     | 0.57              |
| 5:Z:196:VAL:HG13  | 5:Z:283:ILE:HD11  | 1.85                     | 0.57              |
| 5:1:112:VAL:HG12  | 5:1:114:SER:H     | 1.69                     | 0.57              |
| 5:c:122:SER:HB2   | 5:c:127:ASP:HB3   | 1.86                     | 0.57              |
| 5:d:227:LEU:HA    | 5:d:230:CYS:HB3   | 1.86                     | 0.57              |
| 1:A:446:ALA:HA    | 1:A:1094:MET:HG3  | 1.86                     | 0.57              |
| 1:A:534:GLU:OE2   | 1:A:557:ARG:NH1   | 2.33                     | 0.57              |
| 1:A:785:TYR:HD2   | 1:A:786:TYR:CE2   | 2.21                     | 0.57              |
| 1:B:1322:LYS:HG2  | 1:C:1329:LEU:HD22 | 1.86                     | 0.57              |
| 1:D:53:ALA:HA     | 1:E:322:ILE:HB    | 1.85                     | 0.57              |
| 1:F:1243:TYR:OH   | 1:F:1297:LYS:NZ   | 2.36                     | 0.57              |
| 1:G:111:ARG:HG3   | 1:m:40:TYR:HB3    | 1.85                     | 0.57              |
| 1:G:276:SER:HB3   | 1:G:280:VAL:HG13  | 1.85                     | 0.57              |
| 1:H:71:ALA:HB3    | 1:H:371:GLU:HB2   | 1.87                     | 0.57              |
| 1:H:103:THR:OG1   | 1:H:104:GLY:N     | 2.37                     | 0.57              |
| 1:H:1041:VAL:HG12 | 1:H:1067:THR:HG22 | 1.86                     | 0.57              |
| 1:H:1148:LEU:HD13 | 1:H:1153:ARG:HH11 | 1.68                     | 0.57              |
| 1:I:753:SER:CB    | 3:R:83:ASP:OD2    | 2.49                     | 0.57              |
| 1:I:952:ARG:HE    | 1:I:955:GLY:HA2   | 1.69                     | 0.57              |
| 1:I:1179:ARG:NH2  | 1:I:1204:PRO:O    | 2.37                     | 0.57              |
| 1:I:1298:PRO:HB2  | 1:I:1302:LEU:HB2  | 1.85                     | 0.57              |
| 1:l:965:HIS:HB3   | 1:l:968:HIS:HB2   | 1.86                     | 0.57              |
| 1:l:1041:VAL:HG12 | 1:l:1067:THR:HG22 | 1.86                     | 0.57              |
| 1:m:152:LEU:HD12  | 1:n:333:ILE:HG12  | 1.87                     | 0.57              |
| 1:m:448:LYS:HD2   | 1:m:1096:ASP:HB3  | 1.85                     | 0.57              |
| 1:m:925:ARG:NH2   | 1:m:971:HIS:O     | 2.34                     | 0.57              |
| 1:m:1053:ARG:NH1  | 5:W:306:LEU:HD11  | 2.20                     | 0.57              |
| 1:o:560:VAL:HA    | 1:o:999:MET:HE3   | 1.86                     | 0.57              |
| 1:p:717:TRP:HE1   | 1:p:731:VAL:HG11  | 1.69                     | 0.57              |
| 1:q:387:GLU:OE2   | 1:q:1084:ARG:NH2  | 2.38                     | 0.57              |
| 1:q:600:ARG:O     | 1:q:604:THR:HB    | 2.05                     | 0.57              |
| 1:q:611:LEU:HB3   | 1:q:846:VAL:HG11  | 1.87                     | 0.57              |
| 1:q:969:HIS:O     | 1:q:972:ARG:NH2   | 2.37                     | 0.57              |
| 3:J:39:GLU:OE2    | 3:J:43:GLN:NE2    | 2.37                     | 0.57              |
| 4:U:96:ASN:ND2    | 4:U:206:ALA:O     | 2.37                     | 0.57              |
| 1:D:380:THR:O     | 1:E:205:ARG:NH1   | 2.37                     | 0.57              |
| 1:D:501:TYR:CZ    | 1:D:959:LEU:O     | 2.57                     | 0.57              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:F:690:CYS:SG    | 1:F:712:HIS:NE2   | 2.74                     | 0.57              |
| 1:H:667:ALA:HB2   | 1:I:643:GLN:HG2   | 1.87                     | 0.57              |
| 1:k:203:ILE:CG2   | 1:p:383:GLN:CD    | 2.78                     | 0.57              |
| 1:l:914:LEU:HB3   | 1:l:917:TYR:HB2   | 1.85                     | 0.57              |
| 1:m:792:ALA:O     | 1:m:984:HIS:ND1   | 2.31                     | 0.57              |
| 1:n:192:PHE:HB2   | 1:n:223:LYS:HB3   | 1.86                     | 0.57              |
| 1:p:275:VAL:HG12  | 1:p:371:GLU:HB3   | 1.87                     | 0.57              |
| 2:3:258:PHE:CZ    | 3:r:90:ILE:HB     | 2.39                     | 0.57              |
| 2:e:260:ARG:HD3   | 2:e:289:LEU:HD21  | 1.85                     | 0.57              |
| 3:K:49:LEU:HD11   | 3:K:65:ILE:HD11   | 1.86                     | 0.57              |
| 1:A:975:PHE:HE1   | 1:A:995:MET:HB3   | 1.69                     | 0.57              |
| 1:B:929:ASP:HB3   | 1:B:932:LEU:HB3   | 1.87                     | 0.57              |
| 1:C:546:GLU:N     | 1:C:549:GLN:O     | 2.37                     | 0.57              |
| 1:D:897:LEU:O     | 1:D:969:HIS:ND1   | 2.38                     | 0.57              |
| 1:E:12:PRO:HB2    | 1:m:341:LEU:CD1   | 2.35                     | 0.57              |
| 1:E:388:ARG:HD3   | 1:E:1295:VAL:H    | 1.69                     | 0.57              |
| 1:F:513:GLU:HA    | 1:F:973:THR:HG21  | 1.87                     | 0.57              |
| 1:F:1028:THR:HG21 | 1:F:1080:THR:HG23 | 1.87                     | 0.57              |
| 1:F:1045:THR:CB   | 1:l:145:GLU:HG2   | 2.35                     | 0.57              |
| 1:k:135:ALA:HB2   | 4:y:161:LYS:C     | 2.16                     | 0.57              |
| 1:l:1139:ARG:NH1  | 4:T:79:MET:HB2    | 2.19                     | 0.57              |
| 1:q:123:LYS:HG2   | 1:q:1066:ASN:HB3  | 1.85                     | 0.57              |
| 2:g:207:ASP:OD2   | 2:g:209:SER:HB3   | 2.04                     | 0.57              |
| 2:j:66:ARG:O      | 2:j:68:THR:N      | 2.31                     | 0.57              |
| 4:S:74:ASP:HB2    | 4:S:130:VAL:HA    | 1.86                     | 0.57              |
| 5:z:107:THR:HA    | 5:z:292:ALA:HB3   | 1.87                     | 0.57              |
| 5:X:196:VAL:HG13  | 5:X:283:ILE:HD11  | 1.86                     | 0.57              |
| 1:A:381:ASP:HA    | 1:B:205:ARG:HG2   | 1.87                     | 0.57              |
| 1:C:1021:VAL:HG22 | 1:C:1156:CYS:HB3  | 1.87                     | 0.57              |
| 1:F:441:ILE:HD11  | 1:F:1094:MET:HE2  | 1.87                     | 0.57              |
| 1:G:777:GLU:HG3   | 1:H:951:GLN:HE21  | 1.70                     | 0.57              |
| 1:H:311:GLU:OE2   | 1:H:315:THR:OG1   | 2.19                     | 0.57              |
| 1:H:1173:PRO:HB3  | 1:H:1306:LEU:HA   | 1.86                     | 0.57              |
| 1:H:1276:CYS:SG   | 1:H:1277:ILE:N    | 2.78                     | 0.57              |
| 1:k:68:LEU:HD11   | 1:k:301:ALA:O     | 2.00                     | 0.57              |
| 1:m:734:VAL:HG12  | 1:m:739:PRO:HA    | 1.86                     | 0.57              |
| 1:o:710:ALA:C     | 1:o:713:ASP:OD1   | 2.44                     | 0.57              |
| 1:p:606:HIS:HA    | 1:p:909:THR:HG21  | 1.87                     | 0.57              |
| 1:p:659:ILE:O     | 1:p:663:LEU:CB    | 2.51                     | 0.57              |
| 2:g:197:VAL:O     | 2:g:199:ASP:N     | 2.38                     | 0.57              |
| 5:X:29:ILE:HD12   | 5:X:81:LEU:HD21   | 1.84                     | 0.57              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 5:1:206:LEU:HA   | 5:1:209:GLU:HB2   | 1.86                     | 0.57              |
| 1:A:79:ILE:O     | 1:A:1042:ILE:HA   | 2.05                     | 0.57              |
| 1:C:419:ASP:OD1  | 1:C:424:GLN:NE2   | 2.37                     | 0.57              |
| 1:D:1147:ALA:HB1 | 1:E:1206:PRO:HG3  | 1.86                     | 0.57              |
| 1:G:77:HIS:HB3   | 1:G:1040:ALA:HA   | 1.86                     | 0.57              |
| 1:G:497:LEU:HD21 | 1:G:922:PRO:HD2   | 1.86                     | 0.57              |
| 1:H:453:PRO:HG2  | 1:H:1104:HIS:HB3  | 1.87                     | 0.57              |
| 1:I:458:ALA:HB1  | 1:I:461:CYS:HB3   | 1.86                     | 0.57              |
| 1:I:813:PHE:CE2  | 3:R:85:LEU:HG     | 2.40                     | 0.57              |
| 1:k:135:ALA:HA   | 4:y:161:LYS:HB2   | 1.87                     | 0.57              |
| 1:k:722:GLN:NE2  | 1:k:904:GLY:O     | 2.38                     | 0.57              |
| 1:l:638:ASN:ND2  | 1:l:668:VAL:O     | 2.37                     | 0.57              |
| 1:l:925:ARG:NH2  | 1:l:971:HIS:O     | 2.37                     | 0.57              |
| 1:m:220:PHE:HB2  | 1:m:1302:LEU:HD21 | 1.86                     | 0.57              |
| 1:m:1310:THR:HB  | 1:m:1339:ILE:HB   | 1.87                     | 0.57              |
| 1:n:684:ARG:O    | 1:n:688:ARG:HB2   | 2.05                     | 0.57              |
| 1:p:702:GLU:OE2  | 1:p:715:ARG:NH1   | 2.38                     | 0.57              |
| 1:q:433:ASN:O    | 1:q:436:ARG:NH1   | 2.35                     | 0.57              |
| 2:i:111:ALA:CA   | 4:U:232:PHE:CE2   | 2.87                     | 0.57              |
| 3:t:64:MET:HE2   | 3:t:84:LEU:HA     | 1.87                     | 0.57              |
| 5:z:218:LEU:HD21 | 5:1:194:ARG:HE    | 1.68                     | 0.57              |
| 5:z:285:ASP:HA   | 5:z:288:SER:HB3   | 1.86                     | 0.57              |
| 5:b:106:LEU:HB3  | 5:b:133:ILE:HG22  | 1.87                     | 0.57              |
| 1:B:66:THR:HG23  | 1:B:69:GLY:H      | 1.70                     | 0.57              |
| 1:C:193:VAL:HG11 | 1:C:1266:VAL:HG21 | 1.87                     | 0.57              |
| 1:F:207:MET:N    | 1:F:207:MET:SD    | 2.78                     | 0.57              |
| 1:H:722:GLN:NE2  | 1:H:904:GLY:O     | 2.37                     | 0.57              |
| 1:I:419:ASP:OD1  | 1:I:424:GLN:NE2   | 2.37                     | 0.57              |
| 1:l:104:GLY:HA3  | 1:l:107:ILE:HD12  | 1.86                     | 0.57              |
| 1:m:165:VAL:CG1  | 4:S:12:ARG:HB2    | 2.35                     | 0.57              |
| 1:o:796:ASN:HD21 | 1:o:926:PHE:HD1   | 1.53                     | 0.57              |
| 1:p:272:GLY:HA3  | 1:p:1034:SER:O    | 2.04                     | 0.57              |
| 1:p:434:LYS:HE2  | 1:p:1086:VAL:HB   | 1.87                     | 0.57              |
| 4:U:69:LEU:HD11  | 4:U:255:LEU:HD21  | 1.87                     | 0.57              |
| 1:C:1149:LEU:HB3 | 1:D:1207:GLN:HB2  | 1.87                     | 0.57              |
| 1:D:431:PHE:CD1  | 1:D:1309:HIS:O    | 2.57                     | 0.57              |
| 1:D:1171:ARG:NH2 | 1:D:1338:SER:O    | 2.38                     | 0.57              |
| 1:E:725:PRO:HG2  | 1:E:728:ALA:HB2   | 1.87                     | 0.57              |
| 1:E:1297:LYS:HG2 | 1:E:1299:CYS:H    | 1.70                     | 0.57              |
| 1:F:341:LEU:CB   | 1:l:14:LEU:HD21   | 2.35                     | 0.57              |
| 1:F:603:LEU:HD23 | 1:F:794:LEU:HD11  | 1.85                     | 0.57              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:F:1019:THR:CG2  | 1:F:1160:LEU:CD1  | 2.82                     | 0.57              |
| 1:I:539:PHE:O     | 1:I:557:ARG:NH2   | 2.38                     | 0.57              |
| 1:l:584:THR:HG21  | 1:l:689:THR:HG22  | 1.87                     | 0.57              |
| 1:l:795:ASN:ND2   | 1:l:982:CYS:SG    | 2.78                     | 0.57              |
| 1:m:431:PHE:O     | 1:m:438:PRO:HA    | 2.05                     | 0.57              |
| 1:m:748:ARG:NH1   | 2:e:269:ARG:NH2   | 2.51                     | 0.57              |
| 1:p:690:CYS:SG    | 1:p:712:HIS:NE2   | 2.72                     | 0.57              |
| 1:p:726:ARG:HB3   | 1:p:773:ARG:HB2   | 1.87                     | 0.57              |
| 2:j:262:TYR:CD1   | 3:M:87:MET:HE1    | 2.40                     | 0.57              |
| 1:D:14:LEU:HB2    | 1:G:58:TYR:HA     | 1.85                     | 0.56              |
| 1:D:131:GLU:O     | 1:E:112:GLN:NE2   | 2.38                     | 0.56              |
| 1:k:701:ASP:OD2   | 1:k:1108:ASN:ND2  | 2.37                     | 0.56              |
| 1:k:727:ASN:ND2   | 1:k:776:ASP:OD1   | 2.38                     | 0.56              |
| 1:m:713:ASP:O     | 1:m:783:LYS:NZ    | 2.38                     | 0.56              |
| 1:p:643:GLN:HG2   | 1:p:644:ARG:HG2   | 1.86                     | 0.56              |
| 1:q:281:VAL:HG11  | 1:q:372:HIS:HB3   | 1.87                     | 0.56              |
| 2:e:197:VAL:O     | 2:e:199:ASP:N     | 2.38                     | 0.56              |
| 2:h:208:PRO:CG    | 5:a:229:LYS:HZ2   | 2.18                     | 0.56              |
| 4:y:221:ASN:OD1   | 4:y:224:ARG:NH1   | 2.38                     | 0.56              |
| 5:Z:191:ILE:O     | 5:Z:195:ASN:ND2   | 2.37                     | 0.56              |
| 5:b:54:ARG:HD3    | 5:b:58:ARG:HG2    | 1.86                     | 0.56              |
| 5:d:64:ARG:NH1    | 5:d:288:SER:O     | 2.38                     | 0.56              |
| 1:C:1029:ASP:HB2  | 1:C:1082:HIS:HB3  | 1.86                     | 0.56              |
| 1:C:1230:THR:H    | 1:C:1251:THR:HG22 | 1.71                     | 0.56              |
| 1:D:925:ARG:HH12  | 1:D:971:HIS:HB3   | 1.70                     | 0.56              |
| 1:F:786:TYR:O     | 1:F:927:TYR:OH    | 2.22                     | 0.56              |
| 1:H:431:PHE:O     | 1:H:438:PRO:HA    | 2.05                     | 0.56              |
| 1:H:434:LYS:NZ    | 1:I:215:ASN:OD1   | 2.37                     | 0.56              |
| 1:H:877:ILE:HB    | 1:H:898:GLN:HB2   | 1.87                     | 0.56              |
| 1:k:934:ALA:HB2   | 1:k:944:LEU:HD12  | 1.88                     | 0.56              |
| 1:k:1041:VAL:HG12 | 1:k:1067:THR:HG22 | 1.87                     | 0.56              |
| 1:l:292:ILE:HG12  | 1:l:361:LEU:HB3   | 1.87                     | 0.56              |
| 1:l:656:VAL:HG23  | 1:l:676:TYR:HD1   | 1.70                     | 0.56              |
| 1:l:1137:PHE:HB3  | 4:T:55:ARG:HH22   | 1.70                     | 0.56              |
| 1:m:431:PHE:CD1   | 1:m:1309:HIS:O    | 2.58                     | 0.56              |
| 1:m:703:PRO:HG3   | 1:n:948:PRO:HB2   | 1.87                     | 0.56              |
| 1:o:131:GLU:O     | 1:p:112:GLN:NE2   | 2.39                     | 0.56              |
| 1:p:687:ALA:O     | 1:p:691:GLU:HG2   | 2.04                     | 0.56              |
| 1:p:1274:GLN:HE21 | 1:p:1291:THR:H    | 1.53                     | 0.56              |
| 1:q:1179:ARG:NH2  | 1:q:1218:SER:O    | 2.34                     | 0.56              |
| 2:e:197:VAL:C     | 2:e:199:ASP:H     | 2.12                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:618:LEU:HD22  | 1:A:864:LEU:HB3   | 1.87                     | 0.56              |
| 1:B:677:ARG:HH21  | 1:C:604:THR:C     | 2.13                     | 0.56              |
| 1:C:816:LYS:HE2   | 1:C:833:LEU:HG    | 1.87                     | 0.56              |
| 1:D:967:TYR:O     | 1:D:972:ARG:NH2   | 2.36                     | 0.56              |
| 1:E:128:ILE:HG22  | 1:F:102:ALA:HB3   | 1.86                     | 0.56              |
| 1:F:809:LEU:HD21  | 1:F:868:VAL:HG21  | 1.88                     | 0.56              |
| 1:G:329:HIS:HB3   | 1:m:11:LEU:HD22   | 1.87                     | 0.56              |
| 1:G:419:ASP:OD1   | 1:G:424:GLN:NE2   | 2.37                     | 0.56              |
| 1:G:450:LEU:CD2   | 1:G:1018:LEU:HD21 | 2.33                     | 0.56              |
| 1:G:688:ARG:HH12  | 1:H:797:HIS:HE1   | 1.51                     | 0.56              |
| 1:G:885:GLN:O     | 1:G:891:SER:OG    | 2.23                     | 0.56              |
| 1:G:1126:VAL:HB   | 1:G:1130:GLU:HB2  | 1.88                     | 0.56              |
| 1:k:602:SER:HA    | 1:k:646:LEU:HD13  | 1.87                     | 0.56              |
| 1:k:744:HIS:CG    | 2:2:173:MET:O     | 2.58                     | 0.56              |
| 1:k:1021:VAL:HG23 | 1:k:1245:PRO:HB2  | 1.88                     | 0.56              |
| 1:l:66:THR:HG23   | 1:l:69:GLY:H      | 1.70                     | 0.56              |
| 1:l:174:ARG:HH22  | 1:m:99:PRO:CB     | 2.18                     | 0.56              |
| 1:l:659:ILE:O     | 1:l:663:LEU:HB3   | 2.05                     | 0.56              |
| 1:m:432:TYR:CE2   | 1:m:1321:LEU:HD12 | 2.38                     | 0.56              |
| 1:n:587:ARG:HB3   | 1:o:984:HIS:HD2   | 1.71                     | 0.56              |
| 1:n:813:PHE:CD1   | 3:u:85:LEU:HG     | 2.40                     | 0.56              |
| 1:o:191:CYS:SG    | 1:o:243:TYR:OH    | 2.61                     | 0.56              |
| 1:o:483:ARG:HG3   | 1:o:484:GLU:HG2   | 1.86                     | 0.56              |
| 1:o:488:GLU:CD    | 1:o:490:MET:HE2   | 2.25                     | 0.56              |
| 1:q:614:LEU:O     | 1:q:618:LEU:CB    | 2.53                     | 0.56              |
| 2:2:197:VAL:O     | 2:2:199:ASP:N     | 2.38                     | 0.56              |
| 2:3:258:PHE:CZ    | 3:r:90:ILE:HG21   | 2.40                     | 0.56              |
| 2:3:282:ARG:HH21  | 3:r:67:LYS:HG2    | 1.70                     | 0.56              |
| 3:L:60:VAL:HG21   | 3:L:91:ALA:HB2    | 1.88                     | 0.56              |
| 3:Q:71:MET:O      | 3:Q:74:HIS:NE2    | 2.36                     | 0.56              |
| 4:T:6:SER:HB3     | 4:T:9:PRO:HD2     | 1.86                     | 0.56              |
| 4:V:66:LEU:HD21   | 4:V:140:ILE:HG12  | 1.87                     | 0.56              |
| 4:V:69:LEU:HD12   | 4:V:87:LEU:HD22   | 1.88                     | 0.56              |
| 5:W:110:PRO:CB    | 5:W:111:PRO:HD3   | 2.14                     | 0.56              |
| 5:X:31:ILE:HG22   | 5:X:43:VAL:HA     | 1.88                     | 0.56              |
| 1:A:147:THR:C     | 1:A:149:LEU:H     | 2.13                     | 0.56              |
| 1:A:535:LEU:HB2   | 1:A:541:PHE:HE2   | 1.70                     | 0.56              |
| 1:B:722:GLN:NE2   | 1:B:904:GLY:O     | 2.38                     | 0.56              |
| 1:D:818:PHE:CD2   | 3:M:88:LEU:HD22   | 2.41                     | 0.56              |
| 1:G:201:GLY:O     | 1:m:26:LEU:HD23   | 2.04                     | 0.56              |
| 1:G:388:ARG:HD3   | 1:G:1295:VAL:H    | 1.69                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:G:1041:VAL:HG12 | 1:G:1067:THR:HG22 | 1.87                     | 0.56              |
| 1:H:967:TYR:O     | 1:H:972:ARG:NH2   | 2.39                     | 0.56              |
| 1:k:757:ARG:NH2   | 1:k:868:VAL:O     | 2.38                     | 0.56              |
| 1:k:952:ARG:NH2   | 1:k:955:GLY:O     | 2.38                     | 0.56              |
| 1:l:950:TYR:CD1   | 1:l:956:GLY:C     | 2.84                     | 0.56              |
| 1:l:1297:LYS:HE2  | 1:l:1299:CYS:HB2  | 1.87                     | 0.56              |
| 1:m:432:TYR:HH    | 1:m:1321:LEU:CD1  | 1.92                     | 0.56              |
| 2:3:91:HIS:HD2    | 2:3:195:TYR:CG    | 2.08                     | 0.56              |
| 2:f:197:VAL:O     | 2:f:199:ASP:N     | 2.38                     | 0.56              |
| 4:U:64:LYS:HE2    | 4:U:270:SER:HB3   | 1.87                     | 0.56              |
| 4:V:93:VAL:HG21   | 4:V:121:ARG:HE    | 1.70                     | 0.56              |
| 5:X:101:GLU:OE1   | 5:X:174:ARG:NH1   | 2.39                     | 0.56              |
| 1:B:393:THR:OG1   | 1:B:1248:GLN:NE2  | 2.39                     | 0.56              |
| 1:C:534:GLU:OE2   | 1:C:557:ARG:NH1   | 2.39                     | 0.56              |
| 1:F:1171:ARG:NH2  | 1:F:1338:SER:O    | 2.38                     | 0.56              |
| 1:G:118:SER:O     | 1:m:35:ASN:HB3    | 2.04                     | 0.56              |
| 1:H:509:ARG:HB2   | 1:H:513:GLU:HB2   | 1.86                     | 0.56              |
| 1:l:192:PHE:HB2   | 1:l:223:LYS:HB3   | 1.87                     | 0.56              |
| 1:l:688:ARG:HA    | 1:l:691:GLU:CG    | 2.35                     | 0.56              |
| 1:o:392:LEU:HB2   | 1:o:1026:PHE:HE2  | 1.69                     | 0.56              |
| 1:A:539:PHE:O     | 1:A:557:ARG:NH2   | 2.38                     | 0.56              |
| 1:C:986:LEU:O     | 1:C:986:LEU:HD23  | 2.05                     | 0.56              |
| 1:D:30:GLU:HB2    | 1:H:1261:THR:HB   | 1.88                     | 0.56              |
| 1:E:278:HIS:O     | 1:E:282:GLN:NE2   | 2.38                     | 0.56              |
| 1:E:1272:ARG:O    | 1:E:1300:ARG:NH2  | 2.38                     | 0.56              |
| 1:G:112:GLN:O     | 1:m:40:TYR:O      | 2.23                     | 0.56              |
| 1:G:920:VAL:HG12  | 1:G:937:ASN:HD22  | 1.70                     | 0.56              |
| 1:H:77:HIS:HB2    | 1:H:1037:ALA:HB1  | 1.88                     | 0.56              |
| 1:o:509:ARG:HB3   | 1:o:513:GLU:HB2   | 1.86                     | 0.56              |
| 5:z:196:VAL:HG13  | 5:z:283:ILE:HD11  | 1.88                     | 0.56              |
| 5:Z:3:THR:HA      | 5:Z:83:VAL:HB     | 1.87                     | 0.56              |
| 1:A:383:GLN:HA    | 1:B:205:ARG:HH22  | 1.70                     | 0.56              |
| 1:C:1230:THR:HA   | 1:C:1233:ARG:HB3  | 1.87                     | 0.56              |
| 1:E:185:LEU:HD22  | 1:E:388:ARG:HH22  | 1.69                     | 0.56              |
| 1:E:667:ALA:HA    | 1:F:644:ARG:NH2   | 2.20                     | 0.56              |
| 1:E:1132:ILE:HG22 | 4:S:116:ILE:HG23  | 1.86                     | 0.56              |
| 1:E:1276:CYS:SG   | 1:E:1277:ILE:N    | 2.79                     | 0.56              |
| 1:G:120:TYR:CE2   | 1:m:35:ASN:HB2    | 2.33                     | 0.56              |
| 1:H:1016:PHE:CE1  | 1:H:1018:LEU:HD21 | 2.41                     | 0.56              |
| 1:H:1093:ARG:O    | 1:H:1155:THR:HG21 | 2.05                     | 0.56              |
| 1:H:1161:THR:O    | 1:H:1163:VAL:N    | 2.39                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:H:1173:PRO:HD3  | 1:H:1342:THR:HG21 | 1.88                     | 0.56              |
| 1:l:1173:PRO:HD3  | 1:l:1342:THR:HG21 | 1.87                     | 0.56              |
| 1:m:988:SER:HA    | 1:m:991:THR:HG22  | 1.88                     | 0.56              |
| 1:n:1310:THR:HB   | 1:n:1339:ILE:HB   | 1.87                     | 0.56              |
| 1:o:451:CYS:HB3   | 1:o:1098:PHE:HZ   | 1.71                     | 0.56              |
| 1:p:420:THR:HG22  | 1:p:422:GLU:H     | 1.70                     | 0.56              |
| 1:q:534:GLU:OE2   | 1:q:557:ARG:NH1   | 2.39                     | 0.56              |
| 2:e:284:GLU:CA    | 3:t:67:LYS:NZ     | 2.62                     | 0.56              |
| 4:S:109:TYR:HB3   | 4:S:114:GLU:HG3   | 1.88                     | 0.56              |
| 5:W:23:ARG:O      | 5:W:93:ARG:NH2    | 2.39                     | 0.56              |
| 5:a:102:LYS:HG2   | 5:a:297:ASP:HA    | 1.88                     | 0.56              |
| 1:B:952:ARG:NH2   | 1:B:955:GLY:O     | 2.35                     | 0.56              |
| 1:B:1183:MET:SD   | 1:B:1259:ASN:ND2  | 2.79                     | 0.56              |
| 1:D:1041:VAL:HG12 | 1:D:1067:THR:HG22 | 1.86                     | 0.56              |
| 1:F:877:ILE:HB    | 1:F:898:GLN:HB2   | 1.88                     | 0.56              |
| 1:F:1276:CYS:SG   | 1:F:1277:ILE:N    | 2.79                     | 0.56              |
| 1:G:1019:THR:HG23 | 1:G:1160:LEU:HD21 | 1.81                     | 0.56              |
| 1:H:1132:ILE:HG22 | 4:V:116:ILE:HG23  | 1.86                     | 0.56              |
| 1:I:925:ARG:HE    | 1:I:976:SER:HB3   | 1.71                     | 0.56              |
| 1:o:67:PHE:HA     | 1:o:177:ILE:HD11  | 1.87                     | 0.56              |
| 1:o:877:ILE:HB    | 1:o:898:GLN:HB2   | 1.86                     | 0.56              |
| 1:p:787:LEU:HD23  | 1:p:787:LEU:O     | 2.06                     | 0.56              |
| 2:i:272:ASP:OD2   | 2:i:275:THR:CG2   | 2.54                     | 0.56              |
| 4:y:74:ASP:OD2    | 5:1:174:ARG:NH1   | 2.36                     | 0.56              |
| 4:S:215:HIS:CD2   | 5:W:64:ARG:HD3    | 2.41                     | 0.56              |
| 4:U:170:PRO:HA    | 4:U:277:VAL:HA    | 1.87                     | 0.56              |
| 5:W:94:ASN:ND2    | 5:W:302:ASP:O     | 2.39                     | 0.56              |
| 1:A:483:ARG:NH1   | 1:A:509:ARG:O     | 2.39                     | 0.56              |
| 1:A:953:CYS:SG    | 1:F:688:ARG:NH1   | 2.79                     | 0.56              |
| 1:C:1093:ARG:HH11 | 1:C:1153:ARG:HD2  | 1.71                     | 0.56              |
| 1:E:653:TYR:HA    | 1:E:656:VAL:HG12  | 1.88                     | 0.56              |
| 1:E:667:ALA:H     | 1:F:643:GLN:HG3   | 1.70                     | 0.56              |
| 1:E:1144:GLY:HA2  | 1:E:1282:ASP:HB2  | 1.87                     | 0.56              |
| 1:E:1184:LEU:HD21 | 1:E:1265:THR:HG21 | 1.87                     | 0.56              |
| 1:H:1142:ASP:O    | 1:H:1285:TYR:OH   | 2.21                     | 0.56              |
| 1:k:1021:VAL:HG22 | 1:k:1156:CYS:HB3  | 1.87                     | 0.56              |
| 1:k:1260:LYS:HB3  | 1:k:1264:LYS:HB2  | 1.87                     | 0.56              |
| 1:l:207:MET:SD    | 1:l:207:MET:N     | 2.79                     | 0.56              |
| 1:l:379:ASN:HB2   | 1:m:99:PRO:HG2    | 1.87                     | 0.56              |
| 1:l:930:PRO:HG3   | 1:l:957:PHE:HE2   | 1.71                     | 0.56              |
| 1:l:1214:ASN:O    | 1:l:1218:SER:CB   | 2.54                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:m:1205:ASP:H    | 1:m:1211:SER:HA   | 1.71                     | 0.56              |
| 1:o:993:ALA:HA    | 1:o:996:HIS:HD2   | 1.70                     | 0.56              |
| 1:p:1160:LEU:HD23 | 1:p:1214:ASN:CB   | 2.36                     | 0.56              |
| 2:f:206:GLU:HG2   | 2:i:132:TYR:O     | 2.06                     | 0.56              |
| 4:y:69:LEU:HB2    | 4:y:87:LEU:HB2    | 1.88                     | 0.56              |
| 5:X:23:ARG:O      | 5:X:93:ARG:NH2    | 2.38                     | 0.56              |
| 5:c:20:LYS:HE3    | 5:c:121:VAL:HG12  | 1.88                     | 0.56              |
| 1:C:1298:PRO:HB2  | 1:C:1302:LEU:HB2  | 1.87                     | 0.56              |
| 1:D:380:THR:HG22  | 1:E:99:PRO:HB2    | 1.88                     | 0.56              |
| 1:D:664:GLY:O     | 1:D:665:ASP:OD1   | 2.24                     | 0.56              |
| 1:D:749:ASN:HA    | 2:j:269:ARG:HH22  | 1.71                     | 0.56              |
| 1:H:1253:ASP:O    | 1:H:1257:ASN:ND2  | 2.39                     | 0.56              |
| 1:I:393:THR:OG1   | 1:I:1248:GLN:NE2  | 2.39                     | 0.56              |
| 1:I:481:CYS:SG    | 1:I:482:ARG:N     | 2.79                     | 0.56              |
| 1:k:126:ILE:O     | 1:k:126:ILE:HG13  | 2.05                     | 0.56              |
| 1:k:227:THR:HG22  | 1:k:230:LEU:HD21  | 1.87                     | 0.56              |
| 1:k:1313:THR:HG23 | 1:k:1316:LEU:H    | 1.70                     | 0.56              |
| 1:m:87:MET:HE1    | 1:m:1042:ILE:HD12 | 1.87                     | 0.56              |
| 1:m:514:ALA:CA    | 1:m:517:ASP:CG    | 2.57                     | 0.56              |
| 1:n:509:ARG:HB3   | 1:n:513:GLU:HB2   | 1.87                     | 0.56              |
| 1:n:638:ASN:O     | 1:n:642:ARG:HB2   | 2.05                     | 0.56              |
| 1:n:647:LEU:HD11  | 1:n:672:ALA:HB1   | 1.87                     | 0.56              |
| 1:n:1333:HIS:HB3  | 1:n:1336:ASN:HB2  | 1.88                     | 0.56              |
| 1:p:276:SER:HB2   | 1:p:281:VAL:HG23  | 1.88                     | 0.56              |
| 1:p:1298:PRO:O    | 1:p:1303:GLN:N    | 2.38                     | 0.56              |
| 2:j:94:LEU:CD2    | 2:j:222:LEU:HD21  | 2.33                     | 0.56              |
| 2:j:272:ASP:OD2   | 2:j:275:THR:CG2   | 2.54                     | 0.56              |
| 3:v:39:GLU:OE2    | 3:v:43:GLN:NE2    | 2.39                     | 0.56              |
| 4:T:245:SER:O     | 5:X:271:ASN:ND2   | 2.39                     | 0.56              |
| 5:z:281:ARG:HG2   | 5:1:284:THR:HG23  | 1.87                     | 0.56              |
| 5:W:30:PRO:HG3    | 5:W:45:LEU:HD12   | 1.88                     | 0.56              |
| 1:C:172:MET:HE3   | 1:C:1046:PRO:HB3  | 1.88                     | 0.55              |
| 1:C:191:CYS:SG    | 1:C:243:TYR:OH    | 2.61                     | 0.55              |
| 1:C:389:ASP:HA    | 1:C:1027:GLU:HA   | 1.88                     | 0.55              |
| 1:C:663:LEU:HD11  | 1:C:668:VAL:HB    | 1.88                     | 0.55              |
| 1:D:258:ASN:HB2   | 1:D:261:THR:HG22  | 1.87                     | 0.55              |
| 1:E:706:ALA:HB1   | 1:E:713:ASP:HB3   | 1.87                     | 0.55              |
| 1:k:585:LYS:HG3   | 1:l:983:ALA:HB2   | 1.88                     | 0.55              |
| 1:k:795:ASN:ND2   | 1:k:982:CYS:SG    | 2.80                     | 0.55              |
| 1:m:185:LEU:HB3   | 1:m:388:ARG:HH22  | 1.71                     | 0.55              |
| 1:n:534:GLU:OE2   | 1:n:557:ARG:NH1   | 2.39                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:n:1228:TYR:HB2  | 1:n:1250:PHE:HD2  | 1.69                     | 0.55              |
| 1:p:1042:ILE:HD11 | 1:p:1066:ASN:HD22 | 1.71                     | 0.55              |
| 1:q:430:TYR:HA    | 1:q:439:GLN:O     | 2.06                     | 0.55              |
| 2:2:206:GLU:HG2   | 2:3:132:TYR:O     | 2.06                     | 0.55              |
| 2:3:185:VAL:HG13  | 2:3:225:ALA:HB2   | 1.88                     | 0.55              |
| 2:e:206:GLU:HG2   | 2:h:132:TYR:O     | 2.06                     | 0.55              |
| 4:S:217:HIS:HA    | 4:S:220:ILE:HG12  | 1.88                     | 0.55              |
| 5:z:134:VAL:HB    | 5:z:138:LEU:HD23  | 1.89                     | 0.55              |
| 5:d:97:PRO:HG2    | 5:d:98:VAL:HG23   | 1.88                     | 0.55              |
| 1:B:1171:ARG:HE   | 1:B:1339:ILE:HD13 | 1.72                     | 0.55              |
| 1:C:9:GLU:OE2     | 1:C:37:ARG:NH1    | 2.33                     | 0.55              |
| 1:D:285:LEU:HD23  | 1:D:292:ILE:HD13  | 1.87                     | 0.55              |
| 1:D:618:LEU:HD22  | 1:D:864:LEU:HG    | 1.88                     | 0.55              |
| 1:E:332:ARG:HH11  | 1:E:342:PRO:HD3   | 1.70                     | 0.55              |
| 1:F:808:LEU:HD11  | 1:F:914:LEU:HD22  | 1.87                     | 0.55              |
| 1:F:1116:ARG:HB3  | 1:F:1121:ALA:HA   | 1.89                     | 0.55              |
| 1:H:4:ASN:ND2     | 1:I:318:ALA:O     | 2.39                     | 0.55              |
| 1:H:393:THR:HA    | 1:H:1023:THR:HA   | 1.87                     | 0.55              |
| 1:k:131:GLU:OE2   | 1:l:111:ARG:NH1   | 2.40                     | 0.55              |
| 1:k:200:HIS:CE1   | 1:p:1084:ARG:HB3  | 2.41                     | 0.55              |
| 1:k:200:HIS:CE1   | 1:p:1085:ARG:NE   | 2.74                     | 0.55              |
| 1:k:627:GLU:HA    | 1:k:630:ILE:HG13  | 1.88                     | 0.55              |
| 1:k:744:HIS:HA    | 2:2:174:ARG:HA    | 1.88                     | 0.55              |
| 1:l:522:GLU:HG2   | 1:l:525:LYS:HD2   | 1.88                     | 0.55              |
| 1:l:1310:THR:HB   | 1:l:1339:ILE:HB   | 1.88                     | 0.55              |
| 1:n:448:LYS:HD2   | 1:n:1096:ASP:HB3  | 1.88                     | 0.55              |
| 2:3:93:PRO:CG     | 2:3:195:TYR:CZ    | 2.85                     | 0.55              |
| 2:h:238:LEU:HD22  | 2:h:271:VAL:CG2   | 2.36                     | 0.55              |
| 2:h:272:ASP:OD2   | 2:h:275:THR:CG2   | 2.54                     | 0.55              |
| 3:Q:85:LEU:HD22   | 3:Q:88:LEU:HD12   | 1.87                     | 0.55              |
| 4:V:189:TYR:HB2   | 4:V:209:VAL:HG13  | 1.88                     | 0.55              |
| 5:Y:24:LEU:HG     | 5:Y:27:ALA:HB2    | 1.88                     | 0.55              |
| 5:1:112:VAL:HG11  | 5:1:181:PRO:HD3   | 1.87                     | 0.55              |
| 1:A:713:ASP:O     | 1:A:783:LYS:NZ    | 2.36                     | 0.55              |
| 1:D:603:LEU:HB3   | 1:D:794:LEU:HD21  | 1.89                     | 0.55              |
| 1:D:819:LEU:CG    | 3:M:58:GLN:HE21   | 1.91                     | 0.55              |
| 1:H:758:MET:HG3   | 3:Q:83:ASP:HB2    | 1.88                     | 0.55              |
| 1:H:1018:LEU:HD12 | 1:H:1018:LEU:H    | 1.69                     | 0.55              |
| 1:k:419:ASP:OD1   | 1:k:424:GLN:NE2   | 2.39                     | 0.55              |
| 1:k:500:PHE:HZ    | 1:k:507:PRO:HD3   | 1.70                     | 0.55              |
| 1:m:328:GLN:HE21  | 1:m:342:PRO:HD2   | 1.71                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:n:285:LEU:HD23  | 1:n:292:ILE:HD13  | 1.88                     | 0.55              |
| 1:n:695:LEU:O     | 1:o:952:ARG:NH1   | 2.39                     | 0.55              |
| 1:o:808:LEU:HD11  | 1:o:914:LEU:HD13  | 1.87                     | 0.55              |
| 1:p:698:ARG:HG3   | 1:p:703:PRO:HA    | 1.87                     | 0.55              |
| 1:q:139:HIS:O     | 1:q:154:ASN:ND2   | 2.39                     | 0.55              |
| 2:i:66:ARG:HH12   | 2:i:69:GLN:NE2    | 1.89                     | 0.55              |
| 2:i:208:PRO:CB    | 5:c:229:LYS:HZ3   | 2.19                     | 0.55              |
| 2:j:93:PRO:HG3    | 2:j:195:TYR:OH    | 2.03                     | 0.55              |
| 5:l:60:ARG:NH1    | 5:l:286:VAL:O     | 2.38                     | 0.55              |
| 1:B:419:ASP:OD1   | 1:B:424:GLN:NE2   | 2.39                     | 0.55              |
| 1:C:1177:ARG:HG2  | 1:C:1218:SER:HA   | 1.88                     | 0.55              |
| 1:D:925:ARG:HH11  | 1:D:975:PHE:HB2   | 1.70                     | 0.55              |
| 1:E:492:HIS:HD2   | 1:E:495:ARG:HB2   | 1.71                     | 0.55              |
| 1:F:722:GLN:NE2   | 1:F:904:GLY:O     | 2.39                     | 0.55              |
| 1:G:393:THR:HA    | 1:G:1023:THR:HA   | 1.88                     | 0.55              |
| 1:k:71:ALA:HB3    | 1:k:371:GLU:HB2   | 1.88                     | 0.55              |
| 1:k:1042:ILE:HG13 | 1:k:1066:ASN:HB2  | 1.87                     | 0.55              |
| 1:k:1173:PRO:HB3  | 1:k:1306:LEU:HA   | 1.87                     | 0.55              |
| 1:l:278:HIS:HB2   | 1:l:374:ARG:HD2   | 1.88                     | 0.55              |
| 1:l:758:MET:SD    | 3:s:82:LEU:HD23   | 2.46                     | 0.55              |
| 1:l:1031:LEU:HG   | 1:l:1079:CYS:HB3  | 1.88                     | 0.55              |
| 1:m:127:THR:HA    | 1:m:1061:VAL:O    | 2.05                     | 0.55              |
| 1:m:560:VAL:HA    | 1:m:999:MET:HE3   | 1.88                     | 0.55              |
| 2:f:66:ARG:CZ     | 2:f:68:THR:CG2    | 2.77                     | 0.55              |
| 2:i:110:ALA:CB    | 5:c:225:MET:HG2   | 2.37                     | 0.55              |
| 2:i:185:VAL:HG13  | 2:i:225:ALA:HB2   | 1.88                     | 0.55              |
| 4:U:153:ARG:HH21  | 5:c:310:LYS:HE2   | 1.71                     | 0.55              |
| 5:b:129:VAL:O     | 5:b:131:PRO:HD3   | 2.06                     | 0.55              |
| 1:B:626:PHE:HE2   | 1:B:662:ARG:HG2   | 1.69                     | 0.55              |
| 1:D:42:ASP:O      | 1:G:133:SER:OG    | 2.24                     | 0.55              |
| 1:E:665:ASP:OD2   | 1:F:607:GLN:NE2   | 2.37                     | 0.55              |
| 1:G:701:ASP:OD2   | 1:G:1108:ASN:ND2  | 2.39                     | 0.55              |
| 1:H:1256:ILE:HA   | 1:H:1259:ASN:HD22 | 1.70                     | 0.55              |
| 1:k:743:ALA:HB3   | 2:2:173:MET:N     | 2.22                     | 0.55              |
| 1:k:909:THR:HA    | 1:k:932:LEU:HD11  | 1.88                     | 0.55              |
| 1:k:1207:GLN:O    | 1:p:437:ILE:HD13  | 2.06                     | 0.55              |
| 1:l:119:LYS:NZ    | 1:l:1071:GLY:O    | 2.38                     | 0.55              |
| 1:q:1115:VAL:CG1  | 1:q:1119:THR:HG1  | 2.18                     | 0.55              |
| 4:S:199:ASP:OD1   | 4:S:199:ASP:N     | 2.40                     | 0.55              |
| 4:U:74:ASP:OD2    | 4:U:132:HIS:NE2   | 2.39                     | 0.55              |
| 4:U:110:GLY:HA2   | 4:U:114:GLU:HB3   | 1.88                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 5:X:46:ASP:OD2   | 5:X:50:LYS:NZ    | 2.35                     | 0.55              |
| 1:A:128:ILE:CG2  | 1:B:102:ALA:HB3  | 2.27                     | 0.55              |
| 1:A:606:HIS:HA   | 1:A:909:THR:HG21 | 1.88                     | 0.55              |
| 1:A:1104:HIS:O   | 1:A:1116:ARG:NH1 | 2.40                     | 0.55              |
| 1:B:130:PHE:HB2  | 1:B:1059:PHE:HB2 | 1.88                     | 0.55              |
| 1:C:129:PRO:O    | 1:D:100:ARG:NH1  | 2.33                     | 0.55              |
| 1:C:702:GLU:OE2  | 1:C:715:ARG:NH2  | 2.34                     | 0.55              |
| 1:D:24:ILE:HD11  | 1:H:115:VAL:HB   | 1.89                     | 0.55              |
| 1:D:147:THR:HG21 | 1:H:82:HIS:HB2   | 1.88                     | 0.55              |
| 1:D:1297:LYS:H   | 1:D:1297:LYS:HD2 | 1.72                     | 0.55              |
| 1:E:15:ASP:OD1   | 1:l:61:LYS:NZ    | 2.40                     | 0.55              |
| 1:F:1072:LEU:O   | 1:l:33:PHE:CE1   | 2.60                     | 0.55              |
| 1:G:232:ASP:OD1  | 1:G:1352:ASN:ND2 | 2.39                     | 0.55              |
| 1:k:957:PHE:O    | 1:k:959:LEU:HG   | 2.06                     | 0.55              |
| 1:l:1261:THR:O   | 1:l:1265:THR:OG1 | 2.23                     | 0.55              |
| 1:m:602:SER:HA   | 1:m:646:LEU:HD12 | 1.87                     | 0.55              |
| 1:o:276:SER:HB3  | 1:o:280:VAL:HG13 | 1.88                     | 0.55              |
| 1:o:715:ARG:HA   | 1:o:731:VAL:HG21 | 1.87                     | 0.55              |
| 1:p:207:MET:N    | 1:p:207:MET:SD   | 2.79                     | 0.55              |
| 1:q:1231:ARG:NH2 | 1:q:1253:ASP:OD1 | 2.40                     | 0.55              |
| 2:3:238:LEU:HD22 | 2:3:271:VAL:CG2  | 2.36                     | 0.55              |
| 2:3:272:ASP:OD2  | 2:3:275:THR:CG2  | 2.54                     | 0.55              |
| 2:j:185:VAL:HG13 | 2:j:225:ALA:HB2  | 1.88                     | 0.55              |
| 4:y:73:LEU:CD2   | 4:y:130:VAL:HG23 | 2.37                     | 0.55              |
| 1:A:128:ILE:HD11 | 1:A:168:THR:HG23 | 1.87                     | 0.55              |
| 1:A:650:ALA:O    | 1:A:785:TYR:OH   | 2.25                     | 0.55              |
| 1:B:504:ARG:NE   | 1:B:946:ASP:OD2  | 2.39                     | 0.55              |
| 1:D:22:THR:OG1   | 1:D:23:HIS:N     | 2.40                     | 0.55              |
| 1:D:119:LYS:NZ   | 1:D:1071:GLY:O   | 2.35                     | 0.55              |
| 1:E:560:VAL:HG11 | 1:E:576:ARG:HH12 | 1.71                     | 0.55              |
| 1:E:575:LEU:HD12 | 1:E:578:LYS:HD2  | 1.88                     | 0.55              |
| 1:F:104:GLY:HA3  | 1:F:107:ILE:HD12 | 1.88                     | 0.55              |
| 1:G:113:THR:HA   | 1:m:40:TYR:HA    | 1.88                     | 0.55              |
| 1:G:786:TYR:O    | 1:G:927:TYR:OH   | 2.22                     | 0.55              |
| 1:G:1016:PHE:HD2 | 1:G:1018:LEU:CD1 | 2.17                     | 0.55              |
| 1:H:128:ILE:HG22 | 1:I:102:ALA:HB3  | 1.88                     | 0.55              |
| 1:H:727:ASN:ND2  | 1:H:776:ASP:OD1  | 2.40                     | 0.55              |
| 1:I:275:VAL:HA   | 1:I:371:GLU:HB3  | 1.88                     | 0.55              |
| 1:I:1003:SER:O   | 1:I:1007:LEU:HB2 | 2.07                     | 0.55              |
| 1:m:664:GLY:HA2  | 1:n:644:ARG:HH11 | 1.72                     | 0.55              |
| 1:m:702:GLU:OE2  | 1:m:715:ARG:NH2  | 2.38                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:m:1041:VAL:HG12 | 1:m:1067:THR:HG22 | 1.89                     | 0.55              |
| 1:p:1179:ARG:NH1  | 1:p:1211:SER:O    | 2.38                     | 0.55              |
| 1:q:726:ARG:HB3   | 1:q:775:SER:HA    | 1.89                     | 0.55              |
| 2:3:66:ARG:HG3    | 2:3:69:GLN:H      | 1.72                     | 0.55              |
| 2:e:258:PHE:CD2   | 3:t:60:VAL:HG23   | 2.41                     | 0.55              |
| 5:1:31:ILE:O      | 5:1:67:THR:N      | 2.40                     | 0.55              |
| 5:c:146:MET:HG2   | 5:c:180:LEU:HD21  | 1.89                     | 0.55              |
| 1:A:248:THR:O     | 1:A:366:ARG:NH2   | 2.40                     | 0.55              |
| 1:B:605:ASP:OD2   | 1:B:644:ARG:NH2   | 2.39                     | 0.55              |
| 1:B:1219:GLN:HB2  | 1:B:1222:SER:HB3  | 1.89                     | 0.55              |
| 1:F:752:THR:O     | 3:O:86:ARG:NH2    | 2.40                     | 0.55              |
| 1:G:79:ILE:HB     | 1:G:1042:ILE:HG22 | 1.87                     | 0.55              |
| 1:H:603:LEU:HD23  | 1:H:794:LEU:HD11  | 1.89                     | 0.55              |
| 1:I:1166:ASP:HA   | 1:I:1170:PHE:HD2  | 1.71                     | 0.55              |
| 1:k:709:SER:HB3   | 1:k:712:HIS:HD2   | 1.71                     | 0.55              |
| 1:m:419:ASP:OD1   | 1:m:424:GLN:NE2   | 2.38                     | 0.55              |
| 1:m:777:GLU:HG3   | 1:n:951:GLN:HE21  | 1.71                     | 0.55              |
| 1:o:606:HIS:O     | 1:o:912:LYS:NZ    | 2.40                     | 0.55              |
| 1:o:1019:THR:HG23 | 1:o:1160:LEU:CD1  | 2.36                     | 0.55              |
| 1:q:653:TYR:HA    | 1:q:656:VAL:HG12  | 1.88                     | 0.55              |
| 4:y:73:LEU:HD21   | 4:y:131:VAL:CA    | 2.37                     | 0.55              |
| 5:a:89:CYS:HB3    | 5:a:306:LEU:HD11  | 1.89                     | 0.55              |
| 5:b:122:SER:HB2   | 5:b:127:ASP:HB3   | 1.89                     | 0.55              |
| 1:B:967:TYR:O     | 1:B:972:ARG:NH2   | 2.40                     | 0.55              |
| 1:F:820:THR:O     | 1:F:821:ALA:HB3   | 2.06                     | 0.55              |
| 1:G:539:PHE:O     | 1:G:557:ARG:NH2   | 2.40                     | 0.55              |
| 1:G:1195:LEU:HD22 | 1:G:1220:ARG:HH12 | 1.72                     | 0.55              |
| 1:H:709:SER:HB3   | 1:H:712:HIS:HD2   | 1.72                     | 0.55              |
| 1:H:965:HIS:HB3   | 1:H:968:HIS:HB2   | 1.89                     | 0.55              |
| 1:k:486:VAL:O     | 1:k:965:HIS:NE2   | 2.36                     | 0.55              |
| 1:l:225:LEU:O     | 1:l:233:ARG:NH2   | 2.39                     | 0.55              |
| 1:l:677:ARG:HH12  | 1:m:646:LEU:HD13  | 1.71                     | 0.55              |
| 1:l:713:ASP:O     | 1:l:783:LYS:NZ    | 2.39                     | 0.55              |
| 1:l:749:ASN:HD22  | 1:l:757:ARG:HG2   | 1.71                     | 0.55              |
| 1:l:950:TYR:HB3   | 1:l:957:PHE:CG    | 2.41                     | 0.55              |
| 1:l:1116:ARG:NH2  | 1:l:1122:ARG:O    | 2.39                     | 0.55              |
| 1:l:1126:VAL:HB   | 1:l:1130:GLU:HB2  | 1.89                     | 0.55              |
| 1:o:513:GLU:HA    | 1:o:973:THR:HG21  | 1.88                     | 0.55              |
| 2:2:66:ARG:C      | 2:2:67:GLU:HG2    | 2.32                     | 0.55              |
| 2:g:206:GLU:HG2   | 2:j:132:TYR:O     | 2.06                     | 0.55              |
| 3:x:41:ARG:HA     | 3:x:65:ILE:HG21   | 1.88                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:y:103:ASN:HA    | 4:y:106:ALA:HB3   | 1.89                     | 0.55              |
| 5:Y:172:ARG:HG2   | 5:Y:177:THR:HG22  | 1.88                     | 0.55              |
| 1:A:1048:VAL:HG22 | 1:A:1061:VAL:HG12 | 1.88                     | 0.55              |
| 1:F:925:ARG:NH2   | 1:F:971:HIS:O     | 2.38                     | 0.55              |
| 1:G:117:VAL:CG1   | 1:m:36:PHE:HB2    | 2.32                     | 0.55              |
| 1:G:598:VAL:HG11  | 1:G:647:LEU:HD23  | 1.89                     | 0.55              |
| 1:G:1156:CYS:HB2  | 1:G:1245:PRO:HD2  | 1.88                     | 0.55              |
| 1:H:1260:LYS:NZ   | 1:H:1268:GLU:OE1  | 2.33                     | 0.55              |
| 1:I:603:LEU:HD23  | 1:I:794:LEU:HD11  | 1.89                     | 0.55              |
| 1:I:863:HIS:CE1   | 3:R:93:LYS:HA     | 2.41                     | 0.55              |
| 1:k:152:LEU:HD12  | 1:l:333:ILE:HG12  | 1.87                     | 0.55              |
| 1:k:228:ILE:HG22  | 1:k:233:ARG:HH21  | 1.72                     | 0.55              |
| 1:k:758:MET:CG    | 3:r:83:ASP:HB2    | 2.27                     | 0.55              |
| 1:m:836:ASN:HB2   | 1:m:839:LEU:HD12  | 1.89                     | 0.55              |
| 1:n:275:VAL:HG23  | 1:n:1032:LEU:HB3  | 1.89                     | 0.55              |
| 1:n:639:ASN:ND2   | 1:n:848:THR:O     | 2.40                     | 0.55              |
| 1:n:1156:CYS:HB2  | 1:n:1245:PRO:HD2  | 1.88                     | 0.55              |
| 1:o:146:ASP:HA    | 1:o:150:ASP:HB3   | 1.89                     | 0.55              |
| 1:p:64:TRP:HH2    | 1:p:166:LYS:HB3   | 1.71                     | 0.55              |
| 1:p:130:PHE:O     | 1:p:1058:VAL:HA   | 2.07                     | 0.55              |
| 1:p:196:THR:HA    | 1:p:200:HIS:HD2   | 1.72                     | 0.55              |
| 1:q:602:SER:HB2   | 1:q:650:ALA:HA    | 1.89                     | 0.55              |
| 2:h:258:PHE:HZ    | 3:P:87:MET:HE3    | 1.72                     | 0.55              |
| 3:u:72:GLY:O      | 3:u:80:TYR:OH     | 2.25                     | 0.55              |
| 4:y:182:THR:HG21  | 4:y:186:ARG:HD2   | 1.89                     | 0.55              |
| 4:V:249:LEU:HB3   | 4:V:294:ALA:HA    | 1.88                     | 0.55              |
| 1:B:488:GLU:HG3   | 1:B:962:ILE:HG13  | 1.88                     | 0.54              |
| 1:C:183:VAL:HG21  | 1:C:1067:THR:HG21 | 1.89                     | 0.54              |
| 1:C:602:SER:HB3   | 1:C:647:LEU:H     | 1.71                     | 0.54              |
| 1:C:606:HIS:HA    | 1:C:909:THR:HG21  | 1.89                     | 0.54              |
| 1:C:713:ASP:O     | 1:C:783:LYS:NZ    | 2.40                     | 0.54              |
| 1:I:813:PHE:CD2   | 3:R:85:LEU:HB2    | 2.42                     | 0.54              |
| 1:I:957:PHE:CB    | 1:I:959:LEU:HD11  | 2.34                     | 0.54              |
| 1:k:951:GLN:HE21  | 1:p:777:GLU:HG3   | 1.71                     | 0.54              |
| 1:l:752:THR:O     | 3:s:86:ARG:CZ     | 2.55                     | 0.54              |
| 1:m:131:GLU:H     | 1:n:112:GLN:HE22  | 1.54                     | 0.54              |
| 1:m:191:CYS:SG    | 1:m:243:TYR:OH    | 2.64                     | 0.54              |
| 1:n:664:GLY:HA2   | 1:o:644:ARG:NH1   | 2.22                     | 0.54              |
| 1:o:523:PHE:O     | 1:o:528:ASN:ND2   | 2.37                     | 0.54              |
| 1:p:708:VAL:HG22  | 1:p:1003:SER:HA   | 1.88                     | 0.54              |
| 1:p:866:ALA:O     | 3:w:86:ARG:NE     | 2.35                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:q:1173:PRO:HG3  | 1:q:1306:LEU:HD23 | 1.89                     | 0.54              |
| 2:j:238:LEU:HD22  | 2:j:271:VAL:CG2   | 2.36                     | 0.54              |
| 3:J:61:ILE:HG13   | 3:J:84:LEU:HD11   | 1.88                     | 0.54              |
| 4:y:265:SER:HA    | 4:y:278:VAL:HA    | 1.88                     | 0.54              |
| 5:W:196:VAL:HG13  | 5:W:283:ILE:HD11  | 1.89                     | 0.54              |
| 5:d:122:SER:HB2   | 5:d:127:ASP:HB3   | 1.87                     | 0.54              |
| 1:A:1019:THR:CB   | 1:A:1160:LEU:HD11 | 2.37                     | 0.54              |
| 1:A:1166:ASP:HA   | 1:A:1170:PHE:HB2  | 1.89                     | 0.54              |
| 1:B:606:HIS:HA    | 1:B:909:THR:HG21  | 1.89                     | 0.54              |
| 1:C:1009:ARG:NH1  | 1:C:1118:ALA:O    | 2.40                     | 0.54              |
| 1:F:420:THR:HG22  | 1:F:422:GLU:H     | 1.72                     | 0.54              |
| 1:F:639:ASN:OD1   | 1:F:642:ARG:NH1   | 2.40                     | 0.54              |
| 1:G:314:VAL:HB    | 1:n:326:PHE:CE1   | 2.42                     | 0.54              |
| 1:G:1300:ARG:H    | 1:G:1303:GLN:HE21 | 1.56                     | 0.54              |
| 1:I:433:ASN:HD21  | 1:I:439:GLN:HE21  | 1.53                     | 0.54              |
| 1:k:294:ARG:HD2   | 1:k:357:GLN:HB3   | 1.89                     | 0.54              |
| 1:k:688:ARG:O     | 1:k:691:GLU:HG2   | 2.06                     | 0.54              |
| 1:l:950:TYR:C     | 1:l:957:PHE:CE2   | 2.84                     | 0.54              |
| 1:m:400:LEU:HD23  | 1:m:1166:ASP:HB3  | 1.89                     | 0.54              |
| 1:m:1171:ARG:NH2  | 1:m:1338:SER:O    | 2.41                     | 0.54              |
| 1:o:248:THR:O     | 1:o:366:ARG:NH2   | 2.40                     | 0.54              |
| 1:o:309:SER:HB3   | 1:o:312:ASN:HB2   | 1.89                     | 0.54              |
| 1:q:493:ALA:HA    | 1:q:496:ARG:HB2   | 1.89                     | 0.54              |
| 2:i:238:LEU:HD22  | 2:i:271:VAL:CG2   | 2.36                     | 0.54              |
| 5:z:33:TYR:HD2    | 5:z:35:HIS:HB2    | 1.72                     | 0.54              |
| 1:B:1310:THR:HB   | 1:B:1339:ILE:HB   | 1.89                     | 0.54              |
| 1:C:483:ARG:NH2   | 1:C:508:PRO:O     | 2.41                     | 0.54              |
| 1:C:818:PHE:CG    | 3:L:88:LEU:HD13   | 2.41                     | 0.54              |
| 1:E:14:LEU:HB2    | 1:l:58:TYR:HD1    | 1.72                     | 0.54              |
| 1:E:15:ASP:OD2    | 1:l:61:LYS:NZ     | 2.34                     | 0.54              |
| 1:F:587:ARG:NH1   | 1:F:589:PRO:O     | 2.40                     | 0.54              |
| 1:G:813:PHE:CE2   | 3:P:85:LEU:CB     | 2.91                     | 0.54              |
| 1:G:1021:VAL:HG23 | 1:G:1245:PRO:HB2  | 1.89                     | 0.54              |
| 1:I:909:THR:HA    | 1:I:932:LEU:HD11  | 1.89                     | 0.54              |
| 1:k:522:GLU:HG2   | 1:k:525:LYS:HD2   | 1.88                     | 0.54              |
| 1:l:305:LYS:N     | 1:l:349:GLN:OE1   | 2.38                     | 0.54              |
| 1:m:245:ASP:OD1   | 1:m:364:GLY:N     | 2.41                     | 0.54              |
| 1:m:866:ALA:O     | 3:t:86:ARG:NH2    | 2.40                     | 0.54              |
| 1:n:388:ARG:HD3   | 1:n:1295:VAL:H    | 1.72                     | 0.54              |
| 1:n:425:LEU:HD12  | 1:n:575:LEU:HD23  | 1.88                     | 0.54              |
| 1:o:813:PHE:HE2   | 1:o:865:VAL:HG21  | 1.72                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:p:1256:ILE:HA   | 1:p:1259:ASN:HD22 | 1.73                     | 0.54              |
| 2:h:185:VAL:HG13  | 2:h:225:ALA:HB2   | 1.88                     | 0.54              |
| 5:z:296:CYS:N     | 5:z:306:LEU:O     | 2.37                     | 0.54              |
| 5:b:44:GLY:HA3    | 5:b:128:LEU:O     | 2.07                     | 0.54              |
| 1:A:119:LYS:NZ    | 1:A:1072:LEU:O    | 2.41                     | 0.54              |
| 1:A:952:ARG:HH22  | 1:F:696:ASN:HA    | 1.72                     | 0.54              |
| 1:A:1228:TYR:HB2  | 1:A:1250:PHE:HD2  | 1.73                     | 0.54              |
| 1:C:476:ARG:HD3   | 1:C:532:PHE:HZ    | 1.72                     | 0.54              |
| 1:C:500:PHE:HZ    | 1:C:507:PRO:HD3   | 1.72                     | 0.54              |
| 1:D:975:PHE:HE1   | 1:D:995:MET:HB3   | 1.72                     | 0.54              |
| 1:E:37:ARG:NH2    | 1:E:43:ASP:OD2    | 2.40                     | 0.54              |
| 1:E:504:ARG:NH1   | 2:j:135:ASP:OD1   | 2.40                     | 0.54              |
| 1:H:300:PRO:HB3   | 1:H:351:LEU:HD13  | 1.90                     | 0.54              |
| 1:H:777:GLU:HG3   | 1:I:951:GLN:HE21  | 1.72                     | 0.54              |
| 1:I:603:LEU:HB3   | 1:I:794:LEU:HD21  | 1.88                     | 0.54              |
| 1:I:753:SER:HB3   | 3:R:87:MET:HG2    | 1.89                     | 0.54              |
| 1:l:930:PRO:HG3   | 1:l:957:PHE:CE2   | 2.43                     | 0.54              |
| 1:n:708:VAL:HG22  | 1:n:1003:SER:HA   | 1.90                     | 0.54              |
| 2:3:66:ARG:HD2    | 2:3:68:THR:HG23   | 1.89                     | 0.54              |
| 2:j:66:ARG:NH2    | 2:j:294:LEU:O     | 2.40                     | 0.54              |
| 4:y:159:MET:O     | 4:y:160:LEU:HB3   | 2.07                     | 0.54              |
| 5:X:112:VAL:O     | 5:X:113:PHE:CE1   | 2.58                     | 0.54              |
| 1:A:635:ARG:HH11  | 1:A:849:ASP:HB2   | 1.72                     | 0.54              |
| 1:B:285:LEU:HD23  | 1:B:292:ILE:HD13  | 1.90                     | 0.54              |
| 1:D:815:THR:OG1   | 1:D:836:ASN:ND2   | 2.40                     | 0.54              |
| 1:E:13:LYS:HA     | 1:l:57:THR:O      | 2.07                     | 0.54              |
| 1:G:1074:TYR:H    | 1:m:21:LEU:HD21   | 1.72                     | 0.54              |
| 1:G:1097:LEU:HA   | 1:G:1100:VAL:HB   | 1.88                     | 0.54              |
| 1:k:1048:VAL:HG22 | 1:k:1061:VAL:HG12 | 1.90                     | 0.54              |
| 1:l:1148:LEU:HD13 | 1:l:1153:ARG:HH11 | 1.71                     | 0.54              |
| 1:m:343:GLU:HB3   | 1:m:348:ASP:HB3   | 1.88                     | 0.54              |
| 1:m:952:ARG:NH2   | 1:m:955:GLY:O     | 2.41                     | 0.54              |
| 1:n:198:MET:HG3   | 1:n:250:CYS:HA    | 1.89                     | 0.54              |
| 1:q:1018:LEU:HD23 | 1:q:1157:GLU:HB3  | 1.90                     | 0.54              |
| 1:q:1222:SER:H    | 1:q:1226:VAL:HG22 | 1.73                     | 0.54              |
| 4:S:126:ARG:HD3   | 4:S:192:ILE:HD13  | 1.88                     | 0.54              |
| 4:V:186:ARG:HG2   | 4:V:260:SER:HB2   | 1.89                     | 0.54              |
| 5:d:172:ARG:HG3   | 5:d:177:THR:HG22  | 1.88                     | 0.54              |
| 1:A:925:ARG:HE    | 1:A:976:SER:HB3   | 1.72                     | 0.54              |
| 1:C:539:PHE:O     | 1:C:557:ARG:NH2   | 2.41                     | 0.54              |
| 1:C:925:ARG:NH2   | 1:C:966:GLU:OE2   | 2.40                     | 0.54              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:C:1171:ARG:NH2  | 1:C:1330:ASP:OD2 | 2.40                     | 0.54              |
| 1:D:619:ILE:HD12  | 1:D:626:PHE:HA   | 1.90                     | 0.54              |
| 1:E:1322:LYS:HE2  | 1:F:1331:GLU:HG2 | 1.89                     | 0.54              |
| 1:G:952:ARG:HB3   | 1:G:955:GLY:HA2  | 1.90                     | 0.54              |
| 1:I:818:PHE:CD1   | 3:R:88:LEU:HD22  | 2.43                     | 0.54              |
| 1:k:882:ASP:N     | 1:k:882:ASP:OD1  | 2.40                     | 0.54              |
| 1:k:1160:LEU:HD23 | 1:k:1214:ASN:HB2 | 1.89                     | 0.54              |
| 1:l:494:THR:HG23  | 1:l:921:ILE:HD11 | 1.89                     | 0.54              |
| 1:l:606:HIS:HA    | 1:l:909:THR:HG21 | 1.89                     | 0.54              |
| 1:l:1156:CYS:SG   | 1:l:1244:SER:OG  | 2.65                     | 0.54              |
| 1:m:278:HIS:O     | 1:m:282:GLN:NE2  | 2.40                     | 0.54              |
| 1:q:1018:LEU:HA   | 1:q:1158:VAL:O   | 2.08                     | 0.54              |
| 5:W:119:GLY:HA3   | 5:W:129:VAL:HA   | 1.90                     | 0.54              |
| 5:Z:7:VAL:HG22    | 5:Z:38:LEU:HB2   | 1.89                     | 0.54              |
| 1:A:606:HIS:CD2   | 1:F:661:THR:HA   | 2.43                     | 0.54              |
| 1:A:813:PHE:CG    | 3:J:85:LEU:HG    | 2.42                     | 0.54              |
| 1:B:786:TYR:O     | 1:B:927:TYR:OH   | 2.23                     | 0.54              |
| 1:D:481:CYS:SG    | 1:D:482:ARG:N    | 2.81                     | 0.54              |
| 1:D:627:GLU:HA    | 1:D:630:ILE:HG13 | 1.88                     | 0.54              |
| 1:E:71:ALA:HB3    | 1:E:371:GLU:HB2  | 1.89                     | 0.54              |
| 1:E:925:ARG:NH1   | 1:E:972:ARG:O    | 2.41                     | 0.54              |
| 1:G:281:VAL:HG11  | 1:G:372:HIS:HB2  | 1.90                     | 0.54              |
| 1:H:660:ALA:O     | 1:I:606:HIS:NE2  | 2.36                     | 0.54              |
| 1:m:605:ASP:HB3   | 1:m:608:TYR:HB2  | 1.90                     | 0.54              |
| 1:m:882:ASP:N     | 1:m:882:ASP:OD1  | 2.41                     | 0.54              |
| 1:n:539:PHE:HE2   | 1:n:890:PRO:HB2  | 1.71                     | 0.54              |
| 1:o:1171:ARG:HH21 | 1:o:1330:ASP:HB3 | 1.73                     | 0.54              |
| 1:q:1013:HIS:ND1  | 1:q:1014:PRO:O   | 2.37                     | 0.54              |
| 1:q:1094:MET:N    | 1:q:1094:MET:SD  | 2.77                     | 0.54              |
| 4:S:110:GLY:HA2   | 4:S:114:GLU:HB3  | 1.88                     | 0.54              |
| 4:V:190:PHE:HB2   | 4:V:255:LEU:HD22 | 1.90                     | 0.54              |
| 5:X:307:CYS:C     | 5:X:308:ILE:CG1  | 2.77                     | 0.54              |
| 5:1:295:VAL:HA    | 5:1:307:CYS:HA   | 1.90                     | 0.54              |
| 1:A:952:ARG:NH2   | 1:F:695:LEU:O    | 2.40                     | 0.54              |
| 1:A:1167:LEU:HD13 | 1:F:1314:GLN:OE1 | 2.07                     | 0.54              |
| 1:D:389:ASP:N     | 1:D:389:ASP:OD1  | 2.39                     | 0.54              |
| 1:D:463:GLU:OE2   | 1:D:467:GLN:NE2  | 2.41                     | 0.54              |
| 1:E:667:ALA:N     | 1:F:643:GLN:HG3  | 2.23                     | 0.54              |
| 1:F:300:PRO:HB3   | 1:F:351:LEU:HB3  | 1.90                     | 0.54              |
| 1:F:344:SER:H     | 1:F:347:LEU:HD12 | 1.73                     | 0.54              |
| 1:H:535:LEU:HB2   | 1:H:541:PHE:HE2  | 1.73                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:I:446:ALA:HA    | 1:I:1094:MET:HG3  | 1.89                     | 0.54              |
| 1:k:595:THR:HA    | 1:k:675:HIS:HD2   | 1.73                     | 0.54              |
| 1:k:750:PRO:CD    | 2:3:269:ARG:NH2   | 2.70                     | 0.54              |
| 1:k:795:ASN:OD1   | 1:k:984:HIS:CE1   | 2.60                     | 0.54              |
| 1:k:1179:ARG:NH2  | 1:k:1204:PRO:O    | 2.41                     | 0.54              |
| 1:m:309:SER:HB3   | 1:m:312:ASN:HB2   | 1.89                     | 0.54              |
| 1:n:634:THR:HB    | 1:n:668:VAL:HG11  | 1.90                     | 0.54              |
| 1:n:749:ASN:ND2   | 1:n:754:ASP:OD1   | 2.40                     | 0.54              |
| 1:n:813:PHE:CD2   | 3:u:85:LEU:HG     | 2.43                     | 0.54              |
| 1:o:275:VAL:HG12  | 1:o:371:GLU:HB3   | 1.88                     | 0.54              |
| 1:p:497:LEU:HD13  | 1:p:963:PHE:HZ    | 1.73                     | 0.54              |
| 1:q:1313:THR:HG23 | 1:q:1316:LEU:H    | 1.71                     | 0.54              |
| 4:y:141:THR:HG21  | 4:y:147:LEU:H     | 1.73                     | 0.54              |
| 4:y:166:PRO:HG3   | 4:y:279:LYS:HE3   | 1.89                     | 0.54              |
| 4:T:74:ASP:HB2    | 4:T:130:VAL:HA    | 1.90                     | 0.54              |
| 5:z:173:TYR:HB3   | 5:z:176:ALA:HB3   | 1.90                     | 0.54              |
| 1:A:1315:ALA:HB2  | 1:B:408:TYR:CD2   | 2.43                     | 0.54              |
| 1:C:413:ASN:O     | 1:D:413:ASN:ND2   | 2.41                     | 0.54              |
| 1:C:708:VAL:HG22  | 1:C:1003:SER:HA   | 1.88                     | 0.54              |
| 1:F:197:LEU:O     | 1:l:22:THR:HG22   | 2.07                     | 0.54              |
| 1:F:1173:PRO:HB3  | 1:F:1306:LEU:HA   | 1.90                     | 0.54              |
| 1:G:558:ILE:HD13  | 1:G:970:TRP:HA    | 1.90                     | 0.54              |
| 1:G:1314:GLN:HE22 | 1:H:1167:LEU:HD13 | 1.73                     | 0.54              |
| 1:H:480:LEU:HD23  | 1:H:550:VAL:HG11  | 1.89                     | 0.54              |
| 1:I:819:LEU:HD12  | 3:R:58:GLN:HB3    | 1.90                     | 0.54              |
| 1:k:79:ILE:HB     | 1:k:1042:ILE:HG22 | 1.89                     | 0.54              |
| 1:n:1039:THR:HB   | 1:n:1070:MET:HG2  | 1.89                     | 0.54              |
| 1:q:1040:ALA:HB2  | 1:q:1070:MET:HE2  | 1.88                     | 0.54              |
| 2:3:130:ALA:C     | 2:3:132:TYR:N     | 2.66                     | 0.54              |
| 5:z:87:GLY:HA3    | 5:1:86:HIS:HB3    | 1.89                     | 0.54              |
| 1:A:235:ARG:HH12  | 1:A:243:TYR:HB2   | 1.72                     | 0.54              |
| 1:B:924:HIS:HB3   | 1:B:927:TYR:HB2   | 1.89                     | 0.54              |
| 1:C:1344:PRO:HB2  | 1:C:1347:GLN:HB2  | 1.90                     | 0.54              |
| 1:D:632:LEU:O     | 1:D:636:CYS:N     | 2.41                     | 0.54              |
| 1:G:488:GLU:HG3   | 1:G:962:ILE:HA    | 1.89                     | 0.54              |
| 1:k:1195:LEU:HD22 | 1:k:1220:ARG:HH12 | 1.72                     | 0.54              |
| 1:l:929:ASP:HB3   | 1:l:932:LEU:HB3   | 1.89                     | 0.54              |
| 1:l:1025:THR:HB   | 1:l:1087:ARG:HB3  | 1.90                     | 0.54              |
| 1:m:421:ALA:HA    | 1:m:424:GLN:HB2   | 1.90                     | 0.54              |
| 1:n:732:ARG:NH1   | 1:n:895:GLU:OE1   | 2.40                     | 0.54              |
| 1:o:395:TYR:OH    | 1:o:1172:TYR:O    | 2.26                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:p:492:HIS:O     | 1:p:496:ARG:HB2   | 2.08                     | 0.54              |
| 1:p:907:MET:HE2   | 1:p:932:LEU:HD11  | 1.90                     | 0.54              |
| 1:p:1029:ASP:HB2  | 1:p:1082:HIS:HB3  | 1.90                     | 0.54              |
| 1:q:66:THR:O      | 1:q:70:THR:OG1    | 2.26                     | 0.54              |
| 2:j:275:THR:O     | 2:j:279:LEU:CG    | 2.52                     | 0.54              |
| 4:V:61:VAL:HG11   | 4:V:88:PHE:CD2    | 2.28                     | 0.54              |
| 5:z:106:LEU:HD12  | 5:z:133:ILE:HG22  | 1.90                     | 0.54              |
| 5:Z:280:ILE:HA    | 5:Z:283:ILE:HG22  | 1.89                     | 0.54              |
| 5:d:20:LYS:HE3    | 5:d:121:VAL:HG12  | 1.89                     | 0.54              |
| 1:D:159:ASN:ND2   | 1:E:338:GLN:HB2   | 2.24                     | 0.53              |
| 1:D:191:CYS:O     | 1:D:195:ARG:N     | 2.40                     | 0.53              |
| 1:D:539:PHE:O     | 1:D:557:ARG:NH2   | 2.41                     | 0.53              |
| 1:D:639:ASN:ND2   | 1:D:846:VAL:O     | 2.35                     | 0.53              |
| 1:E:15:ASP:CG     | 1:l:61:LYS:NZ     | 2.66                     | 0.53              |
| 1:E:1116:ARG:HD3  | 1:E:1123:ARG:HA   | 1.89                     | 0.53              |
| 1:F:567:LEU:HD22  | 1:F:1161:THR:HG21 | 1.89                     | 0.53              |
| 1:F:921:ILE:HG22  | 1:F:923:PHE:HB3   | 1.90                     | 0.53              |
| 1:G:93:LEU:HA     | 1:G:118:SER:HA    | 1.90                     | 0.53              |
| 1:G:431:PHE:CE1   | 1:G:1310:THR:OG1  | 2.60                     | 0.53              |
| 1:G:495:ARG:NH2   | 1:G:804:ASN:OD1   | 2.41                     | 0.53              |
| 1:G:606:HIS:HA    | 1:G:909:THR:HG21  | 1.90                     | 0.53              |
| 1:G:610:GLU:HG3   | 1:G:911:PRO:HB3   | 1.90                     | 0.53              |
| 1:G:810:VAL:HG21  | 3:P:78:LEU:HD22   | 1.89                     | 0.53              |
| 1:G:1018:LEU:HG   | 1:G:1159:ILE:HD13 | 1.90                     | 0.53              |
| 1:H:819:LEU:HD11  | 3:Q:60:VAL:HG12   | 1.90                     | 0.53              |
| 1:k:695:LEU:HB3   | 1:k:704:LEU:HD23  | 1.90                     | 0.53              |
| 1:l:698:ARG:HB2   | 1:l:703:PRO:HA    | 1.89                     | 0.53              |
| 1:p:500:PHE:HZ    | 1:p:507:PRO:HD3   | 1.74                     | 0.53              |
| 1:p:1320:GLN:HE22 | 1:p:1329:LEU:HB2  | 1.74                     | 0.53              |
| 2:i:130:ALA:C     | 2:i:132:TYR:N     | 2.66                     | 0.53              |
| 3:v:72:GLY:O      | 3:v:80:TYR:OH     | 2.24                     | 0.53              |
| 1:B:415:ILE:HD12  | 1:B:1315:ALA:HB1  | 1.90                     | 0.53              |
| 1:B:446:ALA:HA    | 1:B:1094:MET:HG3  | 1.90                     | 0.53              |
| 1:D:1280:GLU:OE2  | 1:E:206:ARG:NH1   | 2.42                     | 0.53              |
| 1:G:431:PHE:CE1   | 1:G:1310:THR:C    | 2.83                     | 0.53              |
| 1:G:1003:SER:O    | 1:G:1007:LEU:N    | 2.36                     | 0.53              |
| 1:G:1149:LEU:HD11 | 1:H:1182:SER:HB3  | 1.90                     | 0.53              |
| 1:H:210:ARG:NH1   | 1:H:1187:ASP:OD2  | 2.41                     | 0.53              |
| 1:H:1179:ARG:NH2  | 1:H:1204:PRO:O    | 2.42                     | 0.53              |
| 1:l:930:PRO:O     | 1:l:934:ALA:HB2   | 2.08                     | 0.53              |
| 1:m:51:PHE:CD2    | 1:n:87:MET:HB3    | 2.42                     | 0.53              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:m:152:LEU:HG   | 1:n:337:SER:HB2   | 1.90                     | 0.53              |
| 1:m:208:ALA:O    | 1:m:213:ARG:NH1   | 2.39                     | 0.53              |
| 1:m:432:TYR:CE2  | 1:m:1321:LEU:HD11 | 2.43                     | 0.53              |
| 4:T:51:ARG:HD3   | 4:T:147:LEU:HD21  | 1.90                     | 0.53              |
| 4:V:92:MET:HA    | 4:V:102:LYS:HG3   | 1.90                     | 0.53              |
| 5:b:267:THR:HA   | 5:b:270:LEU:HD12  | 1.90                     | 0.53              |
| 1:A:1027:GLU:OE1 | 1:A:1084:ARG:NH2  | 2.41                     | 0.53              |
| 1:C:877:ILE:HB   | 1:C:898:GLN:HB2   | 1.89                     | 0.53              |
| 1:D:877:ILE:HB   | 1:D:898:GLN:HB2   | 1.89                     | 0.53              |
| 1:E:813:PHE:HZ   | 1:E:865:VAL:HG21  | 1.71                     | 0.53              |
| 1:G:390:VAL:HG22 | 1:G:1295:VAL:HB   | 1.91                     | 0.53              |
| 1:H:1093:ARG:HD3 | 1:H:1155:THR:CG2  | 2.39                     | 0.53              |
| 1:I:702:GLU:OE2  | 1:I:715:ARG:NH2   | 2.38                     | 0.53              |
| 1:k:618:LEU:HD22 | 1:k:864:LEU:HB3   | 1.90                     | 0.53              |
| 1:l:749:ASN:ND2  | 1:l:757:ARG:HG2   | 2.22                     | 0.53              |
| 1:m:1233:ARG:O   | 1:m:1238:HIS:ND1  | 2.40                     | 0.53              |
| 1:n:421:ALA:HA   | 1:n:424:GLN:HB2   | 1.90                     | 0.53              |
| 1:n:576:ARG:HH11 | 1:n:1007:LEU:HD21 | 1.72                     | 0.53              |
| 1:o:1097:LEU:HA  | 1:o:1100:VAL:HB   | 1.90                     | 0.53              |
| 1:q:907:MET:HE1  | 1:q:936:ALA:HB2   | 1.89                     | 0.53              |
| 2:f:177:GLU:OE2  | 2:f:214:ASN:ND2   | 2.42                     | 0.53              |
| 3:t:61:ILE:HG13  | 3:t:84:LEU:HD11   | 1.89                     | 0.53              |
| 4:y:92:MET:HA    | 4:y:102:LYS:HG3   | 1.90                     | 0.53              |
| 4:S:63:GLN:HA    | 4:S:140:ILE:HG13  | 1.90                     | 0.53              |
| 4:V:234:PHE:HB2  | 4:V:249:LEU:HD13  | 1.91                     | 0.53              |
| 5:z:109:LEU:HB2  | 5:z:134:VAL:HG22  | 1.90                     | 0.53              |
| 5:z:120:LEU:HD23 | 5:z:121:VAL:HG12  | 1.91                     | 0.53              |
| 5:b:24:LEU:HD11  | 5:b:121:VAL:HG11  | 1.90                     | 0.53              |
| 1:A:638:ASN:ND2  | 1:A:668:VAL:O     | 2.41                     | 0.53              |
| 1:C:587:ARG:NH1  | 1:C:589:PRO:O     | 2.41                     | 0.53              |
| 1:E:31:GLU:OE1   | 1:m:1261:THR:CG2  | 2.56                     | 0.53              |
| 1:G:117:VAL:C    | 1:m:33:PHE:CE2    | 2.87                     | 0.53              |
| 1:G:1064:ASN:OD1 | 5:W:78:GLN:NE2    | 2.40                     | 0.53              |
| 1:I:863:HIS:HE1  | 3:R:93:LYS:HA     | 1.73                     | 0.53              |
| 1:k:1234:GLU:HG2 | 5:z:52:LYS:HB2    | 1.91                     | 0.53              |
| 1:l:1214:ASN:O   | 1:l:1218:SER:HB3  | 2.09                     | 0.53              |
| 1:m:1230:THR:HA  | 1:m:1233:ARG:HB3  | 1.90                     | 0.53              |
| 1:m:1324:THR:H   | 1:n:1326:LYS:NZ   | 2.04                     | 0.53              |
| 1:n:232:ASP:OD1  | 1:n:1352:ASN:ND2  | 2.41                     | 0.53              |
| 1:n:611:LEU:HB3  | 1:n:846:VAL:HG11  | 1.90                     | 0.53              |
| 1:n:888:GLY:O    | 1:n:892:ALA:N     | 2.41                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:o:128:ILE:HD11  | 1:o:168:THR:HG23  | 1.90                     | 0.53              |
| 1:p:1184:LEU:HD21 | 1:p:1265:THR:HG21 | 1.90                     | 0.53              |
| 4:V:232:PHE:HB3   | 5:d:229:LYS:NZ    | 2.23                     | 0.53              |
| 5:Z:216:ARG:HH21  | 5:d:205:ASN:HB3   | 1.74                     | 0.53              |
| 5:d:89:CYS:HA     | 5:d:308:ILE:HA    | 1.90                     | 0.53              |
| 1:A:600:ARG:NH2   | 1:A:793:VAL:O     | 2.41                     | 0.53              |
| 1:A:749:ASN:ND2   | 1:A:754:ASP:OD1   | 2.42                     | 0.53              |
| 1:A:756:ALA:HA    | 1:A:759:ILE:HG12  | 1.91                     | 0.53              |
| 1:D:722:GLN:NE2   | 1:D:904:GLY:O     | 2.41                     | 0.53              |
| 1:E:87:MET:SD     | 1:E:1066:ASN:ND2  | 2.81                     | 0.53              |
| 1:E:664:GLY:HA2   | 1:F:644:ARG:NH1   | 2.24                     | 0.53              |
| 1:F:1017:ALA:N    | 1:F:1160:LEU:O    | 2.41                     | 0.53              |
| 1:m:1117:GLN:HG2  | 1:n:475:ASP:HB2   | 1.89                     | 0.53              |
| 1:n:1147:ALA:HA   | 1:o:1206:PRO:HG3  | 1.90                     | 0.53              |
| 1:o:389:ASP:N     | 1:o:389:ASP:OD1   | 2.40                     | 0.53              |
| 1:o:814:TYR:CZ    | 3:v:81:GLN:HG3    | 2.43                     | 0.53              |
| 1:p:1219:GLN:HB2  | 1:p:1222:SER:HB3  | 1.90                     | 0.53              |
| 1:q:567:LEU:HD22  | 1:q:1161:THR:HG21 | 1.90                     | 0.53              |
| 2:2:177:GLU:OE2   | 2:2:214:ASN:ND2   | 2.42                     | 0.53              |
| 2:i:275:THR:O     | 2:i:279:LEU:CG    | 2.52                     | 0.53              |
| 4:y:71:PHE:N      | 4:y:71:PHE:CD1    | 2.76                     | 0.53              |
| 4:y:130:VAL:HG23  | 4:y:131:VAL:HG13  | 1.90                     | 0.53              |
| 4:S:126:ARG:O     | 4:S:201:GLN:NE2   | 2.41                     | 0.53              |
| 4:V:75:THR:OG1    | 4:V:117:ARG:NH1   | 2.39                     | 0.53              |
| 5:Y:277:PHE:HA    | 5:Y:280:ILE:HG12  | 1.90                     | 0.53              |
| 5:1:29:ILE:HD11   | 5:1:71:MET:HE2    | 1.90                     | 0.53              |
| 5:c:64:ARG:NH1    | 5:c:288:SER:O     | 2.37                     | 0.53              |
| 5:d:4:THR:HG23    | 5:d:80:ILE:HG23   | 1.91                     | 0.53              |
| 1:B:146:ASP:N     | 1:B:146:ASP:OD1   | 2.41                     | 0.53              |
| 1:B:715:ARG:HA    | 1:B:731:VAL:HG21  | 1.90                     | 0.53              |
| 1:C:1156:CYS:HB2  | 1:C:1245:PRO:HD2  | 1.89                     | 0.53              |
| 1:E:5:TRP:CZ3     | 1:m:93:LEU:HD23   | 2.43                     | 0.53              |
| 1:E:434:LYS:HE3   | 1:F:218:GLN:HG2   | 1.91                     | 0.53              |
| 1:F:118:SER:HB2   | 1:l:5:TRP:CH2     | 2.44                     | 0.53              |
| 1:G:400:LEU:HD11  | 1:G:1164:SER:HB2  | 1.90                     | 0.53              |
| 1:G:610:GLU:OE2   | 1:G:914:LEU:N     | 2.40                     | 0.53              |
| 1:G:753:SER:HB2   | 3:P:64:MET:HE1    | 1.90                     | 0.53              |
| 1:G:1297:LYS:H    | 1:G:1297:LYS:HD2  | 1.74                     | 0.53              |
| 1:H:88:THR:HG22   | 1:H:89:THR:HG23   | 1.89                     | 0.53              |
| 1:k:664:GLY:HA2   | 1:l:644:ARG:HH12  | 1.74                     | 0.53              |
| 1:k:786:TYR:O     | 1:k:927:TYR:OH    | 2.24                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:l:1243:TYR:OH  | 1:l:1248:GLN:OE1 | 2.24                     | 0.53              |
| 1:m:611:LEU:HB3  | 1:m:846:VAL:HG11 | 1.90                     | 0.53              |
| 1:m:1276:CYS:SG  | 1:m:1277:ILE:N   | 2.81                     | 0.53              |
| 1:n:757:ARG:NH2  | 1:n:869:PRO:O    | 2.40                     | 0.53              |
| 1:p:482:ARG:HH22 | 1:p:961:PRO:HB3  | 1.73                     | 0.53              |
| 1:q:559:MET:SD   | 1:q:996:HIS:ND1  | 2.73                     | 0.53              |
| 4:y:294:ALA:O    | 5:z:282:GLN:NE2  | 2.34                     | 0.53              |
| 5:X:5:VAL:HB     | 5:X:81:LEU:HB2   | 1.91                     | 0.53              |
| 5:Z:172:ARG:HG2  | 5:Z:177:THR:HG22 | 1.90                     | 0.53              |
| 1:D:10:LEU:HB3   | 1:G:152:LEU:HD21 | 1.91                     | 0.53              |
| 1:D:227:THR:HG23 | 1:D:230:LEU:HD11 | 1.91                     | 0.53              |
| 1:E:5:TRP:CE3    | 1:m:93:LEU:HD23  | 2.44                     | 0.53              |
| 1:G:696:ASN:HA   | 1:H:952:ARG:HH12 | 1.72                     | 0.53              |
| 1:G:1297:LYS:HD3 | 1:G:1299:CYS:HB2 | 1.90                     | 0.53              |
| 1:k:632:LEU:HB2  | 1:k:860:GLU:HB3  | 1.90                     | 0.53              |
| 1:l:126:ILE:O    | 1:l:1062:SER:HA  | 2.09                     | 0.53              |
| 1:n:393:THR:HA   | 1:n:1023:THR:HA  | 1.91                     | 0.53              |
| 1:n:600:ARG:O    | 1:n:604:THR:OG1  | 2.24                     | 0.53              |
| 1:p:627:GLU:HA   | 1:p:630:ILE:HG13 | 1.90                     | 0.53              |
| 1:p:1276:CYS:SG  | 1:p:1277:ILE:N   | 2.80                     | 0.53              |
| 4:y:239:ILE:HA   | 5:z:205:ASN:HD22 | 1.72                     | 0.53              |
| 4:S:160:LEU:HD23 | 4:S:160:LEU:O    | 2.09                     | 0.53              |
| 5:z:94:ASN:HD21  | 5:z:303:LYS:HE2  | 1.74                     | 0.53              |
| 5:X:120:LEU:HD23 | 5:X:121:VAL:HG12 | 1.89                     | 0.53              |
| 1:A:813:PHE:CD2  | 3:J:85:LEU:CD2   | 2.91                     | 0.53              |
| 1:B:325:ASP:HB3  | 1:B:328:GLN:HB3  | 1.91                     | 0.53              |
| 1:B:696:ASN:HA   | 1:C:952:ARG:HH12 | 1.73                     | 0.53              |
| 1:B:856:GLN:NE2  | 1:B:859:GLU:OE1  | 2.42                     | 0.53              |
| 1:E:489:HIS:O    | 1:E:496:ARG:NH1  | 2.42                     | 0.53              |
| 1:F:147:THR:O    | 1:F:148:LEU:HB2  | 2.09                     | 0.53              |
| 1:F:341:LEU:O    | 1:l:14:LEU:HD23  | 2.09                     | 0.53              |
| 1:F:381:ASP:OD1  | 1:F:381:ASP:N    | 2.42                     | 0.53              |
| 1:l:758:MET:HB2  | 3:s:79:ALA:HB1   | 1.91                     | 0.53              |
| 1:m:497:LEU:HD21 | 1:m:922:PRO:HD2  | 1.89                     | 0.53              |
| 1:n:209:THR:HG22 | 1:n:211:VAL:H    | 1.73                     | 0.53              |
| 1:o:768:PHE:HD2  | 1:o:870:GLU:HB2  | 1.74                     | 0.53              |
| 1:o:810:VAL:CG1  | 3:v:81:GLN:HE22  | 2.20                     | 0.53              |
| 1:p:79:ILE:O     | 1:p:1042:ILE:HA  | 2.08                     | 0.53              |
| 2:3:258:PHE:HE1  | 3:r:91:ALA:N     | 2.02                     | 0.53              |
| 2:3:264:ARG:HH22 | 3:r:93:LYS:HZ2   | 1.57                     | 0.53              |
| 2:3:275:THR:O    | 2:3:279:LEU:CG   | 2.52                     | 0.53              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 3:K:71:MET:O      | 3:K:74:HIS:NE2   | 2.42                     | 0.53              |
| 3:R:41:ARG:HH22   | 3:R:62:SER:HA    | 1.74                     | 0.53              |
| 5:a:275:ALA:HA    | 5:a:278:VAL:HG12 | 1.90                     | 0.53              |
| 1:A:481:CYS:SG    | 1:A:482:ARG:N    | 2.81                     | 0.53              |
| 1:B:760:ALA:HA    | 1:B:763:GLN:HB3  | 1.91                     | 0.53              |
| 1:B:1344:PRO:HB2  | 1:B:1347:GLN:HB2 | 1.91                     | 0.53              |
| 1:C:603:LEU:HD23  | 1:C:794:LEU:HD11 | 1.91                     | 0.53              |
| 1:C:1089:ASP:N    | 1:C:1152:GLN:O   | 2.42                     | 0.53              |
| 1:D:558:ILE:HD13  | 1:D:970:TRP:HA   | 1.91                     | 0.53              |
| 1:F:753:SER:HB2   | 3:O:83:ASP:CG    | 2.33                     | 0.53              |
| 1:H:713:ASP:O     | 1:H:783:LYS:NZ   | 2.41                     | 0.53              |
| 1:H:1318:GLU:OE2  | 1:I:1171:ARG:NH2 | 2.42                     | 0.53              |
| 1:k:497:LEU:HD21  | 1:k:922:PRO:HD2  | 1.91                     | 0.53              |
| 1:k:784:VAL:HA    | 1:k:788:CYS:HB2  | 1.89                     | 0.53              |
| 1:l:724:LEU:HB3   | 1:l:772:ARG:HB2  | 1.91                     | 0.53              |
| 1:l:805:LEU:HD23  | 1:l:808:LEU:HD23 | 1.91                     | 0.53              |
| 1:l:1003:SER:O    | 1:l:1007:LEU:HB2 | 2.08                     | 0.53              |
| 1:l:1260:LYS:HD2  | 1:l:1264:LYS:HB3 | 1.91                     | 0.53              |
| 1:m:1093:ARG:NH1  | 1:m:1283:LEU:CD2 | 2.71                     | 0.53              |
| 1:o:98:VAL:HG21   | 1:o:113:THR:HB   | 1.91                     | 0.53              |
| 1:p:605:ASP:OD2   | 1:p:640:TYR:OH   | 2.27                     | 0.53              |
| 1:p:975:PHE:HE1   | 1:p:995:MET:HB3  | 1.74                     | 0.53              |
| 4:T:156:SER:O     | 4:T:165:TYR:N    | 2.42                     | 0.53              |
| 5:X:119:GLY:HA3   | 5:X:129:VAL:HA   | 1.91                     | 0.53              |
| 1:A:717:TRP:HE1   | 1:A:731:VAL:HG11 | 1.74                     | 0.53              |
| 1:D:663:LEU:HB3   | 1:D:673:TYR:CD1  | 2.44                     | 0.53              |
| 1:D:1150:HIS:NE2  | 1:E:1207:GLN:HG2 | 2.24                     | 0.53              |
| 1:E:54:ILE:HG12   | 1:F:91:LYS:HD2   | 1.90                     | 0.53              |
| 1:E:734:VAL:HG12  | 1:E:739:PRO:HA   | 1.90                     | 0.53              |
| 1:E:1175:ASN:ND2  | 1:E:1179:ARG:O   | 2.41                     | 0.53              |
| 1:F:1264:LYS:CG   | 1:l:31:GLU:OE1   | 2.54                     | 0.53              |
| 1:G:119:LYS:HE3   | 1:G:1069:GLU:HB3 | 1.90                     | 0.53              |
| 1:H:156:ASP:OD1   | 1:I:338:GLN:NE2  | 2.42                     | 0.53              |
| 1:m:606:HIS:HA    | 1:m:909:THR:HG21 | 1.91                     | 0.53              |
| 1:n:911:PRO:HG2   | 1:n:914:LEU:HD12 | 1.90                     | 0.53              |
| 1:n:1031:LEU:HD23 | 1:n:1081:ALA:HB2 | 1.90                     | 0.53              |
| 1:p:1269:TYR:OH   | 1:p:1296:GLU:O   | 2.26                     | 0.53              |
| 1:q:584:THR:HB    | 1:q:586:VAL:HG12 | 1.90                     | 0.53              |
| 2:g:177:GLU:OE2   | 2:g:214:ASN:ND2  | 2.42                     | 0.53              |
| 4:S:215:HIS:CG    | 5:W:64:ARG:HD3   | 2.43                     | 0.53              |
| 4:S:228:ARG:CG    | 5:a:224:ASN:HB3  | 2.39                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:V:41:TYR:HE1    | 4:V:160:LEU:HD12  | 1.74                     | 0.53              |
| 1:B:1256:ILE:HA   | 1:B:1259:ASN:HD22 | 1.73                     | 0.52              |
| 1:D:1275:ASP:OD2  | 1:D:1300:ARG:NH2  | 2.42                     | 0.52              |
| 1:E:441:ILE:HG12  | 1:E:1020:VAL:HG21 | 1.91                     | 0.52              |
| 1:E:1180:SER:N    | 1:E:1205:ASP:OD1  | 2.41                     | 0.52              |
| 1:F:1114:TRP:O    | 1:F:1118:ALA:N    | 2.42                     | 0.52              |
| 1:G:330:ALA:CA    | 1:n:314:VAL:HG21  | 2.35                     | 0.52              |
| 1:G:481:CYS:SG    | 1:G:482:ARG:N     | 2.82                     | 0.52              |
| 1:G:602:SER:HA    | 1:G:646:LEU:HD13  | 1.90                     | 0.52              |
| 1:k:258:ASN:HB2   | 1:k:261:THR:HG22  | 1.91                     | 0.52              |
| 1:m:131:GLU:H     | 1:n:112:GLN:NE2   | 2.07                     | 0.52              |
| 1:m:244:LEU:HD23  | 1:m:247:LEU:HD12  | 1.92                     | 0.52              |
| 1:n:127:THR:HA    | 1:n:1061:VAL:O    | 2.09                     | 0.52              |
| 1:n:284:LEU:O     | 1:n:288:LEU:HB2   | 2.09                     | 0.52              |
| 1:o:695:LEU:O     | 1:p:952:ARG:NH1   | 2.42                     | 0.52              |
| 1:p:204:ALA:HB3   | 1:p:212:GLN:HE22  | 1.73                     | 0.52              |
| 1:q:1160:LEU:HD23 | 1:q:1216:TRP:HE1  | 1.74                     | 0.52              |
| 1:q:1188:PRO:O    | 1:q:1260:LYS:HB3  | 2.09                     | 0.52              |
| 2:2:269:ARG:HD3   | 2:2:270:PRO:HD2   | 1.91                     | 0.52              |
| 2:j:258:PHE:CZ    | 3:M:87:MET:HE3    | 2.44                     | 0.52              |
| 4:y:245:SER:HB3   | 5:z:271:ASN:HB3   | 1.91                     | 0.52              |
| 4:S:237:ASN:HA    | 4:S:240:SER:HB2   | 1.91                     | 0.52              |
| 4:T:75:THR:HG21   | 4:T:120:LEU:HD13  | 1.91                     | 0.52              |
| 4:U:197:ASN:H     | 4:U:202:GLY:HA3   | 1.74                     | 0.52              |
| 1:A:965:HIS:O     | 1:A:969:HIS:N     | 2.42                     | 0.52              |
| 1:B:920:VAL:HG21  | 1:B:933:ALA:HA    | 1.91                     | 0.52              |
| 1:B:952:ARG:HE    | 1:B:955:GLY:H     | 1.57                     | 0.52              |
| 1:C:630:ILE:HG23  | 1:C:662:ARG:HH11  | 1.74                     | 0.52              |
| 1:D:79:ILE:HB     | 1:D:1042:ILE:HG22 | 1.89                     | 0.52              |
| 1:F:1072:LEU:O    | 1:l:33:PHE:HZ     | 1.89                     | 0.52              |
| 1:G:313:ALA:HB1   | 1:m:148:LEU:HD13  | 1.90                     | 0.52              |
| 1:k:1228:TYR:HB2  | 1:k:1250:PHE:HD2  | 1.74                     | 0.52              |
| 1:l:87:MET:SD     | 1:l:1066:ASN:ND2  | 2.81                     | 0.52              |
| 1:m:783:LYS:O     | 1:m:787:LEU:HB2   | 2.09                     | 0.52              |
| 1:n:104:GLY:HA3   | 1:n:107:ILE:HD12  | 1.91                     | 0.52              |
| 1:o:1160:LEU:CD2  | 1:o:1214:ASN:HD22 | 2.21                     | 0.52              |
| 1:p:688:ARG:HA    | 1:p:691:GLU:CD    | 2.34                     | 0.52              |
| 1:p:749:ASN:ND2   | 1:p:754:ASP:OD2   | 2.42                     | 0.52              |
| 1:p:1171:ARG:HH12 | 1:p:1337:TYR:HB2  | 1.74                     | 0.52              |
| 1:p:1173:PRO:HD3  | 1:p:1342:THR:HG21 | 1.91                     | 0.52              |
| 1:q:805:LEU:HB3   | 1:q:809:LEU:HD13  | 1.91                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:g:204:LEU:HB2   | 2:g:211:LEU:HD23  | 1.92                     | 0.52              |
| 3:L:72:GLY:O      | 3:L:80:TYR:OH     | 2.27                     | 0.52              |
| 4:T:69:LEU:HB2    | 4:T:87:LEU:HB2    | 1.91                     | 0.52              |
| 5:X:90:TYR:O      | 5:X:307:CYS:N     | 2.39                     | 0.52              |
| 1:C:67:PHE:HA     | 1:C:177:ILE:HD11  | 1.92                     | 0.52              |
| 1:C:296:GLY:HA2   | 1:C:357:GLN:HG2   | 1.91                     | 0.52              |
| 1:D:818:PHE:HB3   | 3:M:88:LEU:HD13   | 1.89                     | 0.52              |
| 1:E:141:LYS:HG3   | 4:S:33:ARG:NH2    | 2.24                     | 0.52              |
| 1:E:183:VAL:HG21  | 1:E:1067:THR:HG21 | 1.91                     | 0.52              |
| 1:E:598:VAL:HG13  | 1:E:646:LEU:HA    | 1.92                     | 0.52              |
| 1:E:1028:THR:HG21 | 1:E:1080:THR:HG23 | 1.91                     | 0.52              |
| 1:F:258:ASN:HB2   | 1:F:261:THR:HG22  | 1.90                     | 0.52              |
| 1:F:634:THR:HG22  | 1:F:663:LEU:HD22  | 1.91                     | 0.52              |
| 1:G:749:ASN:OD1   | 1:G:752:THR:OG1   | 2.26                     | 0.52              |
| 1:G:863:HIS:HE1   | 3:P:93:LYS:CA     | 1.95                     | 0.52              |
| 1:I:257:ASP:HB2   | 1:I:269:ARG:HH12  | 1.74                     | 0.52              |
| 1:k:253:GLU:HA    | 1:k:1035:THR:HG21 | 1.91                     | 0.52              |
| 1:l:749:ASN:H     | 1:l:750:PRO:HD3   | 1.74                     | 0.52              |
| 1:m:1028:THR:HG21 | 1:m:1080:THR:HG23 | 1.91                     | 0.52              |
| 1:o:193:VAL:HG11  | 1:o:1266:VAL:HG21 | 1.90                     | 0.52              |
| 1:o:635:ARG:HH22  | 1:o:860:GLU:HG3   | 1.72                     | 0.52              |
| 1:o:1229:ASN:O    | 1:o:1233:ARG:N    | 2.38                     | 0.52              |
| 1:p:1171:ARG:NH2  | 1:p:1338:SER:O    | 2.38                     | 0.52              |
| 1:q:196:THR:HA    | 1:q:199:GLU:HG2   | 1.89                     | 0.52              |
| 1:q:559:MET:HA    | 1:q:998:LYS:HA    | 1.90                     | 0.52              |
| 1:q:564:PRO:HA    | 1:q:974:PRO:HB3   | 1.89                     | 0.52              |
| 2:e:177:GLU:OE2   | 2:e:214:ASN:ND2   | 2.42                     | 0.52              |
| 2:e:285:GLU:H     | 3:t:67:LYS:CE     | 2.22                     | 0.52              |
| 2:h:110:ALA:HB3   | 5:a:225:MET:CG    | 2.30                     | 0.52              |
| 4:y:71:PHE:N      | 4:y:71:PHE:HD1    | 2.07                     | 0.52              |
| 5:Y:144:GLN:HG2   | 5:Y:148:MET:HE2   | 1.91                     | 0.52              |
| 1:A:54:ILE:HG23   | 1:B:93:LEU:HD13   | 1.91                     | 0.52              |
| 1:A:754:ASP:HB3   | 1:A:757:ARG:HB3   | 1.91                     | 0.52              |
| 1:D:539:PHE:HA    | 1:D:556:PRO:HA    | 1.92                     | 0.52              |
| 1:D:863:HIS:CE1   | 3:M:93:LYS:HA     | 2.45                     | 0.52              |
| 1:E:1310:THR:HB   | 1:E:1339:ILE:HB   | 1.91                     | 0.52              |
| 1:F:419:ASP:OD1   | 1:F:424:GLN:NE2   | 2.42                     | 0.52              |
| 1:F:1095:GLN:HE22 | 1:F:1283:LEU:HD21 | 1.73                     | 0.52              |
| 1:F:1201:HIS:ND1  | 1:F:1212:THR:OG1  | 2.40                     | 0.52              |
| 1:G:753:SER:HB3   | 3:P:87:MET:HE2    | 1.92                     | 0.52              |
| 1:I:192:PHE:HB2   | 1:I:223:LYS:HB3   | 1.92                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:k:126:ILE:HD11  | 1:k:1063:GLN:NE2  | 2.24                     | 0.52              |
| 1:k:1233:ARG:O    | 1:k:1238:HIS:ND1  | 2.43                     | 0.52              |
| 1:l:702:GLU:OE2   | 1:l:715:ARG:NH2   | 2.41                     | 0.52              |
| 1:n:458:ALA:HB1   | 1:n:461:CYS:HB3   | 1.91                     | 0.52              |
| 1:o:390:VAL:HG22  | 1:o:1295:VAL:HB   | 1.90                     | 0.52              |
| 1:p:233:ARG:O     | 1:p:235:ARG:NH2   | 2.40                     | 0.52              |
| 1:q:625:ALA:HA    | 1:q:867:HIS:HE1   | 1.73                     | 0.52              |
| 2:j:88:ARG:NE     | 2:j:132:TYR:OH    | 2.43                     | 0.52              |
| 3:x:39:GLU:OE2    | 3:x:43:GLN:NE2    | 2.43                     | 0.52              |
| 5:z:109:LEU:CB    | 5:z:132:TRP:O     | 2.57                     | 0.52              |
| 1:A:1097:LEU:HA   | 1:A:1100:VAL:HB   | 1.90                     | 0.52              |
| 1:C:662:ARG:HH21  | 1:C:663:LEU:HD12  | 1.73                     | 0.52              |
| 1:C:983:ALA:HB3   | 1:C:987:GLU:HB3   | 1.92                     | 0.52              |
| 1:D:131:GLU:OE1   | 1:G:42:ASP:N      | 2.36                     | 0.52              |
| 1:E:481:CYS:SG    | 1:E:482:ARG:N     | 2.82                     | 0.52              |
| 1:E:1031:LEU:HD12 | 1:E:1031:LEU:O    | 2.09                     | 0.52              |
| 1:F:755:VAL:HB    | 3:O:71:MET:HE2    | 1.92                     | 0.52              |
| 1:G:1275:ASP:OD2  | 1:G:1300:ARG:NH2  | 2.43                     | 0.52              |
| 1:H:1048:VAL:HG12 | 4:V:40:VAL:HG23   | 1.91                     | 0.52              |
| 1:I:104:GLY:HA3   | 1:I:107:ILE:HD12  | 1.90                     | 0.52              |
| 1:k:795:ASN:OD1   | 1:k:984:HIS:HE1   | 1.92                     | 0.52              |
| 1:l:428:THR:HG22  | 1:l:442:SER:HB3   | 1.91                     | 0.52              |
| 1:l:1050:LYS:HB3  | 4:T:42:GLY:HA3    | 1.92                     | 0.52              |
| 1:m:1314:GLN:HG3  | 1:n:1167:LEU:HD13 | 1.92                     | 0.52              |
| 1:n:506:ASP:OD2   | 1:n:949:GLN:NE2   | 2.42                     | 0.52              |
| 1:o:605:ASP:OD2   | 1:o:640:TYR:OH    | 2.28                     | 0.52              |
| 1:p:60:ASN:ND2    | 1:q:44:PRO:O      | 2.42                     | 0.52              |
| 1:q:426:PRO:HB3   | 1:q:1312:THR:HG23 | 1.91                     | 0.52              |
| 2:e:104:LYS:HD3   | 2:h:92:LEU:HD13   | 1.77                     | 0.52              |
| 2:h:88:ARG:NE     | 2:h:132:TYR:OH    | 2.43                     | 0.52              |
| 1:A:1230:THR:HA   | 1:A:1233:ARG:HB3  | 1.92                     | 0.52              |
| 1:C:560:VAL:HA    | 1:C:999:MET:HE3   | 1.91                     | 0.52              |
| 1:C:786:TYR:O     | 1:C:927:TYR:OH    | 2.26                     | 0.52              |
| 1:D:1038:SER:OG   | 1:D:1039:THR:N    | 2.43                     | 0.52              |
| 1:F:98:VAL:HG12   | 1:l:24:ILE:HD13   | 1.92                     | 0.52              |
| 1:F:253:GLU:C     | 1:l:19:ASP:OD2    | 2.52                     | 0.52              |
| 1:I:813:PHE:CE2   | 3:R:85:LEU:CG     | 2.92                     | 0.52              |
| 1:k:483:ARG:HG3   | 1:k:484:GLU:HG2   | 1.90                     | 0.52              |
| 1:m:123:LYS:HA    | 1:m:1066:ASN:HA   | 1.92                     | 0.52              |
| 1:p:724:LEU:HB2   | 1:p:772:ARG:HB2   | 1.91                     | 0.52              |
| 1:q:641:TRP:HA    | 1:q:645:GLY:HA2   | 1.91                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:3:258:PHE:HE1   | 3:r:90:ILE:CA     | 2.23                     | 0.52              |
| 2:f:269:ARG:HD3   | 2:f:270:PRO:HD2   | 1.91                     | 0.52              |
| 2:j:130:ALA:C     | 2:j:132:TYR:N     | 2.66                     | 0.52              |
| 3:R:72:GLY:O      | 3:R:80:TYR:OH     | 2.26                     | 0.52              |
| 3:r:61:ILE:HG13   | 3:r:84:LEU:HD11   | 1.91                     | 0.52              |
| 5:c:146:MET:HE3   | 5:c:180:LEU:HG    | 1.92                     | 0.52              |
| 1:A:130:PHE:HD2   | 1:A:1059:PHE:HB2  | 1.75                     | 0.52              |
| 1:A:656:VAL:HG23  | 1:A:676:TYR:HD1   | 1.74                     | 0.52              |
| 1:A:698:ARG:HG3   | 1:A:703:PRO:HA    | 1.92                     | 0.52              |
| 1:A:1093:ARG:HD3  | 1:A:1155:THR:HG21 | 1.91                     | 0.52              |
| 1:A:1101:PHE:HB3  | 1:A:1104:HIS:HD2  | 1.73                     | 0.52              |
| 1:B:879:ALA:HB3   | 1:B:896:SER:HB2   | 1.92                     | 0.52              |
| 1:C:513:GLU:HA    | 1:C:973:THR:HG21  | 1.91                     | 0.52              |
| 1:D:220:PHE:O     | 1:D:224:MET:N     | 2.41                     | 0.52              |
| 1:D:755:VAL:O     | 1:D:759:ILE:N     | 2.42                     | 0.52              |
| 1:D:1152:GLN:HG3  | 1:D:1284:GLN:HE21 | 1.75                     | 0.52              |
| 1:D:1180:SER:N    | 1:D:1205:ASP:OD1  | 2.42                     | 0.52              |
| 1:E:47:TYR:HE1    | 1:l:156:ASP:OD2   | 1.93                     | 0.52              |
| 1:E:536:HIS:HB3   | 1:E:539:PHE:HB2   | 1.92                     | 0.52              |
| 1:H:450:LEU:HD21  | 1:H:1018:LEU:CD2  | 2.39                     | 0.52              |
| 1:H:1166:ASP:HA   | 1:H:1170:PHE:HD2  | 1.75                     | 0.52              |
| 1:H:1327:LEU:H    | 1:H:1347:GLN:HE21 | 1.58                     | 0.52              |
| 1:k:218:GLN:NE2   | 1:p:435:ASP:HB3   | 2.25                     | 0.52              |
| 1:k:650:ALA:O     | 1:k:785:TYR:OH    | 2.27                     | 0.52              |
| 1:k:1017:ALA:CB   | 1:k:1160:LEU:O    | 2.57                     | 0.52              |
| 1:l:595:THR:HA    | 1:l:675:HIS:HD2   | 1.73                     | 0.52              |
| 1:l:1136:THR:HB   | 4:T:116:ILE:CG1   | 2.37                     | 0.52              |
| 1:n:1314:GLN:HE21 | 1:o:1167:LEU:HD13 | 1.75                     | 0.52              |
| 1:o:734:VAL:HG11  | 1:o:878:ARG:HH11  | 1.75                     | 0.52              |
| 1:o:1148:LEU:HD23 | 1:p:210:ARG:HG2   | 1.90                     | 0.52              |
| 1:p:493:ALA:HB3   | 1:p:874:MET:HB3   | 1.92                     | 0.52              |
| 1:p:967:TYR:O     | 1:p:972:ARG:NH2   | 2.43                     | 0.52              |
| 1:q:692:LEU:HD12  | 1:q:1010:MET:HE3  | 1.90                     | 0.52              |
| 1:q:1230:THR:H    | 1:q:1251:THR:HG22 | 1.73                     | 0.52              |
| 2:j:113:PRO:HG3   | 4:V:229:VAL:HG13  | 1.90                     | 0.52              |
| 4:S:186:ARG:HB2   | 4:S:260:SER:HB2   | 1.90                     | 0.52              |
| 1:B:879:ALA:O     | 1:B:896:SER:N     | 2.38                     | 0.52              |
| 1:C:1041:VAL:HG12 | 1:C:1067:THR:HG22 | 1.91                     | 0.52              |
| 1:E:231:LEU:HG    | 1:E:235:ARG:HH12  | 1.75                     | 0.52              |
| 1:E:388:ARG:HD2   | 1:E:1030:THR:HG21 | 1.92                     | 0.52              |
| 1:E:1055:ILE:HG22 | 5:a:91:THR:HG21   | 1.92                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:I:813:PHE:HE2   | 3:R:82:LEU:HA     | 1.74                     | 0.52              |
| 1:k:448:LYS:HD2   | 1:k:1096:ASP:HB3  | 1.91                     | 0.52              |
| 1:k:656:VAL:HG23  | 1:k:676:TYR:HD1   | 1.75                     | 0.52              |
| 1:k:750:PRO:CD    | 2:3:269:ARG:HH22  | 2.22                     | 0.52              |
| 1:k:1017:ALA:N    | 1:k:1160:LEU:O    | 2.42                     | 0.52              |
| 1:l:703:PRO:HG3   | 1:m:948:PRO:HB2   | 1.92                     | 0.52              |
| 1:l:930:PRO:O     | 1:l:934:ALA:CB    | 2.58                     | 0.52              |
| 1:m:58:TYR:HB2    | 1:n:94:PHE:HD1    | 1.73                     | 0.52              |
| 1:m:147:THR:C     | 1:m:149:LEU:N     | 2.59                     | 0.52              |
| 1:m:182:ARG:NH2   | 1:m:1291:THR:O    | 2.43                     | 0.52              |
| 1:m:207:MET:N     | 1:m:207:MET:SD    | 2.76                     | 0.52              |
| 1:m:522:GLU:HG3   | 1:m:525:LYS:HD2   | 1.91                     | 0.52              |
| 1:m:663:LEU:HD21  | 1:m:669:VAL:H     | 1.75                     | 0.52              |
| 1:n:724:LEU:H     | 1:n:769:VAL:HG21  | 1.75                     | 0.52              |
| 1:p:304:GLY:HA2   | 1:p:351:LEU:HD11  | 1.92                     | 0.52              |
| 1:p:1021:VAL:HG23 | 1:p:1245:PRO:HB2  | 1.91                     | 0.52              |
| 2:e:206:GLU:HB3   | 2:h:132:TYR:CA    | 2.40                     | 0.52              |
| 2:e:285:GLU:N     | 3:t:67:LYS:HE2    | 2.25                     | 0.52              |
| 2:h:93:PRO:CG     | 2:h:195:TYR:CZ    | 2.85                     | 0.52              |
| 2:i:130:ALA:O     | 2:i:132:TYR:N     | 2.43                     | 0.52              |
| 3:J:85:LEU:HD13   | 3:J:88:LEU:HD12   | 1.92                     | 0.52              |
| 3:u:39:GLU:OE2    | 3:u:43:GLN:NE2    | 2.43                     | 0.52              |
| 4:y:69:LEU:HD12   | 4:y:87:LEU:HD13   | 1.92                     | 0.52              |
| 1:B:555:THR:HG21  | 1:B:967:TYR:HB3   | 1.92                     | 0.52              |
| 1:D:1173:PRO:HB3  | 1:D:1306:LEU:HA   | 1.90                     | 0.52              |
| 1:E:30:GLU:HG2    | 1:m:1262:LEU:HB3  | 1.90                     | 0.52              |
| 1:G:815:THR:OG1   | 1:G:836:ASN:OD1   | 2.28                     | 0.52              |
| 1:G:1146:PRO:HA   | 1:H:210:ARG:NH2   | 2.25                     | 0.52              |
| 1:G:1152:GLN:NE2  | 1:G:1281:THR:O    | 2.38                     | 0.52              |
| 1:G:1260:LYS:HB2  | 1:G:1264:LYS:HB2  | 1.91                     | 0.52              |
| 1:H:576:ARG:NE    | 1:H:1013:HIS:O    | 2.40                     | 0.52              |
| 1:H:1021:VAL:HG23 | 1:H:1245:PRO:HB2  | 1.91                     | 0.52              |
| 1:I:1255:ILE:HD12 | 1:I:1258:ALA:HB3  | 1.91                     | 0.52              |
| 1:m:131:GLU:HB3   | 1:n:112:GLN:OE1   | 2.09                     | 0.52              |
| 1:o:220:PHE:HB2   | 1:o:1302:LEU:HD21 | 1.91                     | 0.52              |
| 1:o:1180:SER:N    | 1:o:1205:ASP:OD1  | 2.43                     | 0.52              |
| 1:p:925:ARG:NH1   | 1:p:972:ARG:O     | 2.43                     | 0.52              |
| 1:p:1029:ASP:N    | 1:p:1082:HIS:O    | 2.43                     | 0.52              |
| 1:q:813:PHE:HD1   | 3:x:85:LEU:HD23   | 1.74                     | 0.52              |
| 2:2:197:VAL:C     | 2:2:199:ASP:N     | 2.68                     | 0.52              |
| 2:h:130:ALA:C     | 2:h:132:TYR:N     | 2.66                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:h:216:LEU:HD23  | 2:h:219:LEU:HB2   | 1.92                     | 0.52              |
| 2:g:208:PRO:O     | 2:g:212:VAL:HG23  | 2.10                     | 0.52              |
| 4:S:95:GLU:HG3    | 4:S:203:ARG:HD3   | 1.92                     | 0.52              |
| 5:W:149:LEU:HD21  | 5:W:168:LEU:HD12  | 1.91                     | 0.52              |
| 5:Z:201:SER:OG    | 5:d:211:THR:OG1   | 2.20                     | 0.52              |
| 1:A:440:ARG:HH12  | 1:B:521:LYS:HD2   | 1.73                     | 0.52              |
| 1:A:909:THR:HA    | 1:A:932:LEU:HD11  | 1.90                     | 0.52              |
| 1:B:393:THR:HA    | 1:B:1023:THR:HA   | 1.91                     | 0.52              |
| 1:B:458:ALA:HB1   | 1:B:461:CYS:HB3   | 1.91                     | 0.52              |
| 1:D:819:LEU:CB    | 3:M:58:GLN:NE2    | 2.72                     | 0.52              |
| 1:E:598:VAL:HG12  | 1:E:647:LEU:HB2   | 1.92                     | 0.52              |
| 1:E:1263:PHE:CD2  | 1:G:32:MET:HB2    | 2.45                     | 0.52              |
| 1:F:147:THR:O     | 1:F:148:LEU:CB    | 2.57                     | 0.52              |
| 1:G:117:VAL:CB    | 1:m:33:PHE:CE2    | 2.84                     | 0.52              |
| 1:G:1184:LEU:HD21 | 1:G:1265:THR:HG21 | 1.92                     | 0.52              |
| 1:l:1046:PRO:HA   | 1:l:1062:SER:O    | 2.10                     | 0.52              |
| 1:l:1101:PHE:HB3  | 1:l:1104:HIS:HD2  | 1.74                     | 0.52              |
| 1:m:430:TYR:C     | 1:m:431:PHE:CG    | 2.88                     | 0.52              |
| 1:m:1177:ARG:HH21 | 1:m:1181:SER:HB3  | 1.74                     | 0.52              |
| 1:n:1098:PHE:HE2  | 1:n:1119:THR:HG23 | 1.74                     | 0.52              |
| 1:q:506:ASP:HA    | 1:q:943:PHE:HZ    | 1.75                     | 0.52              |
| 2:h:208:PRO:HD3   | 4:S:236:ASN:HD22  | 1.69                     | 0.52              |
| 2:j:252:PHE:HZ    | 3:M:93:LYS:NZ     | 2.07                     | 0.52              |
| 4:T:167:LEU:HD23  | 4:T:280:LEU:HD12  | 1.92                     | 0.52              |
| 5:b:7:VAL:HG22    | 5:b:38:LEU:HD11   | 1.92                     | 0.52              |
| 1:A:251:VAL:HG11  | 1:A:1033:TYR:HE2  | 1.75                     | 0.51              |
| 1:A:1160:LEU:HD23 | 1:A:1214:ASN:HB2  | 1.91                     | 0.51              |
| 1:A:1275:ASP:OD2  | 1:A:1300:ARG:NH2  | 2.44                     | 0.51              |
| 1:B:925:ARG:NH2   | 1:B:971:HIS:O     | 2.34                     | 0.51              |
| 1:C:476:ARG:HH21  | 1:C:480:LEU:HD12  | 1.75                     | 0.51              |
| 1:D:1021:VAL:HG22 | 1:D:1156:CYS:HB3  | 1.91                     | 0.51              |
| 1:E:480:LEU:HD23  | 1:E:550:VAL:HG11  | 1.92                     | 0.51              |
| 1:G:118:SER:N     | 1:m:5:TRP:CH2     | 2.78                     | 0.51              |
| 1:G:319:HIS:HD2   | 1:n:319:HIS:CE1   | 2.24                     | 0.51              |
| 1:H:328:GLN:HG2   | 1:H:341:LEU:HD22  | 1.90                     | 0.51              |
| 1:k:43:ASP:H      | 1:k:46:ARG:HH12   | 1.57                     | 0.51              |
| 1:k:758:MET:SD    | 3:r:82:LEU:HG     | 2.49                     | 0.51              |
| 1:k:925:ARG:NH2   | 1:k:971:HIS:O     | 2.39                     | 0.51              |
| 1:m:141:LYS:HG2   | 4:S:20:GLU:CG     | 2.40                     | 0.51              |
| 1:m:694:GLY:HA3   | 1:m:1010:MET:HE2  | 1.92                     | 0.51              |
| 1:n:650:ALA:O     | 1:n:785:TYR:OH    | 2.27                     | 0.51              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:p:331:ASP:O    | 1:p:335:GLN:CB    | 2.57                     | 0.51              |
| 1:p:952:ARG:HE   | 1:p:955:GLY:H     | 1.59                     | 0.51              |
| 2:2:206:GLU:HB3  | 2:3:132:TYR:CA    | 2.40                     | 0.51              |
| 2:2:208:PRO:O    | 2:2:212:VAL:HG23  | 2.10                     | 0.51              |
| 2:3:93:PRO:HG3   | 2:3:195:TYR:OH    | 2.03                     | 0.51              |
| 2:e:197:VAL:C    | 2:e:199:ASP:N     | 2.68                     | 0.51              |
| 2:e:204:LEU:HB2  | 2:e:211:LEU:HD23  | 1.91                     | 0.51              |
| 2:h:284:GLU:OE1  | 3:P:70:LYS:NZ     | 2.42                     | 0.51              |
| 2:g:269:ARG:HD3  | 2:g:270:PRO:HD2   | 1.91                     | 0.51              |
| 2:j:130:ALA:O    | 2:j:132:TYR:N     | 2.43                     | 0.51              |
| 3:R:71:MET:O     | 3:R:74:HIS:NE2    | 2.41                     | 0.51              |
| 4:y:85:VAL:HG13  | 4:y:89:PHE:HD2    | 1.74                     | 0.51              |
| 4:y:93:VAL:HB    | 4:y:126:ARG:HH11  | 1.75                     | 0.51              |
| 4:y:267:ILE:HD11 | 4:y:274:GLN:HB3   | 1.91                     | 0.51              |
| 5:Z:31:ILE:HG22  | 5:Z:43:VAL:HG22   | 1.92                     | 0.51              |
| 1:A:100:ARG:NH1  | 1:F:129:PRO:O     | 2.42                     | 0.51              |
| 1:A:982:CYS:HG   | 1:A:988:SER:HG    | 1.52                     | 0.51              |
| 1:A:1201:HIS:ND1 | 1:A:1212:THR:OG1  | 2.42                     | 0.51              |
| 1:C:420:THR:HG22 | 1:C:422:GLU:H     | 1.76                     | 0.51              |
| 1:E:29:GLY:HA2   | 1:m:207:MET:HG3   | 1.84                     | 0.51              |
| 1:F:125:PRO:HB3  | 1:F:1064:ASN:HA   | 1.92                     | 0.51              |
| 1:F:925:ARG:HH11 | 1:F:975:PHE:HB2   | 1.75                     | 0.51              |
| 1:G:1074:TYR:CD2 | 1:m:32:MET:SD     | 3.04                     | 0.51              |
| 1:I:146:ASP:HB2  | 1:I:151:LYS:HG3   | 1.93                     | 0.51              |
| 1:I:757:ARG:HH22 | 1:I:869:PRO:HA    | 1.75                     | 0.51              |
| 1:I:771:ALA:O    | 1:I:773:ARG:CD    | 2.58                     | 0.51              |
| 1:k:390:VAL:HG22 | 1:k:1295:VAL:HB   | 1.92                     | 0.51              |
| 1:k:753:SER:HB2  | 3:r:83:ASP:CG     | 2.35                     | 0.51              |
| 1:k:1261:THR:O   | 1:k:1261:THR:OG1  | 2.26                     | 0.51              |
| 1:l:94:PHE:O     | 1:l:116:MET:HA    | 2.10                     | 0.51              |
| 1:l:493:ALA:HA   | 1:l:496:ARG:HB2   | 1.92                     | 0.51              |
| 1:l:841:ALA:O    | 1:l:845:ASP:HB2   | 2.10                     | 0.51              |
| 1:l:1137:PHE:HE2 | 4:T:117:ARG:HH22  | 1.48                     | 0.51              |
| 1:l:1159:ILE:O   | 1:l:1214:ASN:ND2  | 2.41                     | 0.51              |
| 1:m:1323:GLY:N   | 1:n:1329:LEU:HD23 | 2.25                     | 0.51              |
| 1:n:1179:ARG:NH2 | 1:n:1204:PRO:O    | 2.43                     | 0.51              |
| 1:o:661:THR:HA   | 1:p:606:HIS:CD2   | 2.45                     | 0.51              |
| 1:p:1297:LYS:HD3 | 1:p:1299:CYS:HB2  | 1.90                     | 0.51              |
| 2:h:275:THR:O    | 2:h:279:LEU:CG    | 2.52                     | 0.51              |
| 2:i:88:ARG:NE    | 2:i:132:TYR:OH    | 2.43                     | 0.51              |
| 2:j:83:LYS:O     | 2:j:87:ARG:HG2    | 2.10                     | 0.51              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 4:T:51:ARG:HG2   | 4:T:149:THR:HG23  | 1.93                     | 0.51              |
| 4:T:217:HIS:CE1  | 5:X:286:VAL:HG22  | 2.45                     | 0.51              |
| 5:Y:285:ASP:HA   | 5:Y:288:SER:HB3   | 1.91                     | 0.51              |
| 1:B:416:LYS:O    | 1:C:409:SER:N     | 2.39                     | 0.51              |
| 1:B:1097:LEU:HA  | 1:B:1100:VAL:HB   | 1.91                     | 0.51              |
| 1:D:495:ARG:NH2  | 1:D:762:ASP:OD2   | 2.44                     | 0.51              |
| 1:E:328:GLN:HE21 | 1:E:342:PRO:HD2   | 1.75                     | 0.51              |
| 1:F:232:ASP:HA   | 1:F:1352:ASN:HD22 | 1.75                     | 0.51              |
| 1:G:338:GLN:HG3  | 1:m:10:LEU:O      | 2.11                     | 0.51              |
| 1:k:205:ARG:CB   | 1:p:381:ASP:HB3   | 2.35                     | 0.51              |
| 1:l:1137:PHE:CB  | 4:T:55:ARG:NH2    | 2.73                     | 0.51              |
| 1:n:907:MET:HG3  | 1:n:932:LEU:HD21  | 1.91                     | 0.51              |
| 1:o:64:TRP:HZ3   | 1:o:170:ASP:HB2   | 1.76                     | 0.51              |
| 1:q:504:ARG:NH2  | 1:q:942:VAL:O     | 2.39                     | 0.51              |
| 2:e:285:GLU:N    | 3:t:67:LYS:CE     | 2.73                     | 0.51              |
| 2:h:113:PRO:HG2  | 4:S:233:HIS:NE2   | 2.25                     | 0.51              |
| 2:h:259:ALA:HB3  | 2:h:289:LEU:HD13  | 1.93                     | 0.51              |
| 2:f:197:VAL:C    | 2:f:199:ASP:N     | 2.68                     | 0.51              |
| 3:w:67:LYS:NZ    | 3:w:71:MET:SD     | 2.83                     | 0.51              |
| 4:S:228:ARG:HG2  | 5:a:224:ASN:CA    | 2.40                     | 0.51              |
| 5:W:110:PRO:CG   | 5:W:111:PRO:HD2   | 2.39                     | 0.51              |
| 5:Y:205:ASN:ND2  | 5:c:233:ILE:C     | 2.68                     | 0.51              |
| 5:Z:4:THR:HG23   | 5:Z:80:ILE:HG23   | 1.91                     | 0.51              |
| 5:c:9:PHE:HE1    | 5:c:79:MET:HE3    | 1.75                     | 0.51              |
| 5:c:21:LEU:HB3   | 5:c:74:VAL:HG21   | 1.93                     | 0.51              |
| 1:C:125:PRO:HB3  | 1:C:1064:ASN:HA   | 1.92                     | 0.51              |
| 1:D:330:ALA:HA   | 1:D:333:ILE:HD12  | 1.92                     | 0.51              |
| 1:E:193:VAL:HG11 | 1:E:1266:VAL:HG21 | 1.92                     | 0.51              |
| 1:F:1298:PRO:O   | 1:F:1302:LEU:N    | 2.39                     | 0.51              |
| 1:G:259:PRO:HA   | 1:G:269:ARG:HD3   | 1.92                     | 0.51              |
| 1:G:813:PHE:CZ   | 3:P:85:LEU:CG     | 2.93                     | 0.51              |
| 1:G:882:ASP:N    | 1:G:882:ASP:OD1   | 2.41                     | 0.51              |
| 1:I:284:LEU:O    | 1:I:288:LEU:HB2   | 2.11                     | 0.51              |
| 1:k:275:VAL:HG12 | 1:k:371:GLU:HB3   | 1.92                     | 0.51              |
| 1:k:1310:THR:HB  | 1:k:1339:ILE:HB   | 1.92                     | 0.51              |
| 1:l:19:ASP:OD1   | 1:l:19:ASP:N      | 2.44                     | 0.51              |
| 1:l:392:LEU:HB2  | 1:l:1026:PHE:HE2  | 1.75                     | 0.51              |
| 1:m:200:HIS:HB2  | 1:m:216:ILE:HD13  | 1.93                     | 0.51              |
| 1:m:1179:ARG:NH1 | 1:m:1211:SER:O    | 2.40                     | 0.51              |
| 1:n:1101:PHE:HB3 | 1:n:1104:HIS:HD2  | 1.75                     | 0.51              |
| 1:o:1179:ARG:NH2 | 1:o:1204:PRO:O    | 2.43                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:p:515:LYS:NZ    | 1:p:534:GLU:OE2   | 2.41                     | 0.51              |
| 1:q:542:CYS:SG    | 1:q:967:TYR:OH    | 2.57                     | 0.51              |
| 1:q:871:ASN:O     | 1:q:903:ASN:ND2   | 2.35                     | 0.51              |
| 2:3:88:ARG:NE     | 2:3:132:TYR:OH    | 2.43                     | 0.51              |
| 2:e:269:ARG:HD3   | 2:e:270:PRO:HD2   | 1.91                     | 0.51              |
| 2:i:111:ALA:CB    | 4:U:232:PHE:CZ    | 2.65                     | 0.51              |
| 4:S:69:LEU:HB2    | 4:S:87:LEU:HB2    | 1.92                     | 0.51              |
| 4:U:23:TYR:CE1    | 5:c:2:GLU:HA      | 2.45                     | 0.51              |
| 1:A:62:ILE:HG12   | 1:B:99:PRO:HG3    | 1.91                     | 0.51              |
| 1:B:709:SER:HB3   | 1:B:712:HIS:HD2   | 1.76                     | 0.51              |
| 1:C:53:ALA:HB3    | 1:D:90:GLY:HA2    | 1.92                     | 0.51              |
| 1:C:1048:VAL:HG22 | 1:C:1061:VAL:HG12 | 1.92                     | 0.51              |
| 1:D:879:ALA:HB3   | 1:D:896:SER:HB2   | 1.93                     | 0.51              |
| 1:E:711:LEU:HG    | 1:E:711:LEU:O     | 2.11                     | 0.51              |
| 1:G:537:PRO:O     | 1:G:557:ARG:NH2   | 2.42                     | 0.51              |
| 1:G:539:PHE:HA    | 1:G:556:PRO:HA    | 1.92                     | 0.51              |
| 1:G:1201:HIS:ND1  | 1:G:1212:THR:OG1  | 2.42                     | 0.51              |
| 1:H:411:ALA:HB2   | 1:H:1331:GLU:HB3  | 1.93                     | 0.51              |
| 1:H:1171:ARG:HA   | 1:H:1339:ILE:HG23 | 1.91                     | 0.51              |
| 1:k:813:PHE:CD1   | 3:r:85:LEU:CD2    | 2.87                     | 0.51              |
| 1:l:1199:TYR:HB3  | 1:l:1220:ARG:HB2  | 1.92                     | 0.51              |
| 1:m:1038:SER:OG   | 1:m:1039:THR:N    | 2.43                     | 0.51              |
| 1:o:599:LEU:O     | 1:o:603:LEU:HB2   | 2.11                     | 0.51              |
| 1:o:1171:ARG:HH12 | 1:o:1332:THR:HG22 | 1.75                     | 0.51              |
| 1:p:882:ASP:N     | 1:p:882:ASP:OD1   | 2.43                     | 0.51              |
| 2:i:259:ALA:HB3   | 2:i:289:LEU:HD13  | 1.93                     | 0.51              |
| 2:j:216:LEU:HD23  | 2:j:219:LEU:HB2   | 1.92                     | 0.51              |
| 5:Y:106:LEU:HA    | 5:Y:135:PRO:HA    | 1.91                     | 0.51              |
| 5:a:5:VAL:HB      | 5:a:81:LEU:HB2    | 1.93                     | 0.51              |
| 5:a:51:ASP:CB     | 5:a:54:ARG:HB2    | 2.40                     | 0.51              |
| 1:A:263:THR:HA    | 1:A:269:ARG:HA    | 1.92                     | 0.51              |
| 1:A:410:THR:OG1   | 1:F:1322:LYS:NZ   | 2.31                     | 0.51              |
| 1:A:703:PRO:HG3   | 1:B:948:PRO:HB2   | 1.92                     | 0.51              |
| 1:C:152:LEU:HA    | 1:D:337:SER:HB2   | 1.91                     | 0.51              |
| 1:D:555:THR:HG21  | 1:D:967:TYR:HB3   | 1.92                     | 0.51              |
| 1:D:670:PRO:O     | 1:E:644:ARG:NH2   | 2.43                     | 0.51              |
| 1:D:1230:THR:HA   | 1:D:1233:ARG:HB3  | 1.93                     | 0.51              |
| 1:E:314:VAL:HG22  | 1:H:333:ILE:HD12  | 1.93                     | 0.51              |
| 1:E:755:VAL:HG11  | 3:N:80:TYR:CZ     | 2.45                     | 0.51              |
| 1:F:210:ARG:HA    | 1:F:213:ARG:HG2   | 1.92                     | 0.51              |
| 1:F:748:ARG:NH2   | 1:F:770:ASP:OD1   | 2.42                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:G:607:GLN:OE1   | 1:G:644:ARG:NH1   | 2.43                     | 0.51              |
| 1:H:726:ARG:HB2   | 1:H:773:ARG:HB2   | 1.93                     | 0.51              |
| 1:I:199:GLU:OE1   | 1:I:223:LYS:NZ    | 2.40                     | 0.51              |
| 1:I:711:LEU:HD22  | 1:I:996:HIS:HB2   | 1.93                     | 0.51              |
| 1:k:44:PRO:HB2    | 4:T:162:THR:O     | 2.11                     | 0.51              |
| 1:k:733:VAL:O     | 1:k:740:LEU:N     | 2.41                     | 0.51              |
| 1:l:546:GLU:N     | 1:l:549:GLN:O     | 2.39                     | 0.51              |
| 1:m:430:TYR:O     | 1:m:431:PHE:CD2   | 2.64                     | 0.51              |
| 1:m:512:ASN:HD22  | 1:m:966:GLU:HG2   | 1.75                     | 0.51              |
| 1:o:393:THR:OG1   | 1:o:1248:GLN:NE2  | 2.43                     | 0.51              |
| 1:p:701:ASP:OD2   | 1:p:1108:ASN:ND2  | 2.43                     | 0.51              |
| 1:p:1095:GLN:HE21 | 1:p:1100:VAL:HG21 | 1.75                     | 0.51              |
| 1:p:1160:LEU:HD23 | 1:p:1214:ASN:HB2  | 1.93                     | 0.51              |
| 2:3:130:ALA:O     | 2:3:132:TYR:N     | 2.43                     | 0.51              |
| 2:3:258:PHE:CZ    | 3:r:87:MET:O      | 2.64                     | 0.51              |
| 2:e:204:LEU:HD13  | 2:e:210:VAL:HG12  | 1.92                     | 0.51              |
| 2:g:204:LEU:HD13  | 2:g:210:VAL:HG12  | 1.93                     | 0.51              |
| 1:A:441:ILE:HD13  | 1:A:1092:SER:HB3  | 1.91                     | 0.51              |
| 1:B:492:HIS:HD2   | 1:B:495:ARG:HB2   | 1.76                     | 0.51              |
| 1:B:1175:ASN:ND2  | 1:B:1181:SER:OG   | 2.43                     | 0.51              |
| 1:C:667:ALA:HB2   | 1:D:643:GLN:HG2   | 1.92                     | 0.51              |
| 1:D:86:LYS:HA     | 5:Z:75:GLU:HB3    | 1.92                     | 0.51              |
| 1:D:813:PHE:CE2   | 3:M:82:LEU:HA     | 2.42                     | 0.51              |
| 1:E:20:LEU:HD12   | 1:l:379:ASN:HD21  | 1.71                     | 0.51              |
| 1:F:610:GLU:OE2   | 1:F:914:LEU:N     | 2.43                     | 0.51              |
| 1:G:748:ARG:HH11  | 2:h:275:THR:CB    | 2.23                     | 0.51              |
| 1:H:959:LEU:HB3   | 1:H:963:PHE:HE1   | 1.75                     | 0.51              |
| 1:H:1199:TYR:OH   | 1:H:1252:THR:OG1  | 2.26                     | 0.51              |
| 1:k:930:PRO:CG    | 1:k:957:PHE:HE1   | 2.18                     | 0.51              |
| 1:l:965:HIS:O     | 1:l:969:HIS:N     | 2.42                     | 0.51              |
| 1:l:1298:PRO:O    | 1:l:1303:GLN:N    | 2.34                     | 0.51              |
| 1:m:1230:THR:O    | 1:m:1234:GLU:HB2  | 2.11                     | 0.51              |
| 1:n:424:GLN:CB    | 1:n:575:LEU:HD21  | 2.41                     | 0.51              |
| 1:n:1146:PRO:HB3  | 1:o:1193:ALA:HB1  | 1.92                     | 0.51              |
| 1:n:1148:LEU:HD23 | 1:o:210:ARG:HG2   | 1.93                     | 0.51              |
| 1:o:974:PRO:HA    | 1:o:977:CYS:HB2   | 1.92                     | 0.51              |
| 1:o:1070:MET:SD   | 1:o:1075:GLY:N    | 2.72                     | 0.51              |
| 1:o:1158:VAL:HG12 | 1:o:1160:LEU:HD21 | 1.93                     | 0.51              |
| 1:p:512:ASN:HD21  | 1:p:972:ARG:HB3   | 1.76                     | 0.51              |
| 1:p:876:GLU:HG3   | 1:p:899:HIS:CE1   | 2.45                     | 0.51              |
| 1:q:761:MET:O     | 1:q:871:ASN:ND2   | 2.43                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:q:794:LEU:O     | 1:q:797:HIS:ND1   | 2.38                     | 0.51              |
| 2:2:204:LEU:HB2   | 2:2:211:LEU:HD23  | 1.92                     | 0.51              |
| 2:3:83:LYS:O      | 2:3:87:ARG:HG2    | 2.10                     | 0.51              |
| 2:i:83:LYS:O      | 2:i:87:ARG:HG2    | 2.10                     | 0.51              |
| 4:S:54:VAL:HG21   | 4:S:148:ILE:HD12  | 1.91                     | 0.51              |
| 4:S:254:ARG:HB3   | 4:S:288:GLY:HA3   | 1.93                     | 0.51              |
| 4:V:126:ARG:HD3   | 4:V:192:ILE:HD13  | 1.92                     | 0.51              |
| 1:A:81:PHE:HB2    | 1:A:306:PHE:HB3   | 1.92                     | 0.51              |
| 1:A:696:ASN:HA    | 1:B:952:ARG:HH12  | 1.75                     | 0.51              |
| 1:C:235:ARG:HE    | 1:C:239:GLN:HG3   | 1.76                     | 0.51              |
| 1:C:366:ARG:NH1   | 1:C:1033:TYR:OH   | 2.42                     | 0.51              |
| 1:D:104:GLY:HA3   | 1:D:107:ILE:HD12  | 1.93                     | 0.51              |
| 1:D:786:TYR:O     | 1:D:927:TYR:OH    | 2.28                     | 0.51              |
| 1:G:434:LYS:NZ    | 1:G:1150:HIS:O    | 2.43                     | 0.51              |
| 1:G:446:ALA:HA    | 1:G:1094:MET:HG3  | 1.93                     | 0.51              |
| 1:G:1100:VAL:HG11 | 1:G:1233:ARG:HH11 | 1.76                     | 0.51              |
| 1:I:1022:ARG:NH2  | 1:I:1308:GLN:OE1  | 2.44                     | 0.51              |
| 1:k:393:THR:OG1   | 1:k:1248:GLN:NE2  | 2.42                     | 0.51              |
| 1:l:458:ALA:O     | 1:l:462:LEU:N     | 2.37                     | 0.51              |
| 1:l:709:SER:HB3   | 1:l:712:HIS:HD2   | 1.76                     | 0.51              |
| 1:n:230:LEU:HB3   | 1:n:235:ARG:HH11  | 1.76                     | 0.51              |
| 1:n:262:TYR:HB2   | 1:n:1036:LYS:HD2  | 1.93                     | 0.51              |
| 1:n:1183:MET:SD   | 1:n:1259:ASN:ND2  | 2.84                     | 0.51              |
| 1:o:332:ARG:HB3   | 1:o:337:SER:HA    | 1.93                     | 0.51              |
| 1:p:768:PHE:HB2   | 1:p:870:GLU:HB2   | 1.92                     | 0.51              |
| 1:q:674:THR:O     | 1:q:678:ASN:ND2   | 2.44                     | 0.51              |
| 1:q:897:LEU:HD12  | 1:q:968:HIS:HB2   | 1.92                     | 0.51              |
| 2:2:206:GLU:CB    | 2:3:132:TYR:C     | 2.81                     | 0.51              |
| 2:3:259:ALA:HB3   | 2:3:289:LEU:HD13  | 1.93                     | 0.51              |
| 2:h:83:LYS:O      | 2:h:87:ARG:HG2    | 2.10                     | 0.51              |
| 2:g:197:VAL:C     | 2:g:199:ASP:N     | 2.68                     | 0.51              |
| 4:U:228:ARG:NH2   | 5:c:223:SER:O     | 2.43                     | 0.51              |
| 5:b:49:VAL:HG22   | 5:b:59:MET:HE3    | 1.93                     | 0.51              |
| 1:A:146:ASP:HA    | 1:A:150:ASP:HB3   | 1.92                     | 0.51              |
| 1:A:605:ASP:OD2   | 1:A:640:TYR:OH    | 2.29                     | 0.51              |
| 1:A:1233:ARG:HH22 | 1:A:1244:SER:HB3  | 1.75                     | 0.51              |
| 1:B:273:VAL:HG23  | 1:B:369:ALA:HB3   | 1.93                     | 0.51              |
| 1:E:125:PRO:HA    | 1:E:1064:ASN:HA   | 1.91                     | 0.51              |
| 1:E:866:ALA:O     | 3:N:86:ARG:NH2    | 2.44                     | 0.51              |
| 1:F:119:LYS:HD2   | 1:l:33:PHE:CE1    | 2.46                     | 0.51              |
| 1:F:389:ASP:HA    | 1:F:1027:GLU:HA   | 1.93                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:F:1017:ALA:CB   | 1:F:1160:LEU:O    | 2.56                     | 0.51              |
| 1:H:811:LYS:O     | 1:H:836:ASN:ND2   | 2.41                     | 0.51              |
| 1:k:744:HIS:ND1   | 2:2:175:ALA:N     | 2.55                     | 0.51              |
| 1:m:128:ILE:HD13  | 1:m:171:ALA:HB3   | 1.93                     | 0.51              |
| 1:n:81:PHE:HB2    | 1:n:306:PHE:HB3   | 1.92                     | 0.51              |
| 1:p:88:THR:HG22   | 1:p:89:THR:HG23   | 1.93                     | 0.51              |
| 1:p:576:ARG:HH11  | 1:p:1007:LEU:HD21 | 1.74                     | 0.51              |
| 1:p:692:LEU:CD2   | 1:p:1010:MET:HG3  | 2.29                     | 0.51              |
| 1:p:944:LEU:HD11  | 1:p:951:GLN:HB2   | 1.93                     | 0.51              |
| 1:q:427:THR:HG23  | 1:q:428:THR:HG23  | 1.93                     | 0.51              |
| 1:q:523:PHE:O     | 1:q:528:ASN:ND2   | 2.40                     | 0.51              |
| 1:q:669:VAL:HG12  | 1:q:671:ALA:H     | 1.76                     | 0.51              |
| 2:g:144:LEU:HD11  | 2:g:221:ARG:HE    | 1.76                     | 0.51              |
| 2:g:206:GLU:HB3   | 2:j:132:TYR:CA    | 2.40                     | 0.51              |
| 3:O:71:MET:O      | 3:O:74:HIS:NE2    | 2.44                     | 0.51              |
| 5:b:13:LEU:HD13   | 5:b:123:VAL:HG21  | 1.92                     | 0.51              |
| 5:d:73:ARG:NH2    | 5:d:75:GLU:OE2    | 2.44                     | 0.51              |
| 1:A:1095:GLN:HE21 | 1:A:1100:VAL:HG21 | 1.76                     | 0.51              |
| 1:B:702:GLU:OE2   | 1:B:715:ARG:NH2   | 2.44                     | 0.51              |
| 1:C:882:ASP:OD1   | 1:C:882:ASP:N     | 2.43                     | 0.51              |
| 1:C:1019:THR:HG23 | 1:C:1160:LEU:HD11 | 1.93                     | 0.51              |
| 1:E:30:GLU:CG     | 1:m:1263:PHE:CE2  | 2.93                     | 0.51              |
| 1:E:188:ALA:CB    | 1:E:1032:LEU:HD11 | 2.41                     | 0.51              |
| 1:E:513:GLU:HA    | 1:E:973:THR:HG21  | 1.92                     | 0.51              |
| 1:F:627:GLU:HA    | 1:F:630:ILE:HG13  | 1.93                     | 0.51              |
| 1:G:500:PHE:HZ    | 1:G:507:PRO:HD3   | 1.76                     | 0.51              |
| 1:H:146:ASP:N     | 1:H:146:ASP:OD1   | 2.42                     | 0.51              |
| 1:I:493:ALA:O     | 1:I:497:LEU:HB2   | 2.11                     | 0.51              |
| 1:k:68:LEU:HD12   | 1:k:301:ALA:O     | 2.06                     | 0.51              |
| 1:k:488:GLU:HG3   | 1:k:962:ILE:HB    | 1.93                     | 0.51              |
| 1:l:174:ARG:HH22  | 1:m:99:PRO:HB3    | 1.76                     | 0.51              |
| 1:l:542:CYS:O     | 1:l:552:PRO:HA    | 2.11                     | 0.51              |
| 1:m:152:LEU:HG    | 1:n:337:SER:CB    | 2.41                     | 0.51              |
| 1:m:431:PHE:CE1   | 1:m:1310:THR:OG1  | 2.57                     | 0.51              |
| 1:m:483:ARG:HB2   | 1:m:964:ALA:HB1   | 1.92                     | 0.51              |
| 1:m:757:ARG:HA    | 1:m:768:PHE:HE2   | 1.76                     | 0.51              |
| 1:n:395:TYR:HD1   | 1:n:1305:ALA:HB3  | 1.75                     | 0.51              |
| 1:o:100:ARG:NH2   | 1:o:111:ARG:O     | 2.44                     | 0.51              |
| 1:o:619:ILE:HD11  | 1:o:864:LEU:HD22  | 1.93                     | 0.51              |
| 2:2:144:LEU:HD11  | 2:2:221:ARG:HE    | 1.76                     | 0.51              |
| 2:e:208:PRO:O     | 2:e:212:VAL:HG23  | 2.10                     | 0.51              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:h:130:ALA:O    | 2:h:132:TYR:N     | 2.43                     | 0.51              |
| 2:f:206:GLU:HB3  | 2:i:132:TYR:CA    | 2.40                     | 0.51              |
| 2:i:216:LEU:HD23 | 2:i:219:LEU:HB2   | 1.92                     | 0.51              |
| 2:g:208:PRO:CB   | 2:j:95:LEU:HD12   | 2.40                     | 0.51              |
| 2:j:285:GLU:CG   | 3:M:67:LYS:HE3    | 2.40                     | 0.51              |
| 4:T:217:HIS:HE1  | 5:X:286:VAL:HG22  | 1.74                     | 0.51              |
| 4:V:34:SER:O     | 4:V:38:GLY:N      | 2.41                     | 0.51              |
| 4:V:196:TYR:HA   | 4:V:202:GLY:HA3   | 1.92                     | 0.51              |
| 5:W:152:LEU:HD22 | 5:a:270:LEU:HD11  | 1.92                     | 0.51              |
| 5:Z:106:LEU:CD2  | 5:Z:133:ILE:HG22  | 2.41                     | 0.51              |
| 5:1:191:ILE:HG13 | 5:1:194:ARG:HD3   | 1.93                     | 0.51              |
| 1:A:292:ILE:HG12 | 1:A:361:LEU:HB3   | 1.93                     | 0.50              |
| 1:A:420:THR:HG22 | 1:A:422:GLU:H     | 1.75                     | 0.50              |
| 1:B:650:ALA:O    | 1:B:785:TYR:OH    | 2.27                     | 0.50              |
| 1:C:1314:GLN:HA  | 1:C:1317:MET:HB3  | 1.92                     | 0.50              |
| 1:D:471:PRO:HD2  | 1:D:476:ARG:HG2   | 1.92                     | 0.50              |
| 1:E:483:ARG:NH2  | 1:E:508:PRO:O     | 2.44                     | 0.50              |
| 1:E:601:ALA:O    | 1:E:605:ASP:HB2   | 2.11                     | 0.50              |
| 1:E:694:GLY:HA3  | 1:E:1010:MET:HE2  | 1.92                     | 0.50              |
| 1:F:395:TYR:HE2  | 1:F:1170:PHE:HD1  | 1.59                     | 0.50              |
| 1:F:1262:LEU:HB3 | 1:l:30:GLU:CB     | 2.41                     | 0.50              |
| 1:G:651:ASN:HB3  | 1:G:906:CYS:HB3   | 1.92                     | 0.50              |
| 1:G:691:GLU:HB2  | 1:H:952:ARG:HG3   | 1.93                     | 0.50              |
| 1:I:66:THR:HG23  | 1:I:69:GLY:H      | 1.76                     | 0.50              |
| 1:k:181:LEU:HD21 | 1:k:386:LEU:HG    | 1.93                     | 0.50              |
| 1:k:517:ASP:HB2  | 1:p:696:ASN:HD22  | 1.76                     | 0.50              |
| 1:k:744:HIS:CA   | 2:2:174:ARG:HA    | 2.40                     | 0.50              |
| 1:k:1219:GLN:HB2 | 1:k:1222:SER:HB3  | 1.92                     | 0.50              |
| 1:l:174:ARG:HG2  | 1:l:376:VAL:HB    | 1.93                     | 0.50              |
| 1:m:803:LEU:HD21 | 1:m:914:LEU:HD13  | 1.92                     | 0.50              |
| 1:m:1160:LEU:CD2 | 1:m:1214:ASN:CB   | 2.76                     | 0.50              |
| 1:n:558:ILE:HG22 | 1:n:998:LYS:HD2   | 1.93                     | 0.50              |
| 1:n:925:ARG:HH11 | 1:n:975:PHE:HB2   | 1.76                     | 0.50              |
| 1:o:938:HIS:O    | 1:o:942:VAL:N     | 2.42                     | 0.50              |
| 1:o:1094:MET:HA  | 1:o:1155:THR:HG21 | 1.94                     | 0.50              |
| 1:p:929:ASP:HB3  | 1:p:932:LEU:HB3   | 1.93                     | 0.50              |
| 2:j:259:ALA:HB3  | 2:j:289:LEU:HD13  | 1.93                     | 0.50              |
| 4:U:69:LEU:HD12  | 4:U:87:LEU:HD13   | 1.93                     | 0.50              |
| 4:U:153:ARG:HE   | 5:c:308:ILE:HD11  | 1.76                     | 0.50              |
| 5:z:152:LEU:HD23 | 5:z:161:VAL:HA    | 1.93                     | 0.50              |
| 1:B:292:ILE:HG12 | 1:B:361:LEU:HB3   | 1.92                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:600:ARG:HH11  | 1:B:794:LEU:HD23  | 1.75                     | 0.50              |
| 1:B:842:LEU:C     | 1:B:842:LEU:HD12  | 2.36                     | 0.50              |
| 1:B:1173:PRO:HB3  | 1:B:1306:LEU:HA   | 1.93                     | 0.50              |
| 1:D:1019:THR:HG23 | 1:D:1160:LEU:HD11 | 1.93                     | 0.50              |
| 1:D:1114:TRP:O    | 1:D:1118:ALA:N    | 2.41                     | 0.50              |
| 1:E:506:ASP:OD2   | 1:E:949:GLN:NE2   | 2.45                     | 0.50              |
| 1:E:1256:ILE:HA   | 1:E:1259:ASN:HD22 | 1.77                     | 0.50              |
| 1:F:1019:THR:CA   | 1:F:1160:LEU:HD11 | 2.40                     | 0.50              |
| 1:G:663:LEU:HD12  | 1:G:664:GLY:H     | 1.77                     | 0.50              |
| 1:H:185:LEU:HB3   | 1:H:388:ARG:HH22  | 1.74                     | 0.50              |
| 1:H:598:VAL:HG13  | 1:H:646:LEU:HA    | 1.91                     | 0.50              |
| 1:I:1212:THR:HG21 | 1:I:1219:GLN:HE21 | 1.74                     | 0.50              |
| 1:k:434:LYS:HE3   | 1:l:218:GLN:HG2   | 1.91                     | 0.50              |
| 1:k:907:MET:HE3   | 1:k:932:LEU:HG    | 1.93                     | 0.50              |
| 1:k:948:PRO:HB2   | 1:p:703:PRO:HG3   | 1.93                     | 0.50              |
| 1:k:1161:THR:HG22 | 1:k:1216:TRP:CD2  | 2.45                     | 0.50              |
| 1:k:1168:GLU:HA   | 1:p:438:PRO:HG3   | 1.90                     | 0.50              |
| 1:l:126:ILE:HG22  | 1:m:104:GLY:H     | 1.76                     | 0.50              |
| 1:l:1177:ARG:HH21 | 1:l:1181:SER:HB3  | 1.76                     | 0.50              |
| 1:m:1031:LEU:HD23 | 1:m:1081:ALA:HB2  | 1.93                     | 0.50              |
| 1:n:522:GLU:HG2   | 1:n:525:LYS:HD2   | 1.93                     | 0.50              |
| 1:o:494:THR:HG23  | 1:o:919:THR:HG21  | 1.92                     | 0.50              |
| 1:o:650:ALA:O     | 1:o:785:TYR:OH    | 2.29                     | 0.50              |
| 1:o:1205:ASP:OD2  | 1:o:1208:THR:OG1  | 2.25                     | 0.50              |
| 1:p:71:ALA:HB3    | 1:p:371:GLU:HB2   | 1.92                     | 0.50              |
| 1:p:1166:ASP:HA   | 1:p:1170:PHE:HD2  | 1.76                     | 0.50              |
| 1:q:788:CYS:SG    | 1:q:996:HIS:NE2   | 2.64                     | 0.50              |
| 2:f:204:LEU:HB2   | 2:f:211:LEU:HD23  | 1.92                     | 0.50              |
| 2:f:208:PRO:O     | 2:f:212:VAL:HG23  | 2.10                     | 0.50              |
| 2:g:257:ALA:HB3   | 2:g:260:ARG:HG2   | 1.93                     | 0.50              |
| 3:s:72:GLY:O      | 3:s:80:TYR:OH     | 2.28                     | 0.50              |
| 4:y:159:MET:O     | 4:y:160:LEU:CB    | 2.58                     | 0.50              |
| 4:V:245:SER:O     | 5:Z:271:ASN:ND2   | 2.44                     | 0.50              |
| 5:W:217:LYS:HB3   | 5:a:154:LEU:HD22  | 1.93                     | 0.50              |
| 5:W:297:ASP:HB2   | 5:W:306:LEU:HD12  | 1.93                     | 0.50              |
| 5:1:58:ARG:HE     | 5:1:61:ALA:HB3    | 1.76                     | 0.50              |
| 1:A:504:ARG:NE    | 1:A:946:ASP:OD2   | 2.40                     | 0.50              |
| 1:A:1324:THR:HG23 | 1:B:1326:LYS:HZ1  | 1.74                     | 0.50              |
| 1:B:104:GLY:HA3   | 1:B:107:ILE:HD12  | 1.93                     | 0.50              |
| 1:C:663:LEU:HD21  | 1:D:644:ARG:HH11  | 1.77                     | 0.50              |
| 1:D:431:PHE:O     | 1:D:439:GLN:HB3   | 2.11                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:D:756:ALA:HA    | 1:D:759:ILE:HG12  | 1.92                     | 0.50              |
| 1:F:81:PHE:HB3    | 1:F:84:LEU:HD12   | 1.93                     | 0.50              |
| 1:F:198:MET:CE    | 1:l:21:LEU:HD12   | 2.39                     | 0.50              |
| 1:F:523:PHE:HB2   | 1:F:566:ALA:HB1   | 1.92                     | 0.50              |
| 1:F:986:LEU:HA    | 1:F:989:VAL:HB    | 1.93                     | 0.50              |
| 1:k:949:GLN:HG2   | 1:p:698:ARG:HD3   | 1.94                     | 0.50              |
| 1:k:1199:TYR:HB3  | 1:k:1220:ARG:HB2  | 1.93                     | 0.50              |
| 1:l:603:LEU:HB3   | 1:l:794:LEU:HD21  | 1.93                     | 0.50              |
| 1:l:1233:ARG:HH22 | 1:l:1244:SER:HB3  | 1.76                     | 0.50              |
| 1:m:1261:THR:O    | 1:m:1264:LYS:N    | 2.45                     | 0.50              |
| 1:n:305:LYS:N     | 1:n:349:GLN:OE1   | 2.41                     | 0.50              |
| 1:n:379:ASN:OD1   | 1:o:205:ARG:NH2   | 2.43                     | 0.50              |
| 1:n:435:ASP:OD2   | 1:o:218:GLN:NE2   | 2.45                     | 0.50              |
| 2:i:66:ARG:CG     | 2:i:67:GLU:N      | 2.68                     | 0.50              |
| 4:S:269:ALA:HA    | 4:S:274:GLN:HG3   | 1.93                     | 0.50              |
| 4:U:61:VAL:HG13   | 4:U:64:LYS:HE3    | 1.92                     | 0.50              |
| 5:z:145:ARG:HH12  | 5:z:168:LEU:HD22  | 1.74                     | 0.50              |
| 5:Y:40:SER:HA     | 5:Y:43:VAL:HB     | 1.93                     | 0.50              |
| 5:1:48:VAL:HG22   | 5:1:62:ARG:HE     | 1.75                     | 0.50              |
| 1:A:72:LEU:HD23   | 1:A:180:PHE:HD2   | 1.76                     | 0.50              |
| 1:A:716:LEU:HD21  | 1:A:787:LEU:HD21  | 1.94                     | 0.50              |
| 1:C:818:PHE:CD2   | 3:L:88:LEU:HD13   | 2.47                     | 0.50              |
| 1:D:41:GLY:HA3    | 1:H:111:ARG:HH11  | 1.76                     | 0.50              |
| 1:D:1201:HIS:ND1  | 1:D:1212:THR:OG1  | 2.42                     | 0.50              |
| 1:F:118:SER:HB2   | 1:l:5:TRP:HH2     | 1.75                     | 0.50              |
| 1:G:389:ASP:HA    | 1:G:1027:GLU:HA   | 1.92                     | 0.50              |
| 1:H:523:PHE:HB2   | 1:H:566:ALA:HB1   | 1.93                     | 0.50              |
| 1:I:595:THR:HA    | 1:I:675:HIS:HD2   | 1.75                     | 0.50              |
| 1:I:967:TYR:O     | 1:I:972:ARG:NH2   | 2.44                     | 0.50              |
| 1:k:698:ARG:NH1   | 1:k:701:ASP:O     | 2.45                     | 0.50              |
| 1:k:756:ALA:HA    | 1:k:759:ILE:HG12  | 1.93                     | 0.50              |
| 1:l:450:LEU:HD21  | 1:l:1018:LEU:HD11 | 1.94                     | 0.50              |
| 1:o:251:VAL:HG11  | 1:o:1033:TYR:HE2  | 1.76                     | 0.50              |
| 1:o:1268:GLU:OE2  | 1:o:1300:ARG:NH1  | 2.45                     | 0.50              |
| 1:p:1160:LEU:CD2  | 1:p:1214:ASN:HD22 | 2.24                     | 0.50              |
| 1:q:634:THR:O     | 1:q:638:ASN:HB2   | 2.12                     | 0.50              |
| 1:q:1138:GLY:H    | 5:1:54:ARG:HH21   | 1.59                     | 0.50              |
| 1:q:1161:THR:OG1  | 1:q:1164:SER:OG   | 2.29                     | 0.50              |
| 2:2:262:TYR:CZ    | 3:x:87:MET:HE1    | 2.43                     | 0.50              |
| 2:3:111:ALA:CB    | 4:y:232:PHE:CE1   | 2.88                     | 0.50              |
| 4:U:72:ARG:HD3    | 5:c:102:LYS:O     | 2.11                     | 0.50              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 5:z:29:ILE:HD11  | 5:z:128:LEU:HD21  | 1.94                     | 0.50              |
| 5:X:169:ARG:HA   | 5:X:180:LEU:HD23  | 1.93                     | 0.50              |
| 1:B:439:GLN:HG2  | 1:B:1092:SER:H    | 1.77                     | 0.50              |
| 1:C:921:ILE:HG22 | 1:C:923:PHE:HB3   | 1.94                     | 0.50              |
| 1:C:1180:SER:N   | 1:C:1205:ASP:OD1  | 2.44                     | 0.50              |
| 1:E:82:HIS:CD2   | 1:G:145:GLU:HG2   | 2.46                     | 0.50              |
| 1:E:975:PHE:HE1  | 1:E:995:MET:HB3   | 1.74                     | 0.50              |
| 1:G:888:GLY:O    | 1:G:892:ALA:N     | 2.45                     | 0.50              |
| 1:G:1298:PRO:O   | 1:G:1302:LEU:N    | 2.37                     | 0.50              |
| 1:H:515:LYS:NZ   | 1:H:534:GLU:OE2   | 2.41                     | 0.50              |
| 1:k:48:ASN:HB2   | 4:T:162:THR:HG22  | 1.94                     | 0.50              |
| 1:k:930:PRO:HD3  | 1:k:957:PHE:HZ    | 1.77                     | 0.50              |
| 1:l:232:ASP:HA   | 1:l:1352:ASN:HD22 | 1.77                     | 0.50              |
| 1:l:975:PHE:HE1  | 1:l:995:MET:HB3   | 1.77                     | 0.50              |
| 1:m:804:ASN:HB2  | 1:m:917:TYR:HB3   | 1.93                     | 0.50              |
| 1:m:1229:ASN:O   | 1:m:1233:ARG:HB2  | 2.11                     | 0.50              |
| 1:n:961:PRO:HA   | 1:n:964:ALA:HB3   | 1.92                     | 0.50              |
| 1:n:1097:LEU:HA  | 1:n:1100:VAL:HB   | 1.94                     | 0.50              |
| 1:o:663:LEU:HD11 | 1:o:668:VAL:HB    | 1.93                     | 0.50              |
| 1:o:710:ALA:HA   | 1:o:713:ASP:OD1   | 2.11                     | 0.50              |
| 2:2:257:ALA:HB3  | 2:2:260:ARG:HG2   | 1.93                     | 0.50              |
| 2:e:208:PRO:CB   | 2:h:95:LEU:HD12   | 2.41                     | 0.50              |
| 2:f:144:LEU:HD11 | 2:f:221:ARG:HE    | 1.76                     | 0.50              |
| 2:i:93:PRO:CG    | 2:i:195:TYR:CZ    | 2.85                     | 0.50              |
| 5:Y:85:THR:OG1   | 5:Y:88:GLN:NE2    | 2.45                     | 0.50              |
| 5:Z:154:LEU:HD23 | 5:d:214:TYR:HD1   | 1.76                     | 0.50              |
| 1:A:253:GLU:HA   | 1:A:1035:THR:HG21 | 1.94                     | 0.50              |
| 1:A:309:SER:HB3  | 1:A:312:ASN:HB2   | 1.92                     | 0.50              |
| 1:A:1147:ALA:HA  | 1:B:1206:PRO:HG3  | 1.92                     | 0.50              |
| 1:B:665:ASP:OD2  | 1:C:607:GLN:NE2   | 2.44                     | 0.50              |
| 1:B:1098:PHE:HE2 | 1:B:1119:THR:HG23 | 1.77                     | 0.50              |
| 1:C:104:GLY:HA3  | 1:C:107:ILE:HD12  | 1.94                     | 0.50              |
| 1:D:14:LEU:HD21  | 1:H:341:LEU:HB2   | 1.94                     | 0.50              |
| 1:D:513:GLU:HA   | 1:D:973:THR:HG21  | 1.92                     | 0.50              |
| 1:E:66:THR:HG23  | 1:E:69:GLY:H      | 1.77                     | 0.50              |
| 1:E:602:SER:HA   | 1:E:646:LEU:HD13  | 1.93                     | 0.50              |
| 1:F:329:HIS:ND1  | 1:l:12:PRO:HD2    | 2.26                     | 0.50              |
| 1:G:1018:LEU:HG  | 1:G:1159:ILE:CD1  | 2.41                     | 0.50              |
| 1:H:567:LEU:HD22 | 1:H:1161:THR:HG21 | 1.92                     | 0.50              |
| 1:k:78:ALA:HA    | 1:k:1041:VAL:O    | 2.11                     | 0.50              |
| 1:k:638:ASN:ND2  | 1:k:668:VAL:O     | 2.41                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:l:223:LYS:O     | 1:l:227:THR:OG1   | 2.26                     | 0.50              |
| 1:m:417:LEU:HD23  | 1:n:408:TYR:HB3   | 1.94                     | 0.50              |
| 1:n:492:HIS:HD2   | 1:n:495:ARG:HB2   | 1.77                     | 0.50              |
| 1:q:401:HIS:HB3   | 1:q:1163:VAL:HG22 | 1.94                     | 0.50              |
| 1:q:733:VAL:HA    | 1:q:877:ILE:HG22  | 1.94                     | 0.50              |
| 1:q:813:PHE:HA    | 3:x:85:LEU:HD23   | 1.93                     | 0.50              |
| 4:y:190:PHE:HD2   | 4:y:253:GLN:HE21  | 1.60                     | 0.50              |
| 4:V:81:SER:OG     | 4:V:82:THR:N      | 2.45                     | 0.50              |
| 5:z:296:CYS:HB2   | 5:z:308:ILE:HD11  | 1.93                     | 0.50              |
| 5:Y:107:THR:HG22  | 5:Y:291:PRO:HA    | 1.94                     | 0.50              |
| 5:c:60:ARG:NH1    | 5:c:143:ASN:OD1   | 2.45                     | 0.50              |
| 1:B:934:ALA:HB2   | 1:B:944:LEU:HD12  | 1.93                     | 0.50              |
| 1:C:393:THR:OG1   | 1:C:1248:GLN:NE2  | 2.40                     | 0.50              |
| 1:D:717:TRP:HE1   | 1:D:731:VAL:HG21  | 1.77                     | 0.50              |
| 1:D:726:ARG:NH1   | 1:E:945:ASN:OD1   | 2.43                     | 0.50              |
| 1:E:523:PHE:HE2   | 1:E:1215:PRO:HG3  | 1.75                     | 0.50              |
| 1:E:952:ARG:HG2   | 1:E:954:ASP:H     | 1.77                     | 0.50              |
| 1:F:605:ASP:OD2   | 1:F:640:TYR:OH    | 2.30                     | 0.50              |
| 1:G:665:ASP:OD1   | 1:H:607:GLN:NE2   | 2.45                     | 0.50              |
| 1:I:818:PHE:HB2   | 3:R:88:LEU:HB3    | 1.93                     | 0.50              |
| 1:I:843:VAL:HG13  | 1:I:857:ALA:HB3   | 1.94                     | 0.50              |
| 1:k:191:CYS:SG    | 1:k:243:TYR:OH    | 2.66                     | 0.50              |
| 1:k:965:HIS:HB3   | 1:k:968:HIS:HB2   | 1.94                     | 0.50              |
| 1:l:1147:ALA:HB1  | 1:m:1206:PRO:HG3  | 1.94                     | 0.50              |
| 1:m:839:LEU:O     | 1:m:843:VAL:HB    | 2.12                     | 0.50              |
| 1:n:641:TRP:HZ3   | 1:n:670:PRO:HG2   | 1.77                     | 0.50              |
| 1:n:1009:ARG:HH11 | 1:n:1118:ALA:HA   | 1.75                     | 0.50              |
| 1:o:1101:PHE:HB3  | 1:o:1104:HIS:HD2  | 1.76                     | 0.50              |
| 1:p:546:GLU:N     | 1:p:549:GLN:O     | 2.44                     | 0.50              |
| 1:p:1199:TYR:HB3  | 1:p:1220:ARG:HB2  | 1.94                     | 0.50              |
| 1:q:535:LEU:HD21  | 1:q:1219:GLN:HB2  | 1.94                     | 0.50              |
| 2:2:104:LYS:HD3   | 2:3:92:LEU:HD13   | 1.77                     | 0.50              |
| 2:h:208:PRO:CD    | 4:S:236:ASN:ND2   | 2.67                     | 0.50              |
| 4:T:63:GLN:HA     | 4:T:140:ILE:HG21  | 1.94                     | 0.50              |
| 4:V:72:ARG:HH12   | 5:d:104:ASP:HB2   | 1.76                     | 0.50              |
| 4:V:152:MET:HE3   | 5:d:296:CYS:HB2   | 1.93                     | 0.50              |
| 5:z:199:SER:HB2   | 5:z:283:ILE:HD12  | 1.94                     | 0.50              |
| 5:X:112:VAL:C     | 5:X:113:PHE:CD2   | 2.90                     | 0.50              |
| 5:Z:59:MET:HB3    | 5:Z:63:MET:HE3    | 1.94                     | 0.50              |
| 1:A:1019:THR:HG23 | 1:A:1160:LEU:CD1  | 2.42                     | 0.50              |
| 1:B:678:ASN:O     | 1:B:682:ILE:N     | 2.41                     | 0.50              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:C:577:ALA:HA    | 1:C:994:ILE:HG21 | 1.93                     | 0.50              |
| 1:C:856:GLN:NE2   | 1:C:859:GLU:OE1  | 2.45                     | 0.50              |
| 1:C:1114:TRP:O    | 1:C:1118:ALA:N   | 2.45                     | 0.50              |
| 1:E:19:ASP:OD2    | 1:m:252:THR:HB   | 2.12                     | 0.50              |
| 1:E:660:ALA:O     | 1:F:606:HIS:NE2  | 2.37                     | 0.50              |
| 1:E:749:ASN:H     | 1:E:757:ARG:HH21 | 1.60                     | 0.50              |
| 1:F:165:VAL:HG13  | 4:T:12:ARG:HD2   | 1.93                     | 0.50              |
| 1:F:451:CYS:O     | 1:F:1106:TYR:OH  | 2.27                     | 0.50              |
| 1:F:1262:LEU:HB3  | 1:l:30:GLU:HB2   | 1.94                     | 0.50              |
| 1:G:544:HIS:CE1   | 1:G:553:LEU:HB2  | 2.47                     | 0.50              |
| 1:G:1018:LEU:HB3  | 1:G:1157:GLU:OE2 | 2.12                     | 0.50              |
| 1:G:1166:ASP:HA   | 1:G:1170:PHE:HD2 | 1.76                     | 0.50              |
| 1:H:152:LEU:HD12  | 1:I:333:ILE:HG12 | 1.92                     | 0.50              |
| 1:I:819:LEU:CD1   | 3:R:59:PRO:HD2   | 2.42                     | 0.50              |
| 1:k:1207:GLN:HE21 | 1:p:437:ILE:HG21 | 1.65                     | 0.50              |
| 1:l:557:ARG:HG2   | 1:l:972:ARG:HH12 | 1.77                     | 0.50              |
| 1:m:147:THR:O     | 1:m:150:ASP:N    | 2.45                     | 0.50              |
| 1:m:285:LEU:HD23  | 1:m:292:ILE:HD13 | 1.94                     | 0.50              |
| 1:m:393:THR:OG1   | 1:m:1248:GLN:NE2 | 2.44                     | 0.50              |
| 1:m:664:GLY:HA2   | 1:n:644:ARG:NH1  | 2.27                     | 0.50              |
| 1:n:657:ARG:NH2   | 1:n:778:GLU:OE1  | 2.44                     | 0.50              |
| 1:o:231:LEU:HD22  | 1:o:1082:HIS:HB2 | 1.93                     | 0.50              |
| 1:p:67:PHE:HA     | 1:p:177:ILE:HD11 | 1.92                     | 0.50              |
| 1:q:294:ARG:HG2   | 1:q:359:ASP:HB3  | 1.94                     | 0.50              |
| 2:3:216:LEU:HD23  | 2:3:219:LEU:HB2  | 1.92                     | 0.50              |
| 3:K:40:ARG:HE     | 3:K:69:MET:HG3   | 1.77                     | 0.50              |
| 4:S:49:THR:HA     | 4:S:151:SER:HA   | 1.94                     | 0.50              |
| 4:V:294:ALA:O     | 5:Z:282:GLN:NE2  | 2.44                     | 0.50              |
| 1:A:740:LEU:HD21  | 1:A:767:LEU:HD22 | 1.93                     | 0.50              |
| 1:A:885:GLN:O     | 1:A:891:SER:OG   | 2.29                     | 0.50              |
| 1:B:1180:SER:N    | 1:B:1205:ASP:OD1 | 2.43                     | 0.50              |
| 1:C:754:ASP:N     | 3:L:83:ASP:OD1   | 2.43                     | 0.50              |
| 1:D:391:GLU:HA    | 1:D:1025:THR:HA  | 1.94                     | 0.50              |
| 1:D:651:ASN:HB3   | 1:D:906:CYS:HB3  | 1.94                     | 0.50              |
| 1:E:259:PRO:HA    | 1:E:269:ARG:HD3  | 1.92                     | 0.50              |
| 1:F:30:GLU:HG3    | 1:F:32:MET:HG2   | 1.94                     | 0.50              |
| 1:G:377:TYR:CE1   | 1:H:101:VAL:HG11 | 2.47                     | 0.50              |
| 1:G:1276:CYS:SG   | 1:G:1277:ILE:N   | 2.85                     | 0.50              |
| 1:H:1021:VAL:HG11 | 1:H:1176:PRO:HB3 | 1.93                     | 0.50              |
| 1:H:1053:ARG:HG2  | 5:d:306:LEU:HD22 | 1.93                     | 0.50              |
| 1:H:1087:ARG:NH2  | 1:H:1278:HIS:O   | 2.43                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:H:1313:THR:HG23 | 1:H:1316:LEU:H    | 1.77                     | 0.50              |
| 1:I:813:PHE:CE2   | 3:R:82:LEU:HA     | 2.47                     | 0.50              |
| 1:k:210:ARG:NH1   | 1:k:1187:ASP:OD2  | 2.45                     | 0.50              |
| 1:k:589:PRO:HB2   | 1:k:592:HIS:HB3   | 1.94                     | 0.50              |
| 1:l:390:VAL:HG22  | 1:l:1295:VAL:HB   | 1.93                     | 0.50              |
| 1:l:523:PHE:HZ    | 1:l:534:GLU:HG3   | 1.77                     | 0.50              |
| 1:l:950:TYR:HB3   | 1:l:957:PHE:CE1   | 2.44                     | 0.50              |
| 1:m:172:MET:HE3   | 4:S:12:ARG:NH2    | 2.26                     | 0.50              |
| 1:m:263:THR:HA    | 1:m:269:ARG:HA    | 1.94                     | 0.50              |
| 1:m:493:ALA:O     | 1:m:497:LEU:HB2   | 2.11                     | 0.50              |
| 1:n:309:SER:HB3   | 1:n:312:ASN:HB2   | 1.94                     | 0.50              |
| 1:n:1039:THR:OG1  | 1:n:1068:VAL:O    | 2.29                     | 0.50              |
| 1:o:481:CYS:SG    | 1:o:482:ARG:N     | 2.85                     | 0.50              |
| 1:o:602:SER:HB3   | 1:o:647:LEU:H     | 1.77                     | 0.50              |
| 2:e:257:ALA:HB3   | 2:e:260:ARG:HG2   | 1.93                     | 0.50              |
| 3:N:72:GLY:O      | 3:N:80:TYR:OH     | 2.28                     | 0.50              |
| 3:O:40:ARG:HE     | 3:O:69:MET:HG3    | 1.77                     | 0.50              |
| 4:U:109:TYR:HB3   | 4:U:114:GLU:HG3   | 1.94                     | 0.50              |
| 4:V:18:ASP:HB3    | 4:V:24:LYS:HG2    | 1.94                     | 0.50              |
| 5:d:74:VAL:HG22   | 5:d:79:MET:HG3    | 1.94                     | 0.50              |
| 1:A:453:PRO:HG2   | 1:A:1104:HIS:HB3  | 1.94                     | 0.49              |
| 1:A:813:PHE:CZ    | 3:J:85:LEU:HB3    | 2.44                     | 0.49              |
| 1:C:598:VAL:HG12  | 1:C:647:LEU:HB2   | 1.94                     | 0.49              |
| 1:C:650:ALA:O     | 1:C:785:TYR:OH    | 2.30                     | 0.49              |
| 1:D:476:ARG:HH21  | 1:D:480:LEU:HD12  | 1.77                     | 0.49              |
| 1:D:480:LEU:HD23  | 1:D:550:VAL:HG11  | 1.94                     | 0.49              |
| 1:D:795:ASN:O     | 1:D:797:HIS:ND1   | 2.44                     | 0.49              |
| 1:F:509:ARG:HB3   | 1:F:513:GLU:HB2   | 1.94                     | 0.49              |
| 1:F:759:ILE:HG22  | 3:O:79:ALA:CB     | 2.42                     | 0.49              |
| 1:G:380:THR:HB    | 1:H:101:VAL:HG12  | 1.92                     | 0.49              |
| 1:G:734:VAL:HG12  | 1:G:739:PRO:HA    | 1.93                     | 0.49              |
| 1:H:843:VAL:O     | 1:H:843:VAL:HG12  | 2.12                     | 0.49              |
| 1:I:248:THR:O     | 1:I:366:ARG:NH2   | 2.45                     | 0.49              |
| 1:k:200:HIS:CE1   | 1:p:1085:ARG:HG3  | 2.46                     | 0.49              |
| 1:m:152:LEU:CD1   | 1:n:333:ILE:HG12  | 2.42                     | 0.49              |
| 1:m:417:LEU:HD11  | 1:m:1313:THR:HG21 | 1.92                     | 0.49              |
| 1:m:1101:PHE:HB3  | 1:m:1104:HIS:HD2  | 1.77                     | 0.49              |
| 1:n:833:LEU:N     | 1:n:855:ASN:OD1   | 2.45                     | 0.49              |
| 1:o:998:LYS:HG3   | 1:o:1000:SER:H    | 1.77                     | 0.49              |
| 1:p:534:GLU:OE2   | 1:p:557:ARG:NH1   | 2.45                     | 0.49              |
| 1:p:816:LYS:HD3   | 1:p:833:LEU:HG    | 1.93                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:e:144:LEU:HD11  | 2:e:221:ARG:HE    | 1.76                     | 0.49              |
| 3:J:55:MET:O      | 3:J:62:SER:OG     | 2.30                     | 0.49              |
| 5:z:297:ASP:HB2   | 5:z:306:LEU:HD12  | 1.92                     | 0.49              |
| 1:A:419:ASP:OD1   | 1:A:424:GLN:NE2   | 2.45                     | 0.49              |
| 1:A:1018:LEU:C    | 1:A:1160:LEU:HD12 | 2.37                     | 0.49              |
| 1:A:1160:LEU:HD23 | 1:A:1214:ASN:CB   | 2.42                     | 0.49              |
| 1:B:539:PHE:HA    | 1:B:556:PRO:HA    | 1.94                     | 0.49              |
| 1:B:695:LEU:HD21  | 1:B:1006:ALA:HB1  | 1.94                     | 0.49              |
| 1:B:777:GLU:HG3   | 1:C:951:GLN:HE21  | 1.77                     | 0.49              |
| 1:D:282:GLN:OE1   | 1:D:372:HIS:NE2   | 2.41                     | 0.49              |
| 1:D:1234:GLU:OE1  | 5:Z:52:LYS:HD3    | 2.12                     | 0.49              |
| 1:E:325:ASP:HB3   | 1:E:328:GLN:HB3   | 1.93                     | 0.49              |
| 1:E:409:SER:OG    | 1:E:1333:HIS:ND1  | 2.34                     | 0.49              |
| 1:G:22:THR:OG1    | 1:G:23:HIS:N      | 2.45                     | 0.49              |
| 1:G:925:ARG:HH12  | 1:G:971:HIS:HB3   | 1.78                     | 0.49              |
| 1:I:276:SER:HB3   | 1:I:280:VAL:HG13  | 1.94                     | 0.49              |
| 1:k:184:LEU:O     | 1:k:188:ALA:HB2   | 2.12                     | 0.49              |
| 1:n:100:ARG:HH12  | 1:n:112:GLN:HA    | 1.76                     | 0.49              |
| 1:n:1230:THR:H    | 1:n:1251:THR:HG22 | 1.77                     | 0.49              |
| 1:o:4:ASN:ND2     | 1:p:318:ALA:O     | 2.41                     | 0.49              |
| 1:o:1298:PRO:O    | 1:o:1302:LEU:N    | 2.34                     | 0.49              |
| 1:p:409:SER:OG    | 1:p:1333:HIS:ND1  | 2.39                     | 0.49              |
| 1:p:898:GLN:HE21  | 1:p:970:TRP:CD1   | 2.30                     | 0.49              |
| 1:p:1167:LEU:HD21 | 1:p:1332:THR:HG21 | 1.94                     | 0.49              |
| 1:p:1310:THR:HB   | 1:p:1339:ILE:HB   | 1.94                     | 0.49              |
| 2:2:204:LEU:HD13  | 2:2:210:VAL:HG12  | 1.93                     | 0.49              |
| 2:j:252:PHE:CZ    | 3:M:93:LYS:NZ     | 2.80                     | 0.49              |
| 4:U:294:ALA:O     | 5:Y:282:GLN:NE2   | 2.45                     | 0.49              |
| 5:X:89:CYS:N      | 5:X:308:ILE:HG23  | 2.22                     | 0.49              |
| 1:A:53:ALA:HA     | 1:B:322:ILE:HB    | 1.95                     | 0.49              |
| 1:C:509:ARG:HB2   | 1:C:513:GLU:HB2   | 1.94                     | 0.49              |
| 1:E:46:ARG:NH2    | 1:l:156:ASP:OD1   | 2.43                     | 0.49              |
| 1:E:59:CYS:O      | 1:l:16:VAL:HG12   | 2.11                     | 0.49              |
| 1:E:341:LEU:CD1   | 1:G:12:PRO:HB2    | 2.42                     | 0.49              |
| 1:E:1029:ASP:N    | 1:E:1082:HIS:O    | 2.43                     | 0.49              |
| 1:E:1255:ILE:HD12 | 1:E:1258:ALA:HB3  | 1.94                     | 0.49              |
| 1:F:813:PHE:CE1   | 3:O:85:LEU:HD12   | 2.47                     | 0.49              |
| 1:G:231:LEU:HD22  | 1:G:1082:HIS:HB2  | 1.93                     | 0.49              |
| 1:H:258:ASN:HB2   | 1:H:261:THR:HG22  | 1.94                     | 0.49              |
| 1:H:813:PHE:HZ    | 1:H:865:VAL:HG21  | 1.76                     | 0.49              |
| 1:k:1156:CYS:SG   | 1:k:1157:GLU:N    | 2.83                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:l:1167:LEU:HD23 | 1:l:1171:ARG:HD3  | 1.93                     | 0.49              |
| 1:m:199:GLU:OE1   | 1:m:223:LYS:NZ    | 2.37                     | 0.49              |
| 1:n:596:LEU:HD23  | 1:n:599:LEU:HD12  | 1.94                     | 0.49              |
| 1:o:884:ALA:HA    | 1:o:1111:VAL:HG11 | 1.93                     | 0.49              |
| 1:p:978:TYR:O     | 1:p:982:CYS:HB3   | 2.11                     | 0.49              |
| 1:p:1019:THR:HG1  | 1:p:1160:LEU:HD11 | 1.76                     | 0.49              |
| 1:p:1297:LYS:H    | 1:p:1297:LYS:HD2  | 1.76                     | 0.49              |
| 1:q:71:ALA:HB3    | 1:q:371:GLU:HB2   | 1.92                     | 0.49              |
| 2:f:257:ALA:HB3   | 2:f:260:ARG:HG2   | 1.93                     | 0.49              |
| 3:r:39:GLU:OE2    | 3:r:43:GLN:NE2    | 2.45                     | 0.49              |
| 1:A:1098:PHE:HD2  | 1:A:1120:GLY:HA3  | 1.78                     | 0.49              |
| 1:B:1048:VAL:HG13 | 1:B:1061:VAL:HG12 | 1.94                     | 0.49              |
| 1:D:420:THR:HG21  | 1:E:405:GLY:HA2   | 1.95                     | 0.49              |
| 1:D:1150:HIS:CD2  | 1:E:1207:GLN:HA   | 2.48                     | 0.49              |
| 1:F:251:VAL:HG11  | 1:F:1033:TYR:HE2  | 1.78                     | 0.49              |
| 1:F:653:TYR:HA    | 1:F:656:VAL:HG12  | 1.93                     | 0.49              |
| 1:F:754:ASP:N     | 3:O:83:ASP:OD1    | 2.45                     | 0.49              |
| 1:F:1310:THR:HB   | 1:F:1339:ILE:HB   | 1.94                     | 0.49              |
| 1:G:116:MET:O     | 1:m:37:ARG:O      | 2.30                     | 0.49              |
| 1:G:1130:GLU:HB3  | 1:G:1139:ARG:HH12 | 1.77                     | 0.49              |
| 1:H:1154:ALA:O    | 1:H:1155:THR:HB   | 2.12                     | 0.49              |
| 1:I:1230:THR:H    | 1:I:1251:THR:HG22 | 1.76                     | 0.49              |
| 1:k:888:GLY:O     | 1:k:892:ALA:N     | 2.42                     | 0.49              |
| 1:k:1175:ASN:ND2  | 1:k:1179:ARG:O    | 2.46                     | 0.49              |
| 1:l:243:TYR:OH    | 1:l:1079:CYS:SG   | 2.63                     | 0.49              |
| 1:l:275:VAL:HG12  | 1:l:371:GLU:HB3   | 1.95                     | 0.49              |
| 1:l:1038:SER:OG   | 1:l:1039:THR:N    | 2.45                     | 0.49              |
| 1:m:4:ASN:HD22    | 1:n:319:HIS:HA    | 1.78                     | 0.49              |
| 1:n:613:TYR:HA    | 1:n:616:GLU:HG2   | 1.93                     | 0.49              |
| 1:o:452:HIS:HB3   | 1:o:455:ILE:HG12  | 1.94                     | 0.49              |
| 1:p:192:PHE:HB2   | 1:p:223:LYS:HB3   | 1.94                     | 0.49              |
| 1:q:520:THR:HA    | 1:q:566:ALA:HB2   | 1.94                     | 0.49              |
| 1:q:925:ARG:NH2   | 1:q:972:ARG:O     | 2.46                     | 0.49              |
| 2:h:207:ASP:OD1   | 4:S:197:ASN:OD1   | 2.30                     | 0.49              |
| 2:f:66:ARG:HH21   | 2:f:68:THR:CG2    | 2.25                     | 0.49              |
| 2:j:93:PRO:CG     | 2:j:195:TYR:CZ    | 2.85                     | 0.49              |
| 3:J:72:GLY:O      | 3:J:80:TYR:OH     | 2.29                     | 0.49              |
| 3:M:72:GLY:O      | 3:M:80:TYR:OH     | 2.30                     | 0.49              |
| 3:t:48:VAL:HA     | 3:t:77:LYS:HD2    | 1.94                     | 0.49              |
| 4:y:71:PHE:HD2    | 4:y:131:VAL:HB    | 1.77                     | 0.49              |
| 4:V:54:VAL:HG21   | 4:V:148:ILE:HD12  | 1.94                     | 0.49              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 4:V:197:ASN:H    | 4:V:202:GLY:HA2   | 1.76                     | 0.49              |
| 5:W:46:ASP:OD2   | 5:W:50:LYS:NZ     | 2.41                     | 0.49              |
| 5:X:48:VAL:HG21  | 5:X:62:ARG:HG2    | 1.94                     | 0.49              |
| 5:X:60:ARG:HA    | 5:X:63:MET:HB3    | 1.94                     | 0.49              |
| 1:A:691:GLU:O    | 1:A:692:LEU:HB2   | 2.11                     | 0.49              |
| 1:B:589:PRO:HG2  | 1:B:592:HIS:HB3   | 1.94                     | 0.49              |
| 1:B:812:LEU:HD22 | 1:B:839:LEU:HD13  | 1.94                     | 0.49              |
| 1:D:574:ASP:OD1  | 1:D:978:TYR:OH    | 2.30                     | 0.49              |
| 1:D:802:GLY:HA3  | 1:D:872:ALA:HB2   | 1.94                     | 0.49              |
| 1:G:1146:PRO:HB3 | 1:H:1193:ALA:HB1  | 1.95                     | 0.49              |
| 1:H:79:ILE:HB    | 1:H:1042:ILE:HG22 | 1.92                     | 0.49              |
| 1:I:191:CYS:SG   | 1:I:243:TYR:OH    | 2.66                     | 0.49              |
| 1:I:630:ILE:HA   | 1:I:633:VAL:HG12  | 1.95                     | 0.49              |
| 1:k:97:GLN:HA    | 1:k:114:THR:HA    | 1.94                     | 0.49              |
| 1:k:127:THR:CG2  | 1:k:1060:HIS:HB3  | 2.42                     | 0.49              |
| 1:k:1019:THR:OG1 | 1:k:1160:LEU:CG   | 2.57                     | 0.49              |
| 1:n:558:ILE:HD13 | 1:n:970:TRP:HA    | 1.94                     | 0.49              |
| 1:n:813:PHE:CG   | 3:u:85:LEU:HG     | 2.47                     | 0.49              |
| 1:n:885:GLN:O    | 1:n:891:SER:OG    | 2.28                     | 0.49              |
| 1:o:789:LEU:HD12 | 1:o:989:VAL:HG21  | 1.93                     | 0.49              |
| 1:p:61:LYS:HG3   | 1:q:46:ARG:HA     | 1.95                     | 0.49              |
| 1:q:974:PRO:C    | 1:q:978:TYR:HD2   | 2.13                     | 0.49              |
| 2:3:66:ARG:HG2   | 2:3:69:GLN:CD     | 2.36                     | 0.49              |
| 2:h:93:PRO:HG3   | 2:h:195:TYR:OH    | 2.03                     | 0.49              |
| 2:f:66:ARG:NH2   | 2:f:68:THR:CG2    | 2.75                     | 0.49              |
| 2:f:204:LEU:HD13 | 2:f:210:VAL:HG12  | 1.93                     | 0.49              |
| 3:w:39:GLU:OE2   | 3:w:43:GLN:NE2    | 2.45                     | 0.49              |
| 4:y:64:LYS:HE2   | 4:y:270:SER:HB3   | 1.94                     | 0.49              |
| 4:S:65:ASN:HD22  | 4:S:268:VAL:HG12  | 1.77                     | 0.49              |
| 1:A:785:TYR:CD2  | 1:A:786:TYR:CZ    | 3.00                     | 0.49              |
| 1:D:678:ASN:O    | 1:D:682:ILE:N     | 2.34                     | 0.49              |
| 1:D:1272:ARG:O   | 1:D:1300:ARG:NH1  | 2.46                     | 0.49              |
| 1:E:40:TYR:HB3   | 1:m:111:ARG:CG    | 2.35                     | 0.49              |
| 1:E:61:LYS:HE3   | 1:l:15:ASP:OD2    | 2.13                     | 0.49              |
| 1:E:156:ASP:OD1  | 1:F:338:GLN:NE2   | 2.46                     | 0.49              |
| 1:F:713:ASP:O    | 1:F:783:LYS:NZ    | 2.45                     | 0.49              |
| 1:F:1256:ILE:HA  | 1:F:1259:ASN:HD22 | 1.78                     | 0.49              |
| 1:G:224:MET:HE1  | 1:G:1298:PRO:HG3  | 1.95                     | 0.49              |
| 1:G:653:TYR:HA   | 1:G:656:VAL:HG12  | 1.94                     | 0.49              |
| 1:G:1038:SER:OG  | 1:G:1039:THR:N    | 2.46                     | 0.49              |
| 1:I:245:ASP:OD1  | 1:I:364:GLY:N     | 2.45                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:I:921:ILE:HG22  | 1:I:923:PHE:HB3   | 1.95                     | 0.49              |
| 1:k:393:THR:HA    | 1:k:1023:THR:HA   | 1.94                     | 0.49              |
| 1:k:434:LYS:N     | 1:k:1089:ASP:O    | 2.40                     | 0.49              |
| 1:k:1039:THR:OG1  | 1:k:1068:VAL:O    | 2.26                     | 0.49              |
| 1:k:1156:CYS:HB2  | 1:k:1245:PRO:HD2  | 1.93                     | 0.49              |
| 1:l:689:THR:HG21  | 1:l:990:LEU:HD11  | 1.93                     | 0.49              |
| 1:l:864:LEU:HD22  | 1:l:867:HIS:HE1   | 1.76                     | 0.49              |
| 1:n:609:PRO:HB2   | 1:n:846:VAL:HG13  | 1.94                     | 0.49              |
| 1:o:653:TYR:HA    | 1:o:656:VAL:HG12  | 1.94                     | 0.49              |
| 1:p:650:ALA:O     | 1:p:785:TYR:OH    | 2.25                     | 0.49              |
| 1:p:1070:MET:SD   | 1:p:1070:MET:N    | 2.86                     | 0.49              |
| 5:Z:85:THR:O      | 5:Z:310:LYS:NZ    | 2.41                     | 0.49              |
| 1:A:389:ASP:HA    | 1:A:1027:GLU:HA   | 1.94                     | 0.49              |
| 1:A:1139:ARG:HB2  | 1:A:1141:THR:HG22 | 1.95                     | 0.49              |
| 1:B:227:THR:HG23  | 1:B:230:LEU:HD11  | 1.94                     | 0.49              |
| 1:B:677:ARG:NH2   | 1:C:601:ALA:O     | 2.46                     | 0.49              |
| 1:D:813:PHE:CZ    | 3:M:85:LEU:HG     | 2.29                     | 0.49              |
| 1:D:1309:HIS:CD2  | 1:D:1327:LEU:HB3  | 2.48                     | 0.49              |
| 1:E:587:ARG:HB3   | 1:F:984:HIS:HD2   | 1.77                     | 0.49              |
| 1:G:776:ASP:HB2   | 1:H:951:GLN:OE1   | 2.13                     | 0.49              |
| 1:k:688:ARG:HA    | 1:k:691:GLU:HG2   | 1.95                     | 0.49              |
| 1:l:73:ALA:HA     | 1:l:76:ALA:HB3    | 1.95                     | 0.49              |
| 1:m:248:THR:O     | 1:m:366:ARG:NH2   | 2.46                     | 0.49              |
| 1:m:586:VAL:HG11  | 1:m:688:ARG:HD2   | 1.93                     | 0.49              |
| 1:n:105:ALA:HB2   | 5:a:8:THR:HG21    | 1.95                     | 0.49              |
| 1:n:243:TYR:OH    | 1:n:1079:CYS:SG   | 2.65                     | 0.49              |
| 1:n:438:PRO:HG2   | 1:o:1168:GLU:HA   | 1.94                     | 0.49              |
| 1:n:1321:LEU:HD12 | 1:n:1327:LEU:HD11 | 1.94                     | 0.49              |
| 1:o:219:GLY:O     | 1:o:223:LYS:HB2   | 2.12                     | 0.49              |
| 1:p:47:TYR:OH     | 1:q:59:CYS:SG     | 2.71                     | 0.49              |
| 1:p:818:PHE:HB2   | 3:w:88:LEU:HD22   | 1.95                     | 0.49              |
| 2:i:177:GLU:OE2   | 2:i:214:ASN:ND2   | 2.44                     | 0.49              |
| 4:U:234:PHE:HB2   | 4:U:249:LEU:HD13  | 1.93                     | 0.49              |
| 1:A:1219:GLN:HB2  | 1:A:1222:SER:HB3  | 1.95                     | 0.49              |
| 1:C:1233:ARG:HH22 | 1:C:1244:SER:HB3  | 1.77                     | 0.49              |
| 1:D:37:ARG:NH2    | 1:D:43:ASP:OD2    | 2.46                     | 0.49              |
| 1:D:273:VAL:HG23  | 1:D:369:ALA:HB3   | 1.95                     | 0.49              |
| 1:D:1253:ASP:O    | 1:D:1257:ASN:ND2  | 2.46                     | 0.49              |
| 1:E:34:ASN:CB     | 1:m:1264:LYS:HE3  | 2.42                     | 0.49              |
| 1:E:695:LEU:O     | 1:F:952:ARG:NH2   | 2.45                     | 0.49              |
| 1:E:696:ASN:HA    | 1:F:952:ARG:HH22  | 1.77                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:F:539:PHE:HD1   | 1:F:556:PRO:HA    | 1.78                     | 0.49              |
| 1:k:422:GLU:HA    | 1:k:579:GLN:HE21  | 1.78                     | 0.49              |
| 1:k:438:PRO:HG3   | 1:l:1167:LEU:HD22 | 1.95                     | 0.49              |
| 1:k:446:ALA:HA    | 1:k:1094:MET:HG3  | 1.95                     | 0.49              |
| 1:k:560:VAL:HA    | 1:k:999:MET:HE3   | 1.94                     | 0.49              |
| 1:l:525:LYS:HA    | 1:l:1210:VAL:HG13 | 1.94                     | 0.49              |
| 1:l:749:ASN:ND2   | 1:l:757:ARG:CG    | 2.74                     | 0.49              |
| 1:l:1054:ASP:HB2  | 5:b:91:THR:OG1    | 2.12                     | 0.49              |
| 1:p:83:ASP:HB3    | 1:p:86:LYS:HB2    | 1.95                     | 0.49              |
| 1:p:603:LEU:HD23  | 1:p:794:LEU:HD11  | 1.95                     | 0.49              |
| 2:e:101:ASP:HA    | 2:e:104:LYS:CG    | 2.41                     | 0.49              |
| 4:V:72:ARG:NH2    | 4:V:74:ASP:OD2    | 2.46                     | 0.49              |
| 5:W:102:LYS:HE3   | 5:a:33:TYR:HB2    | 1.94                     | 0.49              |
| 1:A:77:HIS:HB2    | 1:A:1037:ALA:HB1  | 1.95                     | 0.49              |
| 1:B:53:ALA:HA     | 1:C:322:ILE:HB    | 1.94                     | 0.49              |
| 1:B:757:ARG:NH2   | 1:B:868:VAL:O     | 2.45                     | 0.49              |
| 1:C:91:LYS:HE2    | 1:C:120:TYR:HE1   | 1.77                     | 0.49              |
| 1:C:192:PHE:HB2   | 1:C:223:LYS:HB3   | 1.95                     | 0.49              |
| 1:C:416:LYS:HB3   | 1:D:409:SER:HB3   | 1.95                     | 0.49              |
| 1:C:450:LEU:HD21  | 1:C:1018:LEU:HD21 | 1.95                     | 0.49              |
| 1:E:665:ASP:HA    | 1:F:643:GLN:NE2   | 2.28                     | 0.49              |
| 1:F:441:ILE:HD13  | 1:F:1092:SER:HB3  | 1.93                     | 0.49              |
| 1:G:128:ILE:HG22  | 1:H:102:ALA:HB3   | 1.94                     | 0.49              |
| 1:G:330:ALA:HA    | 1:n:314:VAL:CG2   | 2.37                     | 0.49              |
| 1:G:753:SER:H     | 2:h:262:TYR:HE1   | 1.60                     | 0.49              |
| 1:G:1148:LEU:HD21 | 1:H:211:VAL:HG22  | 1.94                     | 0.49              |
| 1:I:185:LEU:HD22  | 1:I:388:ARG:HH22  | 1.78                     | 0.49              |
| 1:I:483:ARG:NH2   | 1:I:508:PRO:O     | 2.44                     | 0.49              |
| 1:I:546:GLU:N     | 1:I:549:GLN:O     | 2.42                     | 0.49              |
| 1:k:400:LEU:HD12  | 1:k:1162:PRO:HA   | 1.95                     | 0.49              |
| 1:k:433:ASN:HD21  | 1:k:439:GLN:HE21  | 1.60                     | 0.49              |
| 1:k:743:ALA:HB3   | 2:2:173:MET:C     | 2.37                     | 0.49              |
| 1:k:988:SER:HA    | 1:k:991:THR:HG22  | 1.93                     | 0.49              |
| 1:l:688:ARG:CA    | 1:l:691:GLU:HG2   | 2.38                     | 0.49              |
| 1:m:1323:GLY:CA   | 1:n:1329:LEU:HD23 | 2.42                     | 0.49              |
| 1:n:667:ALA:HB3   | 1:o:643:GLN:HB3   | 1.94                     | 0.49              |
| 1:n:975:PHE:HE1   | 1:n:995:MET:HB3   | 1.78                     | 0.49              |
| 1:n:1122:ARG:NH1  | 1:n:1141:THR:O    | 2.45                     | 0.49              |
| 1:o:500:PHE:HZ    | 1:o:507:PRO:HD3   | 1.77                     | 0.49              |
| 1:o:520:THR:HG22  | 1:o:566:ALA:HA    | 1.95                     | 0.49              |
| 1:o:662:ARG:O     | 1:p:607:GLN:NE2   | 2.43                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:o:1087:ARG:NH2  | 1:o:1279:GLY:O    | 2.46                     | 0.49              |
| 1:p:1087:ARG:HH21 | 1:p:1152:GLN:HE22 | 1.59                     | 0.49              |
| 1:q:611:LEU:HD13  | 1:q:842:LEU:HD13  | 1.94                     | 0.49              |
| 1:q:901:LEU:HD13  | 1:q:904:GLY:HA3   | 1.95                     | 0.49              |
| 2:h:66:ARG:HG3    | 2:h:69:GLN:OE1    | 2.13                     | 0.49              |
| 5:z:100:TRP:NE1   | 5:z:133:ILE:O     | 2.45                     | 0.49              |
| 5:Z:134:VAL:HB    | 5:Z:138:LEU:HD23  | 1.95                     | 0.49              |
| 5:Z:277:PHE:HA    | 5:Z:280:ILE:HG12  | 1.93                     | 0.49              |
| 5:a:51:ASP:HB3    | 5:a:54:ARG:HB2    | 1.94                     | 0.49              |
| 5:b:107:THR:HG21  | 5:b:289:GLU:HB2   | 1.95                     | 0.49              |
| 5:c:54:ARG:HD2    | 5:c:58:ARG:HG2    | 1.95                     | 0.49              |
| 1:A:191:CYS:HG    | 1:A:243:TYR:HH    | 1.60                     | 0.49              |
| 1:A:602:SER:HA    | 1:A:646:LEU:HD13  | 1.95                     | 0.49              |
| 1:A:1342:THR:OG1  | 1:A:1343:ILE:N    | 2.46                     | 0.49              |
| 1:B:235:ARG:HD3   | 1:B:240:LEU:HD13  | 1.95                     | 0.49              |
| 1:D:67:PHE:HA     | 1:D:177:ILE:HD11  | 1.94                     | 0.49              |
| 1:D:512:ASN:HD21  | 1:D:972:ARG:HB3   | 1.78                     | 0.49              |
| 1:D:816:LYS:HG3   | 1:D:817:PHE:H     | 1.77                     | 0.49              |
| 1:D:1027:GLU:OE1  | 1:D:1085:ARG:NH2  | 2.46                     | 0.49              |
| 1:E:919:THR:HA    | 1:E:937:ASN:HD21  | 1.78                     | 0.49              |
| 1:E:1298:PRO:HB3  | 1:E:1302:LEU:HB2  | 1.95                     | 0.49              |
| 1:G:332:ARG:HG3   | 1:m:12:PRO:HG2    | 1.94                     | 0.49              |
| 1:G:725:PRO:HA    | 1:G:774:THR:H     | 1.77                     | 0.49              |
| 1:G:1028:THR:HG21 | 1:G:1080:THR:HG23 | 1.94                     | 0.49              |
| 1:H:476:ARG:HH21  | 1:H:480:LEU:HD12  | 1.77                     | 0.49              |
| 1:k:203:ILE:HG23  | 1:p:383:GLN:CD    | 2.38                     | 0.49              |
| 1:l:393:THR:HA    | 1:l:1023:THR:HA   | 1.94                     | 0.49              |
| 1:l:451:CYS:O     | 1:l:1106:TYR:OH   | 2.31                     | 0.49              |
| 1:l:611:LEU:HB2   | 1:l:842:LEU:HD13  | 1.94                     | 0.49              |
| 1:l:1048:VAL:HG22 | 1:l:1061:VAL:HG12 | 1.94                     | 0.49              |
| 1:l:1095:GLN:HE21 | 1:l:1100:VAL:HG21 | 1.77                     | 0.49              |
| 1:m:648:ALA:O     | 1:m:676:TYR:OH    | 2.31                     | 0.49              |
| 1:m:775:SER:O     | 1:m:779:MET:HB2   | 2.13                     | 0.49              |
| 1:n:393:THR:OG1   | 1:n:1248:GLN:NE2  | 2.46                     | 0.49              |
| 1:n:608:TYR:HH    | 1:n:649:PHE:H     | 1.58                     | 0.49              |
| 1:o:965:HIS:O     | 1:o:969:HIS:N     | 2.43                     | 0.49              |
| 1:o:1177:ARG:HH21 | 1:o:1181:SER:HB3  | 1.78                     | 0.49              |
| 1:p:840:ALA:O     | 1:p:844:ARG:CB    | 2.61                     | 0.49              |
| 1:p:1228:TYR:HB2  | 1:p:1250:PHE:HD2  | 1.76                     | 0.49              |
| 1:q:600:ARG:O     | 1:q:604:THR:CB    | 2.60                     | 0.49              |
| 1:q:635:ARG:NH1   | 1:q:847:ALA:O     | 2.45                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:q:1221:GLY:H    | 1:q:1226:VAL:HG13 | 1.78                     | 0.49              |
| 2:3:286:ASP:HA    | 2:3:289:LEU:HB3   | 1.95                     | 0.49              |
| 2:g:104:LYS:CG    | 2:j:92:LEU:HD13   | 2.43                     | 0.49              |
| 5:X:89:CYS:HB2    | 5:X:308:ILE:HG12  | 1.95                     | 0.49              |
| 5:Z:212:LEU:HD21  | 5:d:204:ALA:HB3   | 1.94                     | 0.49              |
| 1:A:133:SER:HA    | 1:A:1056:ASN:HA   | 1.94                     | 0.48              |
| 1:A:278:HIS:O     | 1:A:282:GLN:NE2   | 2.45                     | 0.48              |
| 1:B:147:THR:O     | 1:B:148:LEU:CB    | 2.60                     | 0.48              |
| 1:C:725:PRO:HG2   | 1:C:728:ALA:HB2   | 1.93                     | 0.48              |
| 1:E:1029:ASP:HB2  | 1:E:1082:HIS:HB3  | 1.95                     | 0.48              |
| 1:F:276:SER:HB2   | 1:F:281:VAL:HG23  | 1.95                     | 0.48              |
| 1:F:409:SER:OG    | 1:F:1333:HIS:ND1  | 2.44                     | 0.48              |
| 1:H:393:THR:OG1   | 1:H:1248:GLN:NE2  | 2.40                     | 0.48              |
| 1:H:420:THR:HG22  | 1:H:422:GLU:H     | 1.78                     | 0.48              |
| 1:H:595:THR:HA    | 1:H:675:HIS:HD2   | 1.78                     | 0.48              |
| 1:k:262:TYR:HB2   | 1:k:1036:LYS:HD2  | 1.95                     | 0.48              |
| 1:k:516:HIS:CE1   | 1:k:977:CYS:HB3   | 2.48                     | 0.48              |
| 1:l:705:LEU:HD11  | 1:m:952:ARG:HD3   | 1.95                     | 0.48              |
| 1:l:1137:PHE:CB   | 4:T:55:ARG:HH22   | 2.26                     | 0.48              |
| 1:m:726:ARG:NH1   | 1:n:945:ASN:OD1   | 2.46                     | 0.48              |
| 1:n:717:TRP:HE1   | 1:n:731:VAL:HG11  | 1.78                     | 0.48              |
| 1:n:877:ILE:HB    | 1:n:898:GLN:HB2   | 1.95                     | 0.48              |
| 1:p:713:ASP:O     | 1:p:783:LYS:NZ    | 2.46                     | 0.48              |
| 1:q:134:ALA:HA    | 1:q:137:LEU:HB3   | 1.94                     | 0.48              |
| 1:q:182:ARG:HB3   | 1:q:186:ARG:HH12  | 1.78                     | 0.48              |
| 2:2:104:LYS:CG    | 2:3:92:LEU:HD13   | 2.43                     | 0.48              |
| 2:i:111:ALA:CB    | 4:U:232:PHE:CG    | 2.91                     | 0.48              |
| 3:P:85:LEU:O      | 3:P:89:SER:N      | 2.44                     | 0.48              |
| 4:y:70:MET:C      | 4:y:71:PHE:HD1    | 2.20                     | 0.48              |
| 4:y:215:HIS:CE1   | 5:z:290:GLN:HB2   | 2.47                     | 0.48              |
| 5:X:109:LEU:HD12  | 5:X:110:PRO:HD2   | 1.94                     | 0.48              |
| 5:Z:112:VAL:HG11  | 5:Z:178:LEU:HB2   | 1.95                     | 0.48              |
| 5:b:275:ALA:HA    | 5:b:278:VAL:HG12  | 1.95                     | 0.48              |
| 1:A:215:ASN:OD1   | 1:F:434:LYS:NZ    | 2.44                     | 0.48              |
| 1:A:734:VAL:HG11  | 1:A:878:ARG:HH11  | 1.78                     | 0.48              |
| 1:A:789:LEU:HD12  | 1:A:989:VAL:HG21  | 1.95                     | 0.48              |
| 1:A:1031:LEU:HD23 | 1:A:1081:ALA:HB2  | 1.95                     | 0.48              |
| 1:B:1254:ASP:HA   | 1:B:1257:ASN:HD22 | 1.78                     | 0.48              |
| 1:D:428:THR:HG22  | 1:D:442:SER:HB3   | 1.95                     | 0.48              |
| 1:D:702:GLU:OE2   | 1:D:715:ARG:NH2   | 2.45                     | 0.48              |
| 1:F:344:SER:CB    | 1:l:14:LEU:CD1    | 2.64                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:G:924:HIS:HB3   | 1:G:927:TYR:HB2   | 1.95                     | 0.48              |
| 1:H:207:MET:N     | 1:H:207:MET:SD    | 2.85                     | 0.48              |
| 1:H:294:ARG:NE    | 1:H:359:ASP:OD1   | 2.43                     | 0.48              |
| 1:I:278:HIS:HB2   | 1:I:374:ARG:HD3   | 1.94                     | 0.48              |
| 1:I:325:ASP:HB3   | 1:I:328:GLN:HB3   | 1.94                     | 0.48              |
| 1:k:476:ARG:HD3   | 1:k:532:PHE:HZ    | 1.78                     | 0.48              |
| 1:k:600:ARG:NH2   | 1:k:604:THR:OG1   | 2.46                     | 0.48              |
| 1:l:882:ASP:OD1   | 1:l:882:ASP:N     | 2.46                     | 0.48              |
| 1:l:1201:HIS:ND1  | 1:l:1212:THR:OG1  | 2.43                     | 0.48              |
| 1:m:125:PRO:HB3   | 1:m:1064:ASN:HA   | 1.95                     | 0.48              |
| 1:m:134:ALA:HB3   | 1:m:1055:ILE:HD12 | 1.94                     | 0.48              |
| 1:n:740:LEU:HD12  | 1:n:745:ILE:HG22  | 1.94                     | 0.48              |
| 1:n:1021:VAL:HG23 | 1:n:1245:PRO:HB2  | 1.94                     | 0.48              |
| 1:n:1085:ARG:HD3  | 1:o:200:HIS:HA    | 1.94                     | 0.48              |
| 1:n:1298:PRO:HB3  | 1:n:1302:LEU:HD12 | 1.94                     | 0.48              |
| 1:o:804:ASN:O     | 1:o:808:LEU:CB    | 2.61                     | 0.48              |
| 1:p:1179:ARG:NH2  | 1:p:1203:SER:O    | 2.45                     | 0.48              |
| 1:q:187:HIS:HB3   | 1:q:1286:ILE:HD11 | 1.95                     | 0.48              |
| 1:q:557:ARG:HB3   | 1:q:562:ASN:HB3   | 1.95                     | 0.48              |
| 1:q:584:THR:HG21  | 1:q:689:THR:HG23  | 1.95                     | 0.48              |
| 1:q:1123:ARG:NH1  | 5:z:167:GLN:OE1   | 2.46                     | 0.48              |
| 2:h:285:GLU:CD    | 3:P:67:LYS:HE2    | 2.37                     | 0.48              |
| 2:h:285:GLU:O     | 2:h:289:LEU:N     | 2.47                     | 0.48              |
| 2:i:93:PRO:HG3    | 2:i:195:TYR:OH    | 2.03                     | 0.48              |
| 2:g:173:MET:O     | 2:g:173:MET:HG2   | 2.13                     | 0.48              |
| 2:j:177:GLU:OE2   | 2:j:214:ASN:ND2   | 2.44                     | 0.48              |
| 4:U:269:ALA:HA    | 4:U:274:GLN:HG3   | 1.95                     | 0.48              |
| 5:z:35:HIS:ND1    | 5:z:37:LEU:O      | 2.45                     | 0.48              |
| 5:z:148:MET:HA    | 5:z:151:LEU:HD12  | 1.94                     | 0.48              |
| 5:1:72:ARG:HB3    | 5:1:80:ILE:HG22   | 1.95                     | 0.48              |
| 1:A:863:HIS:CE1   | 3:J:93:LYS:HA     | 2.48                     | 0.48              |
| 1:B:422:GLU:HA    | 1:B:579:GLN:HE21  | 1.78                     | 0.48              |
| 1:C:71:ALA:HB3    | 1:C:371:GLU:HG2   | 1.95                     | 0.48              |
| 1:D:509:ARG:HB3   | 1:D:513:GLU:HB2   | 1.95                     | 0.48              |
| 1:D:600:ARG:HH11  | 1:D:794:LEU:HA    | 1.77                     | 0.48              |
| 1:E:389:ASP:HA    | 1:E:1027:GLU:HA   | 1.95                     | 0.48              |
| 1:E:1096:ASP:N    | 1:E:1096:ASP:OD1  | 2.45                     | 0.48              |
| 1:G:326:PHE:CZ    | 1:n:315:THR:HA    | 2.43                     | 0.48              |
| 1:G:641:TRP:CD2   | 1:G:672:ALA:HB2   | 2.48                     | 0.48              |
| 1:G:925:ARG:HH11  | 1:G:975:PHE:HB2   | 1.78                     | 0.48              |
| 1:H:332:ARG:HD2   | 1:H:339:LYS:HB3   | 1.95                     | 0.48              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:k:458:ALA:HB1   | 1:k:461:CYS:HB3  | 1.95                     | 0.48              |
| 1:k:481:CYS:SG    | 1:k:482:ARG:N    | 2.86                     | 0.48              |
| 1:k:1233:ARG:HH22 | 1:k:1244:SER:HB3 | 1.78                     | 0.48              |
| 1:k:1332:THR:HA   | 1:k:1337:TYR:HA  | 1.94                     | 0.48              |
| 1:l:251:VAL:HG11  | 1:l:1033:TYR:HE2 | 1.78                     | 0.48              |
| 1:m:165:VAL:HG12  | 4:S:9:PRO:HA     | 1.95                     | 0.48              |
| 1:m:1059:PHE:CE1  | 4:S:15:MET:O     | 2.66                     | 0.48              |
| 1:o:1179:ARG:NE   | 1:o:1197:THR:O   | 2.40                     | 0.48              |
| 2:3:138:PRO:HA    | 2:3:141:ASP:HB2  | 1.96                     | 0.48              |
| 2:h:286:ASP:HA    | 2:h:289:LEU:HB3  | 1.95                     | 0.48              |
| 2:j:286:ASP:HA    | 2:j:289:LEU:HB3  | 1.95                     | 0.48              |
| 3:v:61:ILE:HG13   | 3:v:84:LEU:HD11  | 1.95                     | 0.48              |
| 4:y:91:SER:HB3    | 4:y:97:VAL:HG21  | 1.94                     | 0.48              |
| 4:y:125:TRP:HE1   | 4:y:201:GLN:HG2  | 1.78                     | 0.48              |
| 5:Z:107:THR:HG22  | 5:Z:291:PRO:HA   | 1.94                     | 0.48              |
| 5:c:145:ARG:NH1   | 5:c:170:VAL:O    | 2.39                     | 0.48              |
| 1:A:71:ALA:HB3    | 1:A:371:GLU:HB2  | 1.95                     | 0.48              |
| 1:A:1175:ASN:HD22 | 1:A:1181:SER:H   | 1.61                     | 0.48              |
| 1:D:235:ARG:HD3   | 1:D:240:LEU:HD13 | 1.94                     | 0.48              |
| 1:D:654:ASP:OD1   | 1:D:782:GLN:NE2  | 2.46                     | 0.48              |
| 1:D:744:HIS:NE2   | 2:g:173:MET:SD   | 2.86                     | 0.48              |
| 1:D:879:ALA:O     | 1:D:896:SER:N    | 2.44                     | 0.48              |
| 1:F:546:GLU:OE1   | 1:F:551:ARG:NH2  | 2.45                     | 0.48              |
| 1:F:638:ASN:ND2   | 1:F:668:VAL:O    | 2.45                     | 0.48              |
| 1:I:589:PRO:HB2   | 1:I:592:HIS:HB3  | 1.94                     | 0.48              |
| 1:k:48:ASN:HB2    | 4:T:162:THR:CG2  | 2.43                     | 0.48              |
| 1:k:1097:LEU:HA   | 1:k:1100:VAL:HB  | 1.95                     | 0.48              |
| 1:l:381:ASP:HA    | 1:m:205:ARG:HD2  | 1.95                     | 0.48              |
| 1:l:598:VAL:HG13  | 1:l:646:LEU:HA   | 1.95                     | 0.48              |
| 1:l:1171:ARG:NH2  | 1:l:1330:ASP:OD2 | 2.46                     | 0.48              |
| 1:m:51:PHE:CD1    | 1:n:87:MET:HA    | 2.47                     | 0.48              |
| 1:m:861:LEU:HD23  | 1:m:864:LEU:HD12 | 1.95                     | 0.48              |
| 1:n:159:ASN:HD22  | 1:o:338:GLN:HB2  | 1.78                     | 0.48              |
| 1:p:72:LEU:HB3    | 1:p:180:PHE:HE2  | 1.77                     | 0.48              |
| 1:p:428:THR:HG22  | 1:p:442:SER:HB3  | 1.95                     | 0.48              |
| 1:p:1160:LEU:CD2  | 1:p:1214:ASN:HB2 | 2.43                     | 0.48              |
| 1:q:969:HIS:H     | 1:q:972:ARG:NH2  | 2.11                     | 0.48              |
| 2:3:136:TYR:HA    | 2:3:139:ARG:HD2  | 1.96                     | 0.48              |
| 2:e:284:GLU:CB    | 3:t:67:LYS:NZ    | 2.60                     | 0.48              |
| 4:U:224:ARG:HH22  | 5:Y:282:GLN:HG3  | 1.78                     | 0.48              |
| 4:V:191:VAL:O     | 4:V:207:PHE:N    | 2.47                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:X:293:PHE:HB3   | 5:X:307:CYS:HB3   | 1.95                     | 0.48              |
| 1:C:603:LEU:HB3   | 1:C:794:LEU:HD21  | 1.95                     | 0.48              |
| 1:C:756:ALA:HA    | 1:C:759:ILE:HG12  | 1.96                     | 0.48              |
| 1:D:392:LEU:HB2   | 1:D:1026:PHE:HE2  | 1.78                     | 0.48              |
| 1:D:882:ASP:OD1   | 1:D:882:ASP:N     | 2.45                     | 0.48              |
| 1:E:25:LYS:HZ2    | 1:m:205:ARG:HH21  | 1.61                     | 0.48              |
| 1:E:1097:LEU:HA   | 1:E:1100:VAL:HB   | 1.94                     | 0.48              |
| 1:G:243:TYR:OH    | 1:G:1079:CYS:SG   | 2.66                     | 0.48              |
| 1:H:1101:PHE:HB3  | 1:H:1104:HIS:HD2  | 1.77                     | 0.48              |
| 1:k:639:ASN:OD1   | 1:k:642:ARG:NH1   | 2.46                     | 0.48              |
| 1:k:713:ASP:O     | 1:k:783:LYS:NZ    | 2.46                     | 0.48              |
| 1:k:1017:ALA:CA   | 1:k:1160:LEU:O    | 2.61                     | 0.48              |
| 1:n:1233:ARG:O    | 1:n:1238:HIS:ND1  | 2.47                     | 0.48              |
| 1:o:660:ALA:O     | 1:o:673:TYR:OH    | 2.31                     | 0.48              |
| 2:i:110:ALA:HB1   | 5:c:225:MET:HG2   | 1.95                     | 0.48              |
| 2:i:285:GLU:O     | 2:i:289:LEU:N     | 2.47                     | 0.48              |
| 4:S:183:ASP:HB2   | 4:S:261:ARG:HE    | 1.77                     | 0.48              |
| 5:Y:25:ILE:HG23   | 5:Y:72:ARG:HA     | 1.95                     | 0.48              |
| 1:A:322:ILE:HB    | 1:F:53:ALA:HA     | 1.96                     | 0.48              |
| 1:A:635:ARG:HG2   | 1:A:639:ASN:HD21  | 1.79                     | 0.48              |
| 1:A:849:ASP:HB3   | 1:A:852:VAL:H     | 1.79                     | 0.48              |
| 1:B:757:ARG:HH22  | 1:B:869:PRO:HA    | 1.78                     | 0.48              |
| 1:D:185:LEU:HD22  | 1:D:388:ARG:HH22  | 1.77                     | 0.48              |
| 1:D:274:ILE:HB    | 1:D:370:LEU:HD23  | 1.96                     | 0.48              |
| 1:E:1085:ARG:HH12 | 1:F:212:GLN:HG3   | 1.78                     | 0.48              |
| 1:F:813:PHE:CE2   | 3:O:82:LEU:HA     | 2.46                     | 0.48              |
| 1:F:957:PHE:HB3   | 1:F:959:LEU:HG    | 1.96                     | 0.48              |
| 1:G:118:SER:N     | 1:m:33:PHE:CE2    | 2.81                     | 0.48              |
| 1:H:726:ARG:NH1   | 1:I:945:ASN:OD1   | 2.47                     | 0.48              |
| 1:H:1177:ARG:NH1  | 1:H:1198:LEU:O    | 2.38                     | 0.48              |
| 1:I:711:LEU:HD13  | 1:I:996:HIS:HD2   | 1.78                     | 0.48              |
| 1:k:644:ARG:HE    | 1:p:664:GLY:HA2   | 1.79                     | 0.48              |
| 1:k:901:LEU:HD11  | 1:k:921:ILE:HD13  | 1.94                     | 0.48              |
| 1:k:930:PRO:CG    | 1:k:957:PHE:CE1   | 2.94                     | 0.48              |
| 1:l:391:GLU:HG3   | 1:l:1297:LYS:HD2  | 1.96                     | 0.48              |
| 1:l:1137:PHE:CE1  | 4:T:55:ARG:HG2    | 2.48                     | 0.48              |
| 1:m:79:ILE:HB     | 1:m:1042:ILE:HG22 | 1.95                     | 0.48              |
| 1:m:381:ASP:N     | 1:m:381:ASP:OD1   | 2.47                     | 0.48              |
| 1:m:755:VAL:HG21  | 3:t:80:TYR:CE1    | 2.48                     | 0.48              |
| 1:m:1043:ILE:HB   | 1:m:1063:GLN:HE21 | 1.79                     | 0.48              |
| 1:n:258:ASN:HB2   | 1:n:261:THR:HG22  | 1.95                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:n:610:GLU:HG3   | 1:n:914:LEU:HG    | 1.94                     | 0.48              |
| 1:n:758:MET:HG3   | 3:u:83:ASP:HB2    | 1.94                     | 0.48              |
| 2:e:207:ASP:CG    | 2:e:208:PRO:HD2   | 2.38                     | 0.48              |
| 2:h:129:ASP:O     | 2:h:131:VAL:N     | 2.47                     | 0.48              |
| 2:h:138:PRO:HA    | 2:h:141:ASP:HB2   | 1.96                     | 0.48              |
| 2:i:74:MET:HE2    | 2:i:267:LEU:HD22  | 1.96                     | 0.48              |
| 3:J:83:ASP:O      | 3:J:86:ARG:HG2    | 2.12                     | 0.48              |
| 4:T:109:TYR:HB3   | 4:T:114:GLU:HG3   | 1.95                     | 0.48              |
| 5:1:114:SER:O     | 5:1:179:THR:OG1   | 2.32                     | 0.48              |
| 5:b:106:LEU:HB2   | 5:b:293:PHE:HB2   | 1.95                     | 0.48              |
| 5:b:170:VAL:HG22  | 5:b:179:THR:HG22  | 1.96                     | 0.48              |
| 5:d:64:ARG:HH12   | 5:d:289:GLU:HA    | 1.78                     | 0.48              |
| 5:d:206:LEU:HD11  | 5:d:272:LYS:HB3   | 1.94                     | 0.48              |
| 1:A:482:ARG:HD3   | 1:A:486:VAL:HB    | 1.94                     | 0.48              |
| 1:A:488:GLU:HG3   | 1:A:962:ILE:HG13  | 1.95                     | 0.48              |
| 1:B:686:VAL:O     | 1:B:690:CYS:N     | 2.45                     | 0.48              |
| 1:E:709:SER:HB3   | 1:E:712:HIS:HD2   | 1.78                     | 0.48              |
| 1:E:1298:PRO:O    | 1:E:1302:LEU:N    | 2.35                     | 0.48              |
| 1:G:703:PRO:HG3   | 1:H:948:PRO:HB2   | 1.95                     | 0.48              |
| 1:G:930:PRO:HD3   | 1:G:957:PHE:HE1   | 1.79                     | 0.48              |
| 1:H:558:ILE:HG22  | 1:H:998:LYS:HD2   | 1.95                     | 0.48              |
| 1:l:71:ALA:HB3    | 1:l:371:GLU:HB2   | 1.96                     | 0.48              |
| 1:l:758:MET:HG3   | 3:s:83:ASP:HB2    | 1.94                     | 0.48              |
| 1:m:380:THR:HG22  | 1:n:99:PRO:HB2    | 1.96                     | 0.48              |
| 1:m:434:LYS:N     | 1:m:1089:ASP:O    | 2.41                     | 0.48              |
| 1:m:1019:THR:HG23 | 1:m:1160:LEU:HD12 | 1.95                     | 0.48              |
| 1:n:126:ILE:O     | 1:n:1062:SER:HA   | 2.14                     | 0.48              |
| 1:n:755:VAL:HG21  | 3:u:71:MET:HG3    | 1.95                     | 0.48              |
| 1:n:1149:LEU:HD13 | 1:o:1207:GLN:HB2  | 1.95                     | 0.48              |
| 1:o:270:LEU:HD13  | 1:o:369:ALA:HB2   | 1.95                     | 0.48              |
| 1:o:863:HIS:CE1   | 3:v:93:LYS:HA     | 2.49                     | 0.48              |
| 1:p:104:GLY:HA3   | 1:p:107:ILE:HD12  | 1.95                     | 0.48              |
| 1:p:804:ASN:O     | 1:p:808:LEU:CB    | 2.62                     | 0.48              |
| 1:p:925:ARG:NH2   | 1:p:966:GLU:OE2   | 2.46                     | 0.48              |
| 1:p:1233:ARG:O    | 1:p:1238:HIS:ND1  | 2.47                     | 0.48              |
| 1:q:447:LEU:HA    | 1:q:450:LEU:HB3   | 1.94                     | 0.48              |
| 2:3:73:GLU:HA     | 2:3:76:LEU:HB2    | 1.96                     | 0.48              |
| 2:e:173:MET:O     | 2:e:173:MET:HG2   | 2.13                     | 0.48              |
| 3:v:41:ARG:HH11   | 3:v:55:MET:HB2    | 1.78                     | 0.48              |
| 5:Z:106:LEU:HD12  | 5:Z:135:PRO:CA    | 2.42                     | 0.48              |
| 5:Z:308:ILE:O     | 5:Z:309:TYR:HB2   | 2.13                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:a:89:CYS:HA     | 5:a:308:ILE:HA    | 1.96                     | 0.48              |
| 5:b:227:LEU:HA    | 5:b:230:CYS:HB3   | 1.94                     | 0.48              |
| 5:d:156:ARG:HG2   | 5:d:184:THR:HG21  | 1.96                     | 0.48              |
| 1:A:458:ALA:HB1   | 1:A:461:CYS:HB3   | 1.96                     | 0.48              |
| 1:B:1330:ASP:OD1  | 1:B:1330:ASP:N    | 2.44                     | 0.48              |
| 1:D:483:ARG:NH2   | 1:D:508:PRO:O     | 2.47                     | 0.48              |
| 1:D:1310:THR:HB   | 1:D:1339:ILE:HB   | 1.95                     | 0.48              |
| 1:E:388:ARG:O     | 1:E:1028:THR:N    | 2.40                     | 0.48              |
| 1:E:920:VAL:HG21  | 1:E:933:ALA:HA    | 1.96                     | 0.48              |
| 1:H:135:ALA:HA    | 1:H:138:THR:HG22  | 1.95                     | 0.48              |
| 1:H:602:SER:HB3   | 1:H:647:LEU:H     | 1.78                     | 0.48              |
| 1:H:627:GLU:HA    | 1:H:630:ILE:HG13  | 1.95                     | 0.48              |
| 1:H:861:LEU:HD12  | 1:H:864:LEU:HD12  | 1.96                     | 0.48              |
| 1:H:1160:LEU:CD2  | 1:H:1214:ASN:ND2  | 2.76                     | 0.48              |
| 1:I:1156:CYS:SG   | 1:I:1157:GLU:N    | 2.86                     | 0.48              |
| 1:k:441:ILE:HD13  | 1:k:1092:SER:HB3  | 1.96                     | 0.48              |
| 1:l:388:ARG:HD2   | 1:l:1030:THR:HG21 | 1.96                     | 0.48              |
| 1:l:600:ARG:O     | 1:l:604:THR:OG1   | 2.24                     | 0.48              |
| 1:m:231:LEU:HD13  | 1:m:1081:ALA:HB1  | 1.96                     | 0.48              |
| 1:o:664:GLY:O     | 1:p:643:GLN:NE2   | 2.47                     | 0.48              |
| 1:p:325:ASP:HB3   | 1:p:328:GLN:HB3   | 1.96                     | 0.48              |
| 1:p:421:ALA:HA    | 1:p:424:GLN:HB2   | 1.96                     | 0.48              |
| 1:q:758:MET:HE1   | 3:x:83:ASP:HB2    | 1.96                     | 0.48              |
| 2:e:174:ARG:NH1   | 2:h:274:THR:HG22  | 2.29                     | 0.48              |
| 2:f:206:GLU:CB    | 2:i:132:TYR:C     | 2.81                     | 0.48              |
| 2:j:285:GLU:O     | 2:j:289:LEU:N     | 2.47                     | 0.48              |
| 4:U:50:ALA:O      | 4:U:150:CYS:N     | 2.46                     | 0.48              |
| 5:Y:198:ILE:HG12  | 5:c:226:LEU:HD11  | 1.95                     | 0.48              |
| 1:A:112:GLN:NE2   | 1:F:131:GLU:O     | 2.46                     | 0.48              |
| 1:A:398:VAL:HG13  | 1:A:1018:LEU:HB2  | 1.95                     | 0.48              |
| 1:B:544:HIS:CE1   | 1:B:553:LEU:HB2   | 2.49                     | 0.48              |
| 1:C:1253:ASP:O    | 1:C:1257:ASN:ND2  | 2.47                     | 0.48              |
| 1:D:177:ILE:HG21  | 1:D:376:VAL:HG21  | 1.96                     | 0.48              |
| 1:D:860:GLU:HA    | 1:D:863:HIS:HD2   | 1.77                     | 0.48              |
| 1:E:131:GLU:OE1   | 1:l:42:ASP:N      | 2.38                     | 0.48              |
| 1:E:395:TYR:HE2   | 1:E:1170:PHE:HD1  | 1.62                     | 0.48              |
| 1:E:1021:VAL:HG11 | 1:E:1176:PRO:HB3  | 1.95                     | 0.48              |
| 1:H:262:TYR:HB3   | 1:H:270:LEU:HB2   | 1.95                     | 0.48              |
| 1:H:559:MET:HE1   | 1:H:970:TRP:HB3   | 1.95                     | 0.48              |
| 1:k:1298:PRO:HB2  | 1:k:1304:GLU:HG2  | 1.95                     | 0.48              |
| 1:k:1320:GLN:NE2  | 1:k:1331:GLU:OE2  | 2.47                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:l:535:LEU:HB2   | 1:l:541:PHE:HE2   | 1.79                     | 0.48              |
| 1:l:1149:LEU:HB2  | 1:m:1206:PRO:HB3  | 1.95                     | 0.48              |
| 1:l:1166:ASP:OD2  | 1:l:1171:ARG:NH1  | 2.46                     | 0.48              |
| 1:m:330:ALA:HA    | 1:m:333:ILE:HD12  | 1.95                     | 0.48              |
| 1:m:397:PRO:HA    | 1:m:1019:THR:HG22 | 1.95                     | 0.48              |
| 1:m:430:TYR:C     | 1:m:431:PHE:CD2   | 2.92                     | 0.48              |
| 1:m:432:TYR:CZ    | 1:m:1321:LEU:HD11 | 2.41                     | 0.48              |
| 1:m:944:LEU:HD22  | 1:m:951:GLN:HB2   | 1.95                     | 0.48              |
| 1:p:753:SER:HB3   | 3:w:87:MET:HE3    | 1.96                     | 0.48              |
| 2:f:174:ARG:NH1   | 2:i:274:THR:HG22  | 2.29                     | 0.48              |
| 2:i:286:ASP:HA    | 2:i:289:LEU:HB3   | 1.95                     | 0.48              |
| 2:j:129:ASP:O     | 2:j:131:VAL:N     | 2.47                     | 0.48              |
| 2:j:138:PRO:HA    | 2:j:141:ASP:HB2   | 1.96                     | 0.48              |
| 3:x:61:ILE:HG13   | 3:x:84:LEU:HD11   | 1.95                     | 0.48              |
| 4:y:173:ILE:O     | 4:y:208:VAL:N     | 2.39                     | 0.48              |
| 4:U:229:VAL:HA    | 4:U:232:PHE:HD2   | 1.78                     | 0.48              |
| 5:Y:215:VAL:O     | 5:Y:219:ALA:N     | 2.43                     | 0.48              |
| 1:A:1137:PHE:CD2  | 4:U:116:ILE:HD12  | 2.49                     | 0.48              |
| 1:C:684:ARG:O     | 1:C:688:ARG:N     | 2.47                     | 0.48              |
| 1:C:920:VAL:HG21  | 1:C:933:ALA:HA    | 1.96                     | 0.48              |
| 1:E:25:LYS:CD     | 1:m:205:ARG:NH2   | 2.77                     | 0.48              |
| 1:E:79:ILE:HB     | 1:E:1042:ILE:HG22 | 1.95                     | 0.48              |
| 1:E:602:SER:HB3   | 1:E:647:LEU:H     | 1.78                     | 0.48              |
| 1:F:734:VAL:HA    | 1:F:739:PRO:HA    | 1.94                     | 0.48              |
| 1:F:1019:THR:CG2  | 1:F:1160:LEU:HD11 | 2.39                     | 0.48              |
| 1:G:326:PHE:HE1   | 1:n:318:ALA:HB2   | 1.79                     | 0.48              |
| 1:G:449:THR:HB    | 1:G:1097:LEU:HD13 | 1.96                     | 0.48              |
| 1:G:611:LEU:HB3   | 1:G:846:VAL:HG11  | 1.95                     | 0.48              |
| 1:G:813:PHE:CE1   | 3:P:85:LEU:HD11   | 2.48                     | 0.48              |
| 1:G:1048:VAL:HG22 | 1:G:1061:VAL:HG12 | 1.96                     | 0.48              |
| 1:H:715:ARG:HA    | 1:H:731:VAL:HG21  | 1.95                     | 0.48              |
| 1:H:755:VAL:HB    | 3:Q:71:MET:HE2    | 1.94                     | 0.48              |
| 1:H:911:PRO:HG2   | 1:H:918:LEU:HD13  | 1.95                     | 0.48              |
| 1:l:874:MET:HB2   | 1:l:874:MET:HE3   | 1.75                     | 0.48              |
| 1:l:957:PHE:O     | 1:l:959:LEU:HD12  | 2.13                     | 0.48              |
| 1:m:275:VAL:HG12  | 1:m:371:GLU:HB3   | 1.96                     | 0.48              |
| 1:m:1147:ALA:HB1  | 1:n:1206:PRO:HG3  | 1.96                     | 0.48              |
| 1:n:148:LEU:HD21  | 1:o:334:GLN:HA    | 1.96                     | 0.48              |
| 1:n:235:ARG:HD3   | 1:n:240:LEU:HD22  | 1.94                     | 0.48              |
| 1:n:813:PHE:CG    | 3:u:85:LEU:CD2    | 2.97                     | 0.48              |
| 1:o:627:GLU:HA    | 1:o:630:ILE:HG13  | 1.96                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:p:752:THR:O     | 3:w:86:ARG:NH1    | 2.47                     | 0.48              |
| 1:q:210:ARG:HG3   | 1:q:1186:VAL:HG11 | 1.96                     | 0.48              |
| 2:3:129:ASP:O     | 2:3:131:VAL:N     | 2.47                     | 0.48              |
| 2:f:104:LYS:CG    | 2:i:92:LEU:HD13   | 2.43                     | 0.48              |
| 2:f:142:VAL:O     | 2:f:146:GLY:N     | 2.47                     | 0.48              |
| 2:j:74:MET:HE2    | 2:j:267:LEU:HD22  | 1.96                     | 0.48              |
| 5:1:32:PRO:HA     | 5:1:66:MET:HG2    | 1.95                     | 0.48              |
| 5:a:64:ARG:NH1    | 5:a:288:SER:O     | 2.40                     | 0.48              |
| 5:c:141:GLU:OE2   | 5:c:145:ARG:NE    | 2.44                     | 0.48              |
| 1:A:129:PRO:HB3   | 1:A:1060:HIS:CE1  | 2.49                     | 0.47              |
| 1:A:183:VAL:HG21  | 1:A:1067:THR:HG21 | 1.95                     | 0.47              |
| 1:A:657:ARG:NH2   | 1:A:778:GLU:OE1   | 2.47                     | 0.47              |
| 1:C:178:ASP:OD1   | 1:C:182:ARG:NE    | 2.45                     | 0.47              |
| 1:C:200:HIS:HB2   | 1:C:216:ILE:HD13  | 1.95                     | 0.47              |
| 1:E:39:TYR:HE1    | 1:m:116:MET:HE2   | 1.78                     | 0.47              |
| 1:E:753:SER:HB2   | 3:N:83:ASP:CG     | 2.35                     | 0.47              |
| 1:F:332:ARG:HH21  | 1:l:12:PRO:CG     | 2.27                     | 0.47              |
| 1:F:815:THR:OG1   | 1:F:836:ASN:ND2   | 2.47                     | 0.47              |
| 1:G:253:GLU:O     | 1:m:19:ASP:CB     | 2.62                     | 0.47              |
| 1:G:763:GLN:HG2   | 1:G:765:GLU:H     | 1.79                     | 0.47              |
| 1:H:494:THR:HG23  | 1:H:921:ILE:HD11  | 1.96                     | 0.47              |
| 1:I:1270:LEU:O    | 1:I:1293:SER:OG   | 2.32                     | 0.47              |
| 1:l:883:PRO:HA    | 1:l:886:ARG:HB2   | 1.96                     | 0.47              |
| 1:l:1179:ARG:NH2  | 1:l:1204:PRO:O    | 2.46                     | 0.47              |
| 1:m:587:ARG:NH1   | 1:m:589:PRO:O     | 2.47                     | 0.47              |
| 1:m:907:MET:HE3   | 1:m:932:LEU:HG    | 1.95                     | 0.47              |
| 1:n:272:GLY:O     | 1:n:368:VAL:HA    | 2.13                     | 0.47              |
| 1:o:695:LEU:HD13  | 1:o:708:VAL:HG21  | 1.96                     | 0.47              |
| 1:p:1105:VAL:HG12 | 1:p:1116:ARG:HH11 | 1.79                     | 0.47              |
| 1:q:441:ILE:HG13  | 1:q:445:GLU:HB2   | 1.95                     | 0.47              |
| 2:3:285:GLU:O     | 2:3:289:LEU:N     | 2.47                     | 0.47              |
| 2:j:136:TYR:HA    | 2:j:139:ARG:HD2   | 1.96                     | 0.47              |
| 4:y:217:HIS:HA    | 4:y:220:ILE:HG12  | 1.96                     | 0.47              |
| 4:U:63:GLN:HA     | 4:U:140:ILE:HG13  | 1.94                     | 0.47              |
| 4:U:153:ARG:NH1   | 4:U:286:ASP:OD1   | 2.46                     | 0.47              |
| 4:U:189:TYR:HD1   | 4:U:254:ARG:HA    | 1.79                     | 0.47              |
| 4:V:78:GLU:O      | 4:V:79:MET:O      | 2.32                     | 0.47              |
| 5:z:45:LEU:HD22   | 5:z:63:MET:HE3    | 1.96                     | 0.47              |
| 5:W:198:ILE:HD13  | 5:a:226:LEU:HD11  | 1.96                     | 0.47              |
| 5:Z:21:LEU:HD11   | 5:Z:120:LEU:HD11  | 1.94                     | 0.47              |
| 1:B:1022:ARG:NH2  | 1:B:1308:GLN:OE1  | 2.47                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:925:ARG:NH1   | 1:C:972:ARG:O     | 2.47                     | 0.47              |
| 1:D:605:ASP:OD2   | 1:D:640:TYR:OH    | 2.32                     | 0.47              |
| 1:E:509:ARG:HB2   | 1:E:513:GLU:HB2   | 1.96                     | 0.47              |
| 1:F:1098:PHE:HE2  | 1:F:1119:THR:HG23 | 1.79                     | 0.47              |
| 1:G:333:ILE:CD1   | 1:n:314:VAL:HG22  | 2.42                     | 0.47              |
| 1:G:434:LYS:N     | 1:G:1089:ASP:O    | 2.40                     | 0.47              |
| 1:I:448:LYS:HD2   | 1:I:1096:ASP:HB3  | 1.96                     | 0.47              |
| 1:I:692:LEU:HD21  | 1:I:1010:MET:HG3  | 1.95                     | 0.47              |
| 1:k:517:ASP:OD2   | 1:p:696:ASN:HB3   | 2.13                     | 0.47              |
| 1:k:643:GLN:HA    | 1:p:667:ALA:HB2   | 1.95                     | 0.47              |
| 1:l:257:ASP:HB2   | 1:l:269:ARG:HH12  | 1.79                     | 0.47              |
| 1:l:492:HIS:HD2   | 1:l:495:ARG:HB2   | 1.79                     | 0.47              |
| 1:m:51:PHE:CE2    | 1:n:87:MET:HB3    | 2.48                     | 0.47              |
| 1:m:126:ILE:O     | 1:m:1062:SER:HA   | 2.14                     | 0.47              |
| 1:m:227:THR:HG22  | 1:m:230:LEU:HD21  | 1.95                     | 0.47              |
| 1:m:476:ARG:HH12  | 1:m:543:PHE:HB2   | 1.78                     | 0.47              |
| 1:n:389:ASP:OD1   | 1:n:389:ASP:N     | 2.47                     | 0.47              |
| 1:n:1029:ASP:HB2  | 1:n:1082:HIS:HB3  | 1.96                     | 0.47              |
| 1:o:395:TYR:HD1   | 1:o:1305:ALA:HB3  | 1.79                     | 0.47              |
| 1:o:844:ARG:HG3   | 1:o:854:ALA:HB2   | 1.95                     | 0.47              |
| 1:p:1126:VAL:HG11 | 1:p:1134:ILE:HD11 | 1.95                     | 0.47              |
| 2:2:105:LEU:HD11  | 2:2:212:VAL:HG13  | 1.86                     | 0.47              |
| 2:2:207:ASP:CG    | 2:2:208:PRO:HD2   | 2.38                     | 0.47              |
| 2:e:104:LYS:CG    | 2:h:92:LEU:HD13   | 2.43                     | 0.47              |
| 2:i:66:ARG:HD3    | 2:i:68:THR:HG22   | 1.96                     | 0.47              |
| 2:i:129:ASP:O     | 2:i:131:VAL:N     | 2.47                     | 0.47              |
| 4:T:234:PHE:HB2   | 4:T:249:LEU:HD13  | 1.95                     | 0.47              |
| 5:z:6:LEU:HD11    | 5:z:78:GLN:HB3    | 1.96                     | 0.47              |
| 5:Y:5:VAL:HB      | 5:Y:81:LEU:HB2    | 1.94                     | 0.47              |
| 5:Y:206:LEU:O     | 5:Y:272:LYS:CE    | 2.58                     | 0.47              |
| 5:1:11:GLN:HG3    | 5:1:123:VAL:HG13  | 1.96                     | 0.47              |
| 1:A:512:ASN:OD1   | 1:A:513:GLU:N     | 2.41                     | 0.47              |
| 1:A:1098:PHE:HE2  | 1:A:1119:THR:HG23 | 1.78                     | 0.47              |
| 1:B:192:PHE:HB2   | 1:B:223:LYS:HB3   | 1.96                     | 0.47              |
| 1:C:257:ASP:OD1   | 1:C:257:ASP:N     | 2.46                     | 0.47              |
| 1:C:392:LEU:HA    | 1:C:1297:LYS:HB3  | 1.95                     | 0.47              |
| 1:D:777:GLU:HG3   | 1:E:951:GLN:HE21  | 1.79                     | 0.47              |
| 1:E:420:THR:HG22  | 1:E:422:GLU:H     | 1.79                     | 0.47              |
| 1:E:726:ARG:NH1   | 1:F:945:ASN:OD1   | 2.47                     | 0.47              |
| 1:E:921:ILE:HG22  | 1:E:923:PHE:HB3   | 1.94                     | 0.47              |
| 1:E:1101:PHE:HB3  | 1:E:1104:HIS:HD2  | 1.80                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:G:192:PHE:HB2   | 1:G:223:LYS:HB3   | 1.96                     | 0.47              |
| 1:G:453:PRO:O     | 1:G:457:ASP:N     | 2.40                     | 0.47              |
| 1:G:639:ASN:HD22  | 1:G:847:ALA:HB1   | 1.78                     | 0.47              |
| 1:H:181:LEU:HD21  | 1:H:386:LEU:HG    | 1.95                     | 0.47              |
| 1:I:396:PHE:HB2   | 1:I:1310:THR:HG21 | 1.96                     | 0.47              |
| 1:I:632:LEU:HB2   | 1:I:860:GLU:HB3   | 1.95                     | 0.47              |
| 1:I:653:TYR:HA    | 1:I:656:VAL:HG12  | 1.95                     | 0.47              |
| 1:I:882:ASP:OD1   | 1:I:882:ASP:N     | 2.45                     | 0.47              |
| 1:k:308:LEU:HB3   | 1:k:310:LYS:HG3   | 1.96                     | 0.47              |
| 1:k:1326:LYS:NZ   | 1:p:1324:THR:H    | 2.10                     | 0.47              |
| 1:l:185:LEU:HB3   | 1:l:388:ARG:HH22  | 1.79                     | 0.47              |
| 1:l:433:ASN:HD21  | 1:l:439:GLN:HG2   | 1.79                     | 0.47              |
| 1:m:67:PHE:O      | 1:m:70:THR:OG1    | 2.32                     | 0.47              |
| 1:o:223:LYS:O     | 1:o:227:THR:CB    | 2.62                     | 0.47              |
| 1:o:659:ILE:HG23  | 1:o:663:LEU:HD23  | 1.97                     | 0.47              |
| 2:3:264:ARG:NH2   | 3:r:93:LYS:NZ     | 2.63                     | 0.47              |
| 2:f:66:ARG:NH2    | 2:f:68:THR:HG21   | 2.27                     | 0.47              |
| 2:f:66:ARG:CD     | 2:f:68:THR:HG22   | 2.34                     | 0.47              |
| 2:f:207:ASP:CG    | 2:f:208:PRO:HD2   | 2.38                     | 0.47              |
| 2:j:92:LEU:N      | 2:j:93:PRO:CD     | 2.77                     | 0.47              |
| 2:j:258:PHE:HZ    | 3:M:87:MET:HE3    | 1.79                     | 0.47              |
| 3:t:69:MET:HE3    | 3:t:70:LYS:CE     | 2.43                     | 0.47              |
| 4:S:71:PHE:N      | 4:S:85:VAL:O      | 2.46                     | 0.47              |
| 4:V:73:LEU:HD11   | 4:V:121:ARG:HD2   | 1.97                     | 0.47              |
| 5:z:120:LEU:HD13  | 5:z:128:LEU:HD13  | 1.95                     | 0.47              |
| 5:Y:87:GLY:HA3    | 5:c:86:HIS:HB3    | 1.96                     | 0.47              |
| 5:c:120:LEU:HB3   | 5:c:121:VAL:H     | 1.56                     | 0.47              |
| 1:A:775:SER:HB2   | 1:A:778:GLU:HG2   | 1.96                     | 0.47              |
| 1:C:433:ASN:ND2   | 1:C:1090:MET:O    | 2.43                     | 0.47              |
| 1:C:486:VAL:O     | 1:C:965:HIS:NE2   | 2.34                     | 0.47              |
| 1:C:761:MET:HB2   | 1:C:806:LYS:HD3   | 1.96                     | 0.47              |
| 1:D:663:LEU:HB3   | 1:D:673:TYR:CE1   | 2.49                     | 0.47              |
| 1:D:1021:VAL:HG23 | 1:D:1245:PRO:HB2  | 1.97                     | 0.47              |
| 1:E:14:LEU:HD21   | 1:m:344:SER:HB2   | 1.96                     | 0.47              |
| 1:E:1106:TYR:HB2  | 1:E:1112:ASP:HB2  | 1.95                     | 0.47              |
| 1:F:596:LEU:HB2   | 1:F:985:THR:HG22  | 1.96                     | 0.47              |
| 1:G:72:LEU:HD23   | 1:G:180:PHE:HD2   | 1.79                     | 0.47              |
| 1:G:118:SER:H     | 1:m:5:TRP:HH2     | 1.62                     | 0.47              |
| 1:G:920:VAL:HG21  | 1:G:933:ALA:HA    | 1.96                     | 0.47              |
| 1:H:1048:VAL:HG22 | 1:H:1061:VAL:HG12 | 1.95                     | 0.47              |
| 1:I:393:THR:HG21  | 1:I:1249:PHE:HE2  | 1.78                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:k:705:LEU:HD11  | 1:l:952:ARG:HD3   | 1.96                     | 0.47              |
| 1:l:1132:ILE:HG22 | 4:T:116:ILE:HG23  | 1.96                     | 0.47              |
| 1:m:753:SER:HB2   | 3:t:83:ASP:HB3    | 1.97                     | 0.47              |
| 1:m:1171:ARG:NH2  | 1:m:1330:ASP:O    | 2.46                     | 0.47              |
| 1:m:1234:GLU:O    | 5:a:52:LYS:HB2    | 2.13                     | 0.47              |
| 1:n:734:VAL:HG23  | 1:n:876:GLU:HB3   | 1.97                     | 0.47              |
| 1:n:1177:ARG:HH21 | 1:n:1181:SER:HB3  | 1.78                     | 0.47              |
| 1:o:435:ASP:OD1   | 1:o:435:ASP:N     | 2.48                     | 0.47              |
| 1:o:1031:LEU:CD1  | 1:o:1079:CYS:HB3  | 2.44                     | 0.47              |
| 1:p:760:ALA:HA    | 1:p:763:GLN:HB3   | 1.95                     | 0.47              |
| 1:p:1272:ARG:O    | 1:p:1300:ARG:NH1  | 2.47                     | 0.47              |
| 2:2:200:VAL:HG21  | 2:2:215:ARG:HG2   | 0.63                     | 0.47              |
| 2:3:74:MET:HE2    | 2:3:267:LEU:HD22  | 1.96                     | 0.47              |
| 2:h:264:ARG:NH1   | 2:h:268:GLU:OE1   | 2.48                     | 0.47              |
| 2:f:208:PRO:CB    | 2:i:95:LEU:HD12   | 2.40                     | 0.47              |
| 2:g:174:ARG:NH1   | 2:j:274:THR:HG22  | 2.29                     | 0.47              |
| 4:y:48:ILE:HD11   | 5:1:296:CYS:HB3   | 1.95                     | 0.47              |
| 5:X:89:CYS:HA     | 5:X:308:ILE:HG13  | 1.93                     | 0.47              |
| 1:A:227:THR:HG23  | 1:A:230:LEU:HD11  | 1.95                     | 0.47              |
| 1:A:924:HIS:HB3   | 1:A:927:TYR:HB2   | 1.96                     | 0.47              |
| 1:C:661:THR:HA    | 1:D:606:HIS:HD2   | 1.79                     | 0.47              |
| 1:F:9:GLU:O       | 1:F:13:LYS:NZ     | 2.47                     | 0.47              |
| 1:F:576:ARG:HH11  | 1:F:1007:LEU:HD21 | 1.79                     | 0.47              |
| 1:H:555:THR:HG22  | 1:H:972:ARG:HH22  | 1.79                     | 0.47              |
| 1:I:447:LEU:HD11  | 1:I:1005:ALA:HA   | 1.95                     | 0.47              |
| 1:I:1177:ARG:NH1  | 1:I:1198:LEU:O    | 2.48                     | 0.47              |
| 1:k:125:PRO:HA    | 1:k:1064:ASN:HA   | 1.95                     | 0.47              |
| 1:k:784:VAL:CA    | 1:k:788:CYS:HB2   | 2.44                     | 0.47              |
| 1:m:429:VAL:HG11  | 1:m:431:PHE:CE2   | 2.41                     | 0.47              |
| 1:m:528:ASN:HB3   | 1:m:531:LEU:HG    | 1.96                     | 0.47              |
| 1:o:733:VAL:HG22  | 1:o:877:ILE:HG23  | 1.95                     | 0.47              |
| 1:q:195:ARG:HH11  | 1:q:247:LEU:HD12  | 1.79                     | 0.47              |
| 1:q:658:LEU:O     | 1:q:662:ARG:HB2   | 2.14                     | 0.47              |
| 1:q:1216:TRP:HB2  | 1:q:1222:SER:HB2  | 1.96                     | 0.47              |
| 2:2:142:VAL:O     | 2:2:146:GLY:N     | 2.47                     | 0.47              |
| 2:e:206:GLU:CB    | 2:h:132:TYR:C     | 2.81                     | 0.47              |
| 2:j:264:ARG:NH1   | 2:j:268:GLU:OE1   | 2.48                     | 0.47              |
| 3:O:49:LEU:O      | 3:O:81:GLN:NE2    | 2.47                     | 0.47              |
| 4:S:83:VAL:HG11   | 4:S:117:ARG:HD2   | 1.95                     | 0.47              |
| 4:U:249:LEU:HB3   | 4:U:294:ALA:HA    | 1.97                     | 0.47              |
| 4:V:183:ASP:HB2   | 4:V:261:ARG:HE    | 1.79                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:1:9:PHE:HZ      | 5:1:79:MET:HE3    | 1.80                     | 0.47              |
| 5:b:14:THR:HG22   | 5:b:16:GLY:H      | 1.78                     | 0.47              |
| 5:c:156:ARG:NH2   | 5:c:165:THR:OG1   | 2.43                     | 0.47              |
| 1:A:715:ARG:HA    | 1:A:731:VAL:HG21  | 1.97                     | 0.47              |
| 1:A:1051:GLU:OE2  | 4:U:51:ARG:NH2    | 2.47                     | 0.47              |
| 1:A:1153:ARG:NH1  | 1:B:1209:PHE:HZ   | 2.01                     | 0.47              |
| 1:B:558:ILE:HD13  | 1:B:970:TRP:HA    | 1.97                     | 0.47              |
| 1:B:1096:ASP:OD1  | 1:B:1096:ASP:N    | 2.47                     | 0.47              |
| 1:C:389:ASP:OD1   | 1:C:389:ASP:N     | 2.41                     | 0.47              |
| 1:C:592:HIS:HE1   | 1:C:986:LEU:HB2   | 1.79                     | 0.47              |
| 1:D:523:PHE:HB2   | 1:D:566:ALA:HB1   | 1.96                     | 0.47              |
| 1:E:232:ASP:OD1   | 1:E:1352:ASN:ND2  | 2.47                     | 0.47              |
| 1:E:777:GLU:HG3   | 1:F:951:GLN:HE21  | 1.80                     | 0.47              |
| 1:E:1168:GLU:O    | 1:E:1172:TYR:OH   | 2.27                     | 0.47              |
| 1:F:37:ARG:NH2    | 1:F:45:GLU:OE2    | 2.47                     | 0.47              |
| 1:F:592:HIS:HB2   | 1:F:682:ILE:HD11  | 1.97                     | 0.47              |
| 1:G:929:ASP:HB3   | 1:G:932:LEU:HB3   | 1.96                     | 0.47              |
| 1:I:734:VAL:HG23  | 1:I:876:GLU:HB3   | 1.96                     | 0.47              |
| 1:I:1041:VAL:HG12 | 1:I:1067:THR:HG22 | 1.96                     | 0.47              |
| 1:k:395:TYR:HE2   | 1:k:1170:PHE:HD1  | 1.63                     | 0.47              |
| 1:k:462:LEU:HD22  | 1:k:890:PRO:HG3   | 1.95                     | 0.47              |
| 1:k:489:HIS:O     | 1:k:496:ARG:NH1   | 2.40                     | 0.47              |
| 1:k:877:ILE:O     | 1:k:897:LEU:HA    | 2.15                     | 0.47              |
| 1:l:510:THR:O     | 1:l:967:TYR:OH    | 2.27                     | 0.47              |
| 1:m:276:SER:HB2   | 1:m:281:VAL:HG23  | 1.96                     | 0.47              |
| 1:m:558:ILE:HD13  | 1:m:970:TRP:HA    | 1.97                     | 0.47              |
| 1:m:1177:ARG:NH1  | 1:m:1218:SER:OG   | 2.47                     | 0.47              |
| 1:m:1228:TYR:HB3  | 1:m:1246:CYS:HB3  | 1.96                     | 0.47              |
| 1:n:248:THR:O     | 1:n:366:ARG:NH2   | 2.48                     | 0.47              |
| 1:n:400:LEU:HD11  | 1:n:1164:SER:HB2  | 1.96                     | 0.47              |
| 1:o:1098:PHE:HE2  | 1:o:1119:THR:HG23 | 1.79                     | 0.47              |
| 1:p:567:LEU:HD22  | 1:p:1161:THR:HG21 | 1.96                     | 0.47              |
| 1:q:398:VAL:HG12  | 1:q:1018:LEU:HB2  | 1.96                     | 0.47              |
| 1:q:748:ARG:HD2   | 1:q:768:PHE:HB3   | 1.97                     | 0.47              |
| 2:2:174:ARG:NH1   | 2:3:274:THR:HG22  | 2.29                     | 0.47              |
| 2:2:208:PRO:CB    | 2:3:95:LEU:HD12   | 2.40                     | 0.47              |
| 1:A:590:GLU:CD    | 1:B:597:GLN:HE22  | 2.23                     | 0.47              |
| 1:A:724:LEU:H     | 1:A:769:VAL:HG21  | 1.80                     | 0.47              |
| 1:A:1194:ALA:O    | 1:A:1197:THR:OG1  | 2.33                     | 0.47              |
| 1:B:392:LEU:HB2   | 1:B:1026:PHE:HE2  | 1.79                     | 0.47              |
| 1:B:687:ALA:HB2   | 1:B:784:VAL:HG21  | 1.95                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:128:ILE:HD11  | 1:C:168:THR:HG23  | 1.96                     | 0.47              |
| 1:C:197:LEU:O     | 1:C:202:THR:OG1   | 2.28                     | 0.47              |
| 1:C:258:ASN:HB2   | 1:C:261:THR:HG22  | 1.97                     | 0.47              |
| 1:C:1307:THR:HG23 | 1:C:1341:GLU:HA   | 1.96                     | 0.47              |
| 1:D:243:TYR:OH    | 1:D:1079:CYS:SG   | 2.71                     | 0.47              |
| 1:D:264:VAL:HG22  | 1:D:297:VAL:HG22  | 1.95                     | 0.47              |
| 1:D:431:PHE:O     | 1:D:439:GLN:N     | 2.48                     | 0.47              |
| 1:D:1177:ARG:NH1  | 1:D:1218:SER:OG   | 2.48                     | 0.47              |
| 1:D:1320:GLN:HE22 | 1:D:1329:LEU:HD12 | 1.80                     | 0.47              |
| 1:E:9:GLU:O       | 1:E:46:ARG:NH2    | 2.37                     | 0.47              |
| 1:E:141:LYS:HG2   | 4:S:29:ARG:HD3    | 1.95                     | 0.47              |
| 1:F:248:THR:O     | 1:F:366:ARG:NH2   | 2.47                     | 0.47              |
| 1:F:314:VAL:HB    | 1:m:326:PHE:CZ    | 2.50                     | 0.47              |
| 1:F:534:GLU:OE2   | 1:F:557:ARG:NH1   | 2.47                     | 0.47              |
| 1:F:1223:LEU:HA   | 1:F:1226:VAL:HG22 | 1.96                     | 0.47              |
| 1:G:748:ARG:CZ    | 2:h:269:ARG:CD    | 2.92                     | 0.47              |
| 1:G:1019:THR:N    | 1:G:1158:VAL:O    | 2.40                     | 0.47              |
| 1:G:1147:ALA:HB1  | 1:H:1206:PRO:N    | 2.30                     | 0.47              |
| 1:H:462:LEU:HD22  | 1:H:890:PRO:HG3   | 1.95                     | 0.47              |
| 1:I:1021:VAL:HG23 | 1:I:1245:PRO:HB2  | 1.95                     | 0.47              |
| 1:I:1230:THR:HA   | 1:I:1233:ARG:HB3  | 1.96                     | 0.47              |
| 1:k:220:PHE:HB2   | 1:k:1302:LEU:HD11 | 1.97                     | 0.47              |
| 1:k:1093:ARG:HH11 | 1:k:1153:ARG:HD2  | 1.78                     | 0.47              |
| 1:k:1269:TYR:HE1  | 1:k:1296:GLU:HB2  | 1.80                     | 0.47              |
| 1:l:300:PRO:HB3   | 1:l:351:LEU:HB2   | 1.96                     | 0.47              |
| 1:l:512:ASN:OD1   | 1:l:513:GLU:N     | 2.46                     | 0.47              |
| 1:l:1179:ARG:NH1  | 1:l:1211:SER:OG   | 2.48                     | 0.47              |
| 1:m:51:PHE:CE1    | 1:n:88:THR:N      | 2.79                     | 0.47              |
| 1:m:141:LYS:CD    | 4:S:20:GLU:CA     | 2.91                     | 0.47              |
| 1:m:272:GLY:H     | 1:m:1036:LYS:HB2  | 1.80                     | 0.47              |
| 1:m:752:THR:O     | 3:t:86:ARG:NE     | 2.47                     | 0.47              |
| 1:m:786:TYR:O     | 1:m:927:TYR:OH    | 2.28                     | 0.47              |
| 1:m:805:LEU:N     | 1:m:871:ASN:OD1   | 2.45                     | 0.47              |
| 1:m:965:HIS:O     | 1:m:969:HIS:N     | 2.48                     | 0.47              |
| 1:n:392:LEU:O     | 1:n:1024:ASP:N    | 2.47                     | 0.47              |
| 1:n:417:LEU:HD13  | 1:n:423:ASN:HB3   | 1.97                     | 0.47              |
| 1:o:74:THR:O      | 1:o:1037:ALA:N    | 2.37                     | 0.47              |
| 1:o:539:PHE:HD1   | 1:o:556:PRO:HA    | 1.79                     | 0.47              |
| 1:o:717:TRP:HE1   | 1:o:731:VAL:HG11  | 1.79                     | 0.47              |
| 1:o:1272:ARG:O    | 1:o:1300:ARG:NH1  | 2.42                     | 0.47              |
| 1:p:458:ALA:HB1   | 1:p:461:CYS:HB3   | 1.97                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:q:231:LEU:HD12  | 1:q:1082:HIS:HB2  | 1.96                     | 0.47              |
| 1:q:698:ARG:HG2   | 1:q:700:CYS:H     | 1.79                     | 0.47              |
| 1:q:791:PRO:HA    | 1:q:794:LEU:HB2   | 1.97                     | 0.47              |
| 1:q:861:LEU:O     | 1:q:865:VAL:HB    | 2.15                     | 0.47              |
| 1:q:966:GLU:O     | 1:q:969:HIS:NE2   | 2.48                     | 0.47              |
| 1:q:1116:ARG:HA   | 1:q:1119:THR:HB   | 1.95                     | 0.47              |
| 2:e:208:PRO:HG3   | 2:h:95:LEU:HD11   | 0.48                     | 0.47              |
| 2:e:261:VAL:CG1   | 3:t:90:ILE:CG2    | 2.91                     | 0.47              |
| 2:h:136:TYR:HA    | 2:h:139:ARG:HD2   | 1.96                     | 0.47              |
| 2:f:200:VAL:HG21  | 2:f:215:ARG:HG2   | 0.63                     | 0.47              |
| 2:f:208:PRO:HG3   | 2:i:95:LEU:HD11   | 0.48                     | 0.47              |
| 2:g:142:VAL:O     | 2:g:146:GLY:N     | 2.47                     | 0.47              |
| 3:O:48:VAL:HA     | 3:O:77:LYS:HD2    | 1.95                     | 0.47              |
| 3:O:85:LEU:O      | 3:O:89:SER:N      | 2.48                     | 0.47              |
| 4:y:61:VAL:O      | 4:y:63:GLN:N      | 2.47                     | 0.47              |
| 4:V:71:PHE:HD2    | 4:V:90:LEU:HD21   | 1.80                     | 0.47              |
| 4:V:159:MET:O     | 4:V:160:LEU:CB    | 2.62                     | 0.47              |
| 4:V:176:ASP:O     | 4:V:226:ARG:NH2   | 2.46                     | 0.47              |
| 5:z:141:GLU:OE2   | 5:z:145:ARG:NE    | 2.48                     | 0.47              |
| 5:X:110:PRO:CB    | 5:X:111:PRO:HD2   | 2.45                     | 0.47              |
| 5:Y:208:SER:HB3   | 5:Y:211:THR:H     | 1.80                     | 0.47              |
| 5:d:49:VAL:HG22   | 5:d:59:MET:HE3    | 1.97                     | 0.47              |
| 5:d:120:LEU:HB3   | 5:d:121:VAL:H     | 1.55                     | 0.47              |
| 5:d:203:ILE:O     | 5:d:207:SER:N     | 2.43                     | 0.47              |
| 1:B:879:ALA:HB2   | 1:B:898:GLN:HE22  | 1.80                     | 0.47              |
| 1:C:920:VAL:HG22  | 1:C:922:PRO:HD3   | 1.97                     | 0.47              |
| 1:C:1309:HIS:CG   | 1:C:1327:LEU:HD12 | 2.50                     | 0.47              |
| 1:D:662:ARG:HD3   | 1:D:663:LEU:HD13  | 1.96                     | 0.47              |
| 1:D:744:HIS:ND1   | 2:g:175:ALA:HA    | 2.29                     | 0.47              |
| 1:D:1255:ILE:HD12 | 1:D:1258:ALA:HB3  | 1.96                     | 0.47              |
| 1:E:23:HIS:NE2    | 1:m:205:ARG:HA    | 2.29                     | 0.47              |
| 1:E:209:THR:HG22  | 1:E:211:VAL:H     | 1.80                     | 0.47              |
| 1:F:417:LEU:HD21  | 1:F:1313:THR:HG21 | 1.97                     | 0.47              |
| 1:G:86:LYS:HZ1    | 1:m:149:LEU:HD13  | 1.80                     | 0.47              |
| 1:G:748:ARG:NH1   | 2:h:275:THR:HG21  | 2.29                     | 0.47              |
| 1:H:319:HIS:CE1   | 1:H:321:ALA:HB3   | 2.50                     | 0.47              |
| 1:l:37:ARG:NH2    | 1:l:43:ASP:OD2    | 2.43                     | 0.47              |
| 1:l:910:VAL:HG22  | 1:l:936:ALA:HB2   | 1.96                     | 0.47              |
| 1:l:1156:CYS:HB2  | 1:l:1245:PRO:HD2  | 1.96                     | 0.47              |
| 1:m:691:GLU:CD    | 1:n:953:CYS:HB2   | 2.37                     | 0.47              |
| 1:n:199:GLU:OE1   | 1:n:223:LYS:NZ    | 2.43                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:n:440:ARG:NH2   | 1:o:521:LYS:HE3   | 2.30                     | 0.47              |
| 1:o:189:PRO:HA    | 1:o:1270:LEU:HD21 | 1.96                     | 0.47              |
| 1:p:1043:ILE:HB   | 1:p:1063:GLN:HE21 | 1.80                     | 0.47              |
| 1:q:192:PHE:HA    | 1:q:195:ARG:HD2   | 1.97                     | 0.47              |
| 2:2:176:GLU:O     | 2:2:177:GLU:C     | 2.58                     | 0.47              |
| 2:h:74:MET:HE2    | 2:h:267:LEU:HD22  | 1.96                     | 0.47              |
| 2:i:136:TYR:HA    | 2:i:139:ARG:HD2   | 1.96                     | 0.47              |
| 2:i:264:ARG:NH1   | 2:i:268:GLU:OE1   | 2.48                     | 0.47              |
| 2:g:208:PRO:HG3   | 2:j:95:LEU:HD11   | 0.48                     | 0.47              |
| 3:P:72:GLY:O      | 3:P:80:TYR:OH     | 2.33                     | 0.47              |
| 4:V:158:ASN:HB3   | 4:V:163:GLU:H     | 1.79                     | 0.47              |
| 5:X:84:PRO:O      | 5:X:310:LYS:NZ    | 2.38                     | 0.47              |
| 5:Y:219:ALA:HB1   | 5:Y:231:GLN:HE21  | 1.79                     | 0.47              |
| 5:Z:293:PHE:HB3   | 5:Z:307:CYS:HB3   | 1.96                     | 0.47              |
| 5:b:120:LEU:CG    | 5:b:129:VAL:HA    | 2.33                     | 0.47              |
| 5:b:145:ARG:NH1   | 5:b:168:LEU:O     | 2.47                     | 0.47              |
| 1:B:276:SER:HB2   | 1:B:281:VAL:HG23  | 1.97                     | 0.47              |
| 1:B:656:VAL:HG23  | 1:B:676:TYR:HD1   | 1.79                     | 0.47              |
| 1:B:713:ASP:O     | 1:B:783:LYS:NZ    | 2.48                     | 0.47              |
| 1:B:734:VAL:HG12  | 1:B:739:PRO:HA    | 1.97                     | 0.47              |
| 1:C:227:THR:HG23  | 1:C:230:LEU:HD11  | 1.97                     | 0.47              |
| 1:C:309:SER:HB3   | 1:C:312:ASN:HB2   | 1.96                     | 0.47              |
| 1:C:993:ALA:HA    | 1:C:996:HIS:HD2   | 1.79                     | 0.47              |
| 1:E:1043:ILE:HG22 | 1:E:1065:ILE:HG22 | 1.96                     | 0.47              |
| 1:F:657:ARG:O     | 1:F:661:THR:N     | 2.47                     | 0.47              |
| 1:G:484:GLU:OE2   | 1:G:966:GLU:N     | 2.48                     | 0.47              |
| 1:H:625:ALA:O     | 1:H:628:THR:OG1   | 2.31                     | 0.47              |
| 1:H:925:ARG:HH12  | 1:H:971:HIS:HB3   | 1.79                     | 0.47              |
| 1:H:1049:THR:HG23 | 1:H:1060:HIS:HB2  | 1.96                     | 0.47              |
| 1:k:80:MET:HA     | 1:k:1043:ILE:O    | 2.15                     | 0.47              |
| 1:k:734:VAL:HG23  | 1:k:876:GLU:HB3   | 1.96                     | 0.47              |
| 1:k:748:ARG:HH11  | 2:3:275:THR:HG21  | 1.80                     | 0.47              |
| 1:l:494:THR:OG1   | 1:l:872:ALA:O     | 2.29                     | 0.47              |
| 1:l:786:TYR:O     | 1:l:927:TYR:OH    | 2.23                     | 0.47              |
| 1:n:641:TRP:CD2   | 1:n:672:ALA:HB2   | 2.50                     | 0.47              |
| 1:n:925:ARG:HH12  | 1:n:971:HIS:HB3   | 1.80                     | 0.47              |
| 1:p:65:VAL:HG11   | 1:p:376:VAL:HG12  | 1.95                     | 0.47              |
| 1:p:331:ASP:O     | 1:p:335:GLN:HB2   | 2.15                     | 0.47              |
| 1:p:819:LEU:HD11  | 3:w:59:PRO:HD2    | 1.97                     | 0.47              |
| 1:q:485:PHE:HA    | 1:q:961:PRO:HB3   | 1.96                     | 0.47              |
| 2:i:73:GLU:HA     | 2:i:76:LEU:HB2    | 1.96                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:S:228:ARG:HG2   | 5:a:224:ASN:CB    | 2.45                     | 0.47              |
| 4:T:87:LEU:HD21   | 4:T:208:VAL:HG21  | 1.96                     | 0.47              |
| 4:T:231:ARG:NH1   | 4:T:294:ALA:OXT   | 2.47                     | 0.47              |
| 4:T:251:THR:HG23  | 4:T:292:GLU:HG3   | 1.97                     | 0.47              |
| 4:U:230:SER:O     | 4:U:234:PHE:N     | 2.48                     | 0.47              |
| 5:X:219:ALA:HA    | 5:X:227:LEU:HD21  | 1.97                     | 0.47              |
| 5:Y:219:ALA:HA    | 5:Y:227:LEU:HD21  | 1.97                     | 0.47              |
| 5:Y:280:ILE:HA    | 5:Y:283:ILE:HG22  | 1.96                     | 0.47              |
| 5:Y:293:PHE:HB3   | 5:Y:307:CYS:HB3   | 1.96                     | 0.47              |
| 5:Z:141:GLU:OE1   | 5:d:281:ARG:NH1   | 2.47                     | 0.47              |
| 5:Z:152:LEU:HD23  | 5:Z:164:ALA:HB2   | 1.96                     | 0.47              |
| 5:l:27:ALA:HA     | 5:l:93:ARG:HB3    | 1.96                     | 0.47              |
| 1:A:390:VAL:HG22  | 1:A:1295:VAL:HB   | 1.97                     | 0.47              |
| 1:B:1166:ASP:HA   | 1:B:1170:PHE:HD2  | 1.79                     | 0.47              |
| 1:D:298:LYS:HA    | 1:D:355:GLU:HG2   | 1.97                     | 0.47              |
| 1:D:429:VAL:HG11  | 1:D:431:PHE:HZ    | 1.63                     | 0.47              |
| 1:D:744:HIS:CE1   | 2:g:175:ALA:HA    | 2.50                     | 0.47              |
| 1:E:33:PHE:HZ     | 1:m:120:TYR:CE2   | 2.33                     | 0.47              |
| 1:E:42:ASP:CG     | 1:m:112:GLN:NE2   | 2.70                     | 0.47              |
| 1:E:196:THR:HA    | 1:E:200:HIS:HD2   | 1.78                     | 0.47              |
| 1:E:393:THR:HA    | 1:E:1023:THR:HA   | 1.97                     | 0.47              |
| 1:F:146:ASP:HB2   | 1:F:151:LYS:HG3   | 1.97                     | 0.47              |
| 1:F:204:ALA:HB3   | 1:l:26:LEU:CD2    | 2.35                     | 0.47              |
| 1:F:388:ARG:HD2   | 1:F:1030:THR:HG21 | 1.96                     | 0.47              |
| 1:F:1101:PHE:HB3  | 1:F:1104:HIS:HD2  | 1.79                     | 0.47              |
| 1:G:441:ILE:HD13  | 1:G:1092:SER:HB3  | 1.96                     | 0.47              |
| 1:G:1019:THR:HG21 | 1:G:1160:LEU:HD21 | 1.94                     | 0.47              |
| 1:H:1161:THR:HG22 | 1:H:1216:TRP:CZ2  | 2.50                     | 0.47              |
| 1:H:1230:THR:H    | 1:H:1251:THR:HG22 | 1.78                     | 0.47              |
| 1:H:1233:ARG:O    | 1:H:1238:HIS:ND1  | 2.47                     | 0.47              |
| 1:I:504:ARG:NE    | 1:I:946:ASP:OD2   | 2.39                     | 0.47              |
| 1:I:637:VAL:HG22  | 1:I:648:ALA:HB3   | 1.96                     | 0.47              |
| 1:I:1101:PHE:HB3  | 1:I:1104:HIS:HD2  | 1.79                     | 0.47              |
| 1:I:1269:TYR:HE1  | 1:I:1296:GLU:HB2  | 1.80                     | 0.47              |
| 1:I:1320:GLN:HG3  | 1:I:1329:LEU:HD12 | 1.97                     | 0.47              |
| 1:k:431:PHE:HB2   | 1:k:439:GLN:HB3   | 1.97                     | 0.47              |
| 1:m:98:VAL:HG21   | 1:m:113:THR:HB    | 1.97                     | 0.47              |
| 1:m:761:MET:HG3   | 1:m:870:GLU:HG3   | 1.97                     | 0.47              |
| 1:m:1226:VAL:HG23 | 1:m:1227:ILE:HG12 | 1.97                     | 0.47              |
| 1:m:1300:ARG:H    | 1:m:1303:GLN:HE21 | 1.63                     | 0.47              |
| 1:n:632:LEU:HD12  | 1:n:635:ARG:HH21  | 1.80                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:n:1093:ARG:HD3  | 1:n:1153:ARG:HD2  | 1.96                     | 0.47              |
| 1:p:58:TYR:HB2    | 1:q:48:ASN:HB2    | 1.96                     | 0.47              |
| 2:2:173:MET:O     | 2:2:173:MET:HG2   | 2.13                     | 0.47              |
| 2:3:93:PRO:HG2    | 2:3:195:TYR:HE2   | 1.78                     | 0.47              |
| 2:3:177:GLU:OE2   | 2:3:214:ASN:ND2   | 2.44                     | 0.47              |
| 2:h:73:GLU:HA     | 2:h:76:LEU:HB2    | 1.96                     | 0.47              |
| 2:h:177:GLU:OE2   | 2:h:214:ASN:ND2   | 2.44                     | 0.47              |
| 2:f:176:GLU:O     | 2:f:177:GLU:C     | 2.58                     | 0.47              |
| 2:j:73:GLU:HA     | 2:j:76:LEU:HB2    | 1.96                     | 0.47              |
| 3:w:85:LEU:HD13   | 3:w:85:LEU:HA     | 1.75                     | 0.47              |
| 4:y:60:GLU:O      | 4:y:62:GLU:N      | 2.47                     | 0.47              |
| 4:T:92:MET:HA     | 4:T:102:LYS:HG2   | 1.96                     | 0.47              |
| 4:U:251:THR:HG23  | 4:U:292:GLU:HG3   | 1.97                     | 0.47              |
| 5:X:172:ARG:HG2   | 5:X:177:THR:HG22  | 1.96                     | 0.47              |
| 5:Z:218:LEU:HD21  | 5:d:194:ARG:HE    | 1.80                     | 0.47              |
| 1:A:813:PHE:CD2   | 3:J:85:LEU:CB     | 2.97                     | 0.46              |
| 1:B:95:TYR:HE2    | 1:B:97:GLN:HE21   | 1.63                     | 0.46              |
| 1:B:1230:THR:HA   | 1:B:1233:ARG:HB3  | 1.96                     | 0.46              |
| 1:C:635:ARG:NH2   | 1:C:849:ASP:HB3   | 2.31                     | 0.46              |
| 1:D:460:PRO:HG2   | 1:D:1236:LEU:HD13 | 1.97                     | 0.46              |
| 1:D:545:THR:HA    | 1:D:550:VAL:HA    | 1.96                     | 0.46              |
| 1:D:941:ARG:O     | 1:D:945:ASN:N     | 2.48                     | 0.46              |
| 1:F:602:SER:HA    | 1:F:646:LEU:HD13  | 1.96                     | 0.46              |
| 1:H:516:HIS:CE1   | 1:H:977:CYS:HB3   | 2.50                     | 0.46              |
| 1:H:1156:CYS:SG   | 1:H:1244:SER:OG   | 2.71                     | 0.46              |
| 1:k:1161:THR:HG22 | 1:k:1216:TRP:CZ2  | 2.50                     | 0.46              |
| 1:k:1320:GLN:HE22 | 1:k:1329:LEU:HD12 | 1.80                     | 0.46              |
| 1:m:441:ILE:HD13  | 1:m:1092:SER:HB3  | 1.95                     | 0.46              |
| 1:m:662:ARG:HD3   | 1:m:663:LEU:HB2   | 1.97                     | 0.46              |
| 1:m:698:ARG:HD3   | 1:n:949:GLN:HG2   | 1.97                     | 0.46              |
| 1:n:978:TYR:O     | 1:n:982:CYS:HB3   | 2.15                     | 0.46              |
| 1:n:1016:PHE:HA   | 1:n:1162:PRO:HD3  | 1.97                     | 0.46              |
| 1:o:609:PRO:O     | 1:o:611:LEU:N     | 2.49                     | 0.46              |
| 1:o:888:GLY:O     | 1:o:892:ALA:N     | 2.44                     | 0.46              |
| 1:o:1147:ALA:HB1  | 1:p:1206:PRO:HG3  | 1.97                     | 0.46              |
| 1:p:126:ILE:O     | 1:p:1062:SER:HA   | 2.14                     | 0.46              |
| 1:p:294:ARG:NE    | 1:p:359:ASP:OD1   | 2.35                     | 0.46              |
| 1:p:519:SER:O     | 1:p:523:PHE:HB2   | 2.15                     | 0.46              |
| 1:q:757:ARG:HD2   | 1:q:870:GLU:HB3   | 1.97                     | 0.46              |
| 1:q:763:GLN:HG2   | 1:q:766:PRO:HD2   | 1.96                     | 0.46              |
| 2:3:264:ARG:NH1   | 2:3:268:GLU:OE1   | 2.48                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:y:127:LEU:HB2   | 4:y:130:VAL:HG13  | 1.97                     | 0.46              |
| 4:T:169:VAL:O     | 4:T:278:VAL:N     | 2.38                     | 0.46              |
| 4:V:31:LEU:O      | 4:V:34:SER:OG     | 2.30                     | 0.46              |
| 5:z:73:ARG:HE     | 5:z:75:GLU:HG3    | 1.79                     | 0.46              |
| 5:b:90:TYR:O      | 5:b:307:CYS:N     | 2.47                     | 0.46              |
| 5:c:102:LYS:HG2   | 5:c:298:VAL:H     | 1.80                     | 0.46              |
| 1:A:595:THR:HA    | 1:A:675:HIS:HD2   | 1.80                     | 0.46              |
| 1:A:1041:VAL:HG12 | 1:A:1067:THR:HG22 | 1.96                     | 0.46              |
| 1:B:625:ALA:O     | 1:B:628:THR:OG1   | 2.31                     | 0.46              |
| 1:C:1327:LEU:H    | 1:C:1347:GLN:HE21 | 1.63                     | 0.46              |
| 1:D:451:CYS:O     | 1:D:1106:TYR:OH   | 2.29                     | 0.46              |
| 1:G:419:ASP:HA    | 1:G:424:GLN:HE22  | 1.80                     | 0.46              |
| 1:G:1272:ARG:O    | 1:G:1300:ARG:NH1  | 2.48                     | 0.46              |
| 1:H:1021:VAL:HG22 | 1:H:1156:CYS:HB3  | 1.96                     | 0.46              |
| 1:H:1161:THR:HG22 | 1:H:1216:TRP:CE2  | 2.49                     | 0.46              |
| 1:I:961:PRO:O     | 1:I:962:ILE:HG13  | 2.14                     | 0.46              |
| 1:k:102:ALA:HB3   | 1:p:175:GLY:HA3   | 1.96                     | 0.46              |
| 1:k:1316:LEU:HD22 | 1:k:1331:GLU:HB3  | 1.96                     | 0.46              |
| 1:l:466:ALA:HA    | 1:l:552:PRO:HG3   | 1.96                     | 0.46              |
| 1:l:618:LEU:HD21  | 1:l:864:LEU:HB3   | 1.97                     | 0.46              |
| 1:l:1093:ARG:HH11 | 1:l:1153:ARG:HD2  | 1.80                     | 0.46              |
| 1:m:210:ARG:NH1   | 1:m:1187:ASP:OD2  | 2.48                     | 0.46              |
| 1:m:584:THR:HG21  | 1:m:689:THR:HA    | 1.97                     | 0.46              |
| 1:n:786:TYR:O     | 1:n:927:TYR:OH    | 2.32                     | 0.46              |
| 1:n:1171:ARG:HE   | 1:n:1339:ILE:HD13 | 1.79                     | 0.46              |
| 1:o:171:ALA:HB2   | 1:p:100:ARG:HB3   | 1.97                     | 0.46              |
| 1:p:559:MET:HE1   | 1:p:970:TRP:HB3   | 1.97                     | 0.46              |
| 1:p:605:ASP:HB3   | 1:p:608:TYR:HB2   | 1.97                     | 0.46              |
| 1:q:393:THR:H     | 1:q:1305:ALA:HB3  | 1.80                     | 0.46              |
| 1:q:948:PRO:HA    | 1:q:951:GLN:HG2   | 1.97                     | 0.46              |
| 2:2:105:LEU:CD1   | 2:2:212:VAL:HG11  | 2.39                     | 0.46              |
| 5:a:120:LEU:HB3   | 5:a:121:VAL:H     | 1.51                     | 0.46              |
| 5:c:197:CYS:HA    | 5:c:200:LEU:HB2   | 1.96                     | 0.46              |
| 1:B:678:ASN:HA    | 1:B:681:SER:HB2   | 1.97                     | 0.46              |
| 1:B:1038:SER:OG   | 1:B:1039:THR:N    | 2.47                     | 0.46              |
| 1:C:52:GLU:H      | 1:D:321:ALA:HA    | 1.80                     | 0.46              |
| 1:C:458:ALA:HB1   | 1:C:461:CYS:HB3   | 1.96                     | 0.46              |
| 1:C:539:PHE:HA    | 1:C:556:PRO:HA    | 1.98                     | 0.46              |
| 1:C:1298:PRO:HA   | 1:C:1301:PHE:HB3  | 1.96                     | 0.46              |
| 1:D:740:LEU:HD21  | 1:D:767:LEU:HD13  | 1.97                     | 0.46              |
| 1:D:745:ILE:HA    | 1:D:766:PRO:HA    | 1.97                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:D:1042:ILE:HG13 | 1:D:1066:ASN:HB2  | 1.98                     | 0.46              |
| 1:G:389:ASP:N     | 1:G:389:ASP:OD1   | 2.47                     | 0.46              |
| 1:G:710:ALA:N     | 1:G:996:HIS:O     | 2.46                     | 0.46              |
| 1:G:1018:LEU:HD21 | 1:G:1159:ILE:HD12 | 1.98                     | 0.46              |
| 1:H:446:ALA:HA    | 1:H:1094:MET:HG3  | 1.96                     | 0.46              |
| 1:H:1296:GLU:OE2  | 1:H:1300:ARG:NH1  | 2.49                     | 0.46              |
| 1:I:853:THR:H     | 1:I:856:GLN:HB3   | 1.80                     | 0.46              |
| 1:k:698:ARG:HG3   | 1:k:703:PRO:HA    | 1.97                     | 0.46              |
| 1:m:93:LEU:HG     | 1:m:118:SER:HB2   | 1.96                     | 0.46              |
| 1:m:723:ALA:HB3   | 1:m:774:THR:HG23  | 1.98                     | 0.46              |
| 1:m:1097:LEU:HA   | 1:m:1100:VAL:HB   | 1.98                     | 0.46              |
| 1:m:1169:PHE:O    | 1:m:1174:ASN:ND2  | 2.47                     | 0.46              |
| 1:n:223:LYS:O     | 1:n:227:THR:CB    | 2.63                     | 0.46              |
| 1:n:727:ASN:ND2   | 1:n:776:ASP:OD1   | 2.48                     | 0.46              |
| 1:o:192:PHE:HB2   | 1:o:223:LYS:HB3   | 1.96                     | 0.46              |
| 1:p:492:HIS:HD2   | 1:p:495:ARG:HB2   | 1.79                     | 0.46              |
| 2:f:101:ASP:HA    | 2:f:104:LYS:CG    | 2.41                     | 0.46              |
| 2:i:138:PRO:HA    | 2:i:141:ASP:HB2   | 1.96                     | 0.46              |
| 2:g:207:ASP:CG    | 2:g:208:PRO:HD2   | 2.38                     | 0.46              |
| 3:L:45:GLY:HA2    | 3:L:49:LEU:HB2    | 1.98                     | 0.46              |
| 3:t:72:GLY:O      | 3:t:80:TYR:OH     | 2.31                     | 0.46              |
| 4:T:62:GLU:OE2    | 4:T:86:SER:OG     | 2.32                     | 0.46              |
| 4:T:141:THR:HB    | 4:T:147:LEU:HB3   | 1.97                     | 0.46              |
| 5:W:145:ARG:HA    | 5:W:148:MET:HB2   | 1.98                     | 0.46              |
| 5:1:277:PHE:HD1   | 5:1:280:ILE:HD12  | 1.80                     | 0.46              |
| 1:C:84:LEU:HG     | 1:C:87:MET:HE2    | 1.97                     | 0.46              |
| 1:E:119:LYS:HD3   | 1:E:1069:GLU:HB3  | 1.96                     | 0.46              |
| 1:E:141:LYS:HD3   | 4:S:29:ARG:HH11   | 1.80                     | 0.46              |
| 1:F:448:LYS:HD2   | 1:F:1096:ASP:HB3  | 1.98                     | 0.46              |
| 1:G:395:TYR:HA    | 1:G:1021:VAL:HA   | 1.96                     | 0.46              |
| 1:H:220:PHE:HB2   | 1:H:1302:LEU:HD11 | 1.96                     | 0.46              |
| 1:H:748:ARG:HG3   | 1:H:771:ALA:H     | 1.79                     | 0.46              |
| 1:I:194:LEU:HD21  | 1:I:251:VAL:HA    | 1.97                     | 0.46              |
| 1:k:91:LYS:HE3    | 1:k:93:LEU:HD11   | 1.97                     | 0.46              |
| 1:k:818:PHE:CZ    | 3:r:58:GLN:CG     | 2.94                     | 0.46              |
| 1:l:64:TRP:HH2    | 1:l:166:LYS:HG2   | 1.81                     | 0.46              |
| 1:o:127:THR:H     | 1:p:103:THR:HA    | 1.80                     | 0.46              |
| 1:o:441:ILE:HG12  | 1:o:1020:VAL:HG21 | 1.97                     | 0.46              |
| 1:o:865:VAL:HA    | 1:o:868:VAL:HG23  | 1.97                     | 0.46              |
| 1:o:1159:ILE:C    | 1:o:1160:LEU:HD23 | 2.34                     | 0.46              |
| 1:p:130:PHE:HB2   | 1:p:1059:PHE:H    | 1.79                     | 0.46              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:p:1096:ASP:N   | 1:p:1096:ASP:OD1  | 2.47                     | 0.46              |
| 1:q:136:CYS:HA   | 1:q:139:HIS:HD2   | 1.81                     | 0.46              |
| 1:q:983:ALA:HB3  | 1:q:988:SER:HB2   | 1.98                     | 0.46              |
| 1:q:1137:PHE:HB2 | 5:1:58:ARG:HD3    | 1.96                     | 0.46              |
| 2:h:258:PHE:CZ   | 3:P:87:MET:HE3    | 2.50                     | 0.46              |
| 2:g:176:GLU:O    | 2:g:177:GLU:C     | 2.58                     | 0.46              |
| 2:g:264:ARG:NH1  | 2:g:268:GLU:OE1   | 2.49                     | 0.46              |
| 3:R:48:VAL:HA    | 3:R:77:LYS:HD2    | 1.97                     | 0.46              |
| 4:y:69:LEU:HB3   | 4:y:71:PHE:HE1    | 1.81                     | 0.46              |
| 4:y:72:ARG:HH22  | 5:1:105:VAL:HG23  | 1.79                     | 0.46              |
| 4:T:229:VAL:HA   | 4:T:232:PHE:HD2   | 1.80                     | 0.46              |
| 4:U:182:THR:H    | 4:U:186:ARG:HH11  | 1.62                     | 0.46              |
| 5:Y:121:VAL:HG13 | 5:Y:123:VAL:HG23  | 1.97                     | 0.46              |
| 1:A:52:GLU:HG2   | 1:B:91:LYS:HE2    | 1.96                     | 0.46              |
| 1:A:191:CYS:SG   | 1:A:243:TYR:OH    | 2.71                     | 0.46              |
| 1:B:523:PHE:HZ   | 1:B:534:GLU:HG3   | 1.80                     | 0.46              |
| 1:C:1201:HIS:ND1 | 1:C:1212:THR:OG1  | 2.48                     | 0.46              |
| 1:D:1009:ARG:NH1 | 1:D:1118:ALA:O    | 2.48                     | 0.46              |
| 1:E:26:LEU:HD22  | 1:m:204:ALA:HB3   | 1.98                     | 0.46              |
| 1:E:654:ASP:OD1  | 1:E:782:GLN:NE2   | 2.49                     | 0.46              |
| 1:G:258:ASN:HB2  | 1:G:261:THR:HG22  | 1.97                     | 0.46              |
| 1:G:819:LEU:HD11 | 3:P:59:PRO:HD2    | 1.92                     | 0.46              |
| 1:G:1201:HIS:CE1 | 1:G:1212:THR:HG1  | 2.33                     | 0.46              |
| 1:H:1031:LEU:HG  | 1:H:1079:CYS:HB3  | 1.98                     | 0.46              |
| 1:l:172:MET:HE3  | 1:l:1046:PRO:HB3  | 1.97                     | 0.46              |
| 1:n:189:PRO:HA   | 1:n:1270:LEU:HD21 | 1.98                     | 0.46              |
| 1:n:413:ASN:O    | 1:o:413:ASN:ND2   | 2.48                     | 0.46              |
| 1:n:539:PHE:HZ   | 1:n:891:SER:HB2   | 1.79                     | 0.46              |
| 1:o:224:MET:HE1  | 1:o:1298:PRO:HD3  | 1.98                     | 0.46              |
| 1:o:1228:TYR:HB2 | 1:o:1250:PHE:HD2  | 1.80                     | 0.46              |
| 1:p:486:VAL:O    | 1:p:965:HIS:NE2   | 2.45                     | 0.46              |
| 1:p:611:LEU:HB3  | 1:p:846:VAL:HG11  | 1.97                     | 0.46              |
| 1:q:439:GLN:HG2  | 1:q:1092:SER:HB3  | 1.98                     | 0.46              |
| 1:q:1049:THR:HB  | 1:q:1060:HIS:HB2  | 1.97                     | 0.46              |
| 2:3:78:LEU:HD13  | 2:3:276:ALA:HB1   | 1.97                     | 0.46              |
| 2:j:78:LEU:HD13  | 2:j:276:ALA:HB1   | 1.97                     | 0.46              |
| 4:S:61:VAL:O     | 4:S:64:LYS:N      | 2.48                     | 0.46              |
| 4:S:61:VAL:O     | 4:S:62:GLU:C      | 2.59                     | 0.46              |
| 5:W:196:VAL:HG22 | 5:W:283:ILE:HG13  | 1.96                     | 0.46              |
| 5:Z:26:GLY:O     | 5:Z:93:ARG:N      | 2.45                     | 0.46              |
| 5:c:227:LEU:HA   | 5:c:230:CYS:HB3   | 1.98                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:66:THR:HG23   | 1:A:69:GLY:H      | 1.81                     | 0.46              |
| 1:A:146:ASP:OD1   | 1:A:146:ASP:N     | 2.48                     | 0.46              |
| 1:B:577:ALA:HA    | 1:B:994:ILE:HG21  | 1.97                     | 0.46              |
| 1:C:48:ASN:ND2    | 5:Z:74:VAL:O      | 2.48                     | 0.46              |
| 1:D:52:GLU:H      | 1:E:321:ALA:HA    | 1.80                     | 0.46              |
| 1:D:1149:LEU:HD13 | 1:E:1207:GLN:HB2  | 1.96                     | 0.46              |
| 1:E:440:ARG:HH22  | 1:F:521:LYS:HE2   | 1.81                     | 0.46              |
| 1:G:1024:ASP:OD1  | 1:G:1088:SER:OG   | 2.26                     | 0.46              |
| 1:G:1260:LYS:O    | 1:G:1263:PHE:N    | 2.48                     | 0.46              |
| 1:H:786:TYR:O     | 1:H:927:TYR:OH    | 2.31                     | 0.46              |
| 1:H:929:ASP:HB3   | 1:H:932:LEU:HB3   | 1.97                     | 0.46              |
| 1:I:1167:LEU:HD23 | 1:I:1171:ARG:HD2  | 1.97                     | 0.46              |
| 1:k:434:LYS:NZ    | 1:l:215:ASN:OD1   | 2.49                     | 0.46              |
| 1:k:683:THR:HA    | 1:k:784:VAL:HG11  | 1.97                     | 0.46              |
| 1:l:950:TYR:HB3   | 1:l:957:PHE:CD1   | 2.51                     | 0.46              |
| 1:m:132:ILE:CD1   | 4:S:16:GLU:HG2    | 2.46                     | 0.46              |
| 1:m:1093:ARG:HG3  | 1:m:1153:ARG:HD3  | 1.97                     | 0.46              |
| 1:n:200:HIS:HB2   | 1:n:216:ILE:HD11  | 1.97                     | 0.46              |
| 1:n:557:ARG:HB3   | 1:n:562:ASN:HB2   | 1.97                     | 0.46              |
| 1:o:301:ALA:N     | 1:o:352:THR:O     | 2.41                     | 0.46              |
| 1:o:497:LEU:HD21  | 1:o:922:PRO:HD2   | 1.97                     | 0.46              |
| 1:p:1156:CYS:SG   | 1:p:1157:GLU:N    | 2.85                     | 0.46              |
| 2:3:92:LEU:N      | 2:3:93:PRO:CD     | 2.77                     | 0.46              |
| 2:i:78:LEU:HD13   | 2:i:276:ALA:HB1   | 1.97                     | 0.46              |
| 4:S:48:ILE:HG22   | 4:S:152:MET:HB2   | 1.98                     | 0.46              |
| 4:T:49:THR:HA     | 4:T:151:SER:HA    | 1.97                     | 0.46              |
| 5:c:106:LEU:HB3   | 5:c:293:PHE:HB2   | 1.98                     | 0.46              |
| 1:A:320:HIS:O     | 1:F:51:PHE:HA     | 2.16                     | 0.46              |
| 1:B:692:LEU:HD22  | 1:B:1010:MET:HG3  | 1.97                     | 0.46              |
| 1:B:969:HIS:ND1   | 1:B:971:HIS:O     | 2.48                     | 0.46              |
| 1:E:596:LEU:HD21  | 1:E:789:LEU:HD11  | 1.98                     | 0.46              |
| 1:E:635:ARG:HH22  | 1:E:847:ALA:HB1   | 1.81                     | 0.46              |
| 1:E:1048:VAL:HG22 | 1:E:1061:VAL:HG12 | 1.98                     | 0.46              |
| 1:F:398:VAL:HG13  | 1:F:1018:LEU:HB2  | 1.96                     | 0.46              |
| 1:F:519:SER:HB2   | 1:F:522:GLU:HG3   | 1.97                     | 0.46              |
| 1:F:715:ARG:HA    | 1:F:731:VAL:HG21  | 1.98                     | 0.46              |
| 1:F:965:HIS:HB3   | 1:F:968:HIS:HB2   | 1.98                     | 0.46              |
| 1:G:1263:PHE:HA   | 1:m:30:GLU:O      | 2.16                     | 0.46              |
| 1:H:484:GLU:OE2   | 1:H:966:GLU:N     | 2.48                     | 0.46              |
| 1:H:734:VAL:HG23  | 1:H:876:GLU:HB3   | 1.98                     | 0.46              |
| 1:I:773:ARG:H     | 1:I:773:ARG:CD    | 2.27                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:k:183:VAL:HG21  | 1:k:1067:THR:HG21 | 1.98                     | 0.46              |
| 1:l:692:LEU:HB3   | 1:l:693:THR:H     | 1.64                     | 0.46              |
| 1:m:193:VAL:HG11  | 1:m:1266:VAL:HG21 | 1.98                     | 0.46              |
| 1:m:223:LYS:O     | 1:m:227:THR:CB    | 2.64                     | 0.46              |
| 1:m:319:HIS:CE1   | 1:m:321:ALA:HB3   | 2.51                     | 0.46              |
| 1:m:1280:GLU:HA   | 1:n:209:THR:HG23  | 1.97                     | 0.46              |
| 1:n:1156:CYS:SG   | 1:n:1157:GLU:N    | 2.86                     | 0.46              |
| 1:n:1297:LYS:HD3  | 1:n:1299:CYS:HB2  | 1.98                     | 0.46              |
| 1:o:909:THR:HA    | 1:o:932:LEU:HD11  | 1.97                     | 0.46              |
| 1:o:961:PRO:HA    | 1:o:964:ALA:HB2   | 1.98                     | 0.46              |
| 1:o:1031:LEU:HD21 | 1:o:1079:CYS:SG   | 2.54                     | 0.46              |
| 1:p:1101:PHE:HB3  | 1:p:1104:HIS:HD2  | 1.81                     | 0.46              |
| 1:q:651:ASN:HD21  | 1:q:790:VAL:HG11  | 1.81                     | 0.46              |
| 2:h:108:PHE:CG    | 2:h:209:SER:HB3   | 2.51                     | 0.46              |
| 4:U:72:ARG:NH1    | 4:U:74:ASP:OD1    | 2.40                     | 0.46              |
| 4:V:80:PRO:O      | 4:V:82:THR:N      | 2.49                     | 0.46              |
| 5:W:3:THR:HA      | 5:W:83:VAL:HB     | 1.97                     | 0.46              |
| 1:A:1133:SER:HA   | 4:U:116:ILE:HG21  | 1.97                     | 0.46              |
| 1:B:1165:ALA:HB3  | 1:B:1168:GLU:HB2  | 1.97                     | 0.46              |
| 1:C:81:PHE:HB2    | 1:C:306:PHE:HB3   | 1.96                     | 0.46              |
| 1:C:388:ARG:HD2   | 1:C:1030:THR:HG21 | 1.98                     | 0.46              |
| 1:D:379:ASN:HA    | 1:G:23:HIS:ND1    | 2.31                     | 0.46              |
| 1:D:692:LEU:HG    | 1:D:695:LEU:CD1   | 2.36                     | 0.46              |
| 1:E:898:GLN:HG2   | 1:E:970:TRP:CD1   | 2.51                     | 0.46              |
| 1:F:116:MET:HE2   | 1:l:37:ARG:HD2    | 1.98                     | 0.46              |
| 1:F:257:ASP:OD1   | 1:F:257:ASP:N     | 2.48                     | 0.46              |
| 1:F:344:SER:OG    | 1:F:345:GLN:N     | 2.48                     | 0.46              |
| 1:F:480:LEU:HD23  | 1:F:550:VAL:HG11  | 1.97                     | 0.46              |
| 1:G:121:SER:HA    | 1:G:1068:VAL:HA   | 1.98                     | 0.46              |
| 1:G:947:PHE:HB3   | 1:G:950:TYR:HD2   | 1.80                     | 0.46              |
| 1:I:182:ARG:NH2   | 1:I:1291:THR:O    | 2.49                     | 0.46              |
| 1:I:982:CYS:SG    | 1:I:988:SER:OG    | 2.69                     | 0.46              |
| 1:k:172:MET:SD    | 1:k:1063:GLN:NE2  | 2.89                     | 0.46              |
| 1:k:537:PRO:O     | 1:k:557:ARG:NH2   | 2.48                     | 0.46              |
| 1:k:1207:GLN:HA   | 1:p:1150:HIS:CD2  | 2.51                     | 0.46              |
| 1:l:181:LEU:HD21  | 1:l:386:LEU:HG    | 1.98                     | 0.46              |
| 1:l:644:ARG:HG2   | 1:l:646:LEU:HG    | 1.97                     | 0.46              |
| 1:l:1132:ILE:CG2  | 4:T:116:ILE:HG23  | 2.46                     | 0.46              |
| 1:l:1230:THR:HA   | 1:l:1233:ARG:HB3  | 1.98                     | 0.46              |
| 1:m:389:ASP:N     | 1:m:389:ASP:OD1   | 2.45                     | 0.46              |
| 1:m:898:GLN:HE22  | 1:m:971:HIS:CD2   | 2.34                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:n:105:ALA:HA    | 5:a:37:LEU:HB3    | 1.98                     | 0.46              |
| 1:n:219:GLY:O     | 1:n:223:LYS:HB2   | 2.16                     | 0.46              |
| 1:o:523:PHE:HE2   | 1:o:1215:PRO:HG3  | 1.80                     | 0.46              |
| 1:o:749:ASN:OD1   | 1:o:752:THR:OG1   | 2.34                     | 0.46              |
| 1:p:389:ASP:HA    | 1:p:1027:GLU:HA   | 1.96                     | 0.46              |
| 1:q:541:PHE:HA    | 1:q:553:LEU:O     | 2.16                     | 0.46              |
| 1:q:1095:GLN:N    | 1:q:1155:THR:O    | 2.44                     | 0.46              |
| 2:f:264:ARG:NH1   | 2:f:268:GLU:OE1   | 2.49                     | 0.46              |
| 2:i:92:LEU:N      | 2:i:93:PRO:CD     | 2.77                     | 0.46              |
| 3:N:64:MET:HG3    | 3:N:87:MET:HG3    | 1.98                     | 0.46              |
| 4:V:60:GLU:O      | 4:V:62:GLU:N      | 2.49                     | 0.46              |
| 5:Z:46:ASP:HA     | 5:Z:49:VAL:HG22   | 1.96                     | 0.46              |
| 5:a:112:VAL:HG12  | 5:a:114:SER:H     | 1.81                     | 0.46              |
| 5:c:218:LEU:HB3   | 5:c:227:LEU:HD13  | 1.98                     | 0.46              |
| 1:A:1133:SER:HA   | 4:U:116:ILE:HD13  | 1.98                     | 0.46              |
| 1:A:1276:CYS:O    | 1:A:1287:CYS:N    | 2.49                     | 0.46              |
| 1:B:200:HIS:HB2   | 1:B:216:ILE:HD13  | 1.98                     | 0.46              |
| 1:B:576:ARG:HH11  | 1:B:1007:LEU:HD21 | 1.81                     | 0.46              |
| 1:C:1177:ARG:NH1  | 1:C:1198:LEU:O    | 2.47                     | 0.46              |
| 1:D:374:ARG:HG2   | 1:D:378:LYS:HG3   | 1.97                     | 0.46              |
| 1:D:1148:LEU:O    | 1:E:1185:GLY:HA3  | 2.16                     | 0.46              |
| 1:E:30:GLU:HG3    | 1:m:1262:LEU:HB3  | 1.98                     | 0.46              |
| 1:E:532:PHE:HA    | 1:E:1219:GLN:HG2  | 1.97                     | 0.46              |
| 1:F:207:MET:HG3   | 1:l:29:GLY:CA     | 2.46                     | 0.46              |
| 1:F:1021:VAL:HG23 | 1:F:1245:PRO:HB2  | 1.98                     | 0.46              |
| 1:H:72:LEU:HD23   | 1:H:180:PHE:HD2   | 1.81                     | 0.46              |
| 1:H:1298:PRO:O    | 1:H:1302:LEU:N    | 2.34                     | 0.46              |
| 1:I:63:GLU:O      | 1:I:174:ARG:NH1   | 2.47                     | 0.46              |
| 1:I:549:GLN:HG3   | 1:I:551:ARG:HG3   | 1.97                     | 0.46              |
| 1:k:743:ALA:C     | 2:2:174:ARG:HA    | 2.41                     | 0.46              |
| 1:l:137:LEU:HD13  | 4:T:33:ARG:HH21   | 1.81                     | 0.46              |
| 1:m:119:LYS:HD3   | 1:m:1069:GLU:HB3  | 1.98                     | 0.46              |
| 1:m:577:ALA:HA    | 1:m:994:ILE:HG13  | 1.98                     | 0.46              |
| 1:n:673:TYR:HB3   | 1:o:644:ARG:HH22  | 1.81                     | 0.46              |
| 1:n:722:GLN:NE2   | 1:n:904:GLY:O     | 2.49                     | 0.46              |
| 1:n:1134:ILE:HG13 | 1:n:1139:ARG:HH11 | 1.81                     | 0.46              |
| 1:o:493:ALA:HA    | 1:o:496:ARG:HB3   | 1.98                     | 0.46              |
| 1:o:538:PHE:HD1   | 1:o:999:MET:HB3   | 1.81                     | 0.46              |
| 1:o:609:PRO:HB2   | 1:o:846:VAL:HG22  | 1.98                     | 0.46              |
| 1:p:1230:THR:H    | 1:p:1251:THR:HG22 | 1.80                     | 0.46              |
| 2:3:108:PHE:CG    | 2:3:209:SER:HB3   | 2.51                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:y:72:ARG:CZ     | 5:1:104:ASP:HA    | 2.45                     | 0.46              |
| 4:y:73:LEU:HD23   | 4:y:130:VAL:CG2   | 2.46                     | 0.46              |
| 4:y:161:LYS:HD3   | 4:y:161:LYS:HA    | 1.67                     | 0.46              |
| 4:S:73:LEU:HD12   | 4:S:83:VAL:HB     | 1.98                     | 0.46              |
| 4:U:215:HIS:CD2   | 5:Y:64:ARG:HD3    | 2.50                     | 0.46              |
| 5:z:295:VAL:HG11  | 5:z:298:VAL:HG23  | 1.98                     | 0.46              |
| 1:A:1344:PRO:HB2  | 1:A:1347:GLN:HB2  | 1.98                     | 0.46              |
| 1:C:865:VAL:HG12  | 3:L:86:ARG:HB3    | 1.98                     | 0.46              |
| 1:D:190:PRO:HA    | 1:D:1078:THR:HB   | 1.98                     | 0.46              |
| 1:D:744:HIS:CD2   | 2:g:173:MET:SD    | 3.09                     | 0.46              |
| 1:E:586:VAL:HG12  | 1:E:588:ALA:H     | 1.80                     | 0.46              |
| 1:F:119:LYS:HD2   | 1:l:33:PHE:CD1    | 2.51                     | 0.46              |
| 1:F:209:THR:HG22  | 1:F:211:VAL:H     | 1.81                     | 0.46              |
| 1:F:232:ASP:OD1   | 1:F:1352:ASN:ND2  | 2.49                     | 0.46              |
| 1:F:818:PHE:CG    | 3:O:88:LEU:HD13   | 2.51                     | 0.46              |
| 1:G:431:PHE:O     | 1:G:438:PRO:HA    | 2.16                     | 0.46              |
| 1:G:1105:VAL:HG12 | 1:G:1116:ARG:HH11 | 1.81                     | 0.46              |
| 1:H:1029:ASP:HB2  | 1:H:1082:HIS:HB3  | 1.97                     | 0.46              |
| 1:l:758:MET:HB3   | 3:s:79:ALA:HA     | 1.98                     | 0.46              |
| 1:n:262:TYR:HB3   | 1:n:270:LEU:HD12  | 1.98                     | 0.46              |
| 1:o:146:ASP:OD1   | 1:o:146:ASP:N     | 2.49                     | 0.46              |
| 1:o:155:ALA:HB3   | 1:p:337:SER:HB2   | 1.98                     | 0.46              |
| 1:o:920:VAL:HG22  | 1:o:922:PRO:HD3   | 1.98                     | 0.46              |
| 1:p:419:ASP:OD1   | 1:p:424:GLN:NE2   | 2.48                     | 0.46              |
| 1:q:270:LEU:HD13  | 1:q:369:ALA:HB2   | 1.97                     | 0.46              |
| 1:q:293:ARG:HG2   | 1:q:295:THR:HG23  | 1.96                     | 0.46              |
| 2:2:101:ASP:HA    | 2:2:104:LYS:CG    | 2.41                     | 0.46              |
| 2:2:208:PRO:HG3   | 2:3:95:LEU:HD11   | 0.48                     | 0.46              |
| 2:g:206:GLU:CB    | 2:j:132:TYR:C     | 2.81                     | 0.46              |
| 3:Q:45:GLY:HA2    | 3:Q:49:LEU:HD12   | 1.98                     | 0.46              |
| 4:U:87:LEU:HD12   | 4:U:90:LEU:HD21   | 1.98                     | 0.46              |
| 5:W:111:PRO:O     | 5:W:113:PHE:HD2   | 1.98                     | 0.46              |
| 5:Z:45:LEU:HD21   | 5:Z:63:MET:HE2    | 1.98                     | 0.46              |
| 5:Z:73:ARG:HG2    | 5:Z:75:GLU:HG2    | 1.98                     | 0.46              |
| 5:Z:148:MET:HE3   | 5:Z:148:MET:HB3   | 1.85                     | 0.46              |
| 5:a:86:HIS:CE1    | 5:a:311:GLY:H     | 2.35                     | 0.46              |
| 1:A:907:MET:HE3   | 1:A:932:LEU:HG    | 1.98                     | 0.45              |
| 1:A:1031:LEU:HG   | 1:A:1079:CYS:O    | 2.16                     | 0.45              |
| 1:B:662:ARG:HH21  | 1:B:663:LEU:HA    | 1.80                     | 0.45              |
| 1:D:44:PRO:HB3    | 1:G:135:ALA:HB3   | 1.99                     | 0.45              |
| 1:E:603:LEU:HB3   | 1:E:908:THR:HG21  | 1.98                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:E:925:ARG:NH2   | 1:E:971:HIS:O     | 2.43                     | 0.45              |
| 1:F:100:ARG:HH22  | 1:F:110:SER:HB2   | 1.81                     | 0.45              |
| 1:F:559:MET:HG2   | 1:F:996:HIS:HA    | 1.98                     | 0.45              |
| 1:G:417:LEU:HD23  | 1:H:408:TYR:HB3   | 1.98                     | 0.45              |
| 1:G:440:ARG:NE    | 1:H:1168:GLU:OE2  | 2.49                     | 0.45              |
| 1:G:1018:LEU:HD23 | 1:G:1159:ILE:HD13 | 1.97                     | 0.45              |
| 1:G:1021:VAL:HG22 | 1:G:1156:CYS:HB3  | 1.98                     | 0.45              |
| 1:G:1333:HIS:HB3  | 1:G:1336:ASN:HB2  | 1.98                     | 0.45              |
| 1:H:389:ASP:OD1   | 1:H:389:ASP:N     | 2.47                     | 0.45              |
| 1:I:119:LYS:HB3   | 1:I:1069:GLU:HB3  | 1.97                     | 0.45              |
| 1:I:937:ASN:HB3   | 1:I:939:ASP:H     | 1.80                     | 0.45              |
| 1:k:258:ASN:HB3   | 1:k:260:GLU:HG2   | 1.97                     | 0.45              |
| 1:k:688:ARG:HH12  | 1:l:797:HIS:CE1   | 2.34                     | 0.45              |
| 1:k:1003:SER:O    | 1:k:1007:LEU:HB2  | 2.15                     | 0.45              |
| 1:k:1148:LEU:HD23 | 1:l:210:ARG:HG2   | 1.97                     | 0.45              |
| 1:l:308:LEU:HD22  | 1:l:312:ASN:HB3   | 1.98                     | 0.45              |
| 1:l:583:LEU:HD11  | 1:l:1012:LEU:HB2  | 1.98                     | 0.45              |
| 1:m:251:VAL:HG11  | 1:m:1033:TYR:CE2  | 2.52                     | 0.45              |
| 1:m:542:CYS:SG    | 1:m:544:HIS:NE2   | 2.89                     | 0.45              |
| 1:m:929:ASP:HB3   | 1:m:932:LEU:HB3   | 1.97                     | 0.45              |
| 1:p:433:ASN:O     | 1:p:436:ARG:NH1   | 2.48                     | 0.45              |
| 1:p:866:ALA:HA    | 3:w:86:ARG:HG3    | 1.98                     | 0.45              |
| 2:3:252:PHE:HB2   | 2:3:264:ARG:HB2   | 1.98                     | 0.45              |
| 2:h:78:LEU:HD13   | 2:h:276:ALA:HB1   | 1.97                     | 0.45              |
| 2:f:173:MET:O     | 2:f:173:MET:HG2   | 2.13                     | 0.45              |
| 4:S:228:ARG:HG2   | 5:a:224:ASN:C     | 2.40                     | 0.45              |
| 4:T:60:GLU:O      | 4:T:63:GLN:N      | 2.36                     | 0.45              |
| 4:U:223:LEU:O     | 4:U:227:PHE:N     | 2.45                     | 0.45              |
| 5:Z:15:THR:O      | 5:Z:19:GLY:N      | 2.44                     | 0.45              |
| 1:B:447:LEU:HD11  | 1:B:1005:ALA:HA   | 1.99                     | 0.45              |
| 1:B:452:HIS:HB3   | 1:B:455:ILE:HG12  | 1.98                     | 0.45              |
| 1:C:276:SER:HB3   | 1:C:280:VAL:HG13  | 1.98                     | 0.45              |
| 1:C:388:ARG:HD3   | 1:C:1295:VAL:H    | 1.81                     | 0.45              |
| 1:C:1156:CYS:SG   | 1:C:1244:SER:OG   | 2.74                     | 0.45              |
| 1:C:1228:TYR:HB2  | 1:C:1250:PHE:HD2  | 1.82                     | 0.45              |
| 1:D:753:SER:HB3   | 3:M:87:MET:HG3    | 1.98                     | 0.45              |
| 1:F:253:GLU:O     | 1:l:19:ASP:CG     | 2.59                     | 0.45              |
| 1:F:310:LYS:O     | 1:m:333:ILE:CD1   | 2.61                     | 0.45              |
| 1:F:651:ASN:OD1   | 1:F:908:THR:OG1   | 2.34                     | 0.45              |
| 1:F:1041:VAL:HG12 | 1:F:1067:THR:HG22 | 1.97                     | 0.45              |
| 1:F:1262:LEU:H    | 1:l:30:GLU:HB2    | 1.81                     | 0.45              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:F:1342:THR:OG1 | 1:F:1343:ILE:N    | 2.49                     | 0.45              |
| 1:G:19:ASP:OD1   | 1:G:19:ASP:N      | 2.48                     | 0.45              |
| 1:G:484:GLU:HB3  | 1:G:968:HIS:CD2   | 2.52                     | 0.45              |
| 1:H:978:TYR:O    | 1:H:982:CYS:HB3   | 2.16                     | 0.45              |
| 1:k:428:THR:HG22 | 1:k:442:SER:HB3   | 1.97                     | 0.45              |
| 1:l:191:CYS:HG   | 1:l:243:TYR:HH    | 1.60                     | 0.45              |
| 1:m:650:ALA:O    | 1:m:785:TYR:OH    | 2.34                     | 0.45              |
| 1:o:1342:THR:OG1 | 1:o:1343:ILE:N    | 2.48                     | 0.45              |
| 1:q:733:VAL:HG12 | 1:q:740:LEU:HB3   | 1.97                     | 0.45              |
| 2:e:285:GLU:CD   | 3:t:67:LYS:HG3    | 2.37                     | 0.45              |
| 2:i:252:PHE:HB2  | 2:i:264:ARG:HB2   | 1.98                     | 0.45              |
| 2:g:101:ASP:HA   | 2:g:104:LYS:CG    | 2.41                     | 0.45              |
| 3:P:49:LEU:HD11  | 3:P:65:ILE:HD11   | 1.98                     | 0.45              |
| 4:T:91:SER:HB3   | 4:T:97:VAL:HG11   | 1.98                     | 0.45              |
| 5:z:2:GLU:HB3    | 5:z:34:ARG:HG2    | 1.97                     | 0.45              |
| 5:z:113:PHE:CG   | 5:z:181:PRO:HG3   | 2.51                     | 0.45              |
| 5:Y:164:ALA:HB1  | 5:c:270:LEU:HD11  | 1.98                     | 0.45              |
| 5:d:40:SER:O     | 5:d:126:TRP:NE1   | 2.49                     | 0.45              |
| 1:A:1320:GLN:NE2 | 1:A:1331:GLU:OE1  | 2.50                     | 0.45              |
| 1:B:539:PHE:O    | 1:B:557:ARG:NH2   | 2.49                     | 0.45              |
| 1:C:389:ASP:OD2  | 1:C:1087:ARG:NH1  | 2.49                     | 0.45              |
| 1:C:630:ILE:HA   | 1:C:633:VAL:HG12  | 1.99                     | 0.45              |
| 1:C:934:ALA:HB2  | 1:C:944:LEU:HD12  | 1.98                     | 0.45              |
| 1:E:1230:THR:H   | 1:E:1251:THR:HG22 | 1.81                     | 0.45              |
| 1:G:650:ALA:O    | 1:G:785:TYR:OH    | 2.28                     | 0.45              |
| 1:G:1243:TYR:HD1 | 1:G:1286:ILE:HG22 | 1.82                     | 0.45              |
| 1:I:392:LEU:HA   | 1:I:1297:LYS:HB3  | 1.99                     | 0.45              |
| 1:I:773:ARG:O    | 1:I:773:ARG:HG2   | 2.16                     | 0.45              |
| 1:k:523:PHE:HE2  | 1:k:1215:PRO:HG3  | 1.81                     | 0.45              |
| 1:k:688:ARG:HH12 | 1:l:797:HIS:HE1   | 1.65                     | 0.45              |
| 1:k:804:ASN:HD22 | 1:k:917:TYR:HA    | 1.82                     | 0.45              |
| 1:l:1139:ARG:CZ  | 4:T:79:MET:HB2    | 2.45                     | 0.45              |
| 1:m:128:ILE:HD11 | 1:m:168:THR:HG23  | 1.97                     | 0.45              |
| 1:m:183:VAL:HG21 | 1:m:1067:THR:HG21 | 1.97                     | 0.45              |
| 1:m:257:ASP:N    | 1:m:257:ASP:OD1   | 2.50                     | 0.45              |
| 1:m:833:LEU:HD11 | 1:m:859:GLU:HB2   | 1.98                     | 0.45              |
| 1:o:391:GLU:O    | 1:o:1297:LYS:HB3  | 2.17                     | 0.45              |
| 1:o:428:THR:HG23 | 1:p:406:ARG:HH22  | 1.81                     | 0.45              |
| 1:p:542:CYS:HB3  | 1:p:967:TYR:CE2   | 2.52                     | 0.45              |
| 1:p:657:ARG:O    | 1:p:661:THR:OG1   | 2.32                     | 0.45              |
| 1:q:130:PHE:HD2  | 1:q:1059:PHE:HB2  | 1.80                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:q:1161:THR:HG23 | 1:q:1214:ASN:HD21 | 1.81                     | 0.45              |
| 2:2:202:ASP:N     | 2:2:203:PRO:HD3   | 2.32                     | 0.45              |
| 2:2:264:ARG:NH1   | 2:2:268:GLU:OE1   | 2.49                     | 0.45              |
| 2:e:264:ARG:NH1   | 2:e:268:GLU:OE1   | 2.49                     | 0.45              |
| 2:h:92:LEU:N      | 2:h:93:PRO:CD     | 2.77                     | 0.45              |
| 2:i:108:PHE:CG    | 2:i:209:SER:HB3   | 2.51                     | 0.45              |
| 3:w:72:GLY:O      | 3:w:80:TYR:OH     | 2.34                     | 0.45              |
| 4:y:188:VAL:HG22  | 4:y:210:VAL:HG12  | 1.99                     | 0.45              |
| 4:y:196:TYR:HB3   | 4:y:237:ASN:HD22  | 1.80                     | 0.45              |
| 4:T:71:PHE:O      | 4:T:85:VAL:N      | 2.50                     | 0.45              |
| 5:W:9:PHE:O       | 5:W:40:SER:OG     | 2.33                     | 0.45              |
| 5:W:26:GLY:H      | 5:W:71:MET:HB3    | 1.81                     | 0.45              |
| 5:W:90:TYR:O      | 5:W:307:CYS:N     | 2.43                     | 0.45              |
| 5:W:199:SER:HB2   | 5:W:283:ILE:HD12  | 1.98                     | 0.45              |
| 5:a:20:LYS:HE3    | 5:a:121:VAL:HG12  | 1.98                     | 0.45              |
| 1:A:1038:SER:OG   | 1:A:1039:THR:N    | 2.49                     | 0.45              |
| 1:C:644:ARG:HB3   | 1:C:646:LEU:HG    | 1.98                     | 0.45              |
| 1:D:132:ILE:HD13  | 1:D:161:VAL:HG22  | 1.99                     | 0.45              |
| 1:D:576:ARG:HH11  | 1:D:1007:LEU:HD21 | 1.81                     | 0.45              |
| 1:D:598:VAL:HG11  | 1:D:647:LEU:HD23  | 1.97                     | 0.45              |
| 1:D:921:ILE:HG22  | 1:D:923:PHE:HB3   | 1.97                     | 0.45              |
| 1:E:14:LEU:HB2    | 1:l:58:TYR:HA     | 1.99                     | 0.45              |
| 1:F:610:GLU:HG3   | 1:F:911:PRO:HB3   | 1.99                     | 0.45              |
| 1:F:882:ASP:OD1   | 1:F:882:ASP:N     | 2.49                     | 0.45              |
| 1:G:400:LEU:HD13  | 1:G:1160:LEU:HD13 | 1.98                     | 0.45              |
| 1:H:1297:LYS:HG2  | 1:H:1299:CYS:H    | 1.81                     | 0.45              |
| 1:I:959:LEU:HB3   | 1:I:963:PHE:CD1   | 2.52                     | 0.45              |
| 1:k:567:LEU:HD13  | 1:k:1216:TRP:HZ2  | 1.81                     | 0.45              |
| 1:k:1038:SER:OG   | 1:k:1039:THR:N    | 2.49                     | 0.45              |
| 1:l:447:LEU:HD11  | 1:l:1005:ALA:HA   | 1.98                     | 0.45              |
| 1:l:794:LEU:O     | 1:l:797:HIS:ND1   | 2.43                     | 0.45              |
| 1:m:51:PHE:CE2    | 1:m:53:ALA:HB2    | 2.52                     | 0.45              |
| 1:m:153:LEU:HA    | 1:m:156:ASP:HB3   | 1.99                     | 0.45              |
| 1:m:429:VAL:HG11  | 1:m:431:PHE:CZ    | 2.46                     | 0.45              |
| 1:m:1229:ASN:O    | 1:m:1233:ARG:CB   | 2.64                     | 0.45              |
| 1:m:1326:LYS:HG3  | 1:m:1328:GLY:H    | 1.82                     | 0.45              |
| 1:n:608:TYR:HA    | 1:n:609:PRO:HD3   | 1.82                     | 0.45              |
| 1:n:713:ASP:O     | 1:n:783:LYS:NZ    | 2.49                     | 0.45              |
| 1:n:813:PHE:CD2   | 3:u:85:LEU:HD23   | 2.52                     | 0.45              |
| 1:o:446:ALA:HA    | 1:o:1094:MET:HG3  | 1.98                     | 0.45              |
| 1:q:257:ASP:HB2   | 1:q:1036:LYS:HD2  | 1.97                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:q:563:LEU:HG    | 1:q:999:MET:HE1   | 1.98                     | 0.45              |
| 2:e:176:GLU:O     | 2:e:177:GLU:C     | 2.58                     | 0.45              |
| 2:j:252:PHE:HB2   | 2:j:264:ARG:HB2   | 1.99                     | 0.45              |
| 3:M:44:PHE:O      | 3:M:49:LEU:N      | 2.33                     | 0.45              |
| 4:T:235:LEU:HD13  | 5:X:202:MET:HE2   | 1.97                     | 0.45              |
| 4:V:129:ARG:O     | 4:V:132:HIS:NE2   | 2.49                     | 0.45              |
| 5:X:29:ILE:O      | 5:X:69:THR:OG1    | 2.32                     | 0.45              |
| 5:c:89:CYS:HA     | 5:c:308:ILE:HA    | 1.98                     | 0.45              |
| 1:A:630:ILE:O     | 1:A:634:THR:OG1   | 2.33                     | 0.45              |
| 1:B:398:VAL:HG13  | 1:B:1018:LEU:HB2  | 1.98                     | 0.45              |
| 1:C:589:PRO:HB2   | 1:C:592:HIS:HB3   | 1.99                     | 0.45              |
| 1:C:803:LEU:HD21  | 1:C:914:LEU:HD13  | 1.98                     | 0.45              |
| 1:D:37:ARG:HD3    | 1:H:116:MET:CE    | 2.46                     | 0.45              |
| 1:D:791:PRO:O     | 1:D:979:SER:OG    | 2.35                     | 0.45              |
| 1:D:1039:THR:HB   | 1:D:1070:MET:HG2  | 1.99                     | 0.45              |
| 1:E:72:LEU:HD23   | 1:E:180:PHE:HD2   | 1.81                     | 0.45              |
| 1:E:691:GLU:HB2   | 1:F:952:ARG:HD2   | 1.99                     | 0.45              |
| 1:E:745:ILE:O     | 1:E:767:LEU:HG    | 2.15                     | 0.45              |
| 1:E:1126:VAL:HB   | 1:E:1130:GLU:HB2  | 1.97                     | 0.45              |
| 1:F:606:HIS:HA    | 1:F:909:THR:HG21  | 1.98                     | 0.45              |
| 1:F:1179:ARG:NH2  | 1:F:1204:PRO:O    | 2.49                     | 0.45              |
| 1:G:184:LEU:O     | 1:G:188:ALA:N     | 2.49                     | 0.45              |
| 1:H:692:LEU:HB3   | 1:H:1010:MET:HE2  | 1.98                     | 0.45              |
| 1:k:592:HIS:HB2   | 1:k:682:ILE:HD11  | 1.99                     | 0.45              |
| 1:k:949:GLN:CG    | 1:p:698:ARG:HD3   | 2.47                     | 0.45              |
| 1:k:1167:LEU:HD23 | 1:k:1171:ARG:HE   | 1.80                     | 0.45              |
| 1:l:482:ARG:HH12  | 1:l:961:PRO:HG3   | 1.81                     | 0.45              |
| 1:m:168:THR:CG2   | 4:S:12:ARG:NE     | 2.80                     | 0.45              |
| 1:m:388:ARG:HD3   | 1:m:1295:VAL:H    | 1.80                     | 0.45              |
| 1:m:462:LEU:HD22  | 1:m:890:PRO:HG3   | 1.98                     | 0.45              |
| 1:m:761:MET:HE3   | 1:m:870:GLU:HB2   | 1.98                     | 0.45              |
| 1:m:911:PRO:HG2   | 1:m:914:LEU:HD12  | 1.97                     | 0.45              |
| 1:n:794:LEU:HA    | 1:n:794:LEU:HD23  | 1.78                     | 0.45              |
| 1:n:1116:ARG:NH2  | 1:n:1122:ARG:O    | 2.50                     | 0.45              |
| 1:o:727:ASN:ND2   | 1:o:776:ASP:OD2   | 2.49                     | 0.45              |
| 1:o:875:LEU:HB2   | 1:o:902:TYR:HB2   | 1.98                     | 0.45              |
| 1:p:756:ALA:HA    | 1:p:759:ILE:HG12  | 1.98                     | 0.45              |
| 1:p:1019:THR:CA   | 1:p:1160:LEU:HD12 | 2.46                     | 0.45              |
| 1:q:428:THR:HG22  | 1:q:442:SER:HB3   | 1.98                     | 0.45              |
| 1:q:657:ARG:HG3   | 1:q:680:LEU:HD22  | 1.99                     | 0.45              |
| 2:f:202:ASP:N     | 2:f:203:PRO:HD3   | 2.32                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:y:191:VAL:HG22  | 4:y:252:LEU:HA    | 1.99                     | 0.45              |
| 4:U:153:ARG:NH2   | 5:c:310:LYS:HE2   | 2.31                     | 0.45              |
| 4:V:61:VAL:O      | 4:V:62:GLU:C      | 2.60                     | 0.45              |
| 5:W:169:ARG:HD3   | 5:W:179:THR:HG23  | 1.98                     | 0.45              |
| 5:X:33:TYR:HD2    | 5:X:35:HIS:HB2    | 1.80                     | 0.45              |
| 5:Y:33:TYR:HD2    | 5:Y:35:HIS:HB2    | 1.81                     | 0.45              |
| 5:a:85:THR:N      | 5:a:90:TYR:OH     | 2.44                     | 0.45              |
| 5:c:63:MET:HE2    | 5:c:63:MET:HB3    | 1.88                     | 0.45              |
| 1:A:1207:GLN:HB2  | 1:F:1149:LEU:HB3  | 1.99                     | 0.45              |
| 1:A:1228:TYR:HB2  | 1:A:1250:PHE:CD2  | 2.51                     | 0.45              |
| 1:B:257:ASP:N     | 1:B:257:ASP:OD1   | 2.49                     | 0.45              |
| 1:C:1219:GLN:HB2  | 1:C:1222:SER:HB3  | 1.98                     | 0.45              |
| 1:D:432:TYR:CE2   | 1:D:1321:LEU:HD13 | 2.52                     | 0.45              |
| 1:D:875:LEU:HB3   | 1:D:900:VAL:HG23  | 1.98                     | 0.45              |
| 1:D:1309:HIS:CG   | 1:D:1327:LEU:HB3  | 2.51                     | 0.45              |
| 1:E:30:GLU:C      | 1:m:1263:PHE:CD2  | 2.93                     | 0.45              |
| 1:E:141:LYS:HG3   | 4:S:33:ARG:HH22   | 1.82                     | 0.45              |
| 1:E:724:LEU:HB3   | 1:E:772:ARG:HB2   | 1.98                     | 0.45              |
| 1:E:1021:VAL:O    | 1:E:1156:CYS:N    | 2.50                     | 0.45              |
| 1:F:191:CYS:SG    | 1:F:243:TYR:OH    | 2.62                     | 0.45              |
| 1:G:625:ALA:HB1   | 1:G:867:HIS:CD2   | 2.52                     | 0.45              |
| 1:G:776:ASP:HB2   | 1:H:951:GLN:CD    | 2.41                     | 0.45              |
| 1:H:1201:HIS:NE2  | 1:H:1219:GLN:HB3  | 2.31                     | 0.45              |
| 1:I:544:HIS:CE1   | 1:I:553:LEU:HB2   | 2.52                     | 0.45              |
| 1:I:596:LEU:HD21  | 1:I:789:LEU:HD11  | 1.99                     | 0.45              |
| 1:I:620:HIS:HB3   | 1:I:869:PRO:HG3   | 1.99                     | 0.45              |
| 1:I:1199:TYR:OH   | 1:I:1252:THR:OG1  | 2.33                     | 0.45              |
| 1:I:1309:HIS:CG   | 1:I:1327:LEU:HD12 | 2.50                     | 0.45              |
| 1:k:82:HIS:CE1    | 1:k:308:LEU:H     | 2.34                     | 0.45              |
| 1:k:558:ILE:HD13  | 1:k:970:TRP:HA    | 1.98                     | 0.45              |
| 1:n:620:HIS:HB3   | 1:n:869:PRO:HG3   | 1.97                     | 0.45              |
| 1:o:194:LEU:HD21  | 1:o:251:VAL:HA    | 1.99                     | 0.45              |
| 1:o:1195:LEU:HD22 | 1:o:1220:ARG:HH12 | 1.81                     | 0.45              |
| 1:p:309:SER:HB3   | 1:p:312:ASN:HB2   | 1.97                     | 0.45              |
| 1:p:1214:ASN:O    | 1:p:1218:SER:CB   | 2.65                     | 0.45              |
| 1:q:44:PRO:O      | 1:q:48:ASN:ND2    | 2.49                     | 0.45              |
| 1:q:182:ARG:HB3   | 1:q:186:ARG:NH1   | 2.32                     | 0.45              |
| 2:2:207:ASP:HB2   | 2:3:130:ALA:HB2   | 1.99                     | 0.45              |
| 2:j:108:PHE:CG    | 2:j:209:SER:HB3   | 2.51                     | 0.45              |
| 3:O:85:LEU:HD22   | 3:O:88:LEU:HD12   | 1.99                     | 0.45              |
| 3:Q:49:LEU:HD11   | 3:Q:65:ILE:HD11   | 1.97                     | 0.45              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 4:V:63:GLN:HA     | 4:V:140:ILE:HG13 | 1.99                     | 0.45              |
| 4:V:79:MET:SD     | 4:V:80:PRO:HD3   | 2.57                     | 0.45              |
| 5:z:280:ILE:O     | 5:z:284:THR:OG1  | 2.30                     | 0.45              |
| 5:d:86:HIS:HA     | 5:d:309:TYR:HD2  | 1.81                     | 0.45              |
| 1:A:603:LEU:HB3   | 1:A:794:LEU:HD21 | 1.99                     | 0.45              |
| 1:B:677:ARG:HH21  | 1:C:605:ASP:N    | 2.15                     | 0.45              |
| 1:C:94:PHE:HB2    | 1:C:117:VAL:HG23 | 1.99                     | 0.45              |
| 1:D:244:LEU:HD23  | 1:D:247:LEU:HD12 | 1.99                     | 0.45              |
| 1:D:517:ASP:OD1   | 1:D:517:ASP:N    | 2.46                     | 0.45              |
| 1:D:559:MET:HG2   | 1:D:996:HIS:HA   | 1.97                     | 0.45              |
| 1:E:52:GLU:H      | 1:F:321:ALA:HA   | 1.80                     | 0.45              |
| 1:E:60:ASN:ND2    | 1:l:18:ILE:HD13  | 2.31                     | 0.45              |
| 1:E:719:PRO:HD2   | 1:E:786:TYR:HB3  | 1.98                     | 0.45              |
| 1:F:202:THR:HA    | 1:l:22:THR:HA    | 1.97                     | 0.45              |
| 1:H:388:ARG:HD3   | 1:H:1295:VAL:H   | 1.82                     | 0.45              |
| 1:I:962:ILE:O     | 1:I:963:PHE:CD1  | 2.70                     | 0.45              |
| 1:k:87:MET:HE2    | 1:k:90:GLY:HA2   | 1.98                     | 0.45              |
| 1:l:809:LEU:HD22  | 3:s:82:LEU:HD11  | 1.99                     | 0.45              |
| 1:m:360:VAL:HA    | 1:m:369:ALA:HA   | 1.99                     | 0.45              |
| 1:n:231:LEU:HD13  | 1:n:1082:HIS:HB2 | 1.99                     | 0.45              |
| 1:n:274:ILE:HB    | 1:n:370:LEU:HD23 | 1.99                     | 0.45              |
| 1:o:544:HIS:CE1   | 1:o:553:LEU:HB2  | 2.52                     | 0.45              |
| 1:q:423:ASN:HB3   | 1:q:575:LEU:HD22 | 1.99                     | 0.45              |
| 1:q:620:HIS:CD2   | 1:q:869:PRO:HD2  | 2.52                     | 0.45              |
| 1:q:1230:THR:HA   | 1:q:1233:ARG:HB3 | 1.98                     | 0.45              |
| 3:Q:85:LEU:O      | 3:Q:89:SER:N     | 2.44                     | 0.45              |
| 4:S:58:LEU:HD23   | 4:S:84:LEU:HB3   | 1.99                     | 0.45              |
| 5:z:280:ILE:HA    | 5:z:283:ILE:HG22 | 1.99                     | 0.45              |
| 5:Z:169:ARG:HA    | 5:Z:180:LEU:HD23 | 1.99                     | 0.45              |
| 5:Z:266:PRO:HB2   | 5:d:168:LEU:HD13 | 1.98                     | 0.45              |
| 1:A:489:HIS:O     | 1:A:496:ARG:NH1  | 2.50                     | 0.45              |
| 1:A:1022:ARG:NH2  | 1:A:1308:GLN:OE1 | 2.49                     | 0.45              |
| 1:C:1025:THR:H    | 1:C:1088:SER:HB2 | 1.81                     | 0.45              |
| 1:C:1183:MET:SD   | 1:C:1259:ASN:ND2 | 2.82                     | 0.45              |
| 1:C:1255:ILE:HD12 | 1:C:1255:ILE:HA  | 1.81                     | 0.45              |
| 1:D:257:ASP:N     | 1:D:257:ASP:OD1  | 2.50                     | 0.45              |
| 1:D:332:ARG:HD2   | 1:D:339:LYS:HB3  | 1.97                     | 0.45              |
| 1:F:539:PHE:O     | 1:F:557:ARG:NH2  | 2.50                     | 0.45              |
| 1:H:380:THR:O     | 1:I:205:ARG:NH1  | 2.50                     | 0.45              |
| 1:I:257:ASP:OD1   | 1:I:257:ASP:N    | 2.49                     | 0.45              |
| 1:k:200:HIS:CD2   | 1:p:1085:ARG:NE  | 2.80                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:k:200:HIS:HE1   | 1:p:1084:ARG:HB3  | 1.81                     | 0.45              |
| 1:k:809:LEU:HG    | 1:k:812:LEU:HD12  | 1.98                     | 0.45              |
| 1:l:715:ARG:HA    | 1:l:731:VAL:HG21  | 1.98                     | 0.45              |
| 1:m:147:THR:C     | 1:m:149:LEU:H     | 2.24                     | 0.45              |
| 1:m:311:GLU:OE2   | 1:m:315:THR:OG1   | 2.34                     | 0.45              |
| 1:m:1199:TYR:OH   | 1:m:1252:THR:OG1  | 2.28                     | 0.45              |
| 1:n:79:ILE:O      | 1:n:1042:ILE:HA   | 2.16                     | 0.45              |
| 1:n:185:LEU:HB3   | 1:n:388:ARG:HH22  | 1.82                     | 0.45              |
| 1:p:651:ASN:OD1   | 1:p:908:THR:OG1   | 2.33                     | 0.45              |
| 1:q:402:VAL:HG12  | 1:q:1167:LEU:HD11 | 1.99                     | 0.45              |
| 1:q:507:PRO:O     | 1:q:950:TYR:OH    | 2.35                     | 0.45              |
| 1:q:726:ARG:HD3   | 1:q:776:ASP:HB2   | 1.99                     | 0.45              |
| 1:q:748:ARG:HH11  | 1:q:768:PHE:HB3   | 1.81                     | 0.45              |
| 2:f:66:ARG:NH1    | 2:f:294:LEU:CB    | 2.68                     | 0.45              |
| 3:M:71:MET:O      | 3:M:74:HIS:NE2    | 2.50                     | 0.45              |
| 3:r:85:LEU:HD12   | 3:r:88:LEU:HD12   | 1.99                     | 0.45              |
| 4:S:215:HIS:CE1   | 5:W:64:ARG:HD3    | 2.52                     | 0.45              |
| 4:T:183:ASP:OD1   | 4:T:183:ASP:N     | 2.50                     | 0.45              |
| 1:B:100:ARG:NH2   | 1:B:101:VAL:O     | 2.49                     | 0.45              |
| 1:B:392:LEU:HA    | 1:B:1297:LYS:HB3  | 1.99                     | 0.45              |
| 1:B:664:GLY:O     | 1:C:644:ARG:NH2   | 2.50                     | 0.45              |
| 1:C:159:ASN:O     | 1:C:163:ARG:N     | 2.50                     | 0.45              |
| 1:D:146:ASP:HB2   | 1:D:151:LYS:HD2   | 1.99                     | 0.45              |
| 1:D:392:LEU:HD23  | 1:D:1306:LEU:HD12 | 1.98                     | 0.45              |
| 1:D:724:LEU:H     | 1:D:769:VAL:HG21  | 1.82                     | 0.45              |
| 1:F:120:TYR:HD2   | 1:l:34:ASN:CG     | 2.25                     | 0.45              |
| 1:F:1263:PHE:HB2  | 1:l:31:GLU:C      | 2.42                     | 0.45              |
| 1:G:923:PHE:HA    | 1:G:963:PHE:CE1   | 2.52                     | 0.45              |
| 1:G:1019:THR:CG2  | 1:G:1160:LEU:CD2  | 2.86                     | 0.45              |
| 1:H:664:GLY:HA3   | 1:I:607:GLN:HB3   | 1.97                     | 0.45              |
| 1:I:724:LEU:HB3   | 1:I:772:ARG:HB2   | 1.99                     | 0.45              |
| 1:k:606:HIS:CD2   | 1:p:661:THR:HA    | 2.51                     | 0.45              |
| 1:k:750:PRO:CG    | 2:3:269:ARG:NH2   | 2.79                     | 0.45              |
| 1:k:1053:ARG:HH12 | 5:z:1:MET:N       | 2.15                     | 0.45              |
| 1:m:126:ILE:HG22  | 1:n:103:THR:HA    | 1.99                     | 0.45              |
| 1:m:949:GLN:O     | 1:m:952:ARG:NH1   | 2.50                     | 0.45              |
| 1:m:1153:ARG:HG3  | 1:m:1283:LEU:HD11 | 1.89                     | 0.45              |
| 1:n:944:LEU:HD22  | 1:n:951:GLN:HB2   | 1.99                     | 0.45              |
| 1:o:600:ARG:NE    | 1:o:793:VAL:O     | 2.50                     | 0.45              |
| 1:o:882:ASP:OD1   | 1:o:882:ASP:N     | 2.50                     | 0.45              |
| 1:p:887:HIS:HD2   | 1:p:1106:TYR:HA   | 1.81                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:q:392:LEU:O     | 1:q:1023:THR:HA   | 2.17                     | 0.45              |
| 2:2:66:ARG:O      | 2:2:67:GLU:CD     | 2.60                     | 0.45              |
| 2:e:142:VAL:O     | 2:e:146:GLY:N     | 2.47                     | 0.45              |
| 2:f:184:ASN:HB2   | 2:f:198:LEU:HD11  | 1.99                     | 0.45              |
| 2:g:66:ARG:HG3    | 2:g:69:GLN:CD     | 2.41                     | 0.45              |
| 5:z:97:PRO:HD3    | 5:z:132:TRP:CE3   | 2.51                     | 0.45              |
| 5:d:147:MET:HG2   | 5:d:196:VAL:HG11  | 1.98                     | 0.45              |
| 1:A:925:ARG:NH2   | 1:A:971:HIS:O     | 2.43                     | 0.45              |
| 1:C:755:VAL:HG12  | 1:C:759:ILE:HG23  | 1.98                     | 0.45              |
| 1:C:1003:SER:O    | 1:C:1007:LEU:N    | 2.41                     | 0.45              |
| 1:D:952:ARG:HE    | 1:D:955:GLY:H     | 1.64                     | 0.45              |
| 1:D:1194:ALA:O    | 1:D:1197:THR:OG1  | 2.27                     | 0.45              |
| 1:F:217:ALA:HB2   | 1:F:1184:LEU:HB2  | 1.99                     | 0.45              |
| 1:F:1180:SER:N    | 1:F:1205:ASP:OD1  | 2.50                     | 0.45              |
| 1:G:152:LEU:HG    | 1:H:337:SER:OG    | 2.17                     | 0.45              |
| 1:G:1019:THR:HG23 | 1:G:1160:LEU:CD1  | 2.42                     | 0.45              |
| 1:H:298:LYS:HE3   | 1:H:353:PHE:CG    | 2.51                     | 0.45              |
| 1:H:428:THR:HG22  | 1:H:442:SER:HB3   | 1.99                     | 0.45              |
| 1:H:595:THR:OG1   | 1:H:678:ASN:ND2   | 2.48                     | 0.45              |
| 1:I:224:MET:HE1   | 1:I:1298:PRO:HG3  | 1.99                     | 0.45              |
| 1:I:421:ALA:HA    | 1:I:424:GLN:HB2   | 1.98                     | 0.45              |
| 1:k:129:PRO:HB3   | 1:k:1060:HIS:CE1  | 2.52                     | 0.45              |
| 1:k:451:CYS:O     | 1:k:1106:TYR:OH   | 2.34                     | 0.45              |
| 1:k:1207:GLN:HG2  | 1:p:1150:HIS:CE1  | 2.50                     | 0.45              |
| 1:l:264:VAL:HG22  | 1:l:297:VAL:HG22  | 1.99                     | 0.45              |
| 1:l:389:ASP:OD1   | 1:l:389:ASP:N     | 2.46                     | 0.45              |
| 1:l:926:PHE:CZ    | 1:l:975:PHE:HB3   | 2.52                     | 0.45              |
| 1:m:51:PHE:CE1    | 1:n:87:MET:O      | 2.69                     | 0.45              |
| 1:m:512:ASN:OD1   | 1:m:513:GLU:N     | 2.50                     | 0.45              |
| 1:m:1029:ASP:HB2  | 1:m:1082:HIS:HB3  | 1.99                     | 0.45              |
| 1:m:1048:VAL:HG21 | 4:S:15:MET:HG3    | 1.98                     | 0.45              |
| 1:n:71:ALA:HB1    | 1:n:273:VAL:HG21  | 1.99                     | 0.45              |
| 1:n:183:VAL:HG21  | 1:n:1067:THR:HG21 | 1.98                     | 0.45              |
| 1:n:458:ALA:O     | 1:n:462:LEU:N     | 2.41                     | 0.45              |
| 1:n:1010:MET:SD   | 1:o:519:SER:OG    | 2.75                     | 0.45              |
| 1:o:263:THR:HA    | 1:o:269:ARG:HA    | 1.99                     | 0.45              |
| 1:p:204:ALA:HB1   | 1:p:206:ARG:HG2   | 1.98                     | 0.45              |
| 1:p:484:GLU:OE2   | 1:p:966:GLU:N     | 2.50                     | 0.45              |
| 1:p:804:ASN:HA    | 1:p:871:ASN:HD21  | 1.81                     | 0.45              |
| 1:p:877:ILE:HB    | 1:p:898:GLN:HB2   | 1.99                     | 0.45              |
| 1:q:607:GLN:HB3   | 1:q:644:ARG:HB3   | 1.98                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:q:1257:ASN:HA   | 1:q:1260:LYS:HG2  | 1.98                     | 0.45              |
| 2:2:206:GLU:O     | 2:3:132:TYR:CG    | 2.69                     | 0.45              |
| 2:h:252:PHE:HB2   | 2:h:264:ARG:HB2   | 1.98                     | 0.45              |
| 2:g:207:ASP:HB2   | 2:j:130:ALA:HB2   | 1.99                     | 0.45              |
| 3:K:85:LEU:O      | 3:K:89:SER:N      | 2.47                     | 0.45              |
| 4:y:73:LEU:HD23   | 4:y:130:VAL:CB    | 2.47                     | 0.45              |
| 4:S:188:VAL:HG22  | 4:S:210:VAL:HG12  | 1.98                     | 0.45              |
| 4:U:72:ARG:HH11   | 4:U:82:THR:HG22   | 1.81                     | 0.45              |
| 4:U:97:VAL:HA     | 4:U:172:GLU:HB3   | 1.99                     | 0.45              |
| 5:W:265:THR:HG22  | 5:W:268:GLU:HB2   | 1.99                     | 0.45              |
| 5:b:120:LEU:HB3   | 5:b:121:VAL:H     | 1.53                     | 0.45              |
| 1:B:251:VAL:HG11  | 1:B:1033:TYR:HE2  | 1.81                     | 0.44              |
| 1:B:567:LEU:HD22  | 1:B:1161:THR:HG21 | 1.99                     | 0.44              |
| 1:B:734:VAL:HG23  | 1:B:876:GLU:HB3   | 1.99                     | 0.44              |
| 1:D:909:THR:HA    | 1:D:932:LEU:HD11  | 1.99                     | 0.44              |
| 1:E:19:ASP:CG     | 1:m:252:THR:HB    | 2.42                     | 0.44              |
| 1:E:760:ALA:HA    | 1:E:763:GLN:HB3   | 1.99                     | 0.44              |
| 1:E:988:SER:HA    | 1:E:991:THR:HG22  | 1.98                     | 0.44              |
| 1:F:75:ALA:O      | 1:F:1038:SER:N    | 2.49                     | 0.44              |
| 1:F:252:THR:HB    | 1:l:19:ASP:CB     | 2.45                     | 0.44              |
| 1:F:806:LYS:HA    | 3:O:82:LEU:HD22   | 1.97                     | 0.44              |
| 1:F:898:GLN:HE21  | 1:F:970:TRP:HB2   | 1.80                     | 0.44              |
| 1:F:1049:THR:HG21 | 5:b:36:HIS:NE2    | 2.32                     | 0.44              |
| 1:G:381:ASP:OD1   | 1:G:381:ASP:N     | 2.49                     | 0.44              |
| 1:G:504:ARG:NE    | 1:G:946:ASP:OD2   | 2.41                     | 0.44              |
| 1:G:699:LEU:HD22  | 1:G:707:TYR:CZ    | 2.52                     | 0.44              |
| 1:I:1099:GLN:O    | 1:I:1239:ASN:ND2  | 2.50                     | 0.44              |
| 1:k:712:HIS:HA    | 1:k:780:VAL:HG22  | 1.98                     | 0.44              |
| 1:k:757:ARG:HH22  | 1:k:869:PRO:HA    | 1.83                     | 0.44              |
| 1:l:813:PHE:HD2   | 3:s:81:GLN:HG3    | 1.82                     | 0.44              |
| 1:l:952:ARG:HG2   | 1:l:955:GLY:H     | 1.82                     | 0.44              |
| 1:m:276:SER:HB3   | 1:m:280:VAL:HG13  | 1.99                     | 0.44              |
| 1:o:1158:VAL:CG1  | 1:o:1160:LEU:HD21 | 2.47                     | 0.44              |
| 1:p:840:ALA:O     | 1:p:844:ARG:HB2   | 2.16                     | 0.44              |
| 1:q:85:ASN:O      | 1:q:88:THR:OG1    | 2.34                     | 0.44              |
| 1:q:1296:GLU:HG2  | 1:q:1299:CYS:HB2  | 1.99                     | 0.44              |
| 2:e:207:ASP:HB2   | 2:h:130:ALA:HB2   | 1.99                     | 0.44              |
| 2:j:285:GLU:OE2   | 3:M:67:LYS:HD2    | 2.16                     | 0.44              |
| 4:y:120:LEU:HA    | 4:y:124:ALA:HB3   | 1.99                     | 0.44              |
| 4:y:251:THR:HA    | 4:y:292:GLU:HA    | 1.99                     | 0.44              |
| 4:V:191:VAL:HB    | 4:V:207:PHE:HB2   | 1.98                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 5:z:24:LEU:HG    | 5:z:120:LEU:HD12 | 1.99                     | 0.44              |
| 5:1:142:ILE:HD13 | 5:1:171:VAL:HG21 | 1.99                     | 0.44              |
| 1:A:691:GLU:O    | 1:A:705:LEU:HD22 | 2.18                     | 0.44              |
| 1:A:1085:ARG:HD3 | 1:B:200:HIS:ND1  | 2.32                     | 0.44              |
| 1:B:748:ARG:NE   | 1:B:770:ASP:HA   | 2.31                     | 0.44              |
| 1:C:657:ARG:NH2  | 1:C:778:GLU:OE1  | 2.48                     | 0.44              |
| 1:C:661:THR:HA   | 1:D:606:HIS:CD2  | 2.52                     | 0.44              |
| 1:C:950:TYR:CE1  | 1:C:958:PRO:HD3  | 2.51                     | 0.44              |
| 1:D:33:PHE:CE1   | 1:H:119:LYS:HG2  | 2.52                     | 0.44              |
| 1:D:62:ILE:HD11  | 1:E:99:PRO:HG3   | 1.99                     | 0.44              |
| 1:D:603:LEU:HD23 | 1:D:794:LEU:HD11 | 1.99                     | 0.44              |
| 1:D:1297:LYS:HD3 | 1:D:1299:CYS:HB2 | 1.98                     | 0.44              |
| 1:E:252:THR:HG21 | 1:G:21:LEU:HD22  | 1.99                     | 0.44              |
| 1:E:294:ARG:HD2  | 1:E:357:GLN:HB3  | 2.00                     | 0.44              |
| 1:E:446:ALA:HA   | 1:E:1094:MET:HG3 | 1.98                     | 0.44              |
| 1:F:333:ILE:CD1  | 1:m:313:ALA:HB3  | 2.48                     | 0.44              |
| 1:F:641:TRP:CD2  | 1:F:672:ALA:HB2  | 2.52                     | 0.44              |
| 1:G:150:ASP:O    | 1:G:154:ASN:N    | 2.41                     | 0.44              |
| 1:G:317:ILE:CD1  | 1:m:148:LEU:HD11 | 2.41                     | 0.44              |
| 1:G:1253:ASP:O   | 1:G:1257:ASN:ND2 | 2.50                     | 0.44              |
| 1:H:517:ASP:N    | 1:H:517:ASP:OD1  | 2.46                     | 0.44              |
| 1:I:391:GLU:HA   | 1:I:1025:THR:HA  | 1.97                     | 0.44              |
| 1:k:215:ASN:OD1  | 1:p:434:LYS:NZ   | 2.50                     | 0.44              |
| 1:k:813:PHE:CG   | 3:r:85:LEU:HD13  | 2.52                     | 0.44              |
| 1:l:888:GLY:O    | 1:l:892:ALA:N    | 2.50                     | 0.44              |
| 1:l:959:LEU:HB3  | 1:l:963:PHE:CE2  | 2.49                     | 0.44              |
| 1:l:1138:GLY:O   | 1:l:1241:SER:OG  | 2.28                     | 0.44              |
| 1:m:332:ARG:HH11 | 1:m:342:PRO:HD3  | 1.82                     | 0.44              |
| 1:m:379:ASN:OD1  | 1:n:205:ARG:NH2  | 2.39                     | 0.44              |
| 1:m:611:LEU:HD11 | 1:m:861:LEU:HD21 | 1.99                     | 0.44              |
| 1:n:608:TYR:OH   | 1:n:649:PHE:N    | 2.36                     | 0.44              |
| 1:o:638:ASN:ND2  | 1:o:668:VAL:O    | 2.41                     | 0.44              |
| 1:p:103:THR:OG1  | 1:p:104:GLY:N    | 2.49                     | 0.44              |
| 1:p:653:TYR:HA   | 1:p:656:VAL:HG12 | 1.99                     | 0.44              |
| 1:p:818:PHE:HZ   | 3:w:61:ILE:HD12  | 1.82                     | 0.44              |
| 1:p:907:MET:HG3  | 1:p:932:LEU:HD21 | 1.98                     | 0.44              |
| 2:3:264:ARG:HH22 | 3:r:93:LYS:NZ    | 2.15                     | 0.44              |
| 2:e:202:ASP:N    | 2:e:203:PRO:HD3  | 2.32                     | 0.44              |
| 2:f:207:ASP:HB2  | 2:i:130:ALA:HB2  | 1.99                     | 0.44              |
| 4:y:111:ARG:NH2  | 4:y:112:GLU:OE2  | 2.45                     | 0.44              |
| 4:y:192:ILE:O    | 4:y:250:GLY:HA2  | 2.16                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:z:29:ILE:O      | 5:z:69:THR:N      | 2.46                     | 0.44              |
| 5:z:170:VAL:HA    | 5:z:178:LEU:O     | 2.17                     | 0.44              |
| 5:Y:134:VAL:HB    | 5:Y:138:LEU:HD23  | 2.00                     | 0.44              |
| 5:Y:195:ASN:HA    | 5:Y:198:ILE:HD12  | 1.98                     | 0.44              |
| 5:Z:147:MET:HE3   | 5:Z:147:MET:HB2   | 1.76                     | 0.44              |
| 1:A:606:HIS:NE2   | 1:F:660:ALA:O     | 2.44                     | 0.44              |
| 1:A:1141:THR:OG1  | 1:A:1142:ASP:N    | 2.49                     | 0.44              |
| 1:C:983:ALA:HB3   | 1:C:987:GLU:OE1   | 2.17                     | 0.44              |
| 1:D:128:ILE:HA    | 1:E:102:ALA:HB3   | 1.98                     | 0.44              |
| 1:D:216:ILE:HG21  | 1:D:1262:LEU:HD11 | 1.98                     | 0.44              |
| 1:D:589:PRO:HB2   | 1:D:592:HIS:HB3   | 1.99                     | 0.44              |
| 1:D:595:THR:HA    | 1:D:675:HIS:HD2   | 1.83                     | 0.44              |
| 1:D:663:LEU:CB    | 1:D:673:TYR:CD1   | 3.01                     | 0.44              |
| 1:D:727:ASN:ND2   | 1:D:776:ASP:OD2   | 2.49                     | 0.44              |
| 1:E:41:GLY:HA3    | 1:m:111:ARG:NH1   | 2.33                     | 0.44              |
| 1:E:755:VAL:HG11  | 3:N:80:TYR:CE1    | 2.52                     | 0.44              |
| 1:F:494:THR:OG1   | 1:F:872:ALA:O     | 2.35                     | 0.44              |
| 1:F:647:LEU:HD11  | 1:F:672:ALA:HB1   | 1.99                     | 0.44              |
| 1:F:678:ASN:HA    | 1:F:681:SER:HB2   | 1.99                     | 0.44              |
| 1:F:818:PHE:O     | 1:F:819:LEU:CG    | 2.63                     | 0.44              |
| 1:F:1262:LEU:HB3  | 1:l:30:GLU:CG     | 2.46                     | 0.44              |
| 1:G:334:GLN:HB3   | 1:n:310:LYS:HG2   | 2.00                     | 0.44              |
| 1:G:819:LEU:HD12  | 3:P:58:GLN:HB3    | 1.99                     | 0.44              |
| 1:G:1043:ILE:HG22 | 1:G:1065:ILE:HB   | 1.99                     | 0.44              |
| 1:H:523:PHE:HZ    | 1:H:534:GLU:HG3   | 1.82                     | 0.44              |
| 1:H:650:ALA:O     | 1:H:785:TYR:OH    | 2.35                     | 0.44              |
| 1:H:959:LEU:HB3   | 1:H:963:PHE:CE1   | 2.52                     | 0.44              |
| 1:I:84:LEU:HG     | 1:I:87:MET:HE2    | 1.98                     | 0.44              |
| 1:I:753:SER:CA    | 3:R:83:ASP:OD1    | 2.65                     | 0.44              |
| 1:I:1298:PRO:O    | 1:I:1302:LEU:N    | 2.38                     | 0.44              |
| 1:k:644:ARG:NE    | 1:p:664:GLY:HA2   | 2.31                     | 0.44              |
| 1:k:784:VAL:O     | 1:k:788:CYS:CA    | 2.65                     | 0.44              |
| 1:l:72:LEU:HD23   | 1:l:180:PHE:HD2   | 1.81                     | 0.44              |
| 1:l:373:LEU:HD12  | 1:l:373:LEU:HA    | 1.87                     | 0.44              |
| 1:m:161:VAL:O     | 1:m:165:VAL:HG23  | 2.16                     | 0.44              |
| 1:n:653:TYR:HA    | 1:n:656:VAL:HG12  | 1.99                     | 0.44              |
| 1:n:711:LEU:HA    | 1:n:716:LEU:HD23  | 1.99                     | 0.44              |
| 1:n:1155:THR:OG1  | 1:n:1156:CYS:N    | 2.51                     | 0.44              |
| 1:o:311:GLU:HA    | 1:o:314:VAL:HB    | 1.99                     | 0.44              |
| 1:o:731:VAL:HG13  | 1:o:879:ALA:HA    | 1.99                     | 0.44              |
| 1:o:1160:LEU:HD23 | 1:o:1214:ASN:HD21 | 1.83                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:o:1171:ARG:NH2  | 1:o:1330:ASP:HB3  | 2.33                     | 0.44              |
| 1:p:216:ILE:HG21  | 1:p:1262:LEU:HD21 | 1.99                     | 0.44              |
| 1:q:656:VAL:HG21  | 1:q:679:LEU:HD12  | 1.99                     | 0.44              |
| 2:f:105:LEU:CD1   | 2:f:212:VAL:HG11  | 2.39                     | 0.44              |
| 2:j:184:ASN:ND2   | 2:j:218:TYR:OH    | 2.51                     | 0.44              |
| 3:r:85:LEU:HA     | 3:r:88:LEU:HG     | 2.00                     | 0.44              |
| 5:1:206:LEU:HD23  | 5:1:276:LEU:HB2   | 1.99                     | 0.44              |
| 1:A:1040:ALA:H    | 1:A:1068:VAL:HG12 | 1.83                     | 0.44              |
| 1:B:965:HIS:HB3   | 1:B:968:HIS:HB2   | 2.00                     | 0.44              |
| 1:B:1233:ARG:HH22 | 1:B:1244:SER:HB3  | 1.82                     | 0.44              |
| 1:D:122:GLU:O     | 1:D:1067:THR:OG1  | 2.31                     | 0.44              |
| 1:D:535:LEU:HB2   | 1:D:541:PHE:HE2   | 1.82                     | 0.44              |
| 1:E:1041:VAL:HG12 | 1:E:1067:THR:HG22 | 1.99                     | 0.44              |
| 1:E:1139:ARG:NH1  | 4:S:80:PRO:HD3    | 2.32                     | 0.44              |
| 1:F:421:ALA:HA    | 1:F:424:GLN:HB2   | 2.00                     | 0.44              |
| 1:F:735:ALA:HB2   | 1:F:740:LEU:HD13  | 1.98                     | 0.44              |
| 1:F:1348:SER:O    | 1:F:1352:ASN:N    | 2.48                     | 0.44              |
| 1:G:319:HIS:CD2   | 1:n:319:HIS:NE2   | 2.86                     | 0.44              |
| 1:G:618:LEU:HD22  | 1:G:864:LEU:HB3   | 1.98                     | 0.44              |
| 1:G:744:HIS:CB    | 2:e:175:ALA:H     | 2.28                     | 0.44              |
| 1:I:511:ALA:HA    | 1:I:514:ALA:HB3   | 1.99                     | 0.44              |
| 1:l:629:GLY:HA3   | 1:l:864:LEU:HD11  | 2.00                     | 0.44              |
| 1:l:643:GLN:OE1   | 1:l:644:ARG:NH1   | 2.51                     | 0.44              |
| 1:l:863:HIS:CE1   | 3:s:93:LYS:HA     | 2.52                     | 0.44              |
| 1:o:458:ALA:HB2   | 1:o:539:PHE:CD2   | 2.53                     | 0.44              |
| 1:o:766:PRO:O     | 1:o:767:LEU:C     | 2.59                     | 0.44              |
| 1:p:197:LEU:O     | 1:p:202:THR:OG1   | 2.36                     | 0.44              |
| 1:p:297:VAL:O     | 1:p:355:GLU:HA    | 2.17                     | 0.44              |
| 1:q:801:ALA:O     | 1:q:904:GLY:HA2   | 2.18                     | 0.44              |
| 2:i:184:ASN:ND2   | 2:i:218:TYR:OH    | 2.51                     | 0.44              |
| 5:W:138:LEU:HD21  | 5:W:178:LEU:HD21  | 1.99                     | 0.44              |
| 5:X:139:ALA:HA    | 5:X:142:ILE:HG22  | 1.99                     | 0.44              |
| 5:d:109:LEU:HD11  | 5:d:139:ALA:HA    | 1.98                     | 0.44              |
| 1:A:785:TYR:HD2   | 1:A:786:TYR:CG    | 2.36                     | 0.44              |
| 1:B:1030:THR:HG22 | 1:B:1080:THR:HA   | 1.99                     | 0.44              |
| 1:B:1297:LYS:H    | 1:B:1297:LYS:HD2  | 1.81                     | 0.44              |
| 1:C:275:VAL:HA    | 1:C:371:GLU:HB2   | 2.00                     | 0.44              |
| 1:D:391:GLU:HG3   | 1:D:1297:LYS:HE3  | 2.00                     | 0.44              |
| 1:D:813:PHE:HZ    | 3:M:85:LEU:HB3    | 1.53                     | 0.44              |
| 1:D:998:LYS:HE3   | 1:D:998:LYS:HB2   | 1.83                     | 0.44              |
| 1:D:1266:VAL:HA   | 1:D:1269:TYR:HB3  | 2.00                     | 0.44              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:G:674:THR:O     | 1:G:678:ASN:N    | 2.48                     | 0.44              |
| 1:G:1027:GLU:OE1  | 1:G:1085:ARG:NH2 | 2.50                     | 0.44              |
| 1:G:1249:PHE:CZ   | 1:G:1305:ALA:HB2 | 2.53                     | 0.44              |
| 1:H:1085:ARG:HD3  | 1:I:200:HIS:HB3  | 2.00                     | 0.44              |
| 1:I:753:SER:HA    | 3:R:83:ASP:OD1   | 2.18                     | 0.44              |
| 1:I:763:GLN:HE21  | 1:I:765:GLU:HB2  | 1.82                     | 0.44              |
| 1:k:240:LEU:HD21  | 1:k:284:LEU:HD23 | 1.98                     | 0.44              |
| 1:l:509:ARG:HH21  | 1:l:514:ALA:HB2  | 1.82                     | 0.44              |
| 1:l:539:PHE:HA    | 1:l:557:ARG:H    | 1.82                     | 0.44              |
| 1:m:281:VAL:HG11  | 1:m:372:HIS:HB2  | 1.99                     | 0.44              |
| 1:m:592:HIS:CE1   | 1:m:986:LEU:HD22 | 2.53                     | 0.44              |
| 1:m:724:LEU:H     | 1:m:769:VAL:HG21 | 1.83                     | 0.44              |
| 1:n:71:ALA:HB3    | 1:n:371:GLU:HB2  | 1.98                     | 0.44              |
| 1:o:53:ALA:HA     | 1:p:322:ILE:HB   | 2.00                     | 0.44              |
| 1:p:712:HIS:HA    | 1:p:780:VAL:HG22 | 2.00                     | 0.44              |
| 1:p:751:GLY:H     | 3:w:86:ARG:NH2   | 2.16                     | 0.44              |
| 1:q:975:PHE:CE1   | 1:q:995:MET:HE2  | 2.53                     | 0.44              |
| 1:q:1115:VAL:HG13 | 1:q:1119:THR:HG1 | 1.82                     | 0.44              |
| 2:g:202:ASP:N     | 2:g:203:PRO:HD3  | 2.32                     | 0.44              |
| 3:L:61:ILE:HG13   | 3:L:84:LEU:HD11  | 2.00                     | 0.44              |
| 3:w:58:GLN:HB2    | 3:w:61:ILE:HG22  | 1.98                     | 0.44              |
| 4:T:254:ARG:HB3   | 4:T:288:GLY:HA3  | 2.00                     | 0.44              |
| 4:V:72:ARG:HH21   | 4:V:132:HIS:CD2  | 2.36                     | 0.44              |
| 5:W:152:LEU:HB2   | 5:a:270:LEU:HD21 | 1.99                     | 0.44              |
| 5:Z:7:VAL:HB      | 5:Z:79:MET:HB2   | 1.99                     | 0.44              |
| 5:a:195:ASN:HA    | 5:a:198:ILE:HD12 | 1.99                     | 0.44              |
| 1:A:613:TYR:HA    | 1:A:616:GLU:HG2  | 2.00                     | 0.44              |
| 1:B:911:PRO:HG2   | 1:B:918:LEU:HD13 | 1.99                     | 0.44              |
| 1:C:515:LYS:HD3   | 1:C:564:PRO:HG3  | 1.99                     | 0.44              |
| 1:C:748:ARG:NH2   | 1:C:771:ALA:H    | 2.15                     | 0.44              |
| 1:C:818:PHE:CD1   | 3:L:88:LEU:HD22  | 2.53                     | 0.44              |
| 1:C:899:HIS:HD2   | 1:C:969:HIS:HE1  | 1.66                     | 0.44              |
| 1:C:1096:ASP:OD1  | 1:C:1096:ASP:N   | 2.51                     | 0.44              |
| 1:D:1231:ARG:HD3  | 5:Z:52:LYS:HE2   | 2.00                     | 0.44              |
| 1:E:275:VAL:HA    | 1:E:371:GLU:HB3  | 1.99                     | 0.44              |
| 1:E:1019:THR:HG23 | 1:E:1160:LEU:HG  | 2.00                     | 0.44              |
| 1:E:1031:LEU:HD23 | 1:E:1081:ALA:CB  | 2.48                     | 0.44              |
| 1:G:68:LEU:HA     | 1:G:73:ALA:HB2   | 2.00                     | 0.44              |
| 1:G:1072:LEU:HD23 | 1:m:19:ASP:OD1   | 2.18                     | 0.44              |
| 1:H:1019:THR:OG1  | 1:H:1158:VAL:HB  | 2.18                     | 0.44              |
| 1:l:276:SER:HB3   | 1:l:280:VAL:HG13 | 2.00                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:m:132:ILE:HD11  | 4:S:16:GLU:OE2    | 2.18                     | 0.44              |
| 1:m:165:VAL:HG13  | 4:S:12:ARG:CB     | 2.46                     | 0.44              |
| 1:n:23:HIS:CD2    | 1:n:25:LYS:H      | 2.36                     | 0.44              |
| 1:n:462:LEU:HD22  | 1:n:890:PRO:HG3   | 2.00                     | 0.44              |
| 1:p:433:ASN:ND2   | 1:p:1089:ASP:O    | 2.42                     | 0.44              |
| 1:p:608:TYR:HA    | 1:p:609:PRO:HD3   | 1.74                     | 0.44              |
| 1:p:1082:HIS:CE1  | 1:p:1352:ASN:HD21 | 2.36                     | 0.44              |
| 1:q:396:PHE:HA    | 1:q:397:PRO:HD3   | 1.85                     | 0.44              |
| 1:q:514:ALA:HB3   | 1:q:530:LEU:HD11  | 1.98                     | 0.44              |
| 1:q:1103:MET:HE3  | 1:q:1127:LEU:HG   | 2.00                     | 0.44              |
| 2:3:184:ASN:ND2   | 2:3:218:TYR:OH    | 2.51                     | 0.44              |
| 2:h:184:ASN:ND2   | 2:h:218:TYR:OH    | 2.51                     | 0.44              |
| 2:j:208:PRO:HD3   | 4:V:236:ASN:HD22  | 1.82                     | 0.44              |
| 2:j:279:LEU:O     | 2:j:283:LEU:HG    | 2.18                     | 0.44              |
| 3:Q:64:MET:HG3    | 3:Q:87:MET:HG3    | 1.99                     | 0.44              |
| 5:1:138:LEU:HD22  | 5:1:173:TYR:CG    | 2.53                     | 0.44              |
| 5:b:96:GLY:HA2    | 5:b:132:TRP:CD1   | 2.53                     | 0.44              |
| 5:d:54:ARG:HD3    | 5:d:54:ARG:HA     | 1.84                     | 0.44              |
| 1:A:421:ALA:HA    | 1:A:424:GLN:HB2   | 1.99                     | 0.44              |
| 1:A:1180:SER:N    | 1:A:1205:ASP:OD1  | 2.49                     | 0.44              |
| 1:B:228:ILE:HG22  | 1:B:233:ARG:HH21  | 1.83                     | 0.44              |
| 1:B:870:GLU:HB2   | 1:B:903:ASN:HD22  | 1.82                     | 0.44              |
| 1:B:920:VAL:HG22  | 1:B:922:PRO:HD3   | 2.00                     | 0.44              |
| 1:C:562:ASN:HD22  | 1:C:972:ARG:HB2   | 1.82                     | 0.44              |
| 1:C:795:ASN:O     | 1:C:797:HIS:ND1   | 2.51                     | 0.44              |
| 1:C:911:PRO:HG2   | 1:C:914:LEU:HD12  | 1.99                     | 0.44              |
| 1:D:416:LYS:HD3   | 1:E:412:GLU:HG3   | 1.99                     | 0.44              |
| 1:D:516:HIS:CE1   | 1:D:977:CYS:HB3   | 2.53                     | 0.44              |
| 1:E:606:HIS:HA    | 1:E:909:THR:HG21  | 1.99                     | 0.44              |
| 1:E:1134:ILE:HG23 | 1:E:1139:ARG:HB3  | 2.00                     | 0.44              |
| 1:E:1318:GLU:O    | 1:E:1322:LYS:HB2  | 2.18                     | 0.44              |
| 1:F:1262:LEU:N    | 1:l:30:GLU:HB2    | 2.33                     | 0.44              |
| 1:G:66:THR:HG23   | 1:G:69:GLY:H      | 1.83                     | 0.44              |
| 1:G:1128:ASP:HB3  | 5:W:187:ASP:OD2   | 2.18                     | 0.44              |
| 1:G:1330:ASP:OD1  | 1:G:1330:ASP:N    | 2.51                     | 0.44              |
| 1:H:257:ASP:OD1   | 1:H:257:ASP:N     | 2.51                     | 0.44              |
| 1:H:328:GLN:HE22  | 1:H:343:GLU:H     | 1.65                     | 0.44              |
| 1:H:618:LEU:HD22  | 1:H:864:LEU:HB3   | 1.98                     | 0.44              |
| 1:H:925:ARG:HH11  | 1:H:975:PHE:HB2   | 1.83                     | 0.44              |
| 1:H:988:SER:HA    | 1:H:991:THR:HG22  | 2.00                     | 0.44              |
| 1:I:451:CYS:O     | 1:I:1106:TYR:OH   | 2.35                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:I:693:THR:HB    | 1:I:1010:MET:HE1  | 2.00                     | 0.44              |
| 1:I:899:HIS:CG    | 1:I:963:PHE:HB3   | 2.53                     | 0.44              |
| 1:k:80:MET:HG2    | 1:k:1043:ILE:HG12 | 2.00                     | 0.44              |
| 1:k:82:HIS:HE1    | 1:k:308:LEU:H     | 1.64                     | 0.44              |
| 1:k:662:ARG:HH22  | 1:k:665:ASP:HB2   | 1.82                     | 0.44              |
| 1:l:484:GLU:OE2   | 1:l:966:GLU:N     | 2.51                     | 0.44              |
| 1:l:750:PRO:HG3   | 1:l:770:ASP:OD1   | 2.17                     | 0.44              |
| 1:l:1261:THR:O    | 1:l:1265:THR:CB   | 2.65                     | 0.44              |
| 1:m:128:ILE:HG22  | 1:n:102:ALA:HB3   | 2.00                     | 0.44              |
| 1:m:727:ASN:ND2   | 1:m:776:ASP:OD1   | 2.50                     | 0.44              |
| 1:m:1309:HIS:CE1  | 1:m:1320:GLN:HG3  | 2.53                     | 0.44              |
| 1:n:1230:THR:HA   | 1:n:1233:ARG:HB3  | 2.00                     | 0.44              |
| 1:o:496:ARG:HG3   | 1:o:962:ILE:HG12  | 2.00                     | 0.44              |
| 1:o:595:THR:HA    | 1:o:675:HIS:HD2   | 1.81                     | 0.44              |
| 1:o:702:GLU:OE2   | 1:o:715:ARG:NH1   | 2.50                     | 0.44              |
| 1:o:1041:VAL:HG12 | 1:o:1067:THR:HG22 | 2.00                     | 0.44              |
| 1:q:534:GLU:HG3   | 1:q:567:LEU:HD11  | 2.00                     | 0.44              |
| 1:q:620:HIS:ND1   | 1:q:903:ASN:OD1   | 2.43                     | 0.44              |
| 5:z:100:TRP:HB3   | 5:z:106:LEU:HD21  | 1.99                     | 0.44              |
| 5:X:106:LEU:HG    | 5:X:133:ILE:HG22  | 1.99                     | 0.44              |
| 1:A:98:VAL:HG21   | 1:A:113:THR:HB    | 2.00                     | 0.44              |
| 1:A:294:ARG:HD2   | 1:A:357:GLN:HB3   | 2.00                     | 0.44              |
| 1:B:258:ASN:HB2   | 1:B:261:THR:HG22  | 2.00                     | 0.44              |
| 1:B:1201:HIS:ND1  | 1:B:1212:THR:OG1  | 2.32                     | 0.44              |
| 1:C:409:SER:OG    | 1:C:1333:HIS:ND1  | 2.51                     | 0.44              |
| 1:C:595:THR:HA    | 1:C:675:HIS:HD2   | 1.83                     | 0.44              |
| 1:D:264:VAL:N     | 1:D:268:GLU:O     | 2.45                     | 0.44              |
| 1:E:595:THR:HA    | 1:E:675:HIS:HD2   | 1.83                     | 0.44              |
| 1:F:144:PHE:N     | 1:F:150:ASP:OD2   | 2.51                     | 0.44              |
| 1:F:396:PHE:CE1   | 1:F:1020:VAL:HB   | 2.53                     | 0.44              |
| 1:F:1156:CYS:SG   | 1:F:1157:GLU:N    | 2.91                     | 0.44              |
| 1:G:755:VAL:O     | 1:G:759:ILE:N     | 2.43                     | 0.44              |
| 1:G:874:MET:HE3   | 1:G:874:MET:HB2   | 1.87                     | 0.44              |
| 1:H:104:GLY:HA3   | 1:H:107:ILE:HD12  | 2.00                     | 0.44              |
| 1:H:137:LEU:HD13  | 1:H:141:LYS:HZ1   | 1.83                     | 0.44              |
| 1:H:698:ARG:HG3   | 1:H:703:PRO:HA    | 1.98                     | 0.44              |
| 1:I:181:LEU:HD21  | 1:I:386:LEU:HG    | 2.00                     | 0.44              |
| 1:I:428:THR:HG22  | 1:I:442:SER:HB3   | 1.99                     | 0.44              |
| 1:I:1276:CYS:SG   | 1:I:1277:ILE:N    | 2.91                     | 0.44              |
| 1:k:276:SER:HB2   | 1:k:281:VAL:HG23  | 2.00                     | 0.44              |
| 1:k:562:ASN:ND2   | 1:k:972:ARG:H     | 2.16                     | 0.44              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:l:794:LEU:HD13  | 1:l:798:ALA:HB2  | 1.99                     | 0.44              |
| 1:m:638:ASN:HD21  | 1:m:668:VAL:HG12 | 1.82                     | 0.44              |
| 1:n:860:GLU:HA    | 1:n:863:HIS:HD2  | 1.83                     | 0.44              |
| 1:q:395:TYR:HE1   | 1:q:1173:PRO:HA  | 1.83                     | 0.44              |
| 1:q:713:ASP:O     | 1:q:783:LYS:NZ   | 2.40                     | 0.44              |
| 2:g:200:VAL:HG21  | 2:g:215:ARG:HG2  | 0.63                     | 0.44              |
| 4:y:51:ARG:HD3    | 4:y:147:LEU:HD13 | 1.99                     | 0.44              |
| 4:S:262:ASP:HB3   | 4:S:281:GLU:HB2  | 1.98                     | 0.44              |
| 5:z:280:ILE:HD12  | 5:1:283:ILE:HG23 | 1.99                     | 0.44              |
| 5:Y:149:LEU:HD21  | 5:Y:168:LEU:HD12 | 2.00                     | 0.44              |
| 5:b:129:VAL:O     | 5:b:129:VAL:HG23 | 2.16                     | 0.44              |
| 1:A:560:VAL:HA    | 1:A:999:MET:HE3  | 1.99                     | 0.44              |
| 1:A:969:HIS:ND1   | 1:A:971:HIS:O    | 2.42                     | 0.44              |
| 1:A:1057:THR:HG21 | 4:U:33:ARG:HH22  | 1.83                     | 0.44              |
| 1:C:227:THR:HG22  | 1:C:230:LEU:HD21 | 2.00                     | 0.44              |
| 1:C:432:TYR:HB3   | 1:C:436:ARG:HA   | 2.00                     | 0.44              |
| 1:C:1021:VAL:HG23 | 1:C:1245:PRO:HB2 | 1.99                     | 0.44              |
| 1:D:119:LYS:HB3   | 1:D:1069:GLU:HB3 | 1.99                     | 0.44              |
| 1:D:605:ASP:HB3   | 1:D:608:TYR:HB2  | 2.00                     | 0.44              |
| 1:D:1054:ASP:OD2  | 4:V:46:GLN:HB2   | 2.17                     | 0.44              |
| 1:D:1064:ASN:OD1  | 5:Z:78:GLN:NE2   | 2.51                     | 0.44              |
| 1:E:258:ASN:HB2   | 1:E:261:THR:HG22 | 2.00                     | 0.44              |
| 1:E:338:GLN:NE2   | 1:G:10:LEU:O     | 2.51                     | 0.44              |
| 1:E:448:LYS:HD2   | 1:E:1096:ASP:HB3 | 2.00                     | 0.44              |
| 1:E:663:LEU:N     | 1:F:607:GLN:OE1  | 2.50                     | 0.44              |
| 1:E:944:LEU:HD11  | 1:E:951:GLN:HB2  | 1.98                     | 0.44              |
| 1:F:92:MET:HE2    | 1:F:346:PHE:HE2  | 1.82                     | 0.44              |
| 1:F:271:ALA:HB1   | 1:F:366:ARG:HH11 | 1.83                     | 0.44              |
| 1:F:600:ARG:HH11  | 1:F:794:LEU:HA   | 1.82                     | 0.44              |
| 1:G:58:TYR:O      | 1:H:94:PHE:HA    | 2.18                     | 0.44              |
| 1:G:96:ILE:HD12   | 1:m:24:ILE:HD11  | 2.00                     | 0.44              |
| 1:G:114:THR:HG22  | 1:G:116:MET:HG3  | 2.00                     | 0.44              |
| 1:G:207:MET:HE1   | 1:m:25:LYS:HE2   | 1.77                     | 0.44              |
| 1:G:437:ILE:HG21  | 1:H:1207:GLN:NE2 | 2.33                     | 0.44              |
| 1:G:635:ARG:HH11  | 1:G:849:ASP:HB2  | 1.81                     | 0.44              |
| 1:H:264:VAL:HG13  | 1:H:295:THR:HG21 | 2.00                     | 0.44              |
| 1:H:390:VAL:HG22  | 1:H:1295:VAL:HB  | 2.00                     | 0.44              |
| 1:H:439:GLN:HG2   | 1:H:1092:SER:H   | 1.83                     | 0.44              |
| 1:H:669:VAL:HB    | 1:H:673:TYR:HB2  | 2.00                     | 0.44              |
| 1:H:1161:THR:HG22 | 1:H:1216:TRP:CH2 | 2.53                     | 0.44              |
| 1:I:100:ARG:HH22  | 1:I:102:ALA:HB2  | 1.82                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:I:540:ASP:HB2   | 1:I:557:ARG:HG3   | 1.99                     | 0.44              |
| 1:m:292:ILE:HG12  | 1:m:361:LEU:HB3   | 1.99                     | 0.44              |
| 1:m:576:ARG:HH11  | 1:m:1007:LEU:HD21 | 1.82                     | 0.44              |
| 1:m:1316:LEU:O    | 1:m:1320:GLN:HG2  | 2.18                     | 0.44              |
| 1:n:146:ASP:N     | 1:n:146:ASP:OD1   | 2.48                     | 0.44              |
| 1:n:223:LYS:O     | 1:n:227:THR:OG1   | 2.25                     | 0.44              |
| 1:n:511:ALA:O     | 1:n:515:LYS:HB2   | 2.18                     | 0.44              |
| 1:n:898:GLN:HE21  | 1:n:970:TRP:HB2   | 1.83                     | 0.44              |
| 1:o:598:VAL:HG12  | 1:o:647:LEU:HB2   | 1.99                     | 0.44              |
| 1:p:159:ASN:ND2   | 1:q:40:TYR:OH     | 2.51                     | 0.44              |
| 1:p:237:ARG:HG3   | 1:p:288:LEU:HD23  | 2.00                     | 0.44              |
| 1:p:633:VAL:HG22  | 1:p:659:ILE:HD11  | 2.00                     | 0.44              |
| 1:q:1085:ARG:HH22 | 1:q:1087:ARG:HG3  | 1.83                     | 0.44              |
| 2:2:204:LEU:HB2   | 2:2:211:LEU:CD2   | 2.48                     | 0.44              |
| 3:s:79:ALA:O      | 3:s:83:ASP:HB2    | 2.18                     | 0.44              |
| 4:S:224:ARG:HH21  | 5:W:282:GLN:NE2   | 2.00                     | 0.44              |
| 4:S:294:ALA:O     | 5:W:282:GLN:NE2   | 2.36                     | 0.44              |
| 4:T:115:ALA:O     | 4:T:118:THR:OG1   | 2.34                     | 0.44              |
| 4:V:52:PHE:HE1    | 5:d:102:LYS:HB3   | 1.82                     | 0.44              |
| 4:V:99:ALA:HA     | 4:V:102:LYS:HB3   | 2.00                     | 0.44              |
| 4:V:215:HIS:HE2   | 4:V:217:HIS:HB3   | 1.83                     | 0.44              |
| 5:W:103:GLY:H     | 5:W:295:VAL:HB    | 1.82                     | 0.44              |
| 1:A:156:ASP:HA    | 1:B:338:GLN:HE22  | 1.83                     | 0.43              |
| 1:A:237:ARG:HG3   | 1:A:288:LEU:HD23  | 2.00                     | 0.43              |
| 1:A:683:THR:HG23  | 1:A:784:VAL:HB    | 2.00                     | 0.43              |
| 1:A:734:VAL:HG12  | 1:A:739:PRO:HA    | 1.99                     | 0.43              |
| 1:A:988:SER:HA    | 1:A:991:THR:HG22  | 2.00                     | 0.43              |
| 1:A:1031:LEU:C    | 1:A:1031:LEU:HD12 | 2.43                     | 0.43              |
| 1:B:602:SER:HB3   | 1:B:647:LEU:H     | 1.84                     | 0.43              |
| 1:C:943:PHE:CE2   | 1:C:958:PRO:HG3   | 2.53                     | 0.43              |
| 1:D:975:PHE:O     | 1:D:979:SER:N     | 2.48                     | 0.43              |
| 1:E:146:ASP:OD1   | 1:E:146:ASP:N     | 2.50                     | 0.43              |
| 1:E:153:LEU:CD1   | 1:l:47:TYR:HD1    | 2.31                     | 0.43              |
| 1:E:440:ARG:HH12  | 1:F:521:LYS:HB3   | 1.82                     | 0.43              |
| 1:E:1031:LEU:HD23 | 1:E:1081:ALA:HB2  | 2.00                     | 0.43              |
| 1:E:1262:LEU:H    | 1:G:30:GLU:HB2    | 1.82                     | 0.43              |
| 1:F:198:MET:SD    | 1:l:21:LEU:HD12   | 2.58                     | 0.43              |
| 1:F:1160:LEU:HD23 | 1:F:1214:ASN:CB   | 2.48                     | 0.43              |
| 1:G:435:ASP:N     | 1:G:435:ASP:OD1   | 2.42                     | 0.43              |
| 1:G:748:ARG:CZ    | 2:h:275:THR:HG21  | 2.47                     | 0.43              |
| 1:G:816:LYS:HG3   | 1:G:817:PHE:H     | 1.83                     | 0.43              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:G:1096:ASP:OD1 | 1:G:1096:ASP:N    | 2.51                     | 0.43              |
| 1:G:1148:LEU:HA  | 1:G:1148:LEU:HD12 | 1.75                     | 0.43              |
| 1:I:756:ALA:HA   | 1:I:759:ILE:HG12  | 2.00                     | 0.43              |
| 1:k:598:VAL:HG11 | 1:k:647:LEU:HD23  | 2.00                     | 0.43              |
| 1:l:567:LEU:HD22 | 1:l:1161:THR:HG21 | 1.99                     | 0.43              |
| 1:l:587:ARG:HH21 | 1:l:589:PRO:HG2   | 1.83                     | 0.43              |
| 1:l:649:PHE:HB3  | 1:l:655:MET:HB3   | 2.00                     | 0.43              |
| 1:m:595:THR:HA   | 1:m:675:HIS:HD2   | 1.83                     | 0.43              |
| 1:m:920:VAL:HG22 | 1:m:922:PRO:HD3   | 2.00                     | 0.43              |
| 1:n:1022:ARG:NH1 | 1:n:1091:GLY:O    | 2.51                     | 0.43              |
| 1:o:67:PHE:O     | 1:o:70:THR:OG1    | 2.31                     | 0.43              |
| 1:o:237:ARG:HG3  | 1:o:288:LEU:HD23  | 1.99                     | 0.43              |
| 1:o:602:SER:HA   | 1:o:646:LEU:HD13  | 1.98                     | 0.43              |
| 1:p:804:ASN:O    | 1:p:808:LEU:HB2   | 2.17                     | 0.43              |
| 1:q:559:MET:HE2  | 1:q:710:ALA:HB3   | 2.01                     | 0.43              |
| 1:q:691:GLU:HB2  | 1:q:705:LEU:HD11  | 1.99                     | 0.43              |
| 1:q:1103:MET:HB2 | 5:z:225:MET:HG3   | 1.99                     | 0.43              |
| 1:q:1177:ARG:HD3 | 1:q:1179:ARG:HH21 | 1.82                     | 0.43              |
| 2:f:204:LEU:HB2  | 2:f:211:LEU:CD2   | 2.48                     | 0.43              |
| 4:T:13:GLU:O     | 4:T:17:PHE:N      | 2.42                     | 0.43              |
| 4:V:65:ASN:HD22  | 4:V:268:VAL:HG12  | 1.83                     | 0.43              |
| 5:X:53:THR:HB    | 5:X:58:ARG:HD2    | 1.99                     | 0.43              |
| 5:Z:288:SER:OG   | 5:Z:289:GLU:N     | 2.51                     | 0.43              |
| 1:A:23:HIS:CD2   | 1:A:25:LYS:H      | 2.36                     | 0.43              |
| 1:B:516:HIS:NE2  | 1:B:977:CYS:HB3   | 2.33                     | 0.43              |
| 1:B:1117:GLN:CD  | 1:C:474:ASP:HB2   | 2.42                     | 0.43              |
| 1:C:174:ARG:NH2  | 1:D:99:PRO:HB3    | 2.33                     | 0.43              |
| 1:C:430:TYR:CG   | 1:C:1314:GLN:HG3  | 2.53                     | 0.43              |
| 1:C:446:ALA:HA   | 1:C:1094:MET:HG3  | 2.00                     | 0.43              |
| 1:D:150:ASP:O    | 1:D:154:ASN:N     | 2.42                     | 0.43              |
| 1:E:1093:ARG:HB2 | 1:E:1153:ARG:HH21 | 1.83                     | 0.43              |
| 1:F:298:LYS:HE3  | 1:F:353:PHE:CG    | 2.53                     | 0.43              |
| 1:F:1101:PHE:HB3 | 1:F:1104:HIS:CD2  | 2.52                     | 0.43              |
| 1:G:458:ALA:HB1  | 1:G:461:CYS:HB3   | 2.00                     | 0.43              |
| 1:G:1230:THR:HA  | 1:G:1233:ARG:HB3  | 2.01                     | 0.43              |
| 1:H:702:GLU:OE2  | 1:H:715:ARG:NH2   | 2.32                     | 0.43              |
| 1:k:231:LEU:HD22 | 1:k:1082:HIS:HB2  | 1.99                     | 0.43              |
| 1:k:504:ARG:NH2  | 1:k:946:ASP:OD1   | 2.46                     | 0.43              |
| 1:k:663:LEU:HD22 | 1:k:663:LEU:HA    | 1.86                     | 0.43              |
| 1:k:688:ARG:HA   | 1:k:691:GLU:CG    | 2.48                     | 0.43              |
| 1:k:1230:THR:O   | 1:k:1234:GLU:HB2  | 2.18                     | 0.43              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:m:129:PRO:HB3   | 1:m:1060:HIS:CE1 | 2.53                     | 0.43              |
| 1:m:278:HIS:HB2   | 1:m:374:ARG:HD3  | 2.01                     | 0.43              |
| 1:m:389:ASP:HA    | 1:m:1027:GLU:HA  | 1.99                     | 0.43              |
| 1:n:213:ARG:HG3   | 1:n:1185:GLY:HA2 | 2.00                     | 0.43              |
| 1:n:898:GLN:HG2   | 1:n:970:TRP:CD1  | 2.54                     | 0.43              |
| 1:o:782:GLN:O     | 1:o:786:TYR:HB2  | 2.19                     | 0.43              |
| 1:p:392:LEU:O     | 1:p:1024:ASP:N   | 2.46                     | 0.43              |
| 1:p:1230:THR:O    | 1:p:1234:GLU:CB  | 2.66                     | 0.43              |
| 1:q:476:ARG:HH11  | 1:q:530:LEU:HD23 | 1.83                     | 0.43              |
| 2:e:184:ASN:HB2   | 2:e:198:LEU:HD11 | 1.99                     | 0.43              |
| 2:e:204:LEU:HB2   | 2:e:211:LEU:CD2  | 2.48                     | 0.43              |
| 2:g:105:LEU:CD1   | 2:g:212:VAL:HG11 | 2.39                     | 0.43              |
| 2:j:93:PRO:HD2    | 2:j:195:TYR:HH   | 1.81                     | 0.43              |
| 3:N:49:LEU:HD11   | 3:N:65:ILE:HD11  | 2.00                     | 0.43              |
| 4:U:71:PHE:O      | 4:U:85:VAL:N     | 2.48                     | 0.43              |
| 4:U:176:ASP:O     | 4:U:226:ARG:NH2  | 2.51                     | 0.43              |
| 5:z:277:PHE:HA    | 5:z:280:ILE:HG12 | 1.99                     | 0.43              |
| 5:W:127:ASP:OD1   | 5:W:127:ASP:N    | 2.45                     | 0.43              |
| 5:Z:109:LEU:HD22  | 5:Z:134:VAL:HG21 | 2.00                     | 0.43              |
| 5:c:227:LEU:HD23  | 5:c:230:CYS:HB3  | 1.99                     | 0.43              |
| 5:d:114:SER:O     | 5:d:179:THR:OG1  | 2.36                     | 0.43              |
| 1:A:380:THR:O     | 1:B:205:ARG:CD   | 2.64                     | 0.43              |
| 1:A:447:LEU:HD11  | 1:A:1005:ALA:HA  | 2.00                     | 0.43              |
| 1:A:910:VAL:HG21  | 1:A:936:ALA:HB2  | 2.01                     | 0.43              |
| 1:B:453:PRO:HG2   | 1:B:1104:HIS:HB3 | 2.00                     | 0.43              |
| 1:B:520:THR:HG22  | 1:B:566:ALA:HA   | 2.01                     | 0.43              |
| 1:B:651:ASN:HB3   | 1:B:906:CYS:HB3  | 2.00                     | 0.43              |
| 1:C:611:LEU:HB3   | 1:C:846:VAL:HG11 | 2.00                     | 0.43              |
| 1:C:865:VAL:HA    | 1:C:868:VAL:HG23 | 1.99                     | 0.43              |
| 1:D:660:ALA:HA    | 1:D:673:TYR:HE1  | 1.83                     | 0.43              |
| 1:E:23:HIS:HB3    | 1:E:26:LEU:HB3   | 1.99                     | 0.43              |
| 1:E:134:ALA:HA    | 1:E:137:LEU:HD12 | 2.01                     | 0.43              |
| 1:E:1142:ASP:O    | 1:E:1285:TYR:OH  | 2.35                     | 0.43              |
| 1:F:210:ARG:NH1   | 1:F:1187:ASP:OD2 | 2.51                     | 0.43              |
| 1:F:630:ILE:HA    | 1:F:633:VAL:HG12 | 1.99                     | 0.43              |
| 1:F:1171:ARG:HH21 | 1:F:1330:ASP:HB2 | 1.82                     | 0.43              |
| 1:G:387:GLU:HB3   | 1:G:1084:ARG:NH1 | 2.34                     | 0.43              |
| 1:G:1255:ILE:HD12 | 1:G:1255:ILE:HA  | 1.89                     | 0.43              |
| 1:k:65:VAL:HG11   | 1:k:376:VAL:HG12 | 1.99                     | 0.43              |
| 1:k:80:MET:HG3    | 1:k:303:TYR:HB2  | 2.01                     | 0.43              |
| 1:k:389:ASP:N     | 1:k:389:ASP:OD1  | 2.41                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:k:748:ARG:NE    | 2:3:269:ARG:NH1   | 2.66                     | 0.43              |
| 1:k:749:ASN:OD1   | 1:k:752:THR:OG1   | 2.36                     | 0.43              |
| 1:k:753:SER:CB    | 3:r:83:ASP:O      | 2.66                     | 0.43              |
| 1:k:1166:ASP:HA   | 1:k:1170:PHE:HB2  | 1.99                     | 0.43              |
| 1:m:81:PHE:HB2    | 1:m:306:PHE:HB3   | 1.99                     | 0.43              |
| 1:m:600:ARG:O     | 1:m:604:THR:OG1   | 2.21                     | 0.43              |
| 1:m:863:HIS:NE2   | 3:t:92:LYS:O      | 2.43                     | 0.43              |
| 1:o:745:ILE:HA    | 1:o:766:PRO:HA    | 2.00                     | 0.43              |
| 1:o:872:ALA:HA    | 1:o:903:ASN:HB2   | 2.00                     | 0.43              |
| 1:o:1026:PHE:HD1  | 1:o:1086:VAL:HG22 | 1.83                     | 0.43              |
| 1:p:481:CYS:SG    | 1:p:482:ARG:N     | 2.89                     | 0.43              |
| 1:p:1156:CYS:SG   | 1:p:1244:SER:OG   | 2.76                     | 0.43              |
| 1:q:462:LEU:HD13  | 1:q:554:CYS:HB2   | 2.01                     | 0.43              |
| 2:e:105:LEU:HD11  | 2:e:212:VAL:HG13  | 1.85                     | 0.43              |
| 2:e:200:VAL:HG21  | 2:e:215:ARG:HG2   | 0.63                     | 0.43              |
| 3:w:48:VAL:HA     | 3:w:77:LYS:HD2    | 1.99                     | 0.43              |
| 4:T:32:GLU:HA     | 4:T:35:ILE:HD12   | 2.00                     | 0.43              |
| 4:U:92:MET:HE2    | 4:U:118:THR:HG21  | 2.00                     | 0.43              |
| 4:V:99:ALA:O      | 4:V:103:ASN:N     | 2.44                     | 0.43              |
| 5:W:71:MET:HG3    | 5:W:79:MET:HE1    | 2.01                     | 0.43              |
| 1:A:87:MET:SD     | 1:A:1066:ASN:ND2  | 2.91                     | 0.43              |
| 1:B:512:ASN:OD1   | 1:B:513:GLU:N     | 2.51                     | 0.43              |
| 1:B:793:VAL:HA    | 1:B:984:HIS:HB2   | 2.00                     | 0.43              |
| 1:B:1316:LEU:O    | 1:B:1320:GLN:HG2  | 2.18                     | 0.43              |
| 1:D:924:HIS:HB3   | 1:D:927:TYR:HB2   | 1.99                     | 0.43              |
| 1:D:1161:THR:OG1  | 1:D:1164:SER:OG   | 2.34                     | 0.43              |
| 1:E:702:GLU:OE2   | 1:E:715:ARG:NH2   | 2.51                     | 0.43              |
| 1:E:734:VAL:HG23  | 1:E:876:GLU:HB3   | 1.99                     | 0.43              |
| 1:E:1297:LYS:HD3  | 1:E:1299:CYS:HB2  | 2.00                     | 0.43              |
| 1:F:695:LEU:HD21  | 1:F:1006:ALA:HB1  | 1.99                     | 0.43              |
| 1:F:1263:PHE:CZ   | 1:l:30:GLU:OE2    | 2.72                     | 0.43              |
| 1:G:1064:ASN:HD22 | 1:G:1065:ILE:N    | 2.16                     | 0.43              |
| 1:H:508:PRO:O     | 1:H:510:THR:OG1   | 2.34                     | 0.43              |
| 1:H:719:PRO:HD2   | 1:H:786:TYR:HB3   | 2.01                     | 0.43              |
| 1:l:11:LEU:HD23   | 1:l:11:LEU:HA     | 1.83                     | 0.43              |
| 1:m:1048:VAL:HG22 | 1:m:1061:VAL:HG12 | 2.01                     | 0.43              |
| 1:n:638:ASN:HD21  | 1:n:668:VAL:HG12  | 1.82                     | 0.43              |
| 1:n:647:LEU:HD13  | 1:n:647:LEU:HA    | 1.82                     | 0.43              |
| 1:n:720:PHE:HB2   | 1:n:786:TYR:CE2   | 2.53                     | 0.43              |
| 1:n:1029:ASP:N    | 1:n:1082:HIS:O    | 2.49                     | 0.43              |
| 1:o:258:ASN:HB3   | 1:o:260:GLU:HG2   | 2.00                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:o:713:ASP:OD1   | 1:o:713:ASP:N     | 2.52                     | 0.43              |
| 1:p:228:ILE:HG22  | 1:p:233:ARG:HH21  | 1.82                     | 0.43              |
| 1:p:482:ARG:HH12  | 1:p:961:PRO:HB3   | 1.83                     | 0.43              |
| 1:p:870:GLU:HB3   | 1:p:903:ASN:HD22  | 1.84                     | 0.43              |
| 1:p:1161:THR:HG22 | 1:p:1216:TRP:CZ3  | 2.54                     | 0.43              |
| 2:2:184:ASN:HB2   | 2:2:198:LEU:HD11  | 1.99                     | 0.43              |
| 2:3:270:PRO:O     | 2:3:271:VAL:C     | 2.62                     | 0.43              |
| 2:h:238:LEU:HB3   | 2:h:271:VAL:HG21  | 2.01                     | 0.43              |
| 2:i:279:LEU:O     | 2:i:283:LEU:HG    | 2.18                     | 0.43              |
| 2:g:204:LEU:HB2   | 2:g:211:LEU:CD2   | 2.48                     | 0.43              |
| 2:j:66:ARG:C      | 2:j:68:THR:N      | 2.74                     | 0.43              |
| 3:N:60:VAL:O      | 3:N:63:THR:OG1    | 2.31                     | 0.43              |
| 4:T:85:VAL:HG13   | 4:T:89:PHE:HB3    | 2.00                     | 0.43              |
| 5:z:3:THR:HA      | 5:z:83:VAL:HB     | 1.99                     | 0.43              |
| 5:z:183:ILE:H     | 5:z:183:ILE:HD12  | 1.82                     | 0.43              |
| 5:X:60:ARG:NH1    | 5:X:143:ASN:OD1   | 2.51                     | 0.43              |
| 5:X:213:ALA:HA    | 5:X:216:ARG:HB2   | 2.00                     | 0.43              |
| 1:A:129:PRO:CD    | 1:B:109:THR:HB    | 2.49                     | 0.43              |
| 1:A:941:ARG:O     | 1:A:945:ASN:N     | 2.51                     | 0.43              |
| 1:A:941:ARG:NH2   | 1:F:726:ARG:HD3   | 2.33                     | 0.43              |
| 1:B:185:LEU:HD22  | 1:B:388:ARG:HH22  | 1.83                     | 0.43              |
| 1:C:404:SER:HA    | 1:C:407:ALA:HB2   | 2.00                     | 0.43              |
| 1:C:625:ALA:HA    | 1:C:867:HIS:CD2   | 2.54                     | 0.43              |
| 1:C:930:PRO:HG2   | 1:C:952:ARG:H     | 1.83                     | 0.43              |
| 1:D:344:SER:HB3   | 1:D:347:LEU:HG    | 2.01                     | 0.43              |
| 1:D:418:VAL:HG21  | 1:E:407:ALA:HB3   | 1.99                     | 0.43              |
| 1:D:577:ALA:HA    | 1:D:994:ILE:HG13  | 2.01                     | 0.43              |
| 1:D:692:LEU:HD12  | 1:D:695:LEU:CB    | 2.28                     | 0.43              |
| 1:D:1034:SER:HA   | 1:D:1076:ALA:HA   | 2.00                     | 0.43              |
| 1:E:688:ARG:HH12  | 1:F:797:HIS:HE1   | 1.66                     | 0.43              |
| 1:E:1256:ILE:HD13 | 1:E:1259:ASN:HD22 | 1.84                     | 0.43              |
| 1:F:202:THR:HA    | 1:l:22:THR:CA     | 2.49                     | 0.43              |
| 1:F:319:HIS:CE1   | 1:F:321:ALA:HB3   | 2.54                     | 0.43              |
| 1:F:598:VAL:HG11  | 1:F:647:LEU:HD23  | 2.01                     | 0.43              |
| 1:F:659:ILE:HG23  | 1:F:663:LEU:HD23  | 1.99                     | 0.43              |
| 1:F:718:PRO:HG3   | 1:F:783:LYS:HG3   | 2.01                     | 0.43              |
| 1:F:756:ALA:HA    | 1:F:759:ILE:HG12  | 2.01                     | 0.43              |
| 1:F:810:VAL:HG21  | 3:O:78:LEU:HD22   | 1.99                     | 0.43              |
| 1:G:119:LYS:HG3   | 1:m:33:PHE:CE1    | 2.54                     | 0.43              |
| 1:G:1073:GLY:HA2  | 1:m:32:MET:CG     | 2.45                     | 0.43              |
| 1:H:928:SER:HB2   | 1:H:959:LEU:HD21  | 2.00                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:I:43:ASP:O      | 1:I:46:ARG:NH1    | 2.50                     | 0.43              |
| 1:I:768:PHE:O     | 1:I:902:TYR:OH    | 2.28                     | 0.43              |
| 1:k:236:ASP:HB3   | 1:k:239:GLN:H     | 1.83                     | 0.43              |
| 1:k:603:LEU:HB3   | 1:k:794:LEU:HD21  | 1.99                     | 0.43              |
| 1:k:1342:THR:OG1  | 1:k:1343:ILE:N    | 2.52                     | 0.43              |
| 1:l:392:LEU:HA    | 1:l:1297:LYS:HB3  | 2.00                     | 0.43              |
| 1:n:220:PHE:HB2   | 1:n:1302:LEU:HD21 | 1.99                     | 0.43              |
| 1:o:556:PRO:HG3   | 1:o:881:LEU:HD11  | 2.00                     | 0.43              |
| 1:q:652:SER:HB3   | 1:q:655:MET:HG2   | 2.00                     | 0.43              |
| 1:q:681:SER:O     | 1:q:685:PHE:HB2   | 2.17                     | 0.43              |
| 2:j:270:PRO:O     | 2:j:271:VAL:C     | 2.62                     | 0.43              |
| 3:r:41:ARG:HA     | 3:r:65:ILE:HG21   | 2.01                     | 0.43              |
| 4:V:45:HIS:HE1    | 4:V:159:MET:HA    | 1.83                     | 0.43              |
| 5:1:34:ARG:HG3    | 5:1:83:VAL:HG21   | 2.00                     | 0.43              |
| 5:a:28:VAL:HG21   | 5:a:133:ILE:HD11  | 1.99                     | 0.43              |
| 5:d:204:ALA:HA    | 5:d:207:SER:HB2   | 2.00                     | 0.43              |
| 1:A:86:LYS:HD3    | 1:F:49:LEU:HB2    | 2.00                     | 0.43              |
| 1:A:210:ARG:HH22  | 1:A:1186:VAL:HA   | 1.83                     | 0.43              |
| 1:A:435:ASP:OD2   | 1:B:218:GLN:NE2   | 2.51                     | 0.43              |
| 1:A:1309:HIS:HD2  | 1:A:1328:GLY:HA2  | 1.82                     | 0.43              |
| 1:B:181:LEU:HD21  | 1:B:386:LEU:HG    | 1.99                     | 0.43              |
| 1:B:815:THR:HG22  | 1:B:816:LYS:HG3   | 2.00                     | 0.43              |
| 1:C:300:PRO:HA    | 1:C:353:PHE:HA    | 2.01                     | 0.43              |
| 1:C:620:HIS:HB2   | 1:C:722:GLN:HB3   | 2.01                     | 0.43              |
| 1:C:677:ARG:HG3   | 1:D:606:HIS:HE1   | 1.84                     | 0.43              |
| 1:C:1179:ARG:HG3  | 1:C:1205:ASP:HB2  | 1.99                     | 0.43              |
| 1:C:1233:ARG:O    | 1:C:1238:HIS:ND1  | 2.48                     | 0.43              |
| 1:E:14:LEU:HB2    | 1:l:58:TYR:CD1    | 2.52                     | 0.43              |
| 1:E:20:LEU:HD13   | 1:l:379:ASN:OD1   | 2.17                     | 0.43              |
| 1:E:152:LEU:HB2   | 1:F:333:ILE:HG23  | 2.00                     | 0.43              |
| 1:F:452:HIS:HD2   | 1:F:1098:PHE:HD1  | 1.66                     | 0.43              |
| 1:F:458:ALA:HB2   | 1:F:539:PHE:CD2   | 2.53                     | 0.43              |
| 1:F:1167:LEU:HD11 | 1:F:1332:THR:HG21 | 2.01                     | 0.43              |
| 1:G:95:TYR:CD2    | 1:m:13:LYS:HE2    | 2.54                     | 0.43              |
| 1:G:455:ILE:HG23  | 1:G:1223:LEU:HD21 | 2.00                     | 0.43              |
| 1:G:744:HIS:CB    | 2:e:175:ALA:N     | 2.70                     | 0.43              |
| 1:H:1159:ILE:HG12 | 1:H:1223:LEU:HD12 | 2.00                     | 0.43              |
| 1:I:294:ARG:HD2   | 1:I:357:GLN:HB3   | 1.99                     | 0.43              |
| 1:I:308:LEU:HD22  | 1:I:322:ILE:HD12  | 2.01                     | 0.43              |
| 1:I:1020:VAL:HG11 | 1:I:1094:MET:HE1  | 2.01                     | 0.43              |
| 1:k:535:LEU:HD12  | 1:k:541:PHE:HE2   | 1.83                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:k:583:LEU:HD11  | 1:k:1012:LEU:HB2  | 2.00                     | 0.43              |
| 1:l:388:ARG:HD3   | 1:l:1295:VAL:HG23 | 2.01                     | 0.43              |
| 1:m:171:ALA:HB2   | 1:n:100:ARG:HB3   | 2.00                     | 0.43              |
| 1:m:278:HIS:HA    | 1:m:372:HIS:CE1   | 2.54                     | 0.43              |
| 1:m:430:TYR:O     | 1:m:431:PHE:CD1   | 2.70                     | 0.43              |
| 1:n:816:LYS:HG2   | 1:n:833:LEU:HD23  | 2.01                     | 0.43              |
| 1:n:1019:THR:HG23 | 1:n:1160:LEU:HD11 | 2.01                     | 0.43              |
| 1:n:1171:ARG:NH1  | 1:n:1332:THR:HG22 | 2.33                     | 0.43              |
| 1:o:128:ILE:HG22  | 1:p:102:ALA:HB3   | 2.00                     | 0.43              |
| 1:o:189:PRO:HA    | 1:o:190:PRO:HD3   | 1.86                     | 0.43              |
| 1:o:577:ALA:HA    | 1:o:994:ILE:HG13  | 2.00                     | 0.43              |
| 1:p:134:ALA:O     | 1:p:138:THR:OG1   | 2.27                     | 0.43              |
| 1:p:528:ASN:HB3   | 1:p:531:LEU:HG    | 1.99                     | 0.43              |
| 1:p:632:LEU:O     | 1:p:636:CYS:HB2   | 2.19                     | 0.43              |
| 1:q:959:LEU:HB3   | 1:q:964:ALA:HB3   | 2.01                     | 0.43              |
| 2:2:104:LYS:HG3   | 2:3:92:LEU:HD13   | 2.01                     | 0.43              |
| 2:3:81:HIS:O      | 2:3:82:GLU:C      | 2.62                     | 0.43              |
| 2:g:104:LYS:HG3   | 2:g:105:LEU:N     | 2.34                     | 0.43              |
| 3:R:85:LEU:HA     | 3:R:88:LEU:HD12   | 2.00                     | 0.43              |
| 4:y:215:HIS:HE1   | 5:z:290:GLN:HB2   | 1.82                     | 0.43              |
| 5:W:5:VAL:HB      | 5:W:81:LEU:HB2    | 2.01                     | 0.43              |
| 5:W:202:MET:HE3   | 5:W:202:MET:HB2   | 1.89                     | 0.43              |
| 5:X:30:PRO:HG2    | 5:X:45:LEU:HB2    | 2.01                     | 0.43              |
| 1:A:37:ARG:NH2    | 1:A:43:ASP:OD2    | 2.52                     | 0.43              |
| 1:A:1230:THR:H    | 1:A:1251:THR:HG22 | 1.84                     | 0.43              |
| 1:B:225:LEU:O     | 1:B:233:ARG:NH2   | 2.52                     | 0.43              |
| 1:B:438:PRO:HD2   | 1:C:1172:TYR:CD1  | 2.54                     | 0.43              |
| 1:C:210:ARG:HH22  | 1:C:1186:VAL:HG23 | 1.82                     | 0.43              |
| 1:C:221:LYS:HE3   | 1:C:1173:PRO:HG2  | 2.01                     | 0.43              |
| 1:C:367:LEU:HD23  | 1:C:367:LEU:HA    | 1.90                     | 0.43              |
| 1:C:724:LEU:HB3   | 1:C:772:ARG:HB2   | 2.00                     | 0.43              |
| 1:F:650:ALA:O     | 1:F:785:TYR:OH    | 2.36                     | 0.43              |
| 1:G:483:ARG:HG3   | 1:G:484:GLU:HG2   | 2.01                     | 0.43              |
| 1:G:1314:GLN:NE2  | 1:H:1167:LEU:HD13 | 2.34                     | 0.43              |
| 1:H:620:HIS:HB3   | 1:H:869:PRO:HG3   | 2.00                     | 0.43              |
| 1:I:146:ASP:OD1   | 1:I:146:ASP:N     | 2.51                     | 0.43              |
| 1:I:184:LEU:O     | 1:I:188:ALA:HB2   | 2.18                     | 0.43              |
| 1:l:208:ALA:HB1   | 1:l:213:ARG:HB3   | 2.01                     | 0.43              |
| 1:m:51:PHE:HD1    | 1:n:87:MET:C      | 1.97                     | 0.43              |
| 1:m:748:ARG:NH1   | 2:e:269:ARG:CZ    | 2.74                     | 0.43              |
| 1:m:816:LYS:HB3   | 1:m:835:ASN:HD22  | 1.82                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:n:231:LEU:HG    | 1:n:235:ARG:HH22  | 1.83                     | 0.43              |
| 1:o:1314:GLN:HB3  | 1:p:1167:LEU:HD13 | 2.00                     | 0.43              |
| 1:p:603:LEU:HB3   | 1:p:794:LEU:HD21  | 2.01                     | 0.43              |
| 1:p:1025:THR:H    | 1:p:1088:SER:HB2  | 1.82                     | 0.43              |
| 1:q:761:MET:HG2   | 1:q:870:GLU:HB2   | 2.01                     | 0.43              |
| 2:3:279:LEU:O     | 2:3:283:LEU:HG    | 2.18                     | 0.43              |
| 2:e:105:LEU:CD1   | 2:e:212:VAL:HG11  | 2.39                     | 0.43              |
| 2:g:104:LYS:HG3   | 2:j:92:LEU:HD13   | 2.01                     | 0.43              |
| 4:S:190:PHE:HD2   | 4:S:253:GLN:HE21  | 1.66                     | 0.43              |
| 4:V:69:LEU:HG     | 4:V:167:LEU:HD11  | 2.00                     | 0.43              |
| 5:W:8:THR:HB      | 5:W:39:GLY:HA2    | 2.01                     | 0.43              |
| 5:X:138:LEU:HD13  | 5:X:173:TYR:HB3   | 1.99                     | 0.43              |
| 5:Z:25:ILE:HG23   | 5:Z:72:ARG:HA     | 2.01                     | 0.43              |
| 5:Z:89:CYS:HA     | 5:Z:308:ILE:CG1   | 2.48                     | 0.43              |
| 5:b:152:LEU:HD22  | 5:b:161:VAL:HG13  | 2.01                     | 0.43              |
| 5:c:86:HIS:HA     | 5:c:309:TYR:HD2   | 1.83                     | 0.43              |
| 5:d:30:PRO:HG3    | 5:d:45:LEU:HD12   | 2.01                     | 0.43              |
| 1:A:395:TYR:HD1   | 1:A:1305:ALA:HB3  | 1.84                     | 0.43              |
| 1:A:648:ALA:O     | 1:A:676:TYR:OH    | 2.26                     | 0.43              |
| 1:B:513:GLU:HA    | 1:B:973:THR:HG21  | 1.99                     | 0.43              |
| 1:B:653:TYR:HA    | 1:B:656:VAL:HG12  | 2.00                     | 0.43              |
| 1:B:724:LEU:HD22  | 1:B:772:ARG:HD2   | 2.00                     | 0.43              |
| 1:C:684:ARG:NH2   | 1:C:778:GLU:OE2   | 2.51                     | 0.43              |
| 1:C:908:THR:HG22  | 1:C:909:THR:HG23  | 2.01                     | 0.43              |
| 1:C:1179:ARG:NH2  | 1:C:1203:SER:O    | 2.44                     | 0.43              |
| 1:D:206:ARG:HH11  | 1:D:209:THR:HG21  | 1.84                     | 0.43              |
| 1:D:431:PHE:N     | 1:D:439:GLN:O     | 2.48                     | 0.43              |
| 1:D:1085:ARG:HD3  | 1:E:200:HIS:HA    | 2.00                     | 0.43              |
| 1:D:1233:ARG:O    | 1:D:1238:HIS:ND1  | 2.52                     | 0.43              |
| 1:D:1322:LYS:HZ3  | 1:E:1331:GLU:HA   | 1.84                     | 0.43              |
| 1:F:558:ILE:HD13  | 1:F:970:TRP:HA    | 1.99                     | 0.43              |
| 1:F:819:LEU:HB2   | 3:O:58:GLN:CD     | 2.43                     | 0.43              |
| 1:H:1093:ARG:HH11 | 1:H:1153:ARG:HD2  | 1.83                     | 0.43              |
| 1:H:1097:LEU:HA   | 1:H:1100:VAL:HB   | 2.01                     | 0.43              |
| 1:I:398:VAL:HG13  | 1:I:1018:LEU:HB2  | 2.01                     | 0.43              |
| 1:I:466:ALA:HA    | 1:I:552:PRO:HG3   | 2.00                     | 0.43              |
| 1:k:1276:CYS:SG   | 1:k:1277:ILE:N    | 2.92                     | 0.43              |
| 1:l:419:ASP:OD1   | 1:l:424:GLN:NE2   | 2.52                     | 0.43              |
| 1:l:805:LEU:HA    | 1:l:808:LEU:HB3   | 2.00                     | 0.43              |
| 1:l:815:THR:HB    | 1:l:833:LEU:HD22  | 2.01                     | 0.43              |
| 1:l:1136:THR:CB   | 4:T:116:ILE:CG1   | 2.97                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:l:1164:SER:HB3  | 1:l:1213:ASN:HD21 | 1.84                     | 0.43              |
| 1:m:73:ALA:HA     | 1:m:76:ALA:HB3    | 1.99                     | 0.43              |
| 1:m:567:LEU:HD22  | 1:m:1161:THR:HG21 | 2.00                     | 0.43              |
| 1:n:482:ARG:HD3   | 1:n:485:PHE:HB3   | 2.00                     | 0.43              |
| 1:o:1048:VAL:HG22 | 1:o:1061:VAL:HG12 | 2.01                     | 0.43              |
| 1:p:299:THR:HA    | 1:p:300:PRO:HD3   | 1.87                     | 0.43              |
| 1:p:433:ASN:OD1   | 1:p:439:GLN:NE2   | 2.39                     | 0.43              |
| 1:p:613:TYR:HA    | 1:p:616:GLU:HG2   | 2.01                     | 0.43              |
| 1:p:1017:ALA:N    | 1:p:1160:LEU:O    | 2.51                     | 0.43              |
| 2:h:81:HIS:O      | 2:h:82:GLU:C      | 2.62                     | 0.43              |
| 2:h:279:LEU:O     | 2:h:283:LEU:HG    | 2.18                     | 0.43              |
| 2:j:81:HIS:O      | 2:j:82:GLU:C      | 2.62                     | 0.43              |
| 4:S:69:LEU:HG     | 4:S:167:LEU:HD11  | 2.00                     | 0.43              |
| 5:z:49:VAL:HG23   | 5:z:50:LYS:HD3    | 2.01                     | 0.43              |
| 5:z:215:VAL:HG11  | 5:1:202:MET:HE3   | 2.01                     | 0.43              |
| 5:Y:277:PHE:CE2   | 5:c:144:GLN:HG2   | 2.54                     | 0.43              |
| 5:1:21:LEU:HB3    | 5:1:74:VAL:HG21   | 2.01                     | 0.43              |
| 1:A:1171:ARG:NH1  | 1:A:1332:THR:HG22 | 2.33                     | 0.43              |
| 1:B:458:ALA:O     | 1:B:462:LEU:N     | 2.41                     | 0.43              |
| 1:B:1320:GLN:HB3  | 1:B:1327:LEU:HA   | 1.99                     | 0.43              |
| 1:C:235:ARG:NH1   | 1:C:239:GLN:O     | 2.52                     | 0.43              |
| 1:C:866:ALA:O     | 3:L:86:ARG:NH2    | 2.52                     | 0.43              |
| 1:C:1149:LEU:HD22 | 1:D:1207:GLN:HG3  | 2.01                     | 0.43              |
| 1:D:818:PHE:O     | 3:M:58:GLN:NE2    | 2.50                     | 0.43              |
| 1:E:458:ALA:HB3   | 1:E:890:PRO:HB2   | 2.01                     | 0.43              |
| 1:E:920:VAL:HG12  | 1:E:937:ASN:HD22  | 1.84                     | 0.43              |
| 1:E:1201:HIS:HE2  | 1:E:1219:GLN:HG3  | 1.83                     | 0.43              |
| 1:G:562:ASN:HD22  | 1:G:972:ARG:HB2   | 1.84                     | 0.43              |
| 1:G:1309:HIS:CG   | 1:G:1327:LEU:HD12 | 2.54                     | 0.43              |
| 1:H:456:HIS:CD2   | 1:H:1001:PRO:HB3  | 2.53                     | 0.43              |
| 1:H:1096:ASP:N    | 1:H:1096:ASP:OD1  | 2.51                     | 0.43              |
| 1:I:92:MET:HE3    | 1:I:1068:VAL:HG11 | 2.01                     | 0.43              |
| 1:k:484:GLU:OE2   | 1:k:966:GLU:N     | 2.51                     | 0.43              |
| 1:k:1034:SER:HA   | 1:k:1076:ALA:HA   | 2.01                     | 0.43              |
| 1:l:272:GLY:H     | 1:l:1036:LYS:HB2  | 1.84                     | 0.43              |
| 1:m:431:PHE:CD1   | 1:m:1310:THR:HA   | 2.39                     | 0.43              |
| 1:m:443:HIS:HA    | 1:m:446:ALA:HB3   | 1.99                     | 0.43              |
| 1:m:608:TYR:HA    | 1:m:609:PRO:HD3   | 1.84                     | 0.43              |
| 1:m:1029:ASP:N    | 1:m:1082:HIS:O    | 2.49                     | 0.43              |
| 1:n:152:LEU:HD12  | 1:o:333:ILE:HA    | 2.01                     | 0.43              |
| 1:o:871:ASN:OD1   | 1:o:872:ALA:N     | 2.48                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:p:170:ASP:OD1   | 1:p:174:ARG:NE    | 2.52                     | 0.43              |
| 1:p:389:ASP:OD1   | 1:p:389:ASP:N     | 2.43                     | 0.43              |
| 2:f:104:LYS:HG3   | 2:f:105:LEU:N     | 2.34                     | 0.43              |
| 2:i:83:LYS:HD2    | 2:i:83:LYS:HA     | 1.88                     | 0.43              |
| 4:S:200:ARG:NH1   | 4:S:245:SER:O     | 2.52                     | 0.43              |
| 4:U:85:VAL:HG13   | 4:U:89:PHE:HD2    | 1.84                     | 0.43              |
| 5:X:21:LEU:HB3    | 5:X:74:VAL:HG21   | 2.01                     | 0.43              |
| 5:X:33:TYR:CD2    | 5:X:35:HIS:HB2    | 2.52                     | 0.43              |
| 5:c:266:PRO:HA    | 5:c:269:GLU:HB3   | 2.01                     | 0.43              |
| 1:A:92:MET:HE3    | 1:A:1068:VAL:HG21 | 2.01                     | 0.43              |
| 1:B:704:LEU:HA    | 1:B:707:TYR:HD2   | 1.84                     | 0.43              |
| 1:B:988:SER:HA    | 1:B:991:THR:HG22  | 2.00                     | 0.43              |
| 1:B:1029:ASP:N    | 1:B:1082:HIS:O    | 2.51                     | 0.43              |
| 1:C:170:ASP:OD2   | 1:C:174:ARG:NH2   | 2.52                     | 0.43              |
| 1:C:544:HIS:ND1   | 1:C:553:LEU:HB2   | 2.33                     | 0.43              |
| 1:C:966:GLU:HA    | 1:C:969:HIS:CD2   | 2.54                     | 0.43              |
| 1:D:656:VAL:HG23  | 1:D:676:TYR:HD1   | 1.84                     | 0.43              |
| 1:D:753:SER:HB3   | 3:M:87:MET:CG     | 2.49                     | 0.43              |
| 1:D:795:ASN:HB3   | 1:D:980:ALA:HA    | 2.00                     | 0.43              |
| 1:E:153:LEU:HD11  | 1:l:47:TYR:HA     | 2.01                     | 0.43              |
| 1:E:849:ASP:HB3   | 1:E:852:VAL:H     | 1.84                     | 0.43              |
| 1:E:1243:TYR:HD1  | 1:E:1286:ILE:HG22 | 1.84                     | 0.43              |
| 1:F:929:ASP:HB3   | 1:F:932:LEU:HB3   | 2.01                     | 0.43              |
| 1:F:1021:VAL:HG22 | 1:F:1156:CYS:HB3  | 2.01                     | 0.43              |
| 1:G:326:PHE:CE1   | 1:n:318:ALA:CB    | 2.98                     | 0.43              |
| 1:G:1034:SER:HA   | 1:G:1076:ALA:HA   | 2.00                     | 0.43              |
| 1:H:493:ALA:HA    | 1:H:496:ARG:HB2   | 2.00                     | 0.43              |
| 1:H:934:ALA:HB2   | 1:H:944:LEU:HD12  | 2.01                     | 0.43              |
| 1:H:1131:ALA:HA   | 1:H:1134:ILE:HD12 | 2.01                     | 0.43              |
| 1:I:258:ASN:HB2   | 1:I:261:THR:HG22  | 2.01                     | 0.43              |
| 1:I:555:THR:HG22  | 1:I:972:ARG:HH22  | 1.83                     | 0.43              |
| 1:I:577:ALA:HA    | 1:I:994:ILE:HG21  | 2.00                     | 0.43              |
| 1:I:753:SER:C     | 3:R:83:ASP:CG     | 2.87                     | 0.43              |
| 1:I:1300:ARG:H    | 1:I:1303:GLN:HE21 | 1.67                     | 0.43              |
| 1:k:67:PHE:N      | 1:k:173:GLU:OE1   | 2.50                     | 0.43              |
| 1:l:282:GLN:O     | 1:l:286:ASN:ND2   | 2.52                     | 0.43              |
| 1:m:168:THR:HG22  | 4:S:12:ARG:NE     | 2.34                     | 0.43              |
| 1:m:493:ALA:O     | 1:m:497:LEU:CB    | 2.67                     | 0.43              |
| 1:n:816:LYS:HE2   | 1:n:833:LEU:HG    | 2.00                     | 0.43              |
| 1:n:966:GLU:HA    | 1:n:969:HIS:HD2   | 1.84                     | 0.43              |
| 1:n:1041:VAL:HG12 | 1:n:1067:THR:HG22 | 2.00                     | 0.43              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:n:1089:ASP:N    | 1:n:1089:ASP:OD1 | 2.51                     | 0.43              |
| 1:o:418:VAL:H     | 1:p:408:TYR:HA   | 1.84                     | 0.43              |
| 1:o:596:LEU:HD22  | 1:o:793:VAL:HG21 | 2.01                     | 0.43              |
| 1:o:1297:LYS:HD3  | 1:o:1299:CYS:HB2 | 2.00                     | 0.43              |
| 1:p:1194:ALA:O    | 1:p:1197:THR:OG1 | 2.32                     | 0.43              |
| 1:q:564:PRO:HD2   | 1:q:567:LEU:HD12 | 2.00                     | 0.43              |
| 2:2:101:ASP:CA    | 2:2:104:LYS:HG2  | 2.43                     | 0.43              |
| 2:2:104:LYS:HG3   | 2:2:105:LEU:N    | 2.34                     | 0.43              |
| 2:3:66:ARG:HD2    | 2:3:69:GLN:HG3   | 2.01                     | 0.43              |
| 2:3:88:ARG:HA     | 2:3:89:PRO:HD3   | 1.69                     | 0.43              |
| 2:e:104:LYS:HG3   | 2:h:92:LEU:HD13  | 2.01                     | 0.43              |
| 5:W:46:ASP:HB2    | 5:W:129:VAL:H    | 1.83                     | 0.43              |
| 5:b:28:VAL:HG21   | 5:b:133:ILE:HD11 | 2.00                     | 0.43              |
| 1:A:54:ILE:HG12   | 1:B:91:LYS:HE3   | 2.01                     | 0.42              |
| 1:B:121:SER:HA    | 1:B:1068:VAL:HA  | 2.00                     | 0.42              |
| 1:C:65:VAL:HG21   | 1:C:376:VAL:HG12 | 2.01                     | 0.42              |
| 1:D:1276:CYS:O    | 1:D:1287:CYS:N   | 2.46                     | 0.42              |
| 1:E:311:GLU:OE2   | 1:E:327:SER:N    | 2.52                     | 0.42              |
| 1:E:813:PHE:CG    | 3:N:85:LEU:HG    | 2.53                     | 0.42              |
| 1:E:1300:ARG:H    | 1:E:1303:GLN:NE2 | 2.17                     | 0.42              |
| 1:F:966:GLU:HA    | 1:F:969:HIS:HD2  | 1.84                     | 0.42              |
| 1:F:1175:ASN:HD22 | 1:F:1180:SER:HA  | 1.84                     | 0.42              |
| 1:G:698:ARG:HG2   | 1:G:699:LEU:O    | 2.18                     | 0.42              |
| 1:H:688:ARG:HH12  | 1:I:797:HIS:CE1  | 2.37                     | 0.42              |
| 1:I:121:SER:HA    | 1:I:1068:VAL:HA  | 2.01                     | 0.42              |
| 1:I:506:ASP:OD2   | 1:I:949:GLN:NE2  | 2.52                     | 0.42              |
| 1:l:453:PRO:HB2   | 1:l:887:HIS:CE1  | 2.53                     | 0.42              |
| 1:l:462:LEU:HD22  | 1:l:890:PRO:HG3  | 2.01                     | 0.42              |
| 1:n:705:LEU:HD23  | 1:n:705:LEU:HA   | 1.79                     | 0.42              |
| 1:o:753:SER:HB2   | 3:v:83:ASP:OD1   | 2.18                     | 0.42              |
| 1:p:558:ILE:HD13  | 1:p:970:TRP:HA   | 2.01                     | 0.42              |
| 1:p:560:VAL:HA    | 1:p:999:MET:HE3  | 2.01                     | 0.42              |
| 2:3:238:LEU:HB3   | 2:3:271:VAL:HG21 | 2.01                     | 0.42              |
| 2:i:110:ALA:HB3   | 5:c:225:MET:HG2  | 2.01                     | 0.42              |
| 4:S:116:ILE:O     | 4:S:120:LEU:N    | 2.52                     | 0.42              |
| 4:S:141:THR:HB    | 4:S:147:LEU:HB3  | 2.01                     | 0.42              |
| 4:U:252:LEU:O     | 4:U:291:VAL:N    | 2.47                     | 0.42              |
| 5:z:98:VAL:HG23   | 5:z:100:TRP:CD1  | 2.53                     | 0.42              |
| 5:Y:97:PRO:HD3    | 5:Y:132:TRP:CE3  | 2.54                     | 0.42              |
| 5:Z:280:ILE:HD11  | 5:d:287:ILE:HG13 | 2.00                     | 0.42              |
| 1:A:1129:SER:HB3  | 4:U:120:LEU:HD21 | 2.00                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1329:LEU:HD23 | 1:A:1329:LEU:HA   | 1.88                     | 0.42              |
| 1:B:441:ILE:HD13  | 1:B:1092:SER:HB3  | 2.00                     | 0.42              |
| 1:C:268:GLU:HB3   | 1:C:367:LEU:HD12  | 2.00                     | 0.42              |
| 1:C:506:ASP:OD2   | 1:C:949:GLN:NE2   | 2.51                     | 0.42              |
| 1:C:1101:PHE:HB3  | 1:C:1104:HIS:HD2  | 1.84                     | 0.42              |
| 1:D:691:GLU:OE1   | 1:E:953:CYS:HB3   | 2.19                     | 0.42              |
| 1:E:589:PRO:HB2   | 1:E:592:HIS:CD2   | 2.54                     | 0.42              |
| 1:E:1274:GLN:HE21 | 1:E:1291:THR:H    | 1.67                     | 0.42              |
| 1:F:115:VAL:HG22  | 1:l:38:LEU:HD13   | 2.01                     | 0.42              |
| 1:F:755:VAL:HG21  | 3:O:71:MET:HG3    | 1.99                     | 0.42              |
| 1:F:1230:THR:H    | 1:F:1251:THR:HG22 | 1.83                     | 0.42              |
| 1:F:1263:PHE:HB2  | 1:l:31:GLU:O      | 2.19                     | 0.42              |
| 1:G:132:ILE:HD13  | 1:G:161:VAL:HG22  | 2.00                     | 0.42              |
| 1:G:258:ASN:HB3   | 1:G:260:GLU:HG2   | 2.00                     | 0.42              |
| 1:G:865:VAL:HA    | 1:G:868:VAL:HG23  | 2.00                     | 0.42              |
| 1:G:982:CYS:HG    | 1:G:988:SER:HG    | 1.66                     | 0.42              |
| 1:G:1018:LEU:CG   | 1:G:1159:ILE:HD13 | 2.48                     | 0.42              |
| 1:H:882:ASP:N     | 1:H:882:ASP:OD1   | 2.53                     | 0.42              |
| 1:k:275:VAL:HG23  | 1:k:1032:LEU:HB3  | 2.01                     | 0.42              |
| 1:l:103:THR:OG1   | 1:l:104:GLY:N     | 2.52                     | 0.42              |
| 1:m:71:ALA:HB3    | 1:m:371:GLU:HB2   | 2.01                     | 0.42              |
| 1:m:1283:LEU:HD12 | 1:m:1283:LEU:HA   | 1.88                     | 0.42              |
| 1:n:899:HIS:HD2   | 1:n:969:HIS:CE1   | 2.37                     | 0.42              |
| 1:o:883:PRO:HA    | 1:o:886:ARG:HB2   | 2.01                     | 0.42              |
| 1:o:1019:THR:CG2  | 1:o:1160:LEU:CD1  | 2.97                     | 0.42              |
| 1:p:224:MET:HE2   | 1:p:224:MET:HB3   | 1.87                     | 0.42              |
| 1:p:274:ILE:HB    | 1:p:370:LEU:HD23  | 2.01                     | 0.42              |
| 1:p:292:ILE:HG12  | 1:p:361:LEU:HB3   | 2.01                     | 0.42              |
| 1:p:750:PRO:HA    | 3:w:86:ARG:HH22   | 1.84                     | 0.42              |
| 1:q:522:GLU:HA    | 1:q:525:LYS:HB2   | 2.01                     | 0.42              |
| 1:q:716:LEU:HB3   | 1:q:783:LYS:HE3   | 2.01                     | 0.42              |
| 1:q:886:ARG:HG3   | 1:q:1107:ARG:HH21 | 1.84                     | 0.42              |
| 2:i:238:LEU:HB3   | 2:i:271:VAL:HG21  | 2.01                     | 0.42              |
| 3:K:39:GLU:OE2    | 3:K:43:GLN:NE2    | 2.48                     | 0.42              |
| 4:y:95:GLU:H      | 4:y:205:SER:HA    | 1.83                     | 0.42              |
| 4:y:129:ARG:O     | 4:y:132:HIS:NE2   | 2.52                     | 0.42              |
| 4:S:69:LEU:HD12   | 4:S:87:LEU:HD22   | 2.01                     | 0.42              |
| 4:V:217:HIS:HA    | 4:V:220:ILE:HG12  | 2.01                     | 0.42              |
| 4:V:232:PHE:HB3   | 5:d:229:LYS:HZ2   | 1.82                     | 0.42              |
| 5:z:101:GLU:O     | 5:z:104:ASP:CG    | 2.63                     | 0.42              |
| 5:W:189:VAL:O     | 5:W:193:MET:N     | 2.45                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:1:149:LEU:O     | 5:1:153:SER:CB    | 2.66                     | 0.42              |
| 5:a:112:VAL:HG11  | 5:a:180:LEU:HD12  | 2.00                     | 0.42              |
| 1:A:103:THR:OG1   | 1:A:104:GLY:N     | 2.52                     | 0.42              |
| 1:B:537:PRO:HG3   | 1:B:1159:ILE:HG21 | 2.01                     | 0.42              |
| 1:B:756:ALA:HA    | 1:B:759:ILE:HG12  | 2.01                     | 0.42              |
| 1:C:68:LEU:HA     | 1:C:73:ALA:HB2    | 2.02                     | 0.42              |
| 1:C:718:PRO:HA    | 1:C:719:PRO:HD3   | 1.92                     | 0.42              |
| 1:C:859:GLU:OE2   | 3:L:92:LYS:HE2    | 2.19                     | 0.42              |
| 1:D:360:VAL:HA    | 1:D:369:ALA:HA    | 2.01                     | 0.42              |
| 1:D:688:ARG:HH12  | 1:E:797:HIS:CE1   | 2.37                     | 0.42              |
| 1:E:276:SER:HB2   | 1:E:281:VAL:HG23  | 2.00                     | 0.42              |
| 1:E:278:HIS:HB2   | 1:E:374:ARG:HD2   | 2.00                     | 0.42              |
| 1:F:400:LEU:HD12  | 1:F:1162:PRO:HA   | 2.00                     | 0.42              |
| 1:F:538:PHE:HD1   | 1:F:999:MET:HB3   | 1.84                     | 0.42              |
| 1:G:262:TYR:HB3   | 1:G:270:LEU:HD12  | 2.00                     | 0.42              |
| 1:G:695:LEU:HB3   | 1:G:704:LEU:HD23  | 2.00                     | 0.42              |
| 1:G:1177:ARG:HH21 | 1:G:1181:SER:HB3  | 1.85                     | 0.42              |
| 1:H:576:ARG:HH11  | 1:H:1014:PRO:HA   | 1.83                     | 0.42              |
| 1:H:652:SER:HB3   | 1:H:655:MET:HG2   | 2.00                     | 0.42              |
| 1:H:1046:PRO:HA   | 1:H:1062:SER:O    | 2.19                     | 0.42              |
| 1:I:393:THR:HA    | 1:I:1023:THR:HA   | 2.01                     | 0.42              |
| 1:I:1333:HIS:HB3  | 1:I:1336:ASN:HB2  | 2.00                     | 0.42              |
| 1:k:1183:MET:HB3  | 1:k:1259:ASN:OD1  | 2.20                     | 0.42              |
| 1:l:619:ILE:HD11  | 1:l:864:LEU:HD13  | 2.00                     | 0.42              |
| 1:l:1050:LYS:NZ   | 4:T:33:ARG:HH11   | 2.16                     | 0.42              |
| 1:l:1139:ARG:NE   | 4:T:79:MET:CB     | 2.82                     | 0.42              |
| 1:l:1228:TYR:HB2  | 1:l:1250:PHE:HD2  | 1.84                     | 0.42              |
| 1:m:184:LEU:O     | 1:m:188:ALA:HB2   | 2.19                     | 0.42              |
| 1:m:558:ILE:HG21  | 1:m:970:TRP:CZ3   | 2.55                     | 0.42              |
| 1:m:815:THR:OG1   | 1:m:836:ASN:ND2   | 2.52                     | 0.42              |
| 1:m:921:ILE:HG22  | 1:m:923:PHE:HB3   | 2.02                     | 0.42              |
| 1:m:1152:GLN:HB2  | 1:m:1283:LEU:O    | 2.18                     | 0.42              |
| 1:m:1194:ALA:O    | 1:m:1197:THR:OG1  | 2.26                     | 0.42              |
| 1:n:863:HIS:CE1   | 3:u:93:LYS:HA     | 2.55                     | 0.42              |
| 1:n:1021:VAL:HG22 | 1:n:1156:CYS:HB3  | 2.02                     | 0.42              |
| 1:n:1117:GLN:NE2  | 1:o:475:ASP:OD2   | 2.52                     | 0.42              |
| 1:n:1278:HIS:HE1  | 1:n:1280:GLU:HB2  | 1.85                     | 0.42              |
| 1:o:1178:GLY:HA3  | 1:o:1214:ASN:H    | 1.85                     | 0.42              |
| 1:p:849:ASP:HB3   | 1:p:852:VAL:H     | 1.83                     | 0.42              |
| 1:p:1153:ARG:NH1  | 1:p:1282:ASP:OD1  | 2.50                     | 0.42              |
| 1:q:629:GLY:HA2   | 1:q:864:LEU:HD11  | 2.02                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:e:252:PHE:HB2   | 2:e:264:ARG:HB2   | 2.01                     | 0.42              |
| 2:h:208:PRO:CG    | 5:a:229:LYS:NZ    | 2.75                     | 0.42              |
| 2:g:184:ASN:HB2   | 2:g:198:LEU:HD11  | 1.99                     | 0.42              |
| 4:y:72:ARG:NH2    | 5:l:105:VAL:H     | 2.17                     | 0.42              |
| 4:T:223:LEU:O     | 4:T:227:PHE:N     | 2.49                     | 0.42              |
| 4:V:215:HIS:CD2   | 4:V:218:THR:H     | 2.32                     | 0.42              |
| 5:z:69:THR:HG22   | 5:z:83:VAL:HG22   | 2.01                     | 0.42              |
| 5:W:267:THR:HA    | 5:W:270:LEU:HD12  | 2.01                     | 0.42              |
| 5:Y:127:ASP:OD1   | 5:Y:127:ASP:N     | 2.48                     | 0.42              |
| 1:A:1249:PHE:HZ   | 1:A:1305:ALA:HB2  | 1.84                     | 0.42              |
| 1:B:210:ARG:NH1   | 1:B:1187:ASP:OD2  | 2.52                     | 0.42              |
| 1:B:506:ASP:OD2   | 1:B:949:GLN:NE2   | 2.52                     | 0.42              |
| 1:B:632:LEU:HD22  | 1:B:860:GLU:HB3   | 2.01                     | 0.42              |
| 1:B:711:LEU:HD22  | 1:B:996:HIS:HB2   | 2.00                     | 0.42              |
| 1:C:273:VAL:HG23  | 1:C:369:ALA:HB3   | 2.01                     | 0.42              |
| 1:D:195:ARG:NH1   | 1:D:199:GLU:OE1   | 2.53                     | 0.42              |
| 1:E:555:THR:HG22  | 1:E:972:ARG:HH12  | 1.85                     | 0.42              |
| 1:E:1038:SER:OG   | 1:E:1039:THR:N    | 2.53                     | 0.42              |
| 1:E:1320:GLN:HE22 | 1:E:1329:LEU:HB2  | 1.85                     | 0.42              |
| 1:F:263:THR:HA    | 1:F:269:ARG:HA    | 2.02                     | 0.42              |
| 1:G:387:GLU:HB3   | 1:G:1084:ARG:HH11 | 1.83                     | 0.42              |
| 1:G:431:PHE:CE1   | 1:G:1311:GLY:N    | 2.87                     | 0.42              |
| 1:G:898:GLN:HG2   | 1:G:970:TRP:CD1   | 2.55                     | 0.42              |
| 1:G:991:THR:O     | 1:G:995:MET:N     | 2.49                     | 0.42              |
| 1:G:1017:ALA:C    | 1:G:1018:LEU:CD1  | 2.71                     | 0.42              |
| 1:G:1060:HIS:NE2  | 5:W:2:GLU:HG2     | 2.33                     | 0.42              |
| 1:H:72:LEU:HD22   | 1:H:177:ILE:HG23  | 2.01                     | 0.42              |
| 1:H:663:LEU:HD23  | 1:H:673:TYR:CG    | 2.54                     | 0.42              |
| 1:H:1166:ASP:HA   | 1:H:1170:PHE:CD2  | 2.54                     | 0.42              |
| 1:I:1096:ASP:OD1  | 1:I:1096:ASP:N    | 2.49                     | 0.42              |
| 1:k:292:ILE:HG12  | 1:k:361:LEU:HB3   | 2.00                     | 0.42              |
| 1:k:693:THR:O     | 1:k:693:THR:HG22  | 2.19                     | 0.42              |
| 1:l:637:VAL:HG22  | 1:l:648:ALA:HB3   | 2.00                     | 0.42              |
| 1:m:1234:GLU:C    | 5:a:52:LYS:HB2    | 2.43                     | 0.42              |
| 1:m:1321:LEU:HD23 | 1:m:1321:LEU:HA   | 1.87                     | 0.42              |
| 1:n:1166:ASP:HA   | 1:n:1170:PHE:HD2  | 1.84                     | 0.42              |
| 1:o:52:GLU:C      | 1:p:89:THR:O      | 2.62                     | 0.42              |
| 1:o:710:ALA:CA    | 1:o:713:ASP:OD1   | 2.67                     | 0.42              |
| 1:p:671:ALA:O     | 1:p:674:THR:OG1   | 2.28                     | 0.42              |
| 1:p:795:ASN:ND2   | 1:p:979:SER:O     | 2.44                     | 0.42              |
| 3:s:61:ILE:HG13   | 3:s:84:LEU:HD11   | 2.01                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:y:68:VAL:HG22   | 4:y:87:LEU:H      | 1.83                     | 0.42              |
| 4:y:217:HIS:NE2   | 5:z:192:ASP:OD2   | 2.49                     | 0.42              |
| 4:V:85:VAL:HG13   | 4:V:89:PHE:HB3    | 2.00                     | 0.42              |
| 5:Z:56:TYR:OH     | 5:Z:289:GLU:OE2   | 2.30                     | 0.42              |
| 5:a:29:ILE:N      | 5:a:69:THR:O      | 2.37                     | 0.42              |
| 5:c:45:LEU:HD23   | 5:c:48:VAL:HB     | 2.01                     | 0.42              |
| 1:A:129:PRO:HD2   | 1:B:100:ARG:HH11  | 1.83                     | 0.42              |
| 1:A:651:ASN:O     | 1:A:786:TYR:CE1   | 2.69                     | 0.42              |
| 1:B:433:ASN:HD21  | 1:B:439:GLN:HE21  | 1.66                     | 0.42              |
| 1:B:519:SER:HB2   | 1:B:522:GLU:HG3   | 2.00                     | 0.42              |
| 1:C:1318:GLU:O    | 1:C:1322:LYS:N    | 2.52                     | 0.42              |
| 1:D:183:VAL:HG21  | 1:D:1067:THR:HG21 | 2.00                     | 0.42              |
| 1:D:207:MET:SD    | 1:D:207:MET:N     | 2.93                     | 0.42              |
| 1:D:209:THR:HB    | 1:D:212:GLN:HB2   | 2.01                     | 0.42              |
| 1:D:430:TYR:C     | 1:D:431:PHE:CD2   | 2.98                     | 0.42              |
| 1:D:622:ASP:HB3   | 1:D:625:ALA:HB3   | 1.99                     | 0.42              |
| 1:D:776:ASP:HA    | 1:D:779:MET:HB3   | 2.01                     | 0.42              |
| 1:E:181:LEU:HD21  | 1:E:386:LEU:HG    | 2.02                     | 0.42              |
| 1:E:257:ASP:N     | 1:E:257:ASP:OD1   | 2.53                     | 0.42              |
| 1:E:884:ALA:HA    | 1:E:1111:VAL:HG11 | 2.01                     | 0.42              |
| 1:G:156:ASP:OD1   | 1:H:338:GLN:NE2   | 2.51                     | 0.42              |
| 1:G:292:ILE:HG12  | 1:G:361:LEU:HB3   | 2.01                     | 0.42              |
| 1:G:319:HIS:CE1   | 1:n:319:HIS:CG    | 3.06                     | 0.42              |
| 1:G:519:SER:H     | 1:G:522:GLU:HB2   | 1.85                     | 0.42              |
| 1:H:379:ASN:C     | 1:I:205:ARG:HH12  | 2.28                     | 0.42              |
| 1:H:411:ALA:HB2   | 1:H:1331:GLU:CB   | 2.49                     | 0.42              |
| 1:H:966:GLU:HA    | 1:H:969:HIS:HD2   | 1.83                     | 0.42              |
| 1:I:773:ARG:HD3   | 1:I:773:ARG:N     | 2.26                     | 0.42              |
| 1:I:1255:ILE:HD12 | 1:I:1255:ILE:HA   | 1.88                     | 0.42              |
| 1:k:717:TRP:HE1   | 1:k:731:VAL:HG11  | 1.85                     | 0.42              |
| 1:k:925:ARG:HH12  | 1:k:971:HIS:HB3   | 1.85                     | 0.42              |
| 1:l:803:LEU:HA    | 1:l:918:LEU:HA    | 2.02                     | 0.42              |
| 1:l:1009:ARG:HH12 | 1:l:1118:ALA:C    | 2.27                     | 0.42              |
| 1:l:1297:LYS:HG2  | 1:l:1299:CYS:H    | 1.84                     | 0.42              |
| 1:m:484:GLU:OE2   | 1:m:966:GLU:N     | 2.52                     | 0.42              |
| 1:m:716:LEU:HD12  | 1:m:716:LEU:HA    | 1.87                     | 0.42              |
| 1:m:1156:CYS:SG   | 1:m:1157:GLU:N    | 2.89                     | 0.42              |
| 1:n:804:ASN:O     | 1:n:808:LEU:CB    | 2.67                     | 0.42              |
| 1:n:1177:ARG:HA   | 1:n:1250:PHE:HE1  | 1.84                     | 0.42              |
| 1:o:54:ILE:HG23   | 1:p:93:LEU:HD13   | 2.02                     | 0.42              |
| 1:p:788:CYS:SG    | 1:p:989:VAL:O     | 2.77                     | 0.42              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:p:1031:LEU:HG  | 1:p:1079:CYS:HB3  | 2.01                     | 0.42              |
| 1:q:592:HIS:CE1  | 1:q:986:LEU:HD22  | 2.55                     | 0.42              |
| 1:q:1101:PHE:HB3 | 1:q:1104:HIS:HD2  | 1.82                     | 0.42              |
| 2:e:258:PHE:CD1  | 3:t:91:ALA:HB2    | 2.54                     | 0.42              |
| 2:h:270:PRO:O    | 2:h:271:VAL:C     | 2.62                     | 0.42              |
| 2:f:259:ALA:HB3  | 2:f:289:LEU:HD13  | 2.01                     | 0.42              |
| 2:i:81:HIS:O     | 2:i:82:GLU:C      | 2.62                     | 0.42              |
| 4:y:48:ILE:HG21  | 5:1:308:ILE:HD12  | 1.99                     | 0.42              |
| 4:U:24:LYS:HE2   | 4:U:24:LYS:HB3    | 1.91                     | 0.42              |
| 5:z:25:ILE:HD12  | 5:z:74:VAL:HG22   | 2.02                     | 0.42              |
| 5:z:226:LEU:HD22 | 5:1:279:MET:HE1   | 2.01                     | 0.42              |
| 1:A:653:TYR:HA   | 1:A:656:VAL:HG12  | 2.01                     | 0.42              |
| 1:A:1179:ARG:HG3 | 1:A:1205:ASP:HB2  | 2.02                     | 0.42              |
| 1:B:232:ASP:OD2  | 1:B:1083:LEU:N    | 2.50                     | 0.42              |
| 1:C:60:ASN:HD22  | 1:D:96:ILE:HG23   | 1.84                     | 0.42              |
| 1:C:146:ASP:HA   | 1:C:150:ASP:HB3   | 2.01                     | 0.42              |
| 1:C:1228:TYR:HB2 | 1:C:1250:PHE:CD2  | 2.55                     | 0.42              |
| 1:D:66:THR:HG23  | 1:D:69:GLY:H      | 1.83                     | 0.42              |
| 1:D:647:LEU:HD13 | 1:D:647:LEU:HA    | 1.77                     | 0.42              |
| 1:E:62:ILE:HD12  | 1:E:62:ILE:HA     | 1.85                     | 0.42              |
| 1:E:231:LEU:HD13 | 1:E:1081:ALA:HB1  | 2.00                     | 0.42              |
| 1:E:276:SER:HB3  | 1:E:280:VAL:HG13  | 2.00                     | 0.42              |
| 1:E:440:ARG:HH22 | 1:F:521:LYS:CD    | 2.32                     | 0.42              |
| 1:E:454:ALA:HB2  | 1:E:1104:HIS:CG   | 2.55                     | 0.42              |
| 1:F:100:ARG:HD3  | 1:F:112:GLN:HA    | 2.01                     | 0.42              |
| 1:F:417:LEU:HD13 | 1:F:423:ASN:HB3   | 2.01                     | 0.42              |
| 1:F:702:GLU:OE2  | 1:F:715:ARG:NH2   | 2.53                     | 0.42              |
| 1:G:437:ILE:HD13 | 1:H:1207:GLN:HE21 | 1.84                     | 0.42              |
| 1:H:184:LEU:O    | 1:H:188:ALA:HB2   | 2.20                     | 0.42              |
| 1:H:602:SER:HB3  | 1:H:646:LEU:HB2   | 2.01                     | 0.42              |
| 1:H:646:LEU:H    | 1:H:646:LEU:HG    | 1.55                     | 0.42              |
| 1:H:1034:SER:HA  | 1:H:1076:ALA:HA   | 2.00                     | 0.42              |
| 1:H:1166:ASP:OD1 | 1:H:1166:ASP:N    | 2.52                     | 0.42              |
| 1:I:1191:GLU:HG3 | 1:I:1256:ILE:HD12 | 2.02                     | 0.42              |
| 1:k:205:ARG:HB3  | 1:p:381:ASP:CB    | 2.41                     | 0.42              |
| 1:k:812:LEU:HD22 | 1:k:839:LEU:HD13  | 2.00                     | 0.42              |
| 1:l:312:ASN:HD22 | 1:l:315:THR:HB    | 1.85                     | 0.42              |
| 1:l:842:LEU:HD12 | 1:l:843:VAL:HG23  | 2.01                     | 0.42              |
| 1:l:920:VAL:HG21 | 1:l:933:ALA:HA    | 2.01                     | 0.42              |
| 1:m:141:LYS:CG   | 4:S:20:GLU:HG2    | 2.49                     | 0.42              |
| 1:m:145:GLU:C    | 1:m:146:ASP:OD1   | 2.62                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:m:431:PHE:HZ    | 1:m:1310:THR:HG23 | 0.75                     | 0.42              |
| 1:m:451:CYS:O     | 1:m:1106:TYR:OH   | 2.29                     | 0.42              |
| 1:m:553:LEU:HD23  | 1:m:553:LEU:HA    | 1.85                     | 0.42              |
| 1:m:1055:ILE:HD12 | 1:m:1055:ILE:HA   | 1.93                     | 0.42              |
| 1:p:511:ALA:HA    | 1:p:514:ALA:HB3   | 2.01                     | 0.42              |
| 1:p:1178:GLY:HA3  | 1:p:1214:ASN:H    | 1.85                     | 0.42              |
| 1:p:1179:ARG:HG3  | 1:p:1205:ASP:HB2  | 2.00                     | 0.42              |
| 1:q:194:LEU:HD12  | 1:q:1077:THR:HG22 | 2.00                     | 0.42              |
| 1:q:395:TYR:HA    | 1:q:1020:VAL:O    | 2.19                     | 0.42              |
| 1:q:952:ARG:HG2   | 1:q:954:ASP:H     | 1.85                     | 0.42              |
| 1:q:1306:LEU:HD13 | 1:q:1343:ILE:HD11 | 2.01                     | 0.42              |
| 2:e:104:LYS:HG3   | 2:e:105:LEU:N     | 2.34                     | 0.42              |
| 4:S:90:LEU:HD22   | 4:S:126:ARG:HH22  | 1.85                     | 0.42              |
| 5:X:89:CYS:HA     | 5:X:308:ILE:HG23  | 2.01                     | 0.42              |
| 5:Y:296:CYS:HB3   | 5:Y:306:LEU:HB2   | 2.01                     | 0.42              |
| 5:Z:33:TYR:HD2    | 5:Z:35:HIS:HB2    | 1.85                     | 0.42              |
| 5:b:45:LEU:O      | 5:b:48:VAL:N      | 2.52                     | 0.42              |
| 1:A:591:GLY:O     | 1:A:595:THR:OG1   | 2.29                     | 0.42              |
| 1:A:1148:LEU:HD23 | 1:B:210:ARG:HG2   | 2.01                     | 0.42              |
| 1:B:400:LEU:HD11  | 1:B:1164:SER:HB2  | 2.01                     | 0.42              |
| 1:C:748:ARG:NH2   | 1:C:770:ASP:OD1   | 2.53                     | 0.42              |
| 1:D:696:ASN:HA    | 1:E:952:ARG:HH12  | 1.85                     | 0.42              |
| 1:E:23:HIS:HD2    | 1:E:26:LEU:H      | 1.66                     | 0.42              |
| 1:F:207:MET:HG3   | 1:l:29:GLY:HA2    | 2.02                     | 0.42              |
| 1:F:395:TYR:OH    | 1:F:1172:TYR:O    | 2.29                     | 0.42              |
| 1:F:969:HIS:O     | 1:F:972:ARG:NE    | 2.50                     | 0.42              |
| 1:G:74:THR:O      | 1:G:1037:ALA:N    | 2.44                     | 0.42              |
| 1:G:600:ARG:HH11  | 1:G:794:LEU:HA    | 1.85                     | 0.42              |
| 1:G:647:LEU:HA    | 1:G:647:LEU:HD13  | 1.78                     | 0.42              |
| 1:H:375:LYS:HA    | 1:H:378:LYS:HG3   | 2.00                     | 0.42              |
| 1:H:392:LEU:HB2   | 1:H:1026:PHE:HE2  | 1.85                     | 0.42              |
| 1:H:619:ILE:HD12  | 1:H:626:PHE:HA    | 2.01                     | 0.42              |
| 1:H:695:LEU:HD21  | 1:H:1006:ALA:HB1  | 2.02                     | 0.42              |
| 1:I:381:ASP:OD1   | 1:I:381:ASP:N     | 2.53                     | 0.42              |
| 1:I:753:SER:C     | 3:R:83:ASP:OD2    | 2.63                     | 0.42              |
| 1:k:975:PHE:HE1   | 1:k:995:MET:HB3   | 1.83                     | 0.42              |
| 1:l:456:HIS:CD2   | 1:l:1001:PRO:HB3  | 2.55                     | 0.42              |
| 1:m:603:LEU:HB3   | 1:m:794:LEU:HD21  | 2.01                     | 0.42              |
| 1:m:1153:ARG:HG2  | 1:m:1283:LEU:HD12 | 1.94                     | 0.42              |
| 1:n:66:THR:HG23   | 1:n:69:GLY:H      | 1.84                     | 0.42              |
| 1:n:273:VAL:HG23  | 1:n:369:ALA:HB3   | 2.01                     | 0.42              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:n:319:HIS:CE1  | 1:n:321:ALA:HB3   | 2.54                     | 0.42              |
| 1:n:605:ASP:HB3  | 1:n:608:TYR:HB2   | 2.02                     | 0.42              |
| 1:n:883:PRO:HA   | 1:n:886:ARG:HB2   | 2.02                     | 0.42              |
| 1:o:421:ALA:HA   | 1:o:424:GLN:HB2   | 2.01                     | 0.42              |
| 1:o:596:LEU:HD21 | 1:o:789:LEU:HD11  | 2.01                     | 0.42              |
| 1:q:262:TYR:HD2  | 1:q:1036:LYS:HE2  | 1.85                     | 0.42              |
| 1:q:862:PHE:CE2  | 3:x:89:SER:HA     | 2.55                     | 0.42              |
| 1:q:1106:TYR:HE2 | 1:q:1115:VAL:HG21 | 1.84                     | 0.42              |
| 2:h:93:PRO:HG2   | 2:h:195:TYR:HE2   | 1.78                     | 0.42              |
| 2:g:259:ALA:HB3  | 2:g:289:LEU:HD13  | 2.02                     | 0.42              |
| 2:j:238:LEU:HB3  | 2:j:271:VAL:HG21  | 2.01                     | 0.42              |
| 3:J:85:LEU:O     | 3:J:85:LEU:HD12   | 2.20                     | 0.42              |
| 3:t:37:GLU:O     | 3:t:40:ARG:HG2    | 2.19                     | 0.42              |
| 4:S:164:ILE:HG21 | 4:S:282:LYS:HA    | 2.02                     | 0.42              |
| 4:S:190:PHE:HB2  | 4:S:255:LEU:HD22  | 2.01                     | 0.42              |
| 4:V:187:PHE:N    | 4:V:211:SER:O     | 2.51                     | 0.42              |
| 5:W:215:VAL:HG23 | 5:a:201:SER:HB3   | 2.02                     | 0.42              |
| 5:a:159:GLU:O    | 5:a:163:ALA:N     | 2.48                     | 0.42              |
| 1:B:576:ARG:NH2  | 1:B:994:ILE:O     | 2.47                     | 0.42              |
| 1:B:626:PHE:CE2  | 1:B:662:ARG:HG2   | 2.54                     | 0.42              |
| 1:B:899:HIS:CG   | 1:B:963:PHE:HB3   | 2.55                     | 0.42              |
| 1:B:1026:PHE:HD1 | 1:B:1086:VAL:HG22 | 1.85                     | 0.42              |
| 1:C:98:VAL:HG11  | 1:C:113:THR:HB    | 2.02                     | 0.42              |
| 1:C:655:MET:O    | 1:C:659:ILE:N     | 2.39                     | 0.42              |
| 1:D:299:THR:HG21 | 1:D:356:THR:HG22  | 2.01                     | 0.42              |
| 1:D:393:THR:HA   | 1:D:1023:THR:HA   | 2.02                     | 0.42              |
| 1:D:698:ARG:HG3  | 1:D:703:PRO:HA    | 2.01                     | 0.42              |
| 1:E:305:LYS:H    | 1:E:349:GLN:NE2   | 2.17                     | 0.42              |
| 1:E:661:THR:HA   | 1:F:606:HIS:CD2   | 2.54                     | 0.42              |
| 1:E:940:ILE:O    | 1:E:944:LEU:N     | 2.50                     | 0.42              |
| 1:E:1309:HIS:NE2 | 1:E:1320:GLN:HG3  | 2.35                     | 0.42              |
| 1:F:796:ASN:HD21 | 1:F:926:PHE:HD1   | 1.67                     | 0.42              |
| 1:F:872:ALA:HB1  | 1:F:901:LEU:HD11  | 2.01                     | 0.42              |
| 1:G:716:LEU:HD23 | 1:G:783:LYS:HD2   | 2.00                     | 0.42              |
| 1:G:1072:LEU:HG  | 1:m:20:LEU:CD2    | 2.50                     | 0.42              |
| 1:H:662:ARG:HH21 | 1:H:663:LEU:HB2   | 1.85                     | 0.42              |
| 1:H:898:GLN:HE21 | 1:H:970:TRP:HB2   | 1.83                     | 0.42              |
| 1:I:431:PHE:O    | 1:I:438:PRO:HA    | 2.19                     | 0.42              |
| 1:I:458:ALA:HB3  | 1:I:539:PHE:CD2   | 2.54                     | 0.42              |
| 1:I:606:HIS:HA   | 1:I:909:THR:HG21  | 2.01                     | 0.42              |
| 1:I:1207:GLN:NE2 | 1:I:1208:THR:OG1  | 2.52                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:k:126:ILE:HG12  | 1:k:1063:GLN:HG2  | 2.02                     | 0.42              |
| 1:k:898:GLN:HE21  | 1:k:970:TRP:HB2   | 1.84                     | 0.42              |
| 1:k:1309:HIS:CG   | 1:k:1327:LEU:HB3  | 2.55                     | 0.42              |
| 1:l:129:PRO:O     | 1:m:100:ARG:NH1   | 2.48                     | 0.42              |
| 1:l:1255:ILE:HD12 | 1:l:1255:ILE:HA   | 1.86                     | 0.42              |
| 1:m:600:ARG:NE    | 1:m:793:VAL:O     | 2.53                     | 0.42              |
| 1:m:1230:THR:H    | 1:m:1251:THR:HG22 | 1.85                     | 0.42              |
| 1:m:1261:THR:O    | 1:m:1263:PHE:N    | 2.53                     | 0.42              |
| 1:o:849:ASP:HB3   | 1:o:852:VAL:H     | 1.84                     | 0.42              |
| 1:p:72:LEU:HB3    | 1:p:180:PHE:CE2   | 2.55                     | 0.42              |
| 1:p:613:TYR:CD2   | 1:p:911:PRO:HG3   | 2.55                     | 0.42              |
| 1:q:809:LEU:HB3   | 1:q:813:PHE:CZ    | 2.55                     | 0.42              |
| 2:2:212:VAL:HG21  | 2:3:92:LEU:HD21   | 2.02                     | 0.42              |
| 2:e:101:ASP:CA    | 2:e:104:LYS:HG2   | 2.43                     | 0.42              |
| 2:e:285:GLU:H     | 3:t:67:LYS:NZ     | 2.18                     | 0.42              |
| 2:g:140:VAL:O     | 2:g:144:LEU:N     | 2.47                     | 0.42              |
| 3:O:61:ILE:HG13   | 3:O:84:LEU:HD11   | 2.01                     | 0.42              |
| 4:y:230:SER:O     | 4:y:234:PHE:CB    | 2.68                     | 0.42              |
| 4:S:159:MET:O     | 4:S:160:LEU:CB    | 2.68                     | 0.42              |
| 4:U:217:HIS:CE1   | 5:Y:286:VAL:HA    | 2.54                     | 0.42              |
| 5:W:277:PHE:HA    | 5:W:280:ILE:HG12  | 2.02                     | 0.42              |
| 5:a:120:LEU:HB2   | 5:a:127:ASP:HB2   | 2.01                     | 0.42              |
| 5:b:11:GLN:NE2    | 5:b:124:SER:O     | 2.50                     | 0.42              |
| 1:A:611:LEU:HB3   | 1:A:846:VAL:HG11  | 2.02                     | 0.42              |
| 1:B:131:GLU:HG3   | 1:C:111:ARG:NH1   | 2.35                     | 0.42              |
| 1:B:562:ASN:ND2   | 1:B:972:ARG:H     | 2.18                     | 0.42              |
| 1:B:717:TRP:CE2   | 1:B:877:ILE:HG21  | 2.54                     | 0.42              |
| 1:C:701:ASP:OD2   | 1:C:1108:ASN:ND2  | 2.49                     | 0.42              |
| 1:C:1085:ARG:HH11 | 1:C:1085:ARG:HD2  | 1.73                     | 0.42              |
| 1:D:635:ARG:HA    | 1:D:638:ASN:HB2   | 2.01                     | 0.42              |
| 1:D:1022:ARG:NH2  | 1:D:1308:GLN:OE1  | 2.53                     | 0.42              |
| 1:E:248:THR:O     | 1:E:366:ARG:NH2   | 2.53                     | 0.42              |
| 1:F:813:PHE:CE1   | 3:O:85:LEU:CG     | 3.03                     | 0.42              |
| 1:F:1191:GLU:HG3  | 1:F:1256:ILE:HG21 | 2.01                     | 0.42              |
| 1:G:65:VAL:HG21   | 1:G:376:VAL:HG23  | 2.00                     | 0.42              |
| 1:G:224:MET:HE2   | 1:G:224:MET:HB3   | 1.84                     | 0.42              |
| 1:G:333:ILE:HD12  | 1:n:314:VAL:HG23  | 2.00                     | 0.42              |
| 1:G:879:ALA:O     | 1:G:896:SER:N     | 2.51                     | 0.42              |
| 1:H:483:ARG:HG3   | 1:H:484:GLU:HG2   | 2.01                     | 0.42              |
| 1:H:819:LEU:HB2   | 3:Q:58:GLN:CD     | 2.45                     | 0.42              |
| 1:I:558:ILE:HG21  | 1:I:970:TRP:CZ3   | 2.55                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:I:678:ASN:O     | 1:I:682:ILE:HG12  | 2.20                     | 0.42              |
| 1:k:64:TRP:HZ3    | 1:k:170:ASP:HB2   | 1.85                     | 0.42              |
| 1:k:298:LYS:HE3   | 1:k:353:PHE:CG    | 2.55                     | 0.42              |
| 1:l:438:PRO:HD2   | 1:m:1172:TYR:CD1  | 2.54                     | 0.42              |
| 1:l:1089:ASP:HB3  | 1:l:1091:GLY:H    | 1.85                     | 0.42              |
| 1:m:541:PHE:HA    | 1:m:553:LEU:O     | 2.20                     | 0.42              |
| 1:m:811:LYS:HD3   | 1:m:917:TYR:HE2   | 1.83                     | 0.42              |
| 1:n:53:ALA:HA     | 1:o:322:ILE:HB    | 2.02                     | 0.42              |
| 1:n:229:PHE:HB3   | 1:n:232:ASP:HB2   | 2.01                     | 0.42              |
| 1:n:434:LYS:HB2   | 1:n:1089:ASP:HA   | 2.01                     | 0.42              |
| 1:n:1316:LEU:O    | 1:n:1320:GLN:HG2  | 2.20                     | 0.42              |
| 1:o:510:THR:O     | 1:o:967:TYR:OH    | 2.27                     | 0.42              |
| 1:o:1156:CYS:HB3  | 1:o:1246:CYS:SG   | 2.60                     | 0.42              |
| 1:q:79:ILE:HD13   | 1:q:304:GLY:HA3   | 2.01                     | 0.42              |
| 1:q:799:CYS:O     | 1:q:906:CYS:HA    | 2.20                     | 0.42              |
| 2:i:111:ALA:HB2   | 4:U:232:PHE:CG    | 2.37                     | 0.42              |
| 2:g:105:LEU:HD11  | 2:g:212:VAL:HG13  | 1.86                     | 0.42              |
| 2:g:206:GLU:HB3   | 2:j:132:TYR:O     | 2.19                     | 0.42              |
| 4:y:62:GLU:OE2    | 4:y:86:SER:OG     | 2.28                     | 0.42              |
| 4:V:170:PRO:HA    | 4:V:277:VAL:HA    | 2.02                     | 0.42              |
| 4:V:254:ARG:HB3   | 4:V:288:GLY:HA3   | 2.01                     | 0.42              |
| 5:z:101:GLU:OE2   | 5:z:173:TYR:OH    | 2.23                     | 0.42              |
| 5:W:112:VAL:HG22  | 5:W:132:TRP:CE2   | 2.55                     | 0.42              |
| 5:Z:29:ILE:HD12   | 5:Z:81:LEU:HD21   | 2.00                     | 0.42              |
| 5:d:45:LEU:HD11   | 5:d:63:MET:HG3    | 2.00                     | 0.42              |
| 1:A:818:PHE:CG    | 3:J:88:LEU:HD13   | 2.54                     | 0.42              |
| 1:A:1059:PHE:HZ   | 4:U:33:ARG:HD3    | 1.85                     | 0.42              |
| 1:B:177:ILE:HG21  | 1:B:376:VAL:HG21  | 2.01                     | 0.42              |
| 1:B:507:PRO:HD2   | 1:B:958:PRO:HB3   | 2.01                     | 0.42              |
| 1:D:123:LYS:HE3   | 1:D:1066:ASN:OD1  | 2.20                     | 0.42              |
| 1:E:25:LYS:HD2    | 1:m:205:ARG:NH2   | 2.34                     | 0.42              |
| 1:E:310:LYS:HA    | 1:G:148:LEU:HD21  | 2.02                     | 0.42              |
| 1:F:925:ARG:HH12  | 1:F:971:HIS:HB3   | 1.85                     | 0.42              |
| 1:G:86:LYS:HZ1    | 1:m:149:LEU:CG    | 2.33                     | 0.42              |
| 1:G:484:GLU:HG3   | 1:G:967:TYR:HB2   | 2.01                     | 0.42              |
| 1:H:188:ALA:O     | 1:H:1078:THR:OG1  | 2.36                     | 0.42              |
| 1:I:309:SER:HB3   | 1:I:312:ASN:HB2   | 2.01                     | 0.42              |
| 1:I:753:SER:HB2   | 3:R:83:ASP:CG     | 2.41                     | 0.42              |
| 1:I:786:TYR:O     | 1:I:927:TYR:OH    | 2.31                     | 0.42              |
| 1:I:1028:THR:HG21 | 1:I:1080:THR:HG23 | 2.02                     | 0.42              |
| 1:I:1043:ILE:HB   | 1:I:1063:GLN:HE21 | 1.85                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:k:6:THR:HG23    | 1:k:46:ARG:HA     | 2.02                     | 0.42              |
| 1:k:818:PHE:CE2   | 3:r:60:VAL:CG1    | 3.03                     | 0.42              |
| 1:k:1031:LEU:HG   | 1:k:1079:CYS:HB3  | 2.02                     | 0.42              |
| 1:l:423:ASN:ND2   | 1:m:405:GLY:O     | 2.53                     | 0.42              |
| 1:l:872:ALA:HB1   | 1:l:901:LEU:HD11  | 2.02                     | 0.42              |
| 1:l:914:LEU:HD22  | 1:l:917:TYR:HD2   | 1.84                     | 0.42              |
| 1:m:51:PHE:HE1    | 1:n:87:MET:C      | 2.20                     | 0.42              |
| 1:n:73:ALA:HA     | 1:n:76:ALA:HB3    | 2.01                     | 0.42              |
| 1:n:492:HIS:O     | 1:n:496:ARG:HB2   | 2.20                     | 0.42              |
| 1:n:882:ASP:OD1   | 1:n:882:ASP:N     | 2.52                     | 0.42              |
| 1:o:564:PRO:O     | 1:o:568:ALA:N     | 2.51                     | 0.42              |
| 1:o:860:GLU:HA    | 1:o:863:HIS:HD2   | 1.85                     | 0.42              |
| 1:p:394:PHE:O     | 1:p:1022:ARG:N    | 2.53                     | 0.42              |
| 2:h:84:LEU:CG     | 2:h:230:TRP:CH2   | 2.97                     | 0.42              |
| 2:i:270:PRO:O     | 2:i:271:VAL:C     | 2.62                     | 0.42              |
| 3:v:82:LEU:HA     | 3:v:85:LEU:HB2    | 2.01                     | 0.42              |
| 5:1:183:ILE:HG21  | 5:1:193:MET:HB2   | 2.00                     | 0.42              |
| 5:a:70:ILE:HD12   | 5:a:84:PRO:HB3    | 2.01                     | 0.42              |
| 1:A:6:THR:HG23    | 1:A:46:ARG:HA     | 2.02                     | 0.41              |
| 1:A:141:LYS:HE3   | 4:U:32:GLU:HB2    | 2.02                     | 0.41              |
| 1:A:373:LEU:HD12  | 1:A:373:LEU:HA    | 1.84                     | 0.41              |
| 1:A:395:TYR:HE2   | 1:A:1170:PHE:HD1  | 1.68                     | 0.41              |
| 1:B:185:LEU:CD2   | 1:B:1032:LEU:HD22 | 2.50                     | 0.41              |
| 1:B:328:GLN:HG2   | 1:B:341:LEU:HD22  | 2.02                     | 0.41              |
| 1:B:662:ARG:HH22  | 1:B:668:VAL:HG21  | 1.85                     | 0.41              |
| 1:B:1155:THR:OG1  | 1:B:1156:CYS:N    | 2.53                     | 0.41              |
| 1:B:1156:CYS:SG   | 1:B:1157:GLU:N    | 2.93                     | 0.41              |
| 1:B:1298:PRO:O    | 1:B:1303:GLN:N    | 2.42                     | 0.41              |
| 1:B:1309:HIS:CD2  | 1:B:1327:LEU:HB3  | 2.55                     | 0.41              |
| 1:C:520:THR:HB    | 1:C:1163:VAL:HG21 | 2.02                     | 0.41              |
| 1:C:775:SER:O     | 1:C:779:MET:N     | 2.46                     | 0.41              |
| 1:E:815:THR:OG1   | 1:E:836:ASN:ND2   | 2.53                     | 0.41              |
| 1:E:1072:LEU:HD23 | 1:G:18:ILE:HB     | 2.02                     | 0.41              |
| 1:F:253:GLU:O     | 1:l:19:ASP:OD2    | 2.37                     | 0.41              |
| 1:F:332:ARG:HH12  | 1:F:341:LEU:HG    | 1.85                     | 0.41              |
| 1:F:647:LEU:HD13  | 1:F:647:LEU:HA    | 1.76                     | 0.41              |
| 1:F:809:LEU:HD22  | 3:O:82:LEU:HD11   | 2.02                     | 0.41              |
| 1:F:1017:ALA:CA   | 1:F:1160:LEU:O    | 2.68                     | 0.41              |
| 1:G:572:PHE:O     | 1:G:576:ARG:N     | 2.50                     | 0.41              |
| 1:G:630:ILE:HA    | 1:G:633:VAL:HG12  | 2.01                     | 0.41              |
| 1:G:726:ARG:HD3   | 1:H:941:ARG:NH2   | 2.34                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:G:819:LEU:HD12  | 3:P:59:PRO:HD2    | 1.97                     | 0.41              |
| 1:G:1134:ILE:HG23 | 1:G:1139:ARG:HB2  | 2.02                     | 0.41              |
| 1:G:1323:GLY:HA2  | 1:H:1326:LYS:NZ   | 2.35                     | 0.41              |
| 1:H:228:ILE:HG22  | 1:H:233:ARG:HH21  | 1.85                     | 0.41              |
| 1:I:388:ARG:HD3   | 1:I:1295:VAL:H    | 1.85                     | 0.41              |
| 1:I:567:LEU:HD22  | 1:I:1161:THR:HG21 | 2.01                     | 0.41              |
| 1:I:600:ARG:O     | 1:I:604:THR:OG1   | 2.24                     | 0.41              |
| 1:I:773:ARG:CD    | 1:I:773:ARG:N     | 2.83                     | 0.41              |
| 1:k:135:ALA:CA    | 4:y:161:LYS:CB    | 2.98                     | 0.41              |
| 1:k:556:PRO:O     | 1:k:972:ARG:NH2   | 2.52                     | 0.41              |
| 1:k:653:TYR:HA    | 1:k:656:VAL:HG12  | 2.01                     | 0.41              |
| 1:k:725:PRO:HA    | 1:k:774:THR:H     | 1.84                     | 0.41              |
| 1:k:744:HIS:CE1   | 2:2:174:ARG:C     | 2.80                     | 0.41              |
| 1:k:753:SER:HB2   | 3:r:83:ASP:O      | 2.20                     | 0.41              |
| 1:l:1177:ARG:HG2  | 1:l:1218:SER:HA   | 2.00                     | 0.41              |
| 1:m:49:LEU:HB3    | 1:m:50:SER:H      | 1.79                     | 0.41              |
| 1:m:53:ALA:HB3    | 1:n:90:GLY:HA2    | 2.01                     | 0.41              |
| 1:m:54:ILE:HG23   | 1:n:93:LEU:HD13   | 2.02                     | 0.41              |
| 1:m:141:LYS:HD3   | 4:S:20:GLU:CA     | 2.50                     | 0.41              |
| 1:m:271:ALA:O     | 1:m:1033:TYR:OH   | 2.32                     | 0.41              |
| 1:m:446:ALA:HA    | 1:m:1094:MET:HG3  | 2.02                     | 0.41              |
| 1:m:1021:VAL:HG23 | 1:m:1156:CYS:HB3  | 2.01                     | 0.41              |
| 1:n:53:ALA:HA     | 1:o:322:ILE:O     | 2.20                     | 0.41              |
| 1:o:535:LEU:HB2   | 1:o:541:PHE:HE2   | 1.85                     | 0.41              |
| 1:p:181:LEU:HD21  | 1:p:386:LEU:HG    | 2.02                     | 0.41              |
| 1:p:562:ASN:ND2   | 1:p:972:ARG:H     | 2.18                     | 0.41              |
| 1:p:1164:SER:HB3  | 1:p:1213:ASN:HD21 | 1.85                     | 0.41              |
| 2:f:252:PHE:HB2   | 2:f:264:ARG:HB2   | 2.01                     | 0.41              |
| 2:i:282:ARG:HA    | 2:i:282:ARG:HD2   | 1.83                     | 0.41              |
| 3:R:45:GLY:HA2    | 3:R:49:LEU:HD12   | 2.01                     | 0.41              |
| 4:V:258:PHE:HE2   | 4:V:263:SER:HB2   | 1.84                     | 0.41              |
| 5:z:194:ARG:HG2   | 5:1:218:LEU:HB3   | 2.01                     | 0.41              |
| 5:W:97:PRO:HD2    | 5:W:132:TRP:CZ2   | 2.55                     | 0.41              |
| 5:W:154:LEU:HD23  | 5:a:214:TYR:CD1   | 2.55                     | 0.41              |
| 5:Y:277:PHE:HE2   | 5:c:144:GLN:HG2   | 1.85                     | 0.41              |
| 5:Z:87:GLY:HA3    | 5:d:86:HIS:HB3    | 2.02                     | 0.41              |
| 5:1:59:MET:HE2    | 5:1:110:PRO:HB2   | 2.01                     | 0.41              |
| 5:c:45:LEU:CD2    | 5:c:48:VAL:HB     | 2.49                     | 0.41              |
| 5:c:49:VAL:HG22   | 5:c:59:MET:HE3    | 2.01                     | 0.41              |
| 5:c:90:TYR:O      | 5:c:307:CYS:N     | 2.45                     | 0.41              |
| 1:A:779:MET:HG3   | 1:A:783:LYS:HE2   | 2.02                     | 0.41              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:A:1126:VAL:HB   | 1:A:1130:GLU:HB2 | 2.02                     | 0.41              |
| 1:B:434:LYS:HE3   | 1:C:218:GLN:HG2  | 2.01                     | 0.41              |
| 1:B:1095:GLN:HE22 | 1:B:1242:PHE:HB3 | 1.85                     | 0.41              |
| 1:C:816:LYS:HG2   | 1:C:833:LEU:HD23 | 2.01                     | 0.41              |
| 1:F:476:ARG:HD3   | 1:F:532:PHE:HZ   | 1.85                     | 0.41              |
| 1:F:546:GLU:N     | 1:F:549:GLN:O    | 2.53                     | 0.41              |
| 1:F:600:ARG:O     | 1:F:604:THR:N    | 2.53                     | 0.41              |
| 1:G:777:GLU:H     | 1:H:951:GLN:NE2  | 2.18                     | 0.41              |
| 1:G:787:LEU:HD21  | 1:G:971:HIS:CE1  | 2.55                     | 0.41              |
| 1:G:1188:PRO:HB3  | 1:G:1261:THR:N   | 2.29                     | 0.41              |
| 1:H:492:HIS:CD2   | 1:H:495:ARG:HB2  | 2.55                     | 0.41              |
| 1:H:1148:LEU:HD12 | 1:H:1148:LEU:HA  | 1.82                     | 0.41              |
| 1:I:481:CYS:HB2   | 1:I:508:PRO:HB2  | 2.01                     | 0.41              |
| 1:I:711:LEU:HD13  | 1:I:996:HIS:CD2  | 2.54                     | 0.41              |
| 1:I:817:PHE:HD2   | 1:I:819:LEU:H    | 1.65                     | 0.41              |
| 1:k:215:ASN:HB3   | 1:p:1085:ARG:HD2 | 2.02                     | 0.41              |
| 1:k:391:GLU:O     | 1:k:1297:LYS:HB3 | 2.19                     | 0.41              |
| 1:k:1161:THR:HG22 | 1:k:1216:TRP:CE2 | 2.54                     | 0.41              |
| 1:l:156:ASP:O     | 1:l:160:THR:OG1  | 2.31                     | 0.41              |
| 1:l:197:LEU:O     | 1:l:202:THR:OG1  | 2.31                     | 0.41              |
| 1:l:813:PHE:CZ    | 3:s:82:LEU:CD1   | 2.99                     | 0.41              |
| 1:l:954:ASP:HA    | 1:l:980:ALA:HB1  | 2.01                     | 0.41              |
| 1:l:1269:TYR:HE1  | 1:l:1296:GLU:HB2 | 1.85                     | 0.41              |
| 1:m:446:ALA:HB2   | 1:m:1094:MET:HE3 | 2.01                     | 0.41              |
| 1:n:811:LYS:HD3   | 1:n:917:TYR:HE2  | 1.85                     | 0.41              |
| 1:n:1201:HIS:ND1  | 1:n:1212:THR:OG1 | 2.48                     | 0.41              |
| 1:o:611:LEU:HD11  | 1:o:861:LEU:HD21 | 2.01                     | 0.41              |
| 1:p:647:LEU:HD12  | 1:p:676:TYR:CZ   | 2.54                     | 0.41              |
| 1:p:1022:ARG:NH1  | 1:p:1091:GLY:O   | 2.51                     | 0.41              |
| 1:p:1314:GLN:O    | 1:p:1318:GLU:HG2 | 2.20                     | 0.41              |
| 1:q:273:VAL:O     | 1:q:1033:TYR:HA  | 2.20                     | 0.41              |
| 2:2:140:VAL:O     | 2:2:144:LEU:N    | 2.47                     | 0.41              |
| 2:3:70:LEU:HD22   | 2:3:247:ARG:HB3  | 2.02                     | 0.41              |
| 2:e:258:PHE:CE1   | 3:t:91:ALA:HB2   | 2.55                     | 0.41              |
| 2:h:70:LEU:HD22   | 2:h:247:ARG:HB3  | 2.02                     | 0.41              |
| 2:f:101:ASP:CA    | 2:f:104:LYS:HG2  | 2.43                     | 0.41              |
| 5:z:104:ASP:OD1   | 5:z:104:ASP:N    | 2.45                     | 0.41              |
| 5:W:69:THR:HB     | 5:W:81:LEU:HB3   | 2.02                     | 0.41              |
| 5:X:149:LEU:HD13  | 5:X:165:THR:HA   | 2.02                     | 0.41              |
| 5:X:295:VAL:HG11  | 5:X:298:VAL:HG23 | 2.01                     | 0.41              |
| 5:Y:309:TYR:HE1   | 5:c:86:HIS:HB2   | 1.84                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:Z:94:ASN:HD21   | 5:Z:303:LYS:HE2   | 1.85                     | 0.41              |
| 5:Z:195:ASN:HA    | 5:Z:198:ILE:HD12  | 2.01                     | 0.41              |
| 5:a:155:ASP:HB3   | 5:a:161:VAL:HG11  | 2.01                     | 0.41              |
| 1:A:107:ILE:HG12  | 1:F:1291:THR:HG22 | 2.02                     | 0.41              |
| 1:A:389:ASP:OD1   | 1:A:389:ASP:N     | 2.53                     | 0.41              |
| 1:A:400:LEU:HD23  | 1:A:1166:ASP:HB3  | 2.02                     | 0.41              |
| 1:A:577:ALA:HA    | 1:A:994:ILE:HG21  | 2.02                     | 0.41              |
| 1:A:614:LEU:O     | 1:A:618:LEU:HB2   | 2.19                     | 0.41              |
| 1:A:1148:LEU:HD12 | 1:A:1148:LEU:HA   | 1.80                     | 0.41              |
| 1:C:516:HIS:NE2   | 1:C:977:CYS:HB3   | 2.35                     | 0.41              |
| 1:C:899:HIS:CD2   | 1:C:969:HIS:HE1   | 2.38                     | 0.41              |
| 1:C:1278:HIS:CE1  | 1:C:1280:GLU:HB2  | 2.56                     | 0.41              |
| 1:D:692:LEU:CB    | 1:D:705:LEU:HD21  | 2.42                     | 0.41              |
| 1:E:379:ASN:HD22  | 1:l:24:ILE:H      | 1.68                     | 0.41              |
| 1:E:523:PHE:HB2   | 1:E:566:ALA:HB1   | 2.01                     | 0.41              |
| 1:E:532:PHE:HE2   | 1:E:543:PHE:HE2   | 1.68                     | 0.41              |
| 1:E:640:TYR:HD2   | 1:E:648:ALA:HB2   | 1.85                     | 0.41              |
| 1:E:696:ASN:ND2   | 1:F:509:ARG:HH11  | 2.18                     | 0.41              |
| 1:F:72:LEU:HG     | 1:F:275:VAL:HG11  | 2.02                     | 0.41              |
| 1:F:1082:HIS:CE1  | 1:F:1352:ASN:HD21 | 2.38                     | 0.41              |
| 1:G:749:ASN:ND2   | 1:G:754:ASP:OD2   | 2.48                     | 0.41              |
| 1:H:1039:THR:HB   | 1:H:1070:MET:HG2  | 2.02                     | 0.41              |
| 1:I:1199:TYR:HB3  | 1:I:1220:ARG:HB2  | 2.01                     | 0.41              |
| 1:k:126:ILE:HG22  | 1:l:103:THR:OG1   | 2.20                     | 0.41              |
| 1:k:901:LEU:HD12  | 1:k:901:LEU:HA    | 1.92                     | 0.41              |
| 1:k:1087:ARG:NH2  | 1:k:1279:GLY:HA2  | 2.35                     | 0.41              |
| 1:k:1168:GLU:OE2  | 1:p:440:ARG:HD3   | 2.20                     | 0.41              |
| 1:l:316:ALA:O     | 1:l:320:HIS:HA    | 2.19                     | 0.41              |
| 1:l:755:VAL:HG11  | 3:s:80:TYR:CZ     | 2.55                     | 0.41              |
| 1:l:1139:ARG:HH11 | 4:T:79:MET:HB2    | 1.85                     | 0.41              |
| 1:m:391:GLU:HA    | 1:m:1025:THR:HA   | 2.01                     | 0.41              |
| 1:n:129:PRO:HB3   | 1:n:1060:HIS:CE1  | 2.56                     | 0.41              |
| 1:n:870:GLU:HB3   | 1:n:903:ASN:HD22  | 1.84                     | 0.41              |
| 1:n:971:HIS:CE1   | 1:n:996:HIS:HE1   | 2.38                     | 0.41              |
| 1:o:231:LEU:HD12  | 1:o:235:ARG:HH22  | 1.85                     | 0.41              |
| 1:o:611:LEU:HB3   | 1:o:846:VAL:HG21  | 2.02                     | 0.41              |
| 1:p:212:GLN:O     | 1:p:216:ILE:HG12  | 2.20                     | 0.41              |
| 1:p:1233:ARG:HH22 | 1:p:1244:SER:HB3  | 1.85                     | 0.41              |
| 1:q:395:TYR:OH    | 1:q:1172:TYR:O    | 2.34                     | 0.41              |
| 1:q:881:LEU:HB2   | 1:q:886:ARG:HB3   | 2.02                     | 0.41              |
| 2:2:260:ARG:HG2   | 2:2:289:LEU:HD11  | 2.02                     | 0.41              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:e:285:GLU:OE2   | 3:t:67:LYS:CG    | 2.51                     | 0.41              |
| 2:j:83:LYS:HD2    | 2:j:83:LYS:HA    | 1.88                     | 0.41              |
| 3:u:68:TYR:OH     | 3:u:83:ASP:OD2   | 2.33                     | 0.41              |
| 4:y:234:PHE:CE2   | 5:z:202:MET:HE1  | 2.56                     | 0.41              |
| 4:T:54:VAL:HB     | 4:T:146:CYS:HB2  | 2.02                     | 0.41              |
| 5:z:112:VAL:C     | 5:z:113:PHE:CG   | 2.97                     | 0.41              |
| 5:X:310:LYS:HB2   | 5:X:310:LYS:HE2  | 1.85                     | 0.41              |
| 5:Z:113:PHE:CD1   | 5:Z:181:PRO:HG3  | 2.55                     | 0.41              |
| 5:Z:144:GLN:HG3   | 5:d:277:PHE:HD2  | 1.85                     | 0.41              |
| 5:1:143:ASN:ND2   | 5:1:147:MET:HE2  | 2.35                     | 0.41              |
| 5:1:153:SER:OG    | 5:1:184:THR:OG1  | 2.32                     | 0.41              |
| 5:b:45:LEU:HG     | 5:b:48:VAL:HB    | 2.02                     | 0.41              |
| 5:d:138:LEU:HD12  | 5:d:141:GLU:HB3  | 2.03                     | 0.41              |
| 1:A:813:PHE:CG    | 3:J:85:LEU:CG    | 3.03                     | 0.41              |
| 1:C:278:HIS:HA    | 1:C:372:HIS:CE1  | 2.55                     | 0.41              |
| 1:D:24:ILE:HG21   | 1:H:98:VAL:HG12  | 2.02                     | 0.41              |
| 1:D:65:VAL:HG21   | 1:D:376:VAL:HG12 | 2.02                     | 0.41              |
| 1:D:296:GLY:HA2   | 1:D:357:GLN:HA   | 2.02                     | 0.41              |
| 1:D:458:ALA:HB1   | 1:D:461:CYS:HB3  | 2.02                     | 0.41              |
| 1:D:485:PHE:HB2   | 1:D:544:HIS:CD2  | 2.55                     | 0.41              |
| 1:D:555:THR:HG22  | 1:D:972:ARG:HH22 | 1.85                     | 0.41              |
| 1:D:603:LEU:C     | 1:D:908:THR:HG23 | 2.45                     | 0.41              |
| 1:D:1171:ARG:NH2  | 1:D:1330:ASP:HB2 | 2.35                     | 0.41              |
| 1:D:1269:TYR:CE1  | 1:D:1296:GLU:HB2 | 2.56                     | 0.41              |
| 1:E:59:CYS:HA     | 1:F:95:TYR:O     | 2.20                     | 0.41              |
| 1:E:129:PRO:HB3   | 1:E:1060:HIS:CE1 | 2.56                     | 0.41              |
| 1:E:453:PRO:HB2   | 1:E:887:HIS:CE1  | 2.56                     | 0.41              |
| 1:F:761:MET:HE3   | 1:F:871:ASN:HB2  | 2.02                     | 0.41              |
| 1:F:1055:ILE:HD13 | 5:X:72:ARG:HG2   | 2.02                     | 0.41              |
| 1:F:1175:ASN:ND2  | 1:F:1179:ARG:O   | 2.54                     | 0.41              |
| 1:G:577:ALA:HA    | 1:G:994:ILE:HG21 | 2.01                     | 0.41              |
| 1:G:1314:GLN:O    | 1:G:1318:GLU:N   | 2.50                     | 0.41              |
| 1:H:373:LEU:HD12  | 1:H:373:LEU:HA   | 1.89                     | 0.41              |
| 1:H:630:ILE:HA    | 1:H:633:VAL:HG12 | 2.02                     | 0.41              |
| 1:I:600:ARG:HH11  | 1:I:794:LEU:HD23 | 1.85                     | 0.41              |
| 1:I:1016:PHE:HA   | 1:I:1162:PRO:HD3 | 2.03                     | 0.41              |
| 1:I:1330:ASP:OD1  | 1:I:1330:ASP:N   | 2.49                     | 0.41              |
| 1:k:547:ASN:OD1   | 1:k:547:ASN:N    | 2.53                     | 0.41              |
| 1:k:698:ARG:HG2   | 1:k:699:LEU:O    | 2.20                     | 0.41              |
| 1:l:1020:VAL:HG11 | 1:l:1094:MET:HE1 | 2.03                     | 0.41              |
| 1:m:192:PHE:HB2   | 1:m:223:LYS:HB3  | 2.03                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:m:374:ARG:HG2   | 1:m:378:LYS:HG3   | 2.03                     | 0.41              |
| 1:m:794:LEU:HA    | 1:m:794:LEU:HD23  | 1.84                     | 0.41              |
| 1:m:1183:MET:SD   | 1:m:1259:ASN:ND2  | 2.93                     | 0.41              |
| 1:n:84:LEU:O      | 1:n:87:MET:N      | 2.52                     | 0.41              |
| 1:n:630:ILE:HA    | 1:n:662:ARG:NH1   | 2.35                     | 0.41              |
| 1:o:379:ASN:OD1   | 1:p:205:ARG:NH2   | 2.41                     | 0.41              |
| 1:o:589:PRO:HB2   | 1:o:592:HIS:CD2   | 2.55                     | 0.41              |
| 1:o:696:ASN:HA    | 1:p:952:ARG:HH12  | 1.85                     | 0.41              |
| 1:o:753:SER:HB2   | 3:v:83:ASP:CG     | 2.45                     | 0.41              |
| 1:q:1031:LEU:HB2  | 1:q:1079:CYS:HB3  | 2.02                     | 0.41              |
| 2:e:140:VAL:O     | 2:e:144:LEU:N     | 2.47                     | 0.41              |
| 2:h:88:ARG:HA     | 2:h:89:PRO:HD3    | 1.69                     | 0.41              |
| 2:f:66:ARG:HE     | 2:f:68:THR:HG21   | 1.61                     | 0.41              |
| 2:i:88:ARG:HA     | 2:i:89:PRO:HD3    | 1.69                     | 0.41              |
| 2:j:255:ARG:HA    | 2:j:256:PRO:HD3   | 1.94                     | 0.41              |
| 4:S:136:CYS:O     | 4:S:151:SER:N     | 2.44                     | 0.41              |
| 4:S:238:SER:HB3   | 5:W:205:ASN:HD22  | 1.85                     | 0.41              |
| 4:S:258:PHE:HE2   | 4:S:263:SER:HB2   | 1.84                     | 0.41              |
| 5:W:33:TYR:CD2    | 5:W:35:HIS:HB2    | 2.55                     | 0.41              |
| 5:X:195:ASN:HA    | 5:X:198:ILE:HD12  | 2.02                     | 0.41              |
| 5:a:214:TYR:HE2   | 5:a:273:LEU:HD11  | 1.85                     | 0.41              |
| 5:b:89:CYS:HA     | 5:b:308:ILE:HA    | 2.03                     | 0.41              |
| 5:d:120:LEU:HD23  | 5:d:129:VAL:HA    | 2.02                     | 0.41              |
| 1:A:129:PRO:HD2   | 1:B:100:ARG:NH1   | 2.35                     | 0.41              |
| 1:A:391:GLU:HA    | 1:A:1025:THR:HA   | 2.03                     | 0.41              |
| 1:A:1019:THR:N    | 1:A:1160:LEU:HD12 | 2.36                     | 0.41              |
| 1:A:1034:SER:HA   | 1:A:1076:ALA:HA   | 2.02                     | 0.41              |
| 1:B:795:ASN:O     | 1:B:797:HIS:ND1   | 2.53                     | 0.41              |
| 1:C:235:ARG:HH11  | 1:C:239:GLN:HE21  | 1.67                     | 0.41              |
| 1:C:244:LEU:HD23  | 1:C:244:LEU:HA    | 1.89                     | 0.41              |
| 1:C:818:PHE:CE1   | 3:L:88:LEU:HD22   | 2.56                     | 0.41              |
| 1:D:275:VAL:HG23  | 1:D:1032:LEU:HB3  | 2.00                     | 0.41              |
| 1:D:638:ASN:HD21  | 1:D:668:VAL:HG12  | 1.85                     | 0.41              |
| 1:D:965:HIS:O     | 1:D:969:HIS:N     | 2.53                     | 0.41              |
| 1:E:13:LYS:HB3    | 1:I:59:CYS:HB3    | 2.02                     | 0.41              |
| 1:E:251:VAL:HG11  | 1:E:1033:TYR:CE2  | 2.54                     | 0.41              |
| 1:E:882:ASP:N     | 1:E:882:ASP:OD1   | 2.54                     | 0.41              |
| 1:E:1031:LEU:HD12 | 1:E:1031:LEU:C    | 2.46                     | 0.41              |
| 1:F:562:ASN:HD22  | 1:F:972:ARG:HB2   | 1.85                     | 0.41              |
| 1:G:1136:THR:HA   | 5:W:58:ARG:NH2    | 2.35                     | 0.41              |
| 1:H:293:ARG:HH11  | 1:H:367:LEU:HD21  | 1.85                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:H:346:PHE:HA    | 1:H:349:GLN:HE21  | 1.84                     | 0.41              |
| 1:H:1017:ALA:O    | 1:H:1160:LEU:CA   | 2.69                     | 0.41              |
| 1:I:251:VAL:HG11  | 1:I:1033:TYR:CE2  | 2.55                     | 0.41              |
| 1:I:535:LEU:HB2   | 1:I:541:PHE:HE2   | 1.84                     | 0.41              |
| 1:k:1096:ASP:OD1  | 1:k:1096:ASP:N    | 2.54                     | 0.41              |
| 1:l:452:HIS:CD2   | 1:l:1097:LEU:HB3  | 2.55                     | 0.41              |
| 1:l:516:HIS:CE1   | 1:l:977:CYS:HB3   | 2.55                     | 0.41              |
| 1:l:657:ARG:NH2   | 1:l:778:GLU:OE1   | 2.54                     | 0.41              |
| 1:l:1274:GLN:HE21 | 1:l:1291:THR:HA   | 1.85                     | 0.41              |
| 1:m:520:THR:HG22  | 1:m:566:ALA:HA    | 2.02                     | 0.41              |
| 1:n:277:THR:HG21  | 1:n:387:GLU:HG3   | 2.01                     | 0.41              |
| 1:n:294:ARG:NE    | 1:n:359:ASP:OD1   | 2.48                     | 0.41              |
| 1:n:693:THR:HG21  | 1:o:981:ALA:HB2   | 2.02                     | 0.41              |
| 1:o:925:ARG:HH12  | 1:o:971:HIS:HB3   | 1.85                     | 0.41              |
| 1:p:50:SER:O      | 1:q:56:GLY:HA2    | 2.20                     | 0.41              |
| 1:q:506:ASP:OD1   | 1:q:506:ASP:N     | 2.52                     | 0.41              |
| 1:q:598:VAL:HG13  | 1:q:647:LEU:HD11  | 2.02                     | 0.41              |
| 1:q:610:GLU:HB3   | 1:q:911:PRO:HB3   | 2.02                     | 0.41              |
| 2:3:134:ASP:OD1   | 2:3:231:GLN:NE2   | 2.53                     | 0.41              |
| 2:g:260:ARG:HG2   | 2:g:289:LEU:HD11  | 2.02                     | 0.41              |
| 3:O:72:GLY:O      | 3:O:80:TYR:OH     | 2.38                     | 0.41              |
| 4:S:61:VAL:O      | 4:S:63:GLN:N      | 2.53                     | 0.41              |
| 4:S:96:ASN:ND2    | 4:S:205:SER:OG    | 2.53                     | 0.41              |
| 5:Z:54:ARG:NH2    | 5:Z:116:GLU:HB2   | 2.35                     | 0.41              |
| 5:d:275:ALA:HA    | 5:d:278:VAL:HG12  | 2.01                     | 0.41              |
| 1:A:262:TYR:CZ    | 1:A:300:PRO:HD2   | 2.56                     | 0.41              |
| 1:A:604:THR:HB    | 1:F:677:ARG:HH21  | 1.86                     | 0.41              |
| 1:B:128:ILE:HD11  | 1:B:1061:VAL:HG22 | 2.02                     | 0.41              |
| 1:B:1297:LYS:HD3  | 1:B:1299:CYS:HB2  | 2.02                     | 0.41              |
| 1:D:663:LEU:HD12  | 1:D:663:LEU:HA    | 1.83                     | 0.41              |
| 1:D:775:SER:O     | 1:D:779:MET:N     | 2.46                     | 0.41              |
| 1:D:1269:TYR:O    | 1:D:1273:SER:OG   | 2.22                     | 0.41              |
| 1:E:11:LEU:HD13   | 1:m:323:MET:HE1   | 1.98                     | 0.41              |
| 1:E:65:VAL:HG11   | 1:E:376:VAL:HG12  | 2.03                     | 0.41              |
| 1:E:712:HIS:HA    | 1:E:780:VAL:HG22  | 2.01                     | 0.41              |
| 1:F:433:ASN:HD21  | 1:F:439:GLN:HE21  | 1.67                     | 0.41              |
| 1:H:1038:SER:OG   | 1:H:1039:THR:N    | 2.53                     | 0.41              |
| 1:I:196:THR:HA    | 1:I:200:HIS:HD2   | 1.84                     | 0.41              |
| 1:I:240:LEU:HD21  | 1:I:284:LEU:HD23  | 2.02                     | 0.41              |
| 1:I:274:ILE:HB    | 1:I:370:LEU:HD23  | 2.02                     | 0.41              |
| 1:k:77:HIS:HE1    | 1:k:79:ILE:HD11   | 1.84                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:k:398:VAL:HG13  | 1:k:1018:LEU:HB2  | 2.02                     | 0.41              |
| 1:k:1177:ARG:HH21 | 1:k:1181:SER:HB3  | 1.84                     | 0.41              |
| 1:l:544:HIS:CE1   | 1:l:553:LEU:HB2   | 2.54                     | 0.41              |
| 1:l:608:TYR:HA    | 1:l:609:PRO:HD3   | 1.74                     | 0.41              |
| 1:l:1300:ARG:H    | 1:l:1303:GLN:HE21 | 1.68                     | 0.41              |
| 1:m:141:LYS:CB    | 4:S:20:GLU:HG2    | 2.49                     | 0.41              |
| 1:m:622:ASP:O     | 1:m:626:PHE:HB2   | 2.21                     | 0.41              |
| 1:m:626:PHE:HE2   | 1:m:662:ARG:HG2   | 1.85                     | 0.41              |
| 1:m:748:ARG:NH2   | 1:m:771:ALA:H     | 2.19                     | 0.41              |
| 1:n:907:MET:HE3   | 1:n:932:LEU:HG    | 2.03                     | 0.41              |
| 1:n:1048:VAL:HA   | 1:n:1061:VAL:HG12 | 2.03                     | 0.41              |
| 1:o:77:HIS:CE1    | 1:o:349:GLN:HG3   | 2.55                     | 0.41              |
| 1:o:802:GLY:N     | 1:o:919:THR:O     | 2.48                     | 0.41              |
| 1:o:1031:LEU:HD23 | 1:o:1081:ALA:HB1  | 2.02                     | 0.41              |
| 1:o:1069:GLU:HG2  | 1:o:1070:MET:H    | 1.86                     | 0.41              |
| 1:o:1232:ASN:HD22 | 1:o:1235:LYS:HD2  | 1.86                     | 0.41              |
| 1:o:1309:HIS:CG   | 1:o:1327:LEU:HD12 | 2.55                     | 0.41              |
| 1:o:1320:GLN:HE22 | 1:o:1329:LEU:HD23 | 1.85                     | 0.41              |
| 1:p:715:ARG:NE    | 1:p:880:ALA:O     | 2.48                     | 0.41              |
| 1:q:398:VAL:HG23  | 1:q:429:VAL:HG23  | 2.02                     | 0.41              |
| 1:q:898:GLN:HB3   | 1:q:970:TRP:HZ3   | 1.85                     | 0.41              |
| 2:f:104:LYS:HG3   | 2:i:92:LEU:HD13   | 2.01                     | 0.41              |
| 2:j:285:GLU:CD    | 3:M:67:LYS:CE     | 2.76                     | 0.41              |
| 4:S:87:LEU:HD21   | 4:S:208:VAL:HG21  | 2.03                     | 0.41              |
| 4:T:189:TYR:HB2   | 4:T:209:VAL:HG13  | 2.02                     | 0.41              |
| 4:U:198:SER:H     | 4:U:202:GLY:HA2   | 1.86                     | 0.41              |
| 5:1:45:LEU:HB3    | 5:1:129:VAL:HG23  | 2.03                     | 0.41              |
| 5:b:266:PRO:O     | 5:b:270:LEU:N     | 2.47                     | 0.41              |
| 1:A:626:PHE:HB2   | 1:A:658:LEU:HD13  | 2.02                     | 0.41              |
| 1:B:720:PHE:HB2   | 1:B:786:TYR:CE2   | 2.55                     | 0.41              |
| 1:C:698:ARG:HG3   | 1:C:703:PRO:HA    | 2.03                     | 0.41              |
| 1:D:12:PRO:O      | 1:G:57:THR:OG1    | 2.38                     | 0.41              |
| 1:D:42:ASP:N      | 1:G:131:GLU:OE1   | 2.41                     | 0.41              |
| 1:D:146:ASP:OD1   | 1:D:146:ASP:N     | 2.52                     | 0.41              |
| 1:D:438:PRO:HD2   | 1:E:1172:TYR:CD1  | 2.55                     | 0.41              |
| 1:D:663:LEU:HD23  | 1:D:673:TYR:CD1   | 2.55                     | 0.41              |
| 1:D:689:THR:HG21  | 1:D:990:LEU:HD11  | 2.03                     | 0.41              |
| 1:E:319:HIS:CE1   | 1:E:321:ALA:HB3   | 2.56                     | 0.41              |
| 1:E:982:CYS:SG    | 1:E:988:SER:OG    | 2.67                     | 0.41              |
| 1:E:1053:ARG:HG3  | 5:a:306:LEU:HD22  | 2.03                     | 0.41              |
| 1:E:1228:TYR:HB2  | 1:E:1250:PHE:CD2  | 2.52                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:116:MET:HE1  | 1:l:5:TRP:O      | 2.19                     | 0.41              |
| 1:F:1309:HIS:CD2 | 1:F:1327:LEU:HB3 | 2.56                     | 0.41              |
| 1:H:81:PHE:HB2   | 1:H:306:PHE:HB3  | 2.03                     | 0.41              |
| 1:H:453:PRO:HB2  | 1:H:887:HIS:CE1  | 2.56                     | 0.41              |
| 1:I:555:THR:HG21 | 1:I:967:TYR:HB3  | 2.03                     | 0.41              |
| 1:I:1097:LEU:HA  | 1:I:1100:VAL:HB  | 2.03                     | 0.41              |
| 1:k:538:PHE:O    | 1:k:557:ARG:HB2  | 2.20                     | 0.41              |
| 1:k:1207:GLN:O   | 1:p:437:ILE:CD1  | 2.69                     | 0.41              |
| 1:l:404:SER:HA   | 1:l:407:ALA:HB2  | 2.02                     | 0.41              |
| 1:l:434:LYS:NZ   | 1:m:215:ASN:OD1  | 2.53                     | 0.41              |
| 1:l:635:ARG:HH22 | 1:l:847:ALA:HB1  | 1.85                     | 0.41              |
| 1:l:950:TYR:O    | 1:l:957:PHE:CZ   | 2.68                     | 0.41              |
| 1:l:1332:THR:O   | 1:l:1332:THR:OG1 | 2.36                     | 0.41              |
| 1:m:141:LYS:CG   | 4:S:20:GLU:CG    | 2.98                     | 0.41              |
| 1:m:231:LEU:HD22 | 1:m:280:VAL:HG23 | 2.02                     | 0.41              |
| 1:m:698:ARG:HB2  | 1:n:949:GLN:HB3  | 2.01                     | 0.41              |
| 1:n:923:PHE:HA   | 1:n:963:PHE:HE1  | 1.85                     | 0.41              |
| 1:n:1166:ASP:HA  | 1:n:1170:PHE:HB2 | 2.02                     | 0.41              |
| 1:o:181:LEU:HD11 | 1:o:386:LEU:HD21 | 2.02                     | 0.41              |
| 1:p:361:LEU:HD23 | 1:p:370:LEU:HD11 | 2.03                     | 0.41              |
| 1:p:678:ASN:O    | 1:p:682:ILE:HG12 | 2.21                     | 0.41              |
| 2:2:252:PHE:HB2  | 2:2:264:ARG:HB2  | 2.01                     | 0.41              |
| 2:e:260:ARG:HG2  | 2:e:289:LEU:HD11 | 2.02                     | 0.41              |
| 2:h:246:ARG:HA   | 2:h:249:ILE:HD12 | 2.03                     | 0.41              |
| 2:i:66:ARG:HH11  | 2:i:69:GLN:CD    | 2.21                     | 0.41              |
| 2:j:70:LEU:HD22  | 2:j:247:ARG:HB3  | 2.02                     | 0.41              |
| 2:j:134:ASP:OD1  | 2:j:231:GLN:NE2  | 2.53                     | 0.41              |
| 2:j:246:ARG:HA   | 2:j:249:ILE:HD12 | 2.03                     | 0.41              |
| 2:j:282:ARG:HA   | 2:j:282:ARG:HD2  | 1.83                     | 0.41              |
| 3:u:44:PHE:CZ    | 3:u:55:MET:HE2   | 2.56                     | 0.41              |
| 4:y:173:ILE:HG12 | 4:y:208:VAL:HG23 | 2.01                     | 0.41              |
| 4:U:75:THR:HG22  | 4:U:77:ILE:HG12  | 2.02                     | 0.41              |
| 5:Z:219:ALA:HA   | 5:Z:227:LEU:HD21 | 2.03                     | 0.41              |
| 1:A:256:LEU:HG   | 1:A:347:LEU:HD23 | 2.02                     | 0.41              |
| 1:A:678:ASN:O    | 1:A:682:ILE:HG12 | 2.20                     | 0.41              |
| 1:B:750:PRO:HA   | 3:K:86:ARG:HH22  | 1.86                     | 0.41              |
| 1:B:757:ARG:HA   | 1:B:768:PHE:HE2  | 1.86                     | 0.41              |
| 1:C:88:THR:HG22  | 1:C:89:THR:HG23  | 2.03                     | 0.41              |
| 1:C:1156:CYS:SG  | 1:C:1157:GLU:N   | 2.94                     | 0.41              |
| 1:E:52:GLU:HG2   | 1:F:91:LYS:NZ    | 2.27                     | 0.41              |
| 1:F:119:LYS:CD   | 1:l:33:PHE:HD1   | 2.34                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:F:139:HIS:CE1   | 1:F:153:LEU:HD23  | 2.55                     | 0.41              |
| 1:F:313:ALA:HB3   | 1:m:333:ILE:HD13  | 2.03                     | 0.41              |
| 1:F:683:THR:HA    | 1:F:784:VAL:HG11  | 2.02                     | 0.41              |
| 1:F:1048:VAL:HG22 | 1:F:1061:VAL:HG12 | 2.02                     | 0.41              |
| 1:G:561:GLY:HA3   | 1:G:975:PHE:CE1   | 2.56                     | 0.41              |
| 1:H:757:ARG:NH1   | 1:H:868:VAL:O     | 2.41                     | 0.41              |
| 1:I:190:PRO:HA    | 1:I:1078:THR:HB   | 2.02                     | 0.41              |
| 1:I:231:LEU:HD22  | 1:I:280:VAL:HG23  | 2.02                     | 0.41              |
| 1:I:768:PHE:HD2   | 1:I:870:GLU:HB2   | 1.85                     | 0.41              |
| 1:k:185:LEU:HD23  | 1:k:1032:LEU:HD13 | 2.02                     | 0.41              |
| 1:k:209:THR:HG21  | 1:p:1280:GLU:HA   | 2.02                     | 0.41              |
| 1:k:221:LYS:NZ    | 1:k:1304:GLU:OE1  | 2.37                     | 0.41              |
| 1:l:80:MET:HB2    | 1:l:303:TYR:HD2   | 1.85                     | 0.41              |
| 1:l:244:LEU:HA    | 1:l:247:LEU:HD12  | 2.02                     | 0.41              |
| 1:l:725:PRO:HA    | 1:l:774:THR:H     | 1.85                     | 0.41              |
| 1:l:950:TYR:C     | 1:l:957:PHE:CZ    | 2.98                     | 0.41              |
| 1:l:1179:ARG:HG3  | 1:l:1205:ASP:HB2  | 2.02                     | 0.41              |
| 1:m:441:ILE:HD11  | 1:m:1094:MET:HE2  | 2.03                     | 0.41              |
| 1:m:531:LEU:HD13  | 1:m:1201:HIS:HB3  | 2.01                     | 0.41              |
| 1:n:507:PRO:HD2   | 1:n:958:PRO:HB3   | 2.03                     | 0.41              |
| 1:n:1009:ARG:HB3  | 1:o:522:GLU:OE2   | 2.20                     | 0.41              |
| 1:o:126:ILE:O     | 1:o:1062:SER:HA   | 2.20                     | 0.41              |
| 1:o:1029:ASP:N    | 1:o:1082:HIS:O    | 2.51                     | 0.41              |
| 1:p:497:LEU:HD13  | 1:p:963:PHE:CZ    | 2.55                     | 0.41              |
| 1:p:649:PHE:HB3   | 1:p:655:MET:HB3   | 2.03                     | 0.41              |
| 1:p:1165:ALA:O    | 1:p:1169:PHE:N    | 2.53                     | 0.41              |
| 1:q:1037:ALA:HB1  | 1:q:1070:MET:HE3  | 2.03                     | 0.41              |
| 2:3:73:GLU:HG2    | 2:3:77:TRP:CD1    | 2.56                     | 0.41              |
| 2:h:98:ILE:O      | 2:h:102:TYR:N     | 2.44                     | 0.41              |
| 2:h:285:GLU:CD    | 3:P:67:LYS:HZ1    | 2.20                     | 0.41              |
| 3:r:87:MET:HA     | 3:r:90:ILE:HD12   | 2.03                     | 0.41              |
| 4:S:189:TYR:HB2   | 4:S:209:VAL:HG13  | 2.02                     | 0.41              |
| 4:S:268:VAL:HG22  | 4:S:275:LEU:HB3   | 2.01                     | 0.41              |
| 5:z:89:CYS:SG     | 5:z:306:LEU:HB3   | 2.60                     | 0.41              |
| 5:W:309:TYR:OH    | 5:a:311:GLY:O     | 2.33                     | 0.41              |
| 5:X:112:VAL:HG21  | 5:X:132:TRP:CE2   | 2.56                     | 0.41              |
| 5:Y:147:MET:HB2   | 5:Y:147:MET:HE3   | 1.79                     | 0.41              |
| 5:Y:194:ARG:NH1   | 5:c:221:GLU:O     | 2.54                     | 0.41              |
| 5:a:51:ASP:HB2    | 5:a:54:ARG:HB2    | 2.03                     | 0.41              |
| 1:A:428:THR:HG22  | 1:A:442:SER:HB3   | 2.03                     | 0.41              |
| 1:A:429:VAL:HG13  | 1:A:1310:THR:HG23 | 2.02                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:647:LEU:HA    | 1:A:647:LEU:HD13  | 1.80                     | 0.41              |
| 1:A:865:VAL:HA    | 1:A:868:VAL:HG23  | 2.01                     | 0.41              |
| 1:A:1289:GLU:HG3  | 4:U:144:ALA:HB1   | 2.02                     | 0.41              |
| 1:B:389:ASP:OD1   | 1:B:389:ASP:N     | 2.39                     | 0.41              |
| 1:B:401:HIS:HB3   | 1:B:1162:PRO:HB2  | 2.03                     | 0.41              |
| 1:B:757:ARG:HA    | 1:B:768:PHE:CE2   | 2.56                     | 0.41              |
| 1:B:794:LEU:HD23  | 1:B:794:LEU:HA    | 1.89                     | 0.41              |
| 1:B:923:PHE:HA    | 1:B:963:PHE:CZ    | 2.56                     | 0.41              |
| 1:B:1093:ARG:HH11 | 1:B:1153:ARG:HD2  | 1.85                     | 0.41              |
| 1:B:1321:LEU:HD12 | 1:B:1327:LEU:HD21 | 2.02                     | 0.41              |
| 1:C:592:HIS:HB2   | 1:C:682:ILE:HD11  | 2.02                     | 0.41              |
| 1:C:966:GLU:HA    | 1:C:969:HIS:HD2   | 1.86                     | 0.41              |
| 1:D:6:THR:HG23    | 1:D:46:ARG:HA     | 2.03                     | 0.41              |
| 1:D:11:LEU:HD23   | 1:D:11:LEU:HA     | 1.93                     | 0.41              |
| 1:D:62:ILE:HD12   | 1:D:62:ILE:HA     | 1.85                     | 0.41              |
| 1:D:194:LEU:HG    | 1:D:250:CYS:HB3   | 2.03                     | 0.41              |
| 1:D:637:VAL:HG22  | 1:D:648:ALA:HB3   | 2.02                     | 0.41              |
| 1:D:982:CYS:SG    | 1:D:988:SER:OG    | 2.63                     | 0.41              |
| 1:D:1172:TYR:HE2  | 1:D:1207:GLN:HE22 | 1.67                     | 0.41              |
| 1:E:251:VAL:HG11  | 1:E:1033:TYR:HE2  | 1.85                     | 0.41              |
| 1:E:396:PHE:HB2   | 1:E:1310:THR:HG21 | 2.02                     | 0.41              |
| 1:F:361:LEU:HD23  | 1:F:370:LEU:HD11  | 2.02                     | 0.41              |
| 1:F:470:PRO:HG2   | 1:F:480:LEU:HD21  | 2.03                     | 0.41              |
| 1:F:544:HIS:ND1   | 1:F:553:LEU:HB2   | 2.36                     | 0.41              |
| 1:F:804:ASN:HA    | 1:F:871:ASN:HD21  | 1.85                     | 0.41              |
| 1:F:816:LYS:HE3   | 1:F:835:ASN:HD22  | 1.85                     | 0.41              |
| 1:F:943:PHE:CE2   | 1:F:958:PRO:HG3   | 2.56                     | 0.41              |
| 1:F:1327:LEU:H    | 1:F:1347:GLN:HE21 | 1.68                     | 0.41              |
| 1:G:124:SER:O     | 1:G:1065:ILE:HG12 | 2.21                     | 0.41              |
| 1:G:437:ILE:HG21  | 1:H:1207:GLN:HE21 | 1.85                     | 0.41              |
| 1:G:638:ASN:ND2   | 1:G:668:VAL:O     | 2.53                     | 0.41              |
| 1:G:975:PHE:HE1   | 1:G:995:MET:HB3   | 1.86                     | 0.41              |
| 1:G:1064:ASN:OD1  | 5:W:77:ASN:ND2    | 2.54                     | 0.41              |
| 1:H:92:MET:HE2    | 1:H:346:PHE:HD2   | 1.86                     | 0.41              |
| 1:H:505:ILE:HD11  | 2:h:141:ASP:HB3   | 2.03                     | 0.41              |
| 1:H:715:ARG:HB3   | 1:H:970:TRP:CZ2   | 2.55                     | 0.41              |
| 1:H:1146:PRO:O    | 1:I:210:ARG:NH2   | 2.54                     | 0.41              |
| 1:H:1184:LEU:HD23 | 1:H:1184:LEU:HA   | 1.86                     | 0.41              |
| 1:H:1273:SER:OG   | 1:H:1293:SER:OG   | 2.36                     | 0.41              |
| 1:I:344:SER:H     | 1:I:347:LEU:HD12  | 1.85                     | 0.41              |
| 1:I:456:HIS:CD2   | 1:I:1001:PRO:HB3  | 2.56                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:I:656:VAL:HG23  | 1:I:676:TYR:HD1   | 1.84                     | 0.41              |
| 1:I:682:ILE:HD13  | 1:I:682:ILE:HA    | 1.90                     | 0.41              |
| 1:I:898:GLN:HG2   | 1:I:970:TRP:CD1   | 2.56                     | 0.41              |
| 1:I:1165:ALA:HB3  | 1:I:1168:GLU:HB2  | 2.03                     | 0.41              |
| 1:I:1166:ASP:N    | 1:I:1166:ASP:OD1  | 2.54                     | 0.41              |
| 1:I:1312:THR:HG21 | 1:I:1336:ASN:HD22 | 1.86                     | 0.41              |
| 1:k:504:ARG:NE    | 1:k:946:ASP:OD2   | 2.46                     | 0.41              |
| 1:k:860:GLU:HA    | 1:k:863:HIS:HD2   | 1.85                     | 0.41              |
| 1:k:932:LEU:HA    | 1:k:932:LEU:HD12  | 1.90                     | 0.41              |
| 1:k:943:PHE:CE2   | 1:k:958:PRO:HG3   | 2.56                     | 0.41              |
| 1:l:64:TRP:CH2    | 1:l:166:LYS:HG2   | 2.56                     | 0.41              |
| 1:l:88:THR:HG22   | 1:l:89:THR:HG23   | 2.02                     | 0.41              |
| 1:l:174:ARG:HH22  | 1:m:99:PRO:HA     | 1.83                     | 0.41              |
| 1:l:546:GLU:HB3   | 1:l:547:ASN:H     | 1.75                     | 0.41              |
| 1:l:753:SER:CB    | 3:s:86:ARG:HD3    | 2.50                     | 0.41              |
| 1:l:810:VAL:HG21  | 3:s:78:LEU:HD22   | 2.03                     | 0.41              |
| 1:l:1096:ASP:OD1  | 1:l:1096:ASP:N    | 2.51                     | 0.41              |
| 1:m:51:PHE:CG     | 1:n:87:MET:CB     | 2.93                     | 0.41              |
| 1:m:149:LEU:HD12  | 1:m:153:LEU:HB2   | 2.02                     | 0.41              |
| 1:m:349:GLN:HB3   | 1:m:351:LEU:HG    | 2.03                     | 0.41              |
| 1:m:481:CYS:O     | 1:m:545:THR:N     | 2.50                     | 0.41              |
| 1:m:730:LEU:HB2   | 1:m:731:VAL:HG23  | 2.03                     | 0.41              |
| 1:m:1323:GLY:CA   | 1:n:1329:LEU:CD2  | 2.99                     | 0.41              |
| 1:m:1324:THR:H    | 1:n:1326:LYS:HZ2  | 1.69                     | 0.41              |
| 1:n:373:LEU:HD12  | 1:n:373:LEU:HA    | 1.87                     | 0.41              |
| 1:n:877:ILE:O     | 1:n:897:LEU:HA    | 2.21                     | 0.41              |
| 1:n:1003:SER:O    | 1:n:1007:LEU:HB2  | 2.20                     | 0.41              |
| 1:o:129:PRO:HA    | 1:o:1059:PHE:O    | 2.20                     | 0.41              |
| 1:o:661:THR:HA    | 1:p:606:HIS:NE2   | 2.36                     | 0.41              |
| 1:o:1038:SER:OG   | 1:o:1039:THR:N    | 2.54                     | 0.41              |
| 1:p:66:THR:HG23   | 1:p:69:GLY:H      | 1.85                     | 0.41              |
| 1:p:901:LEU:HD12  | 1:p:901:LEU:HA    | 1.86                     | 0.41              |
| 1:p:925:ARG:NH2   | 1:p:971:HIS:O     | 2.36                     | 0.41              |
| 1:p:1019:THR:HG23 | 1:p:1160:LEU:HD12 | 1.89                     | 0.41              |
| 1:q:81:PHE:HD2    | 1:q:84:LEU:HG     | 1.84                     | 0.41              |
| 1:q:482:ARG:HD2   | 1:q:485:PHE:HB2   | 2.02                     | 0.41              |
| 1:q:482:ARG:HG2   | 1:q:544:HIS:HA    | 2.03                     | 0.41              |
| 1:q:858:ALA:O     | 1:q:862:PHE:HB2   | 2.20                     | 0.41              |
| 1:q:889:ALA:HB1   | 1:q:892:ALA:HB3   | 2.03                     | 0.41              |
| 2:2:259:ALA:HB3   | 2:2:289:LEU:HD13  | 2.01                     | 0.41              |
| 2:3:246:ARG:HA    | 2:3:249:ILE:HD12  | 2.03                     | 0.41              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:h:134:ASP:OD1  | 2:h:231:GLN:NE2   | 2.53                     | 0.41              |
| 2:i:93:PRO:HD2   | 2:i:195:TYR:HH    | 1.83                     | 0.41              |
| 2:i:260:ARG:HD3  | 2:i:289:LEU:HD21  | 2.03                     | 0.41              |
| 2:g:101:ASP:CA   | 2:g:104:LYS:HG2   | 2.43                     | 0.41              |
| 2:g:252:PHE:HB2  | 2:g:264:ARG:HB2   | 2.01                     | 0.41              |
| 2:j:77:TRP:O     | 2:j:81:HIS:N      | 2.54                     | 0.41              |
| 2:j:187:ASP:O    | 2:j:191:ARG:N     | 2.54                     | 0.41              |
| 3:M:68:TYR:HE2   | 3:M:84:LEU:HD12   | 1.86                     | 0.41              |
| 3:x:58:GLN:HB2   | 3:x:61:ILE:HG22   | 2.03                     | 0.41              |
| 4:y:245:SER:OG   | 4:y:246:THR:N     | 2.53                     | 0.41              |
| 4:S:60:GLU:O     | 4:S:62:GLU:N      | 2.54                     | 0.41              |
| 5:z:31:ILE:H     | 5:z:31:ILE:HG13   | 1.76                     | 0.41              |
| 5:z:106:LEU:N    | 5:z:293:PHE:O     | 2.48                     | 0.41              |
| 5:X:56:TYR:OH    | 5:X:289:GLU:OE2   | 2.35                     | 0.41              |
| 5:X:69:THR:HG22  | 5:X:83:VAL:HG22   | 2.03                     | 0.41              |
| 5:X:113:PHE:CG   | 5:X:181:PRO:HG3   | 2.55                     | 0.41              |
| 5:Z:33:TYR:CD2   | 5:Z:35:HIS:HB2    | 2.56                     | 0.41              |
| 5:1:33:TYR:CE2   | 5:1:35:HIS:HB2    | 2.56                     | 0.41              |
| 5:d:63:MET:HE2   | 5:d:63:MET:HB3    | 1.87                     | 0.41              |
| 5:d:71:MET:HA    | 5:d:81:LEU:HD23   | 2.03                     | 0.41              |
| 1:A:99:PRO:HG2   | 1:F:379:ASN:HB2   | 2.02                     | 0.41              |
| 1:A:901:LEU:HD12 | 1:A:901:LEU:HA    | 1.93                     | 0.41              |
| 1:A:1330:ASP:OD1 | 1:A:1330:ASP:N    | 2.41                     | 0.41              |
| 1:B:646:LEU:H    | 1:B:646:LEU:HG    | 1.80                     | 0.41              |
| 1:D:233:ARG:HH22 | 1:D:1343:ILE:HG23 | 1.86                     | 0.41              |
| 1:D:754:ASP:N    | 3:M:83:ASP:OD1    | 2.54                     | 0.41              |
| 1:E:282:GLN:HE22 | 1:E:372:HIS:CE1   | 2.38                     | 0.41              |
| 1:E:562:ASN:ND2  | 1:E:972:ARG:H     | 2.19                     | 0.41              |
| 1:E:664:GLY:HA2  | 1:F:644:ARG:CZ    | 2.51                     | 0.41              |
| 1:E:930:PRO:O    | 1:E:934:ALA:CB    | 2.68                     | 0.41              |
| 1:F:83:ASP:OD2   | 1:l:147:THR:OG1   | 2.35                     | 0.41              |
| 1:F:310:LYS:HB2  | 1:m:330:ALA:O     | 2.20                     | 0.41              |
| 1:G:586:VAL:HG11 | 1:G:688:ARG:HD2   | 2.03                     | 0.41              |
| 1:G:608:TYR:HA   | 1:G:609:PRO:HD3   | 1.90                     | 0.41              |
| 1:G:1025:THR:H   | 1:G:1088:SER:HB2  | 1.86                     | 0.41              |
| 1:H:316:ALA:HB2  | 1:H:322:ILE:HD11  | 2.02                     | 0.41              |
| 1:H:396:PHE:CZ   | 1:H:1020:VAL:HB   | 2.56                     | 0.41              |
| 1:H:794:LEU:O    | 1:H:797:HIS:ND1   | 2.46                     | 0.41              |
| 1:k:131:GLU:O    | 1:l:112:GLN:NE2   | 2.53                     | 0.41              |
| 1:k:388:ARG:HH12 | 1:k:1078:THR:HG21 | 1.86                     | 0.41              |
| 1:k:702:GLU:OE1  | 1:k:715:ARG:NH1   | 2.45                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:k:920:VAL:HG21 | 1:k:933:ALA:HA   | 2.02                     | 0.41              |
| 1:l:528:ASN:OD1  | 1:l:529:TYR:N    | 2.53                     | 0.41              |
| 1:l:558:ILE:HG12 | 1:l:881:LEU:HD21 | 2.03                     | 0.41              |
| 1:l:599:LEU:HD23 | 1:l:793:VAL:HG21 | 2.02                     | 0.41              |
| 1:l:753:SER:HB2  | 3:s:83:ASP:OD1   | 2.21                     | 0.41              |
| 1:m:19:ASP:OD1   | 1:m:19:ASP:N     | 2.54                     | 0.41              |
| 1:m:23:HIS:HD2   | 1:m:25:LYS:HB3   | 1.86                     | 0.41              |
| 1:n:389:ASP:HB3  | 1:n:1027:GLU:HG2 | 2.03                     | 0.41              |
| 1:n:757:ARG:HH21 | 1:n:869:PRO:C    | 2.29                     | 0.41              |
| 1:o:585:LYS:HE3  | 1:o:585:LYS:HB2  | 1.94                     | 0.41              |
| 1:o:600:ARG:HH11 | 1:o:794:LEU:HD23 | 1.86                     | 0.41              |
| 1:p:555:THR:HG21 | 1:p:967:TYR:HB3  | 2.03                     | 0.41              |
| 1:p:639:ASN:OD1  | 1:p:642:ARG:NH1  | 2.41                     | 0.41              |
| 1:p:808:LEU:HD13 | 1:p:917:TYR:HB3  | 2.02                     | 0.41              |
| 1:q:443:HIS:HA   | 1:q:446:ALA:HB3  | 2.03                     | 0.41              |
| 1:q:497:LEU:HA   | 1:q:500:PHE:HE1  | 1.86                     | 0.41              |
| 3:K:65:ILE:HD13  | 3:K:65:ILE:HA    | 1.92                     | 0.41              |
| 3:R:85:LEU:HD22  | 3:R:88:LEU:HD12  | 2.02                     | 0.41              |
| 4:y:73:LEU:CG    | 4:y:131:VAL:HA   | 2.50                     | 0.41              |
| 4:S:166:PRO:HB3  | 4:S:281:GLU:HA   | 2.01                     | 0.41              |
| 4:U:83:VAL:HG11  | 4:U:117:ARG:HD2  | 2.03                     | 0.41              |
| 4:U:93:VAL:HG21  | 4:U:121:ARG:HE   | 1.85                     | 0.41              |
| 5:W:277:PHE:HE2  | 5:a:144:GLN:HG2  | 1.86                     | 0.41              |
| 5:Y:17:ASP:CG    | 5:Y:121:VAL:HG11 | 2.45                     | 0.41              |
| 5:Y:29:ILE:HG12  | 5:Y:130:LEU:HD21 | 2.01                     | 0.41              |
| 5:Y:284:THR:O    | 5:Y:288:SER:N    | 2.49                     | 0.41              |
| 5:Z:60:ARG:HH11  | 5:Z:64:ARG:HH22  | 1.69                     | 0.41              |
| 5:a:2:GLU:OE2    | 5:a:72:ARG:NH1   | 2.52                     | 0.41              |
| 5:c:89:CYS:HB3   | 5:c:306:LEU:HD11 | 2.02                     | 0.41              |
| 5:c:226:LEU:HD12 | 5:c:230:CYS:HB2  | 2.03                     | 0.41              |
| 1:A:1149:LEU:O   | 1:B:214:ALA:HB1  | 2.21                     | 0.40              |
| 1:B:493:ALA:HB3  | 1:B:874:MET:HB3  | 2.03                     | 0.40              |
| 1:C:228:ILE:HG22 | 1:C:233:ARG:HH21 | 1.86                     | 0.40              |
| 1:D:57:THR:HA    | 1:E:93:LEU:O     | 2.21                     | 0.40              |
| 1:D:602:SER:HA   | 1:D:646:LEU:HD13 | 2.03                     | 0.40              |
| 1:E:559:MET:HE2  | 1:E:975:PHE:HE2  | 1.86                     | 0.40              |
| 1:E:701:ASP:OD2  | 1:E:1108:ASN:ND2 | 2.47                     | 0.40              |
| 1:F:483:ARG:HH12 | 1:F:513:GLU:CD   | 2.30                     | 0.40              |
| 1:G:725:PRO:HG2  | 1:G:728:ALA:HB2  | 2.02                     | 0.40              |
| 1:G:802:GLY:O    | 1:G:919:THR:N    | 2.41                     | 0.40              |
| 1:H:1344:PRO:HB2 | 1:H:1347:GLN:HB2 | 2.03                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:k:500:PHE:CZ    | 1:k:507:PRO:HD3   | 2.54                     | 0.40              |
| 1:k:665:ASP:OD1   | 1:l:607:GLN:NE2   | 2.54                     | 0.40              |
| 1:k:1322:LYS:HE2  | 1:l:1331:GLU:HB3  | 2.03                     | 0.40              |
| 1:l:229:PHE:HB3   | 1:l:232:ASP:HB2   | 2.02                     | 0.40              |
| 1:l:802:GLY:HA3   | 1:l:872:ALA:HB2   | 2.02                     | 0.40              |
| 1:m:388:ARG:HD2   | 1:m:1030:THR:HG21 | 2.04                     | 0.40              |
| 1:m:888:GLY:O     | 1:m:892:ALA:N     | 2.46                     | 0.40              |
| 1:n:119:LYS:NZ    | 1:n:1071:GLY:O    | 2.40                     | 0.40              |
| 1:n:603:LEU:HB3   | 1:n:794:LEU:HD21  | 2.04                     | 0.40              |
| 1:n:998:LYS:HE3   | 1:n:998:LYS:HB2   | 1.93                     | 0.40              |
| 1:o:195:ARG:HH12  | 1:o:199:GLU:HB2   | 1.85                     | 0.40              |
| 1:o:298:LYS:HE3   | 1:o:353:PHE:CG    | 2.56                     | 0.40              |
| 1:o:644:ARG:HD3   | 1:o:644:ARG:HA    | 1.82                     | 0.40              |
| 1:o:678:ASN:O     | 1:o:682:ILE:HG12  | 2.22                     | 0.40              |
| 1:p:390:VAL:HG22  | 1:p:1295:VAL:HB   | 2.02                     | 0.40              |
| 1:p:813:PHE:CD2   | 3:w:85:LEU:HD23   | 2.56                     | 0.40              |
| 1:q:140:LEU:HD21  | 1:q:161:VAL:HG11  | 2.02                     | 0.40              |
| 2:3:260:ARG:HD3   | 2:3:289:LEU:HD21  | 2.03                     | 0.40              |
| 2:3:282:ARG:HD2   | 2:3:282:ARG:HA    | 1.83                     | 0.40              |
| 2:e:212:VAL:HG21  | 2:h:92:LEU:HD21   | 2.02                     | 0.40              |
| 2:e:259:ALA:HB3   | 2:e:289:LEU:HD13  | 2.02                     | 0.40              |
| 2:i:133:GLY:O     | 2:i:136:TYR:CB    | 2.69                     | 0.40              |
| 2:i:134:ASP:OD1   | 2:i:231:GLN:NE2   | 2.53                     | 0.40              |
| 2:g:212:VAL:HG21  | 2:j:92:LEU:HD21   | 2.02                     | 0.40              |
| 4:y:66:LEU:HD21   | 4:y:140:ILE:HA    | 2.02                     | 0.40              |
| 4:U:95:GLU:OE2    | 4:U:203:ARG:NH2   | 2.54                     | 0.40              |
| 4:U:99:ALA:O      | 4:U:103:ASN:ND2   | 2.54                     | 0.40              |
| 5:W:149:LEU:HD13  | 5:W:165:THR:HG22  | 2.02                     | 0.40              |
| 5:X:192:ASP:HA    | 5:X:195:ASN:HD22  | 1.85                     | 0.40              |
| 5:1:106:LEU:HG    | 5:1:133:ILE:HG22  | 2.03                     | 0.40              |
| 5:d:19:GLY:O      | 5:d:22:SER:OG     | 2.37                     | 0.40              |
| 1:A:1055:ILE:HD12 | 1:A:1055:ILE:HA   | 1.96                     | 0.40              |
| 1:B:62:ILE:HD12   | 1:B:62:ILE:HA     | 1.89                     | 0.40              |
| 1:B:119:LYS:NZ    | 1:B:1071:GLY:O    | 2.35                     | 0.40              |
| 1:B:603:LEU:HB3   | 1:B:794:LEU:HD21  | 2.03                     | 0.40              |
| 1:B:1300:ARG:H    | 1:B:1303:GLN:NE2  | 2.19                     | 0.40              |
| 1:C:181:LEU:HD22  | 1:C:373:LEU:HD21  | 2.03                     | 0.40              |
| 1:C:985:THR:O     | 1:C:986:LEU:C     | 2.65                     | 0.40              |
| 1:D:359:ASP:O     | 1:D:370:LEU:N     | 2.40                     | 0.40              |
| 1:D:706:ALA:HB1   | 1:D:713:ASP:HB3   | 2.04                     | 0.40              |
| 1:D:743:ALA:C     | 2:g:174:ARG:HA    | 2.47                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:D:1322:LYS:HE2  | 1:E:1330:ASP:OD1  | 2.21                     | 0.40              |
| 1:E:141:LYS:HE3   | 4:S:33:ARG:HH22   | 1.87                     | 0.40              |
| 1:E:429:VAL:HG22  | 1:E:1312:THR:HA   | 2.03                     | 0.40              |
| 1:E:967:TYR:O     | 1:E:972:ARG:NH2   | 2.55                     | 0.40              |
| 1:E:1179:ARG:HD2  | 1:E:1201:HIS:CE1  | 2.56                     | 0.40              |
| 1:F:113:THR:CG2   | 1:l:38:LEU:HD11   | 2.50                     | 0.40              |
| 1:F:120:TYR:HD2   | 1:l:34:ASN:ND2    | 2.19                     | 0.40              |
| 1:G:605:ASP:OD2   | 1:G:640:TYR:OH    | 2.39                     | 0.40              |
| 1:G:744:HIS:HB2   | 2:e:174:ARG:C     | 2.43                     | 0.40              |
| 1:G:1344:PRO:HB2  | 1:G:1347:GLN:HB2  | 2.03                     | 0.40              |
| 1:H:248:THR:HG22  | 1:H:1033:TYR:CZ   | 2.56                     | 0.40              |
| 1:H:483:ARG:NH2   | 1:H:508:PRO:O     | 2.55                     | 0.40              |
| 1:H:492:HIS:HD2   | 1:H:495:ARG:HB2   | 1.86                     | 0.40              |
| 1:H:1175:ASN:HD22 | 1:H:1180:SER:HA   | 1.85                     | 0.40              |
| 1:I:412:GLU:HG2   | 1:I:1333:HIS:HE1  | 1.86                     | 0.40              |
| 1:I:576:ARG:HH11  | 1:I:1007:LEU:HD21 | 1.85                     | 0.40              |
| 1:k:98:VAL:HG12   | 1:k:114:THR:H     | 1.87                     | 0.40              |
| 1:k:1166:ASP:HA   | 1:k:1170:PHE:HD2  | 1.86                     | 0.40              |
| 1:l:125:PRO:HB3   | 1:l:1064:ASN:HA   | 2.03                     | 0.40              |
| 1:l:659:ILE:O     | 1:l:663:LEU:CB    | 2.69                     | 0.40              |
| 1:l:1142:ASP:O    | 1:l:1285:TYR:OH   | 2.25                     | 0.40              |
| 1:l:1175:ASN:HB3  | 1:l:1180:SER:HA   | 2.02                     | 0.40              |
| 1:m:486:VAL:O     | 1:m:965:HIS:NE2   | 2.46                     | 0.40              |
| 1:m:1324:THR:N    | 1:n:1326:LYS:HZ2  | 2.20                     | 0.40              |
| 1:n:91:LYS:HA     | 1:n:119:LYS:O     | 2.20                     | 0.40              |
| 1:n:231:LEU:HD12  | 1:n:235:ARG:HH12  | 1.87                     | 0.40              |
| 1:o:254:SER:OG    | 1:o:1036:LYS:O    | 2.39                     | 0.40              |
| 2:3:187:ASP:O     | 2:3:191:ARG:N     | 2.54                     | 0.40              |
| 2:f:66:ARG:CG     | 2:f:69:GLN:HG3    | 2.43                     | 0.40              |
| 2:j:88:ARG:HA     | 2:j:89:PRO:HD3    | 1.69                     | 0.40              |
| 3:u:48:VAL:HA     | 3:u:77:LYS:HD2    | 2.02                     | 0.40              |
| 4:U:69:LEU:HG     | 4:U:167:LEU:HD11  | 2.03                     | 0.40              |
| 4:U:99:ALA:HA     | 4:U:102:LYS:HB3   | 2.03                     | 0.40              |
| 5:z:168:LEU:HD12  | 5:1:270:LEU:HD13  | 2.03                     | 0.40              |
| 5:W:109:LEU:O     | 5:W:110:PRO:O     | 2.39                     | 0.40              |
| 5:b:5:VAL:HB      | 5:b:81:LEU:HB2    | 2.02                     | 0.40              |
| 1:A:59:CYS:HA     | 1:B:95:TYR:O      | 2.20                     | 0.40              |
| 1:A:193:VAL:HG11  | 1:A:1266:VAL:HG21 | 2.02                     | 0.40              |
| 1:A:236:ASP:HB3   | 1:A:239:GLN:H     | 1.86                     | 0.40              |
| 1:D:678:ASN:HA    | 1:D:681:SER:HB2   | 2.04                     | 0.40              |
| 1:D:794:LEU:HA    | 1:D:794:LEU:HD23  | 1.88                     | 0.40              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:D:1146:PRO:O   | 1:E:1197:THR:HG21 | 2.21                     | 0.40              |
| 1:D:1309:HIS:CE1 | 1:D:1327:LEU:HD12 | 2.57                     | 0.40              |
| 1:E:724:LEU:HB2  | 1:E:769:VAL:HG21  | 2.03                     | 0.40              |
| 1:F:1297:LYS:HD3 | 1:F:1299:CYS:HB2  | 2.04                     | 0.40              |
| 1:G:622:ASP:HB3  | 1:G:625:ALA:HB3   | 2.03                     | 0.40              |
| 1:H:381:ASP:OD1  | 1:H:381:ASP:N     | 2.53                     | 0.40              |
| 1:H:1269:TYR:CE1 | 1:H:1296:GLU:HB2  | 2.55                     | 0.40              |
| 1:k:401:HIS:HB3  | 1:k:1162:PRO:HB2  | 2.02                     | 0.40              |
| 1:k:523:PHE:CG   | 1:k:566:ALA:HB1   | 2.56                     | 0.40              |
| 1:k:544:HIS:CE1  | 1:k:553:LEU:HB2   | 2.55                     | 0.40              |
| 1:k:744:HIS:HA   | 2:2:175:ALA:N     | 2.37                     | 0.40              |
| 1:l:415:ILE:HD12 | 1:l:1315:ALA:HB1  | 2.03                     | 0.40              |
| 1:l:1156:CYS:SG  | 1:l:1157:GLU:N    | 2.95                     | 0.40              |
| 1:l:1298:PRO:O   | 1:l:1302:LEU:N    | 2.47                     | 0.40              |
| 1:m:688:ARG:HH22 | 1:n:797:HIS:CE1   | 2.39                     | 0.40              |
| 1:n:452:HIS:CD2  | 1:n:453:PRO:HD2   | 2.57                     | 0.40              |
| 1:o:65:VAL:HG11  | 1:o:376:VAL:HG12  | 2.04                     | 0.40              |
| 1:o:1093:ARG:HG3 | 1:o:1153:ARG:HG3  | 2.04                     | 0.40              |
| 1:p:663:LEU:HD21 | 1:p:669:VAL:HB    | 2.03                     | 0.40              |
| 1:q:632:LEU:HD23 | 1:q:635:ARG:HH21  | 1.86                     | 0.40              |
| 1:q:715:ARG:HG2  | 1:q:730:LEU:HD22  | 2.03                     | 0.40              |
| 2:j:73:GLU:HG2   | 2:j:77:TRP:CD1    | 2.56                     | 0.40              |
| 3:N:48:VAL:HA    | 3:N:77:LYS:HD2    | 2.02                     | 0.40              |
| 3:v:85:LEU:HA    | 3:v:88:LEU:HD12   | 2.02                     | 0.40              |
| 3:w:68:TYR:HE2   | 3:w:84:LEU:HD23   | 1.86                     | 0.40              |
| 4:S:115:ALA:O    | 4:S:118:THR:OG1   | 2.35                     | 0.40              |
| 4:S:185:ILE:HD12 | 4:S:259:CYS:HA    | 2.04                     | 0.40              |
| 5:z:110:PRO:CB   | 5:z:111:PRO:CD    | 2.95                     | 0.40              |
| 5:W:158:HIS:CD2  | 5:W:159:GLU:HG2   | 2.56                     | 0.40              |
| 5:X:180:LEU:HB3  | 5:X:183:ILE:HD11  | 2.03                     | 0.40              |
| 5:Y:3:THR:HA     | 5:Y:83:VAL:HB     | 2.03                     | 0.40              |
| 5:Z:138:LEU:HD11 | 5:Z:178:LEU:HD21  | 2.02                     | 0.40              |
| 5:Z:147:MET:SD   | 5:Z:196:VAL:HG21  | 2.62                     | 0.40              |
| 5:a:120:LEU:HB2  | 5:a:128:LEU:H     | 1.86                     | 0.40              |
| 5:c:107:THR:N    | 5:c:134:VAL:O     | 2.50                     | 0.40              |
| 1:A:128:ILE:HG22 | 1:B:102:ALA:CA    | 2.50                     | 0.40              |
| 1:A:132:ILE:HD13 | 1:A:161:VAL:HG22  | 2.03                     | 0.40              |
| 1:A:537:PRO:HG3  | 1:A:1159:ILE:HG21 | 2.04                     | 0.40              |
| 1:A:1021:VAL:CG2 | 1:A:1156:CYS:HB3  | 2.48                     | 0.40              |
| 1:B:564:PRO:HD2  | 1:B:567:LEU:HD12  | 2.02                     | 0.40              |
| 1:B:836:ASN:HB3  | 1:B:839:LEU:HB3   | 2.02                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:1309:HIS:CE1  | 1:B:1327:LEU:HD12 | 2.57                     | 0.40              |
| 1:C:60:ASN:HB3    | 1:D:97:GLN:H      | 1.87                     | 0.40              |
| 1:C:839:LEU:HD23  | 1:C:839:LEU:HA    | 1.93                     | 0.40              |
| 1:C:1179:ARG:NH1  | 1:C:1211:SER:O    | 2.51                     | 0.40              |
| 1:D:44:PRO:HB2    | 4:S:162:THR:O     | 2.20                     | 0.40              |
| 1:D:345:GLN:O     | 1:D:349:GLN:NE2   | 2.54                     | 0.40              |
| 1:D:679:LEU:HD23  | 1:D:679:LEU:HA    | 1.90                     | 0.40              |
| 1:D:692:LEU:HD22  | 1:D:692:LEU:HA    | 1.78                     | 0.40              |
| 1:D:1043:ILE:HB   | 1:D:1063:GLN:HE21 | 1.87                     | 0.40              |
| 1:E:323:MET:HE3   | 1:E:323:MET:HB2   | 1.91                     | 0.40              |
| 1:E:652:SER:HB3   | 1:E:655:MET:HB2   | 2.04                     | 0.40              |
| 1:E:755:VAL:HG21  | 3:N:80:TYR:CE1    | 2.57                     | 0.40              |
| 1:E:813:PHE:CZ    | 3:N:85:LEU:HD12   | 2.56                     | 0.40              |
| 1:F:476:ARG:HH21  | 1:F:480:LEU:HD12  | 1.86                     | 0.40              |
| 1:F:537:PRO:HD3   | 1:F:1216:TRP:CG   | 2.56                     | 0.40              |
| 1:F:620:HIS:HE1   | 1:F:770:ASP:HB3   | 1.86                     | 0.40              |
| 1:F:1264:LYS:HG2  | 1:l:31:GLU:HB2    | 2.04                     | 0.40              |
| 1:G:163:ARG:HD2   | 1:H:97:GLN:NE2    | 2.37                     | 0.40              |
| 1:G:247:LEU:HA    | 1:G:247:LEU:HD23  | 1.88                     | 0.40              |
| 1:G:733:VAL:O     | 1:G:740:LEU:N     | 2.53                     | 0.40              |
| 1:G:1017:ALA:O    | 1:G:1018:LEU:CD1  | 2.60                     | 0.40              |
| 1:H:62:ILE:HD12   | 1:H:62:ILE:HA     | 1.96                     | 0.40              |
| 1:H:78:ALA:HA     | 1:H:1041:VAL:HG23 | 2.04                     | 0.40              |
| 1:H:140:LEU:HG    | 1:H:157:ALA:HB1   | 2.04                     | 0.40              |
| 1:H:662:ARG:HH12  | 1:H:668:VAL:HG21  | 1.87                     | 0.40              |
| 1:H:761:MET:HB2   | 1:H:806:LYS:HD3   | 2.02                     | 0.40              |
| 1:k:356:THR:HG23  | 1:k:358:MET:HG3   | 2.02                     | 0.40              |
| 1:k:521:LYS:CD    | 1:p:440:ARG:NH2   | 2.76                     | 0.40              |
| 1:k:955:GLY:HA3   | 1:k:957:PHE:CE2   | 2.56                     | 0.40              |
| 1:l:813:PHE:CD2   | 3:s:81:GLN:HG3    | 2.57                     | 0.40              |
| 1:l:813:PHE:CE2   | 3:s:82:LEU:HA     | 2.56                     | 0.40              |
| 1:l:887:HIS:NE2   | 1:l:1105:VAL:O    | 2.50                     | 0.40              |
| 1:l:1175:ASN:HD22 | 1:l:1181:SER:H    | 1.69                     | 0.40              |
| 1:m:901:LEU:HD11  | 1:m:921:ILE:HD13  | 2.04                     | 0.40              |
| 1:n:193:VAL:HG11  | 1:n:1266:VAL:HG21 | 2.04                     | 0.40              |
| 1:n:271:ALA:HA    | 1:n:1036:LYS:HB2  | 2.03                     | 0.40              |
| 1:n:484:GLU:OE2   | 1:n:966:GLU:N     | 2.54                     | 0.40              |
| 1:o:452:HIS:CE1   | 1:o:1101:PHE:HB2  | 2.57                     | 0.40              |
| 1:o:547:ASN:N     | 1:o:547:ASN:OD1   | 2.53                     | 0.40              |
| 1:o:792:ALA:HB2   | 1:o:992:LEU:HD12  | 2.04                     | 0.40              |
| 1:o:964:ALA:O     | 1:o:966:GLU:N     | 2.55                     | 0.40              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:p:51:PHE:HA     | 1:q:55:PHE:O     | 2.22                     | 0.40              |
| 1:p:391:GLU:O     | 1:p:1297:LYS:HB3 | 2.21                     | 0.40              |
| 1:p:612:PHE:CE1   | 1:p:648:ALA:HB1  | 2.57                     | 0.40              |
| 1:p:943:PHE:CE2   | 1:p:958:PRO:HG3  | 2.56                     | 0.40              |
| 1:q:299:THR:O     | 1:q:354:THR:N    | 2.46                     | 0.40              |
| 1:q:618:LEU:HD11  | 1:q:865:VAL:HA   | 2.03                     | 0.40              |
| 2:3:248:LEU:HA    | 2:3:248:LEU:HD23 | 1.91                     | 0.40              |
| 2:f:212:VAL:HG21  | 2:i:92:LEU:HD21  | 2.02                     | 0.40              |
| 2:f:245:ARG:HH21  | 2:f:268:GLU:C    | 2.30                     | 0.40              |
| 2:j:133:GLY:O     | 2:j:136:TYR:CB   | 2.69                     | 0.40              |
| 5:X:21:LEU:HB2    | 5:X:74:VAL:HG11  | 2.03                     | 0.40              |
| 5:Z:198:ILE:HD13  | 5:d:226:LEU:HD21 | 2.04                     | 0.40              |
| 5:b:45:LEU:CG     | 5:b:48:VAL:HB    | 2.51                     | 0.40              |
| 1:A:95:TYR:HD1    | 1:A:116:MET:HG2  | 1.87                     | 0.40              |
| 1:A:434:LYS:N     | 1:A:1089:ASP:O   | 2.53                     | 0.40              |
| 1:A:683:THR:HA    | 1:A:784:VAL:HG11 | 2.03                     | 0.40              |
| 1:A:754:ASP:HB2   | 3:J:86:ARG:HH12  | 1.84                     | 0.40              |
| 1:B:608:TYR:HA    | 1:B:609:PRO:HD3  | 1.88                     | 0.40              |
| 1:B:780:VAL:HA    | 1:B:783:LYS:HE3  | 2.02                     | 0.40              |
| 1:C:251:VAL:HG11  | 1:C:1033:TYR:HE2 | 1.86                     | 0.40              |
| 1:C:415:ILE:HD12  | 1:C:1315:ALA:HB1 | 2.04                     | 0.40              |
| 1:C:618:LEU:HD22  | 1:C:864:LEU:HB3  | 2.03                     | 0.40              |
| 1:D:77:HIS:CE1    | 1:D:79:ILE:HD11  | 2.56                     | 0.40              |
| 1:D:181:LEU:HD22  | 1:D:373:LEU:HD21 | 2.04                     | 0.40              |
| 1:D:544:HIS:ND1   | 1:D:553:LEU:HB2  | 2.37                     | 0.40              |
| 1:E:285:LEU:HD23  | 1:E:292:ILE:HD13 | 2.03                     | 0.40              |
| 1:E:292:ILE:HG12  | 1:E:361:LEU:HB3  | 2.03                     | 0.40              |
| 1:F:740:LEU:HD22  | 1:F:875:LEU:HD11 | 2.03                     | 0.40              |
| 1:F:1096:ASP:N    | 1:F:1096:ASP:OD1 | 2.52                     | 0.40              |
| 1:G:326:PHE:CE1   | 1:n:318:ALA:HB2  | 2.57                     | 0.40              |
| 1:G:1018:LEU:HG   | 1:G:1159:ILE:HA  | 2.03                     | 0.40              |
| 1:H:116:MET:HE3   | 1:H:116:MET:HB2  | 2.00                     | 0.40              |
| 1:H:184:LEU:O     | 1:H:188:ALA:CB   | 2.69                     | 0.40              |
| 1:H:224:MET:SD    | 1:H:1298:PRO:HD3 | 2.62                     | 0.40              |
| 1:H:1003:SER:O    | 1:H:1007:LEU:CB  | 2.69                     | 0.40              |
| 1:I:1164:SER:OG   | 1:I:1213:ASN:O   | 2.31                     | 0.40              |
| 1:k:127:THR:HG21  | 1:k:1060:HIS:HB3 | 2.03                     | 0.40              |
| 1:k:135:ALA:CA    | 4:y:161:LYS:HB3  | 2.51                     | 0.40              |
| 1:k:408:TYR:CE2   | 1:p:1315:ALA:HA  | 2.56                     | 0.40              |
| 1:k:537:PRO:HB3   | 1:k:1216:TRP:CE3 | 2.56                     | 0.40              |
| 1:k:1345:LEU:HD23 | 1:k:1345:LEU:HA  | 1.91                     | 0.40              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:l:852:VAL:HG12 | 1:l:857:ALA:HB2   | 2.04                     | 0.40              |
| 1:l:1228:TYR:HB2 | 1:l:1250:PHE:CD2  | 2.56                     | 0.40              |
| 1:n:245:ASP:OD1  | 1:n:364:GLY:N     | 2.54                     | 0.40              |
| 1:n:1027:GLU:N   | 1:n:1085:ARG:O    | 2.54                     | 0.40              |
| 1:n:1096:ASP:OD1 | 1:n:1096:ASP:N    | 2.54                     | 0.40              |
| 1:n:1330:ASP:OD1 | 1:n:1330:ASP:N    | 2.47                     | 0.40              |
| 1:o:183:VAL:HG21 | 1:o:1067:THR:HG21 | 2.03                     | 0.40              |
| 1:o:1310:THR:HB  | 1:o:1339:ILE:HB   | 2.03                     | 0.40              |
| 1:p:762:ASP:OD1  | 1:p:871:ASN:ND2   | 2.55                     | 0.40              |
| 1:p:1022:ARG:NH2 | 1:p:1308:GLN:OE1  | 2.54                     | 0.40              |
| 1:q:128:ILE:HG23 | 1:q:1061:VAL:HG23 | 2.03                     | 0.40              |
| 2:h:133:GLY:O    | 2:h:136:TYR:CB    | 2.69                     | 0.40              |
| 2:f:260:ARG:HG2  | 2:f:289:LEU:HD11  | 2.03                     | 0.40              |
| 2:i:107:GLY:O    | 4:U:232:PHE:CD1   | 2.65                     | 0.40              |
| 4:T:262:ASP:HB3  | 4:T:281:GLU:HB2   | 2.04                     | 0.40              |
| 4:V:235:LEU:HD21 | 5:Z:202:MET:HE2   | 2.03                     | 0.40              |
| 5:X:148:MET:HE3  | 5:X:148:MET:HB3   | 1.96                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

| Mol | Chain | Analysed        | Favoured   | Allowed   | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|-----------|----------|-------------|----|
| 1   | A     | 1331/1353 (98%) | 1204 (90%) | 126 (10%) | 1 (0%)   | 48          | 83 |
| 1   | B     | 1304/1353 (96%) | 1209 (93%) | 92 (7%)   | 3 (0%)   | 43          | 77 |
| 1   | C     | 1304/1353 (96%) | 1182 (91%) | 119 (9%)  | 3 (0%)   | 43          | 77 |
| 1   | D     | 1308/1353 (97%) | 1184 (90%) | 123 (9%)  | 1 (0%)   | 48          | 83 |
| 1   | E     | 1326/1353 (98%) | 1186 (89%) | 138 (10%) | 2 (0%)   | 43          | 77 |
| 1   | F     | 1313/1353 (97%) | 1216 (93%) | 92 (7%)   | 5 (0%)   | 30          | 67 |
| 1   | G     | 1337/1353 (99%) | 1223 (92%) | 112 (8%)  | 2 (0%)   | 48          | 83 |

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| Mol | Chain | Analysed        | Favoured   | Allowed   | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|-----------|----------|-------------|-----|
| 1   | H     | 1337/1353 (99%) | 1193 (89%) | 142 (11%) | 2 (0%)   | 48          | 83  |
| 1   | I     | 1315/1353 (97%) | 1190 (90%) | 123 (9%)  | 2 (0%)   | 43          | 77  |
| 1   | k     | 1287/1353 (95%) | 1164 (90%) | 117 (9%)  | 6 (0%)   | 24          | 63  |
| 1   | l     | 1332/1353 (98%) | 1211 (91%) | 120 (9%)  | 1 (0%)   | 48          | 83  |
| 1   | m     | 1306/1353 (96%) | 1175 (90%) | 125 (10%) | 6 (0%)   | 24          | 63  |
| 1   | n     | 1331/1353 (98%) | 1202 (90%) | 128 (10%) | 1 (0%)   | 48          | 83  |
| 1   | o     | 1307/1353 (97%) | 1173 (90%) | 130 (10%) | 4 (0%)   | 36          | 72  |
| 1   | p     | 1297/1353 (96%) | 1167 (90%) | 127 (10%) | 3 (0%)   | 43          | 77  |
| 1   | q     | 1201/1353 (89%) | 1058 (88%) | 143 (12%) | 0        | 100         | 100 |
| 2   | 2     | 166/718 (23%)   | 153 (92%)  | 9 (5%)    | 4 (2%)   | 4           | 26  |
| 2   | 3     | 194/718 (27%)   | 177 (91%)  | 13 (7%)   | 4 (2%)   | 5           | 29  |
| 2   | e     | 166/718 (23%)   | 153 (92%)  | 10 (6%)   | 3 (2%)   | 6           | 32  |
| 2   | f     | 166/718 (23%)   | 154 (93%)  | 9 (5%)    | 3 (2%)   | 6           | 32  |
| 2   | g     | 166/718 (23%)   | 154 (93%)  | 9 (5%)    | 3 (2%)   | 6           | 32  |
| 2   | h     | 194/718 (27%)   | 177 (91%)  | 13 (7%)   | 4 (2%)   | 5           | 29  |
| 2   | i     | 194/718 (27%)   | 176 (91%)  | 14 (7%)   | 4 (2%)   | 5           | 29  |
| 2   | j     | 194/718 (27%)   | 176 (91%)  | 14 (7%)   | 4 (2%)   | 5           | 29  |
| 3   | J     | 58/98 (59%)     | 54 (93%)   | 4 (7%)    | 0        | 100         | 100 |
| 3   | K     | 57/98 (58%)     | 55 (96%)   | 2 (4%)    | 0        | 100         | 100 |
| 3   | L     | 57/98 (58%)     | 57 (100%)  | 0         | 0        | 100         | 100 |
| 3   | M     | 57/98 (58%)     | 57 (100%)  | 0         | 0        | 100         | 100 |
| 3   | N     | 57/98 (58%)     | 54 (95%)   | 3 (5%)    | 0        | 100         | 100 |
| 3   | O     | 57/98 (58%)     | 56 (98%)   | 1 (2%)    | 0        | 100         | 100 |
| 3   | P     | 57/98 (58%)     | 56 (98%)   | 1 (2%)    | 0        | 100         | 100 |
| 3   | Q     | 57/98 (58%)     | 54 (95%)   | 3 (5%)    | 0        | 100         | 100 |
| 3   | R     | 57/98 (58%)     | 56 (98%)   | 1 (2%)    | 0        | 100         | 100 |
| 3   | r     | 58/98 (59%)     | 57 (98%)   | 1 (2%)    | 0        | 100         | 100 |
| 3   | s     | 57/98 (58%)     | 55 (96%)   | 2 (4%)    | 0        | 100         | 100 |
| 3   | t     | 57/98 (58%)     | 56 (98%)   | 1 (2%)    | 0        | 100         | 100 |
| 3   | u     | 58/98 (59%)     | 54 (93%)   | 4 (7%)    | 0        | 100         | 100 |
| 3   | v     | 58/98 (59%)     | 56 (97%)   | 2 (3%)    | 0        | 100         | 100 |

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| Mol | Chain | Analysed          | Favoured    | Allowed   | Outliers | Percentiles |     |
|-----|-------|-------------------|-------------|-----------|----------|-------------|-----|
| 3   | w     | 58/98 (59%)       | 56 (97%)    | 2 (3%)    | 0        | 100         | 100 |
| 3   | x     | 55/98 (56%)       | 52 (94%)    | 3 (6%)    | 0        | 100         | 100 |
| 4   | S     | 287/294 (98%)     | 254 (88%)   | 30 (10%)  | 3 (1%)   | 12          | 47  |
| 4   | T     | 287/294 (98%)     | 255 (89%)   | 30 (10%)  | 2 (1%)   | 18          | 55  |
| 4   | U     | 287/294 (98%)     | 256 (89%)   | 28 (10%)  | 3 (1%)   | 12          | 47  |
| 4   | V     | 287/294 (98%)     | 242 (84%)   | 40 (14%)  | 5 (2%)   | 7           | 34  |
| 4   | y     | 247/294 (84%)     | 211 (85%)   | 33 (13%)  | 3 (1%)   | 10          | 42  |
| 5   | l     | 251/311 (81%)     | 233 (93%)   | 17 (7%)   | 1 (0%)   | 30          | 67  |
| 5   | W     | 277/311 (89%)     | 239 (86%)   | 36 (13%)  | 2 (1%)   | 18          | 55  |
| 5   | X     | 273/311 (88%)     | 250 (92%)   | 21 (8%)   | 2 (1%)   | 18          | 55  |
| 5   | Y     | 278/311 (89%)     | 251 (90%)   | 27 (10%)  | 0        | 100         | 100 |
| 5   | Z     | 277/311 (89%)     | 253 (91%)   | 23 (8%)   | 1 (0%)   | 30          | 67  |
| 5   | a     | 261/311 (84%)     | 241 (92%)   | 20 (8%)   | 0        | 100         | 100 |
| 5   | b     | 264/311 (85%)     | 249 (94%)   | 14 (5%)   | 1 (0%)   | 30          | 67  |
| 5   | c     | 268/311 (86%)     | 248 (92%)   | 20 (8%)   | 0        | 100         | 100 |
| 5   | d     | 268/311 (86%)     | 253 (94%)   | 15 (6%)   | 0        | 100         | 100 |
| 5   | z     | 280/311 (90%)     | 255 (91%)   | 23 (8%)   | 2 (1%)   | 18          | 55  |
| All | All   | 27383/33540 (82%) | 24832 (91%) | 2455 (9%) | 96 (0%)  | 31          | 67  |

All (96) Ramachandran outliers are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 692  | LEU  |
| 1   | E     | 960  | SER  |
| 1   | k     | 1262 | LEU  |
| 1   | l     | 750  | PRO  |
| 1   | m     | 148  | LEU  |
| 1   | m     | 1262 | LEU  |
| 1   | o     | 610  | GLU  |
| 2   | 2     | 198  | LEU  |
| 2   | 2     | 256  | PRO  |
| 2   | 3     | 130  | ALA  |
| 2   | e     | 198  | LEU  |
| 2   | e     | 256  | PRO  |
| 2   | h     | 130  | ALA  |
| 2   | f     | 198  | LEU  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | f     | 256  | PRO  |
| 2   | i     | 130  | ALA  |
| 2   | g     | 198  | LEU  |
| 2   | g     | 256  | PRO  |
| 2   | j     | 130  | ALA  |
| 4   | y     | 62   | GLU  |
| 4   | U     | 60   | GLU  |
| 4   | V     | 60   | GLU  |
| 4   | V     | 79   | MET  |
| 5   | z     | 111  | PRO  |
| 5   | W     | 110  | PRO  |
| 5   | W     | 111  | PRO  |
| 5   | X     | 111  | PRO  |
| 5   | l     | 169  | ARG  |
| 1   | I     | 959  | LEU  |
| 1   | m     | 146  | ASP  |
| 1   | m     | 1283 | LEU  |
| 1   | o     | 766  | PRO  |
| 2   | 2     | 255  | ARG  |
| 2   | 3     | 131  | VAL  |
| 2   | 3     | 271  | VAL  |
| 2   | e     | 255  | ARG  |
| 2   | h     | 131  | VAL  |
| 2   | h     | 271  | VAL  |
| 2   | f     | 255  | ARG  |
| 2   | i     | 131  | VAL  |
| 2   | i     | 271  | VAL  |
| 2   | g     | 255  | ARG  |
| 2   | j     | 131  | VAL  |
| 2   | j     | 271  | VAL  |
| 4   | y     | 61   | VAL  |
| 4   | S     | 61   | VAL  |
| 4   | S     | 62   | GLU  |
| 4   | V     | 61   | VAL  |
| 4   | V     | 62   | GLU  |
| 1   | B     | 1334 | TYR  |
| 1   | C     | 1334 | TYR  |
| 1   | D     | 691  | GLU  |
| 1   | F     | 819  | LEU  |
| 1   | F     | 1322 | LYS  |
| 1   | k     | 985  | THR  |
| 1   | o     | 960  | SER  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | p     | 960  | SER  |
| 4   | T     | 204  | PRO  |
| 4   | U     | 80   | PRO  |
| 4   | V     | 81   | SER  |
| 5   | X     | 309  | TYR  |
| 1   | B     | 930  | PRO  |
| 1   | C     | 986  | LEU  |
| 1   | F     | 148  | LEU  |
| 1   | F     | 821  | ALA  |
| 1   | F     | 960  | SER  |
| 1   | G     | 960  | SER  |
| 1   | H     | 1155 | THR  |
| 1   | H     | 1162 | PRO  |
| 1   | k     | 960  | SER  |
| 1   | m     | 960  | SER  |
| 1   | p     | 1335 | GLY  |
| 2   | 2     | 67   | GLU  |
| 2   | 3     | 129  | ASP  |
| 2   | h     | 129  | ASP  |
| 2   | i     | 129  | ASP  |
| 2   | j     | 129  | ASP  |
| 4   | S     | 60   | GLU  |
| 5   | Z     | 309  | TYR  |
| 1   | B     | 959  | LEU  |
| 1   | C     | 958  | PRO  |
| 1   | k     | 313  | ALA  |
| 1   | n     | 960  | SER  |
| 1   | o     | 765  | GLU  |
| 4   | y     | 60   | GLU  |
| 5   | z     | 101  | GLU  |
| 5   | b     | 129  | VAL  |
| 1   | E     | 959  | LEU  |
| 1   | I     | 960  | SER  |
| 1   | m     | 869  | PRO  |
| 1   | p     | 1071 | GLY  |
| 1   | G     | 961  | PRO  |
| 4   | T     | 61   | VAL  |
| 1   | k     | 961  | PRO  |
| 4   | U     | 22   | PRO  |
| 1   | k     | 1298 | PRO  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed        | Rotameric   | Outliers | Percentiles |     |
|-----|-------|-----------------|-------------|----------|-------------|-----|
| 1   | A     | 1142/1156 (99%) | 1132 (99%)  | 10 (1%)  | 70          | 77  |
| 1   | B     | 1123/1156 (97%) | 1114 (99%)  | 9 (1%)   | 73          | 78  |
| 1   | C     | 1123/1156 (97%) | 1111 (99%)  | 12 (1%)  | 65          | 74  |
| 1   | D     | 1125/1156 (97%) | 1112 (99%)  | 13 (1%)  | 63          | 74  |
| 1   | E     | 1138/1156 (98%) | 1134 (100%) | 4 (0%)   | 84          | 83  |
| 1   | F     | 1128/1156 (98%) | 1120 (99%)  | 8 (1%)   | 76          | 80  |
| 1   | G     | 1147/1156 (99%) | 1139 (99%)  | 8 (1%)   | 76          | 80  |
| 1   | H     | 1147/1156 (99%) | 1138 (99%)  | 9 (1%)   | 73          | 78  |
| 1   | I     | 1130/1156 (98%) | 1123 (99%)  | 7 (1%)   | 78          | 81  |
| 1   | k     | 1105/1156 (96%) | 1093 (99%)  | 12 (1%)  | 65          | 74  |
| 1   | l     | 1144/1156 (99%) | 1140 (100%) | 4 (0%)   | 86          | 84  |
| 1   | m     | 1124/1156 (97%) | 1115 (99%)  | 9 (1%)   | 73          | 78  |
| 1   | n     | 1143/1156 (99%) | 1130 (99%)  | 13 (1%)  | 65          | 74  |
| 1   | o     | 1124/1156 (97%) | 1119 (100%) | 5 (0%)   | 84          | 83  |
| 1   | p     | 1110/1156 (96%) | 1103 (99%)  | 7 (1%)   | 78          | 81  |
| 1   | q     | 1042/1156 (90%) | 1037 (100%) | 5 (0%)   | 81          | 82  |
| 2   | 2     | 159/596 (27%)   | 156 (98%)   | 3 (2%)   | 50          | 66  |
| 2   | 3     | 177/596 (30%)   | 173 (98%)   | 4 (2%)   | 44          | 63  |
| 2   | e     | 159/596 (27%)   | 156 (98%)   | 3 (2%)   | 50          | 66  |
| 2   | f     | 159/596 (27%)   | 156 (98%)   | 3 (2%)   | 50          | 66  |
| 2   | g     | 159/596 (27%)   | 156 (98%)   | 3 (2%)   | 50          | 66  |
| 2   | h     | 177/596 (30%)   | 173 (98%)   | 4 (2%)   | 44          | 63  |
| 2   | i     | 177/596 (30%)   | 173 (98%)   | 4 (2%)   | 44          | 63  |
| 2   | j     | 177/596 (30%)   | 173 (98%)   | 4 (2%)   | 44          | 63  |
| 3   | J     | 50/71 (70%)     | 49 (98%)    | 1 (2%)   | 48          | 66  |
| 3   | K     | 49/71 (69%)     | 49 (100%)   | 0        | 100         | 100 |

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| Mol | Chain | Analysed          | Rotameric   | Outliers | Percentiles |     |
|-----|-------|-------------------|-------------|----------|-------------|-----|
| 3   | L     | 49/71 (69%)       | 49 (100%)   | 0        | 100         | 100 |
| 3   | M     | 49/71 (69%)       | 49 (100%)   | 0        | 100         | 100 |
| 3   | N     | 49/71 (69%)       | 48 (98%)    | 1 (2%)   | 48          | 66  |
| 3   | O     | 49/71 (69%)       | 48 (98%)    | 1 (2%)   | 48          | 66  |
| 3   | P     | 49/71 (69%)       | 48 (98%)    | 1 (2%)   | 48          | 66  |
| 3   | Q     | 49/71 (69%)       | 48 (98%)    | 1 (2%)   | 48          | 66  |
| 3   | R     | 49/71 (69%)       | 49 (100%)   | 0        | 100         | 100 |
| 3   | r     | 50/71 (70%)       | 48 (96%)    | 2 (4%)   | 28          | 49  |
| 3   | s     | 49/71 (69%)       | 48 (98%)    | 1 (2%)   | 48          | 66  |
| 3   | t     | 49/71 (69%)       | 47 (96%)    | 2 (4%)   | 27          | 49  |
| 3   | u     | 50/71 (70%)       | 49 (98%)    | 1 (2%)   | 48          | 66  |
| 3   | v     | 50/71 (70%)       | 49 (98%)    | 1 (2%)   | 48          | 66  |
| 3   | w     | 50/71 (70%)       | 49 (98%)    | 1 (2%)   | 48          | 66  |
| 3   | x     | 48/71 (68%)       | 48 (100%)   | 0        | 100         | 100 |
| 4   | S     | 251/255 (98%)     | 250 (100%)  | 1 (0%)   | 84          | 83  |
| 4   | T     | 251/255 (98%)     | 251 (100%)  | 0        | 100         | 100 |
| 4   | U     | 251/255 (98%)     | 248 (99%)   | 3 (1%)   | 63          | 74  |
| 4   | V     | 251/255 (98%)     | 244 (97%)   | 7 (3%)   | 38          | 59  |
| 4   | y     | 216/255 (85%)     | 212 (98%)   | 4 (2%)   | 50          | 66  |
| 5   | l     | 229/275 (83%)     | 229 (100%)  | 0        | 100         | 100 |
| 5   | W     | 253/275 (92%)     | 251 (99%)   | 2 (1%)   | 73          | 78  |
| 5   | X     | 249/275 (90%)     | 247 (99%)   | 2 (1%)   | 73          | 78  |
| 5   | Y     | 254/275 (92%)     | 253 (100%)  | 1 (0%)   | 84          | 83  |
| 5   | Z     | 253/275 (92%)     | 251 (99%)   | 2 (1%)   | 73          | 78  |
| 5   | a     | 238/275 (86%)     | 233 (98%)   | 5 (2%)   | 47          | 65  |
| 5   | b     | 241/275 (88%)     | 235 (98%)   | 6 (2%)   | 42          | 62  |
| 5   | c     | 245/275 (89%)     | 242 (99%)   | 3 (1%)   | 63          | 74  |
| 5   | d     | 245/275 (89%)     | 242 (99%)   | 3 (1%)   | 63          | 74  |
| 5   | z     | 256/275 (93%)     | 250 (98%)   | 6 (2%)   | 44          | 63  |
| All | All   | 23810/28425 (84%) | 23589 (99%) | 221 (1%) | 68          | 77  |

All (221) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 312  | ASN  |
| 1   | A     | 398  | VAL  |
| 1   | A     | 429  | VAL  |
| 1   | A     | 555  | THR  |
| 1   | A     | 618  | LEU  |
| 1   | A     | 663  | LEU  |
| 1   | A     | 787  | LEU  |
| 1   | A     | 788  | CYS  |
| 1   | A     | 1019 | THR  |
| 1   | A     | 1021 | VAL  |
| 1   | B     | 126  | ILE  |
| 1   | B     | 148  | LEU  |
| 1   | B     | 168  | THR  |
| 1   | B     | 312  | ASN  |
| 1   | B     | 662  | ARG  |
| 1   | B     | 1019 | THR  |
| 1   | B     | 1061 | VAL  |
| 1   | B     | 1163 | VAL  |
| 1   | B     | 1297 | LYS  |
| 1   | C     | 51   | PHE  |
| 1   | C     | 128  | ILE  |
| 1   | C     | 148  | LEU  |
| 1   | C     | 275  | VAL  |
| 1   | C     | 363  | VAL  |
| 1   | C     | 429  | VAL  |
| 1   | C     | 515  | LYS  |
| 1   | C     | 663  | LEU  |
| 1   | C     | 769  | VAL  |
| 1   | C     | 962  | ILE  |
| 1   | C     | 1019 | THR  |
| 1   | C     | 1021 | VAL  |
| 1   | D     | 128  | ILE  |
| 1   | D     | 429  | VAL  |
| 1   | D     | 618  | LEU  |
| 1   | D     | 647  | LEU  |
| 1   | D     | 662  | ARG  |
| 1   | D     | 663  | LEU  |
| 1   | D     | 691  | GLU  |
| 1   | D     | 692  | LEU  |
| 1   | D     | 731  | VAL  |
| 1   | D     | 834  | THR  |
| 1   | D     | 1019 | THR  |
| 1   | D     | 1021 | VAL  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | D     | 1321 | LEU  |
| 1   | E     | 128  | ILE  |
| 1   | E     | 312  | ASN  |
| 1   | E     | 646  | LEU  |
| 1   | E     | 1032 | LEU  |
| 1   | F     | 128  | ILE  |
| 1   | F     | 148  | LEU  |
| 1   | F     | 280  | VAL  |
| 1   | F     | 312  | ASN  |
| 1   | F     | 647  | LEU  |
| 1   | F     | 1019 | THR  |
| 1   | F     | 1160 | LEU  |
| 1   | F     | 1321 | LEU  |
| 1   | G     | 101  | VAL  |
| 1   | G     | 128  | ILE  |
| 1   | G     | 363  | VAL  |
| 1   | G     | 398  | VAL  |
| 1   | G     | 662  | ARG  |
| 1   | G     | 834  | THR  |
| 1   | G     | 1021 | VAL  |
| 1   | G     | 1065 | ILE  |
| 1   | H     | 179  | THR  |
| 1   | H     | 312  | ASN  |
| 1   | H     | 646  | LEU  |
| 1   | H     | 662  | ARG  |
| 1   | H     | 842  | LEU  |
| 1   | H     | 1018 | LEU  |
| 1   | H     | 1021 | VAL  |
| 1   | H     | 1159 | ILE  |
| 1   | H     | 1331 | GLU  |
| 1   | I     | 312  | ASN  |
| 1   | I     | 398  | VAL  |
| 1   | I     | 692  | LEU  |
| 1   | I     | 959  | LEU  |
| 1   | I     | 1019 | THR  |
| 1   | I     | 1021 | VAL  |
| 1   | I     | 1163 | VAL  |
| 1   | k     | 101  | VAL  |
| 1   | k     | 280  | VAL  |
| 1   | k     | 302  | SER  |
| 1   | k     | 647  | LEU  |
| 1   | k     | 662  | ARG  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | k     | 663  | LEU  |
| 1   | k     | 788  | CYS  |
| 1   | k     | 820  | THR  |
| 1   | k     | 1019 | THR  |
| 1   | k     | 1021 | VAL  |
| 1   | k     | 1160 | LEU  |
| 1   | k     | 1297 | LYS  |
| 1   | l     | 128  | ILE  |
| 1   | l     | 312  | ASN  |
| 1   | l     | 1021 | VAL  |
| 1   | l     | 1332 | THR  |
| 1   | m     | 117  | VAL  |
| 1   | m     | 147  | THR  |
| 1   | m     | 312  | ASN  |
| 1   | m     | 517  | ASP  |
| 1   | m     | 647  | LEU  |
| 1   | m     | 662  | ARG  |
| 1   | m     | 663  | LEU  |
| 1   | m     | 842  | LEU  |
| 1   | m     | 1032 | LEU  |
| 1   | n     | 128  | ILE  |
| 1   | n     | 312  | ASN  |
| 1   | n     | 429  | VAL  |
| 1   | n     | 575  | LEU  |
| 1   | n     | 618  | LEU  |
| 1   | n     | 691  | GLU  |
| 1   | n     | 962  | ILE  |
| 1   | n     | 1019 | THR  |
| 1   | n     | 1021 | VAL  |
| 1   | n     | 1163 | VAL  |
| 1   | n     | 1297 | LYS  |
| 1   | n     | 1321 | LEU  |
| 1   | n     | 1332 | THR  |
| 1   | o     | 429  | VAL  |
| 1   | o     | 488  | GLU  |
| 1   | o     | 765  | GLU  |
| 1   | o     | 1021 | VAL  |
| 1   | o     | 1298 | PRO  |
| 1   | p     | 312  | ASN  |
| 1   | p     | 376  | VAL  |
| 1   | p     | 398  | VAL  |
| 1   | p     | 646  | LEU  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | p     | 734  | VAL  |
| 1   | p     | 1019 | THR  |
| 1   | p     | 1021 | VAL  |
| 1   | q     | 225  | LEU  |
| 1   | q     | 373  | LEU  |
| 1   | q     | 598  | VAL  |
| 1   | q     | 852  | VAL  |
| 1   | q     | 1010 | MET  |
| 2   | 2     | 173  | MET  |
| 2   | 2     | 200  | VAL  |
| 2   | 2     | 202  | ASP  |
| 2   | 3     | 94   | LEU  |
| 2   | 3     | 271  | VAL  |
| 2   | 3     | 272  | ASP  |
| 2   | 3     | 295  | ARG  |
| 2   | e     | 173  | MET  |
| 2   | e     | 200  | VAL  |
| 2   | e     | 202  | ASP  |
| 2   | h     | 94   | LEU  |
| 2   | h     | 271  | VAL  |
| 2   | h     | 272  | ASP  |
| 2   | h     | 295  | ARG  |
| 2   | f     | 173  | MET  |
| 2   | f     | 200  | VAL  |
| 2   | f     | 202  | ASP  |
| 2   | i     | 94   | LEU  |
| 2   | i     | 271  | VAL  |
| 2   | i     | 272  | ASP  |
| 2   | i     | 295  | ARG  |
| 2   | g     | 173  | MET  |
| 2   | g     | 200  | VAL  |
| 2   | g     | 202  | ASP  |
| 2   | j     | 94   | LEU  |
| 2   | j     | 271  | VAL  |
| 2   | j     | 272  | ASP  |
| 2   | j     | 295  | ARG  |
| 3   | J     | 85   | LEU  |
| 3   | N     | 85   | LEU  |
| 3   | O     | 60   | VAL  |
| 3   | P     | 85   | LEU  |
| 3   | Q     | 85   | LEU  |
| 3   | r     | 60   | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | r     | 85  | LEU  |
| 3   | s     | 85  | LEU  |
| 3   | t     | 85  | LEU  |
| 3   | t     | 87  | MET  |
| 3   | u     | 85  | LEU  |
| 3   | v     | 85  | LEU  |
| 3   | w     | 85  | LEU  |
| 4   | y     | 75  | THR  |
| 4   | y     | 105 | LEU  |
| 4   | y     | 185 | ILE  |
| 4   | y     | 209 | VAL  |
| 4   | S     | 64  | LYS  |
| 4   | U     | 60  | GLU  |
| 4   | U     | 160 | LEU  |
| 4   | U     | 209 | VAL  |
| 4   | V     | 6   | SER  |
| 4   | V     | 64  | LYS  |
| 4   | V     | 79  | MET  |
| 4   | V     | 85  | VAL  |
| 4   | V     | 105 | LEU  |
| 4   | V     | 160 | LEU  |
| 4   | V     | 209 | VAL  |
| 5   | z     | 25  | ILE  |
| 5   | z     | 31  | ILE  |
| 5   | z     | 74  | VAL  |
| 5   | z     | 102 | LYS  |
| 5   | z     | 112 | VAL  |
| 5   | z     | 308 | ILE  |
| 5   | W     | 109 | LEU  |
| 5   | W     | 308 | ILE  |
| 5   | X     | 21  | LEU  |
| 5   | X     | 308 | ILE  |
| 5   | Y     | 308 | ILE  |
| 5   | Z     | 13  | LEU  |
| 5   | Z     | 308 | ILE  |
| 5   | a     | 45  | LEU  |
| 5   | a     | 50  | LYS  |
| 5   | a     | 51  | ASP  |
| 5   | a     | 169 | ARG  |
| 5   | a     | 295 | VAL  |
| 5   | b     | 38  | LEU  |
| 5   | b     | 45  | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5   | b     | 120 | LEU  |
| 5   | b     | 123 | VAL  |
| 5   | b     | 128 | LEU  |
| 5   | b     | 129 | VAL  |
| 5   | c     | 45  | LEU  |
| 5   | c     | 226 | LEU  |
| 5   | c     | 295 | VAL  |
| 5   | d     | 120 | LEU  |
| 5   | d     | 123 | VAL  |
| 5   | d     | 295 | VAL  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (528) such sidechains are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 23   | HIS  |
| 1   | A     | 77   | HIS  |
| 1   | A     | 112  | GLN  |
| 1   | A     | 218  | GLN  |
| 1   | A     | 278  | HIS  |
| 1   | A     | 312  | ASN  |
| 1   | A     | 349  | GLN  |
| 1   | A     | 424  | GLN  |
| 1   | A     | 439  | GLN  |
| 1   | A     | 492  | HIS  |
| 1   | A     | 549  | GLN  |
| 1   | A     | 607  | GLN  |
| 1   | A     | 639  | ASN  |
| 1   | A     | 675  | HIS  |
| 1   | A     | 712  | HIS  |
| 1   | A     | 749  | ASN  |
| 1   | A     | 863  | HIS  |
| 1   | A     | 867  | HIS  |
| 1   | A     | 984  | HIS  |
| 1   | A     | 1060 | HIS  |
| 1   | A     | 1064 | ASN  |
| 1   | A     | 1095 | GLN  |
| 1   | A     | 1104 | HIS  |
| 1   | A     | 1207 | GLN  |
| 1   | A     | 1274 | GLN  |
| 1   | A     | 1347 | GLN  |
| 1   | B     | 23   | HIS  |
| 1   | B     | 77   | HIS  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | B     | 82   | HIS  |
| 1   | B     | 97   | GLN  |
| 1   | B     | 159  | ASN  |
| 1   | B     | 218  | GLN  |
| 1   | B     | 338  | GLN  |
| 1   | B     | 372  | HIS  |
| 1   | B     | 439  | GLN  |
| 1   | B     | 443  | HIS  |
| 1   | B     | 492  | HIS  |
| 1   | B     | 562  | ASN  |
| 1   | B     | 597  | GLN  |
| 1   | B     | 795  | ASN  |
| 1   | B     | 856  | GLN  |
| 1   | B     | 903  | ASN  |
| 1   | B     | 996  | HIS  |
| 1   | B     | 1060 | HIS  |
| 1   | B     | 1063 | GLN  |
| 1   | B     | 1064 | ASN  |
| 1   | B     | 1095 | GLN  |
| 1   | B     | 1207 | GLN  |
| 1   | B     | 1248 | GLN  |
| 1   | B     | 1257 | ASN  |
| 1   | B     | 1309 | HIS  |
| 1   | C     | 23   | HIS  |
| 1   | C     | 82   | HIS  |
| 1   | C     | 200  | HIS  |
| 1   | C     | 239  | GLN  |
| 1   | C     | 282  | GLN  |
| 1   | C     | 338  | GLN  |
| 1   | C     | 349  | GLN  |
| 1   | C     | 372  | HIS  |
| 1   | C     | 439  | GLN  |
| 1   | C     | 562  | ASN  |
| 1   | C     | 592  | HIS  |
| 1   | C     | 675  | HIS  |
| 1   | C     | 712  | HIS  |
| 1   | C     | 795  | ASN  |
| 1   | C     | 863  | HIS  |
| 1   | C     | 873  | GLN  |
| 1   | C     | 899  | HIS  |
| 1   | C     | 951  | GLN  |
| 1   | C     | 996  | HIS  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | C     | 1060 | HIS  |
| 1   | C     | 1064 | ASN  |
| 1   | C     | 1095 | GLN  |
| 1   | C     | 1278 | HIS  |
| 1   | C     | 1336 | ASN  |
| 1   | C     | 1347 | GLN  |
| 1   | D     | 82   | HIS  |
| 1   | D     | 112  | GLN  |
| 1   | D     | 312  | ASN  |
| 1   | D     | 328  | GLN  |
| 1   | D     | 439  | GLN  |
| 1   | D     | 443  | HIS  |
| 1   | D     | 512  | ASN  |
| 1   | D     | 549  | GLN  |
| 1   | D     | 597  | GLN  |
| 1   | D     | 675  | HIS  |
| 1   | D     | 678  | ASN  |
| 1   | D     | 782  | GLN  |
| 1   | D     | 836  | ASN  |
| 1   | D     | 863  | HIS  |
| 1   | D     | 887  | HIS  |
| 1   | D     | 898  | GLN  |
| 1   | D     | 899  | HIS  |
| 1   | D     | 951  | GLN  |
| 1   | D     | 996  | HIS  |
| 1   | D     | 1060 | HIS  |
| 1   | D     | 1095 | GLN  |
| 1   | D     | 1309 | HIS  |
| 1   | D     | 1320 | GLN  |
| 1   | E     | 82   | HIS  |
| 1   | E     | 200  | HIS  |
| 1   | E     | 218  | GLN  |
| 1   | E     | 282  | GLN  |
| 1   | E     | 312  | ASN  |
| 1   | E     | 328  | GLN  |
| 1   | E     | 349  | GLN  |
| 1   | E     | 372  | HIS  |
| 1   | E     | 379  | ASN  |
| 1   | E     | 439  | GLN  |
| 1   | E     | 492  | HIS  |
| 1   | E     | 592  | HIS  |
| 1   | E     | 607  | GLN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | E     | 639  | ASN  |
| 1   | E     | 675  | HIS  |
| 1   | E     | 712  | HIS  |
| 1   | E     | 763  | GLN  |
| 1   | E     | 797  | HIS  |
| 1   | E     | 836  | ASN  |
| 1   | E     | 863  | HIS  |
| 1   | E     | 867  | HIS  |
| 1   | E     | 899  | HIS  |
| 1   | E     | 937  | ASN  |
| 1   | E     | 971  | HIS  |
| 1   | E     | 1063 | GLN  |
| 1   | E     | 1095 | GLN  |
| 1   | E     | 1219 | GLN  |
| 1   | E     | 1259 | ASN  |
| 1   | E     | 1274 | GLN  |
| 1   | E     | 1352 | ASN  |
| 1   | F     | 23   | HIS  |
| 1   | F     | 77   | HIS  |
| 1   | F     | 139  | HIS  |
| 1   | F     | 159  | ASN  |
| 1   | F     | 278  | HIS  |
| 1   | F     | 282  | GLN  |
| 1   | F     | 328  | GLN  |
| 1   | F     | 383  | GLN  |
| 1   | F     | 439  | GLN  |
| 1   | F     | 456  | HIS  |
| 1   | F     | 492  | HIS  |
| 1   | F     | 549  | GLN  |
| 1   | F     | 643  | GLN  |
| 1   | F     | 675  | HIS  |
| 1   | F     | 795  | ASN  |
| 1   | F     | 796  | ASN  |
| 1   | F     | 807  | HIS  |
| 1   | F     | 835  | ASN  |
| 1   | F     | 898  | GLN  |
| 1   | F     | 899  | HIS  |
| 1   | F     | 915  | GLN  |
| 1   | F     | 951  | GLN  |
| 1   | F     | 969  | HIS  |
| 1   | F     | 984  | HIS  |
| 1   | F     | 1063 | GLN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | F     | 1064 | ASN  |
| 1   | F     | 1095 | GLN  |
| 1   | F     | 1259 | ASN  |
| 1   | F     | 1303 | GLN  |
| 1   | F     | 1309 | HIS  |
| 1   | F     | 1336 | ASN  |
| 1   | F     | 1347 | GLN  |
| 1   | F     | 1352 | ASN  |
| 1   | G     | 282  | GLN  |
| 1   | G     | 312  | ASN  |
| 1   | G     | 372  | HIS  |
| 1   | G     | 472  | GLN  |
| 1   | G     | 499  | HIS  |
| 1   | G     | 562  | ASN  |
| 1   | G     | 639  | ASN  |
| 1   | G     | 675  | HIS  |
| 1   | G     | 678  | ASN  |
| 1   | G     | 722  | GLN  |
| 1   | G     | 863  | HIS  |
| 1   | G     | 867  | HIS  |
| 1   | G     | 873  | GLN  |
| 1   | G     | 899  | HIS  |
| 1   | G     | 937  | ASN  |
| 1   | G     | 997  | HIS  |
| 1   | G     | 1060 | HIS  |
| 1   | G     | 1064 | ASN  |
| 1   | G     | 1066 | ASN  |
| 1   | G     | 1082 | HIS  |
| 1   | G     | 1152 | GLN  |
| 1   | G     | 1214 | ASN  |
| 1   | G     | 1278 | HIS  |
| 1   | G     | 1336 | ASN  |
| 1   | G     | 1347 | GLN  |
| 1   | H     | 60   | ASN  |
| 1   | H     | 154  | ASN  |
| 1   | H     | 159  | ASN  |
| 1   | H     | 328  | GLN  |
| 1   | H     | 338  | GLN  |
| 1   | H     | 424  | GLN  |
| 1   | H     | 439  | GLN  |
| 1   | H     | 443  | HIS  |
| 1   | H     | 492  | HIS  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | H     | 712  | HIS  |
| 1   | H     | 863  | HIS  |
| 1   | H     | 898  | GLN  |
| 1   | H     | 899  | HIS  |
| 1   | H     | 903  | ASN  |
| 1   | H     | 951  | GLN  |
| 1   | H     | 969  | HIS  |
| 1   | H     | 996  | HIS  |
| 1   | H     | 1063 | GLN  |
| 1   | H     | 1064 | ASN  |
| 1   | H     | 1066 | ASN  |
| 1   | H     | 1257 | ASN  |
| 1   | H     | 1259 | ASN  |
| 1   | H     | 1274 | GLN  |
| 1   | H     | 1347 | GLN  |
| 1   | I     | 77   | HIS  |
| 1   | I     | 82   | HIS  |
| 1   | I     | 218  | GLN  |
| 1   | I     | 282  | GLN  |
| 1   | I     | 312  | ASN  |
| 1   | I     | 349  | GLN  |
| 1   | I     | 372  | HIS  |
| 1   | I     | 439  | GLN  |
| 1   | I     | 443  | HIS  |
| 1   | I     | 492  | HIS  |
| 1   | I     | 544  | HIS  |
| 1   | I     | 675  | HIS  |
| 1   | I     | 807  | HIS  |
| 1   | I     | 863  | HIS  |
| 1   | I     | 899  | HIS  |
| 1   | I     | 951  | GLN  |
| 1   | I     | 996  | HIS  |
| 1   | I     | 1060 | HIS  |
| 1   | I     | 1063 | GLN  |
| 1   | I     | 1064 | ASN  |
| 1   | I     | 1104 | HIS  |
| 1   | I     | 1150 | HIS  |
| 1   | I     | 1207 | GLN  |
| 1   | I     | 1219 | GLN  |
| 1   | I     | 1232 | ASN  |
| 1   | I     | 1238 | HIS  |
| 1   | I     | 1336 | ASN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | I     | 1347 | GLN  |
| 1   | k     | 77   | HIS  |
| 1   | k     | 82   | HIS  |
| 1   | k     | 97   | GLN  |
| 1   | k     | 159  | ASN  |
| 1   | k     | 372  | HIS  |
| 1   | k     | 439  | GLN  |
| 1   | k     | 544  | HIS  |
| 1   | k     | 675  | HIS  |
| 1   | k     | 712  | HIS  |
| 1   | k     | 763  | GLN  |
| 1   | k     | 795  | ASN  |
| 1   | k     | 855  | ASN  |
| 1   | k     | 863  | HIS  |
| 1   | k     | 885  | GLN  |
| 1   | k     | 887  | HIS  |
| 1   | k     | 899  | HIS  |
| 1   | k     | 951  | GLN  |
| 1   | k     | 984  | HIS  |
| 1   | k     | 996  | HIS  |
| 1   | k     | 1060 | HIS  |
| 1   | k     | 1063 | GLN  |
| 1   | k     | 1064 | ASN  |
| 1   | k     | 1066 | ASN  |
| 1   | k     | 1082 | HIS  |
| 1   | k     | 1174 | ASN  |
| 1   | k     | 1239 | ASN  |
| 1   | k     | 1320 | GLN  |
| 1   | l     | 23   | HIS  |
| 1   | l     | 159  | ASN  |
| 1   | l     | 200  | HIS  |
| 1   | l     | 239  | GLN  |
| 1   | l     | 286  | ASN  |
| 1   | l     | 312  | ASN  |
| 1   | l     | 372  | HIS  |
| 1   | l     | 433  | ASN  |
| 1   | l     | 439  | GLN  |
| 1   | l     | 492  | HIS  |
| 1   | l     | 499  | HIS  |
| 1   | l     | 607  | GLN  |
| 1   | l     | 638  | ASN  |
| 1   | l     | 675  | HIS  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | l     | 749  | ASN  |
| 1   | l     | 795  | ASN  |
| 1   | l     | 863  | HIS  |
| 1   | l     | 873  | GLN  |
| 1   | l     | 899  | HIS  |
| 1   | l     | 903  | ASN  |
| 1   | l     | 937  | ASN  |
| 1   | l     | 951  | GLN  |
| 1   | l     | 1063 | GLN  |
| 1   | l     | 1064 | ASN  |
| 1   | l     | 1082 | HIS  |
| 1   | l     | 1274 | GLN  |
| 1   | l     | 1278 | HIS  |
| 1   | l     | 1303 | GLN  |
| 1   | l     | 1309 | HIS  |
| 1   | l     | 1333 | HIS  |
| 1   | l     | 1352 | ASN  |
| 1   | m     | 4    | ASN  |
| 1   | m     | 23   | HIS  |
| 1   | m     | 85   | ASN  |
| 1   | m     | 112  | GLN  |
| 1   | m     | 312  | ASN  |
| 1   | m     | 319  | HIS  |
| 1   | m     | 328  | GLN  |
| 1   | m     | 345  | GLN  |
| 1   | m     | 372  | HIS  |
| 1   | m     | 424  | GLN  |
| 1   | m     | 492  | HIS  |
| 1   | m     | 592  | HIS  |
| 1   | m     | 675  | HIS  |
| 1   | m     | 712  | HIS  |
| 1   | m     | 835  | ASN  |
| 1   | m     | 836  | ASN  |
| 1   | m     | 863  | HIS  |
| 1   | m     | 898  | GLN  |
| 1   | m     | 899  | HIS  |
| 1   | m     | 937  | ASN  |
| 1   | m     | 968  | HIS  |
| 1   | m     | 969  | HIS  |
| 1   | m     | 996  | HIS  |
| 1   | m     | 997  | HIS  |
| 1   | m     | 1060 | HIS  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | m     | 1063 | GLN  |
| 1   | m     | 1064 | ASN  |
| 1   | m     | 1082 | HIS  |
| 1   | m     | 1104 | HIS  |
| 1   | m     | 1274 | GLN  |
| 1   | m     | 1303 | GLN  |
| 1   | m     | 1333 | HIS  |
| 1   | m     | 1347 | GLN  |
| 1   | n     | 23   | HIS  |
| 1   | n     | 77   | HIS  |
| 1   | n     | 112  | GLN  |
| 1   | n     | 159  | ASN  |
| 1   | n     | 282  | GLN  |
| 1   | n     | 286  | ASN  |
| 1   | n     | 312  | ASN  |
| 1   | n     | 319  | HIS  |
| 1   | n     | 433  | ASN  |
| 1   | n     | 439  | GLN  |
| 1   | n     | 492  | HIS  |
| 1   | n     | 712  | HIS  |
| 1   | n     | 863  | HIS  |
| 1   | n     | 899  | HIS  |
| 1   | n     | 903  | ASN  |
| 1   | n     | 951  | GLN  |
| 1   | n     | 969  | HIS  |
| 1   | n     | 971  | HIS  |
| 1   | n     | 996  | HIS  |
| 1   | n     | 1060 | HIS  |
| 1   | n     | 1063 | GLN  |
| 1   | n     | 1064 | ASN  |
| 1   | n     | 1082 | HIS  |
| 1   | n     | 1095 | GLN  |
| 1   | n     | 1099 | GLN  |
| 1   | n     | 1104 | HIS  |
| 1   | n     | 1248 | GLN  |
| 1   | n     | 1259 | ASN  |
| 1   | n     | 1314 | GLN  |
| 1   | n     | 1352 | ASN  |
| 1   | o     | 23   | HIS  |
| 1   | o     | 77   | HIS  |
| 1   | o     | 112  | GLN  |
| 1   | o     | 282  | GLN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | o     | 312  | ASN  |
| 1   | o     | 328  | GLN  |
| 1   | o     | 349  | GLN  |
| 1   | o     | 357  | GLN  |
| 1   | o     | 372  | HIS  |
| 1   | o     | 439  | GLN  |
| 1   | o     | 499  | HIS  |
| 1   | o     | 549  | GLN  |
| 1   | o     | 562  | ASN  |
| 1   | o     | 579  | GLN  |
| 1   | o     | 675  | HIS  |
| 1   | o     | 863  | HIS  |
| 1   | o     | 899  | HIS  |
| 1   | o     | 968  | HIS  |
| 1   | o     | 969  | HIS  |
| 1   | o     | 971  | HIS  |
| 1   | o     | 996  | HIS  |
| 1   | o     | 997  | HIS  |
| 1   | o     | 1064 | ASN  |
| 1   | o     | 1104 | HIS  |
| 1   | o     | 1271 | ASN  |
| 1   | o     | 1274 | GLN  |
| 1   | o     | 1303 | GLN  |
| 1   | o     | 1320 | GLN  |
| 1   | p     | 82   | HIS  |
| 1   | p     | 139  | HIS  |
| 1   | p     | 159  | ASN  |
| 1   | p     | 167  | ASN  |
| 1   | p     | 212  | GLN  |
| 1   | p     | 218  | GLN  |
| 1   | p     | 286  | ASN  |
| 1   | p     | 312  | ASN  |
| 1   | p     | 328  | GLN  |
| 1   | p     | 349  | GLN  |
| 1   | p     | 357  | GLN  |
| 1   | p     | 372  | HIS  |
| 1   | p     | 383  | GLN  |
| 1   | p     | 424  | GLN  |
| 1   | p     | 472  | GLN  |
| 1   | p     | 492  | HIS  |
| 1   | p     | 512  | ASN  |
| 1   | p     | 549  | GLN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | p     | 696  | ASN  |
| 1   | p     | 863  | HIS  |
| 1   | p     | 899  | HIS  |
| 1   | p     | 903  | ASN  |
| 1   | p     | 951  | GLN  |
| 1   | p     | 997  | HIS  |
| 1   | p     | 1063 | GLN  |
| 1   | p     | 1064 | ASN  |
| 1   | p     | 1066 | ASN  |
| 1   | p     | 1082 | HIS  |
| 1   | p     | 1095 | GLN  |
| 1   | p     | 1104 | HIS  |
| 1   | p     | 1152 | GLN  |
| 1   | p     | 1214 | ASN  |
| 1   | p     | 1257 | ASN  |
| 1   | p     | 1274 | GLN  |
| 1   | p     | 1278 | HIS  |
| 1   | q     | 77   | HIS  |
| 1   | q     | 82   | HIS  |
| 1   | q     | 154  | ASN  |
| 1   | q     | 167  | ASN  |
| 1   | q     | 212  | GLN  |
| 1   | q     | 401  | HIS  |
| 1   | q     | 423  | ASN  |
| 1   | q     | 424  | GLN  |
| 1   | q     | 433  | ASN  |
| 1   | q     | 443  | HIS  |
| 1   | q     | 472  | GLN  |
| 1   | q     | 639  | ASN  |
| 1   | q     | 675  | HIS  |
| 1   | q     | 678  | ASN  |
| 1   | q     | 712  | HIS  |
| 1   | q     | 796  | ASN  |
| 1   | q     | 851  | ASN  |
| 1   | q     | 885  | GLN  |
| 1   | q     | 887  | HIS  |
| 1   | q     | 945  | ASN  |
| 1   | q     | 1063 | GLN  |
| 1   | q     | 1303 | GLN  |
| 1   | q     | 1320 | GLN  |
| 2   | 2     | 81   | HIS  |
| 2   | 3     | 91   | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | 3     | 184 | ASN  |
| 2   | e     | 81  | HIS  |
| 2   | e     | 214 | ASN  |
| 2   | h     | 91  | HIS  |
| 2   | h     | 184 | ASN  |
| 2   | h     | 231 | GLN  |
| 2   | h     | 265 | ASN  |
| 2   | f     | 81  | HIS  |
| 2   | f     | 214 | ASN  |
| 2   | i     | 69  | GLN  |
| 2   | i     | 91  | HIS  |
| 2   | i     | 184 | ASN  |
| 2   | i     | 265 | ASN  |
| 2   | g     | 81  | HIS  |
| 2   | g     | 214 | ASN  |
| 2   | j     | 91  | HIS  |
| 2   | j     | 184 | ASN  |
| 3   | J     | 43  | GLN  |
| 3   | J     | 50  | ASN  |
| 3   | K     | 58  | GLN  |
| 3   | L     | 43  | GLN  |
| 3   | L     | 58  | GLN  |
| 3   | M     | 58  | GLN  |
| 3   | M     | 81  | GLN  |
| 3   | P     | 50  | ASN  |
| 3   | R     | 58  | GLN  |
| 3   | R     | 81  | GLN  |
| 3   | r     | 50  | ASN  |
| 3   | t     | 43  | GLN  |
| 3   | v     | 43  | GLN  |
| 3   | v     | 81  | GLN  |
| 3   | w     | 43  | GLN  |
| 3   | w     | 50  | ASN  |
| 3   | w     | 58  | GLN  |
| 3   | x     | 50  | ASN  |
| 4   | y     | 215 | HIS  |
| 4   | y     | 236 | ASN  |
| 4   | y     | 237 | ASN  |
| 4   | y     | 253 | GLN  |
| 4   | S     | 96  | ASN  |
| 4   | S     | 132 | HIS  |
| 4   | S     | 155 | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | S     | 197 | ASN  |
| 4   | S     | 217 | HIS  |
| 4   | T     | 155 | HIS  |
| 4   | U     | 103 | ASN  |
| 4   | U     | 237 | ASN  |
| 4   | V     | 46  | GLN  |
| 4   | V     | 155 | HIS  |
| 4   | V     | 237 | ASN  |
| 5   | z     | 94  | ASN  |
| 5   | z     | 231 | GLN  |
| 5   | z     | 290 | GLN  |
| 5   | W     | 78  | GLN  |
| 5   | W     | 144 | GLN  |
| 5   | W     | 158 | HIS  |
| 5   | X     | 231 | GLN  |
| 5   | Y     | 88  | GLN  |
| 5   | Y     | 144 | GLN  |
| 5   | Y     | 205 | ASN  |
| 5   | Y     | 231 | GLN  |
| 5   | Y     | 282 | GLN  |
| 5   | Z     | 78  | GLN  |
| 5   | Z     | 86  | HIS  |
| 5   | Z     | 94  | ASN  |
| 5   | Z     | 271 | ASN  |
| 5   | Z     | 282 | GLN  |
| 5   | Z     | 290 | GLN  |
| 5   | 1     | 11  | GLN  |
| 5   | 1     | 36  | HIS  |
| 5   | a     | 86  | HIS  |
| 5   | a     | 143 | ASN  |
| 5   | a     | 167 | GLN  |
| 5   | b     | 78  | GLN  |
| 5   | c     | 11  | GLN  |
| 5   | c     | 36  | HIS  |
| 5   | d     | 11  | GLN  |
| 5   | d     | 36  | HIS  |
| 5   | d     | 86  | HIS  |
| 5   | d     | 143 | ASN  |

### 5.3.3 RNA ⓘ

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](#)

There are no chain breaks in this entry.

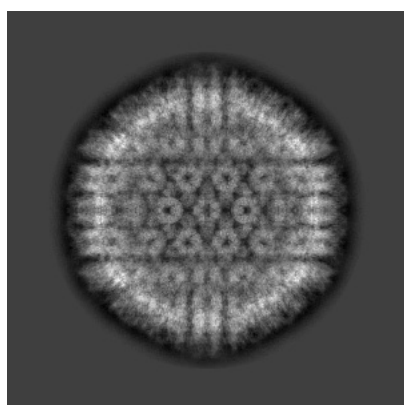
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-9366. These allow visual inspection of the internal detail of the map and identification of artifacts.

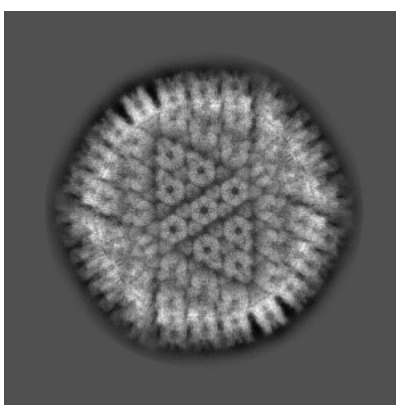
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

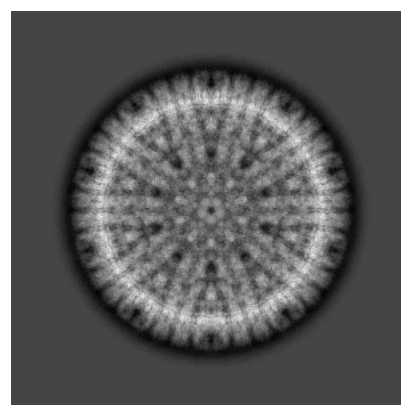
#### 6.1.1 Primary map



X



Y

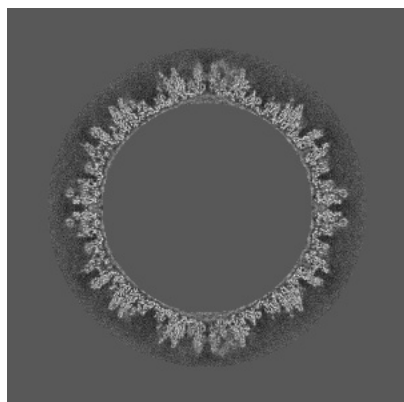


Z

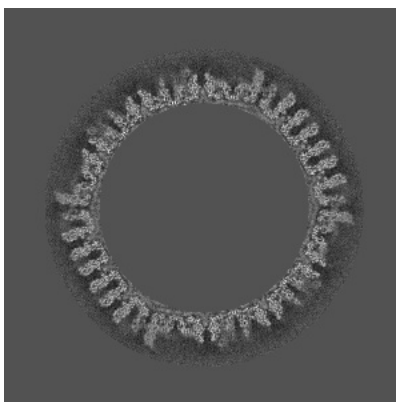
The images above show the map projected in three orthogonal directions.

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

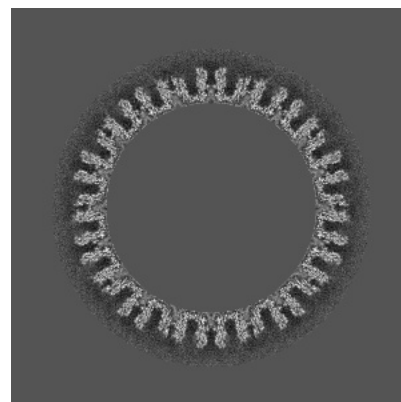
#### 6.2.1 Primary map



X Index: 640



Y Index: 640

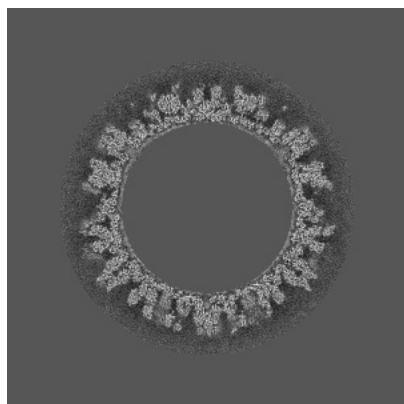


Z Index: 640

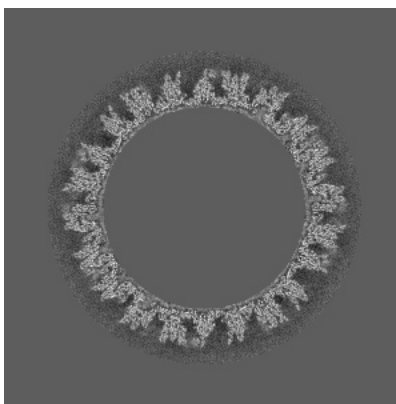
The images above show central slices of the map in three orthogonal directions.

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

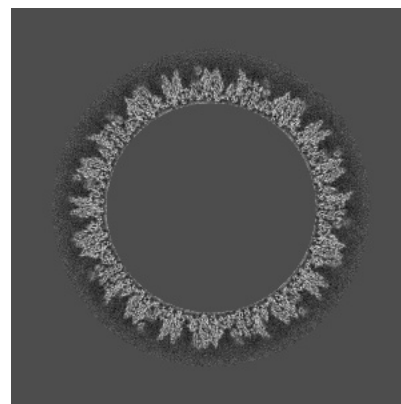
### 6.3.1 Primary map



X Index: 445



Y Index: 731

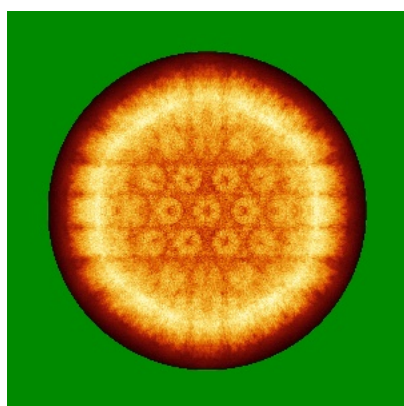


Z Index: 618

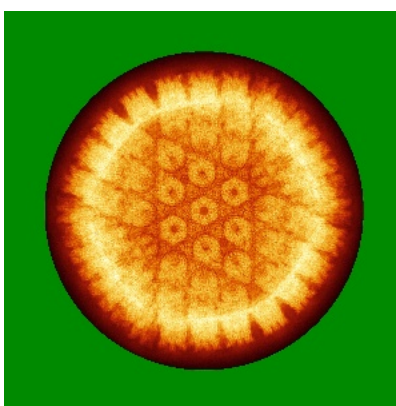
The images above show the largest variance slices of the map in three orthogonal directions.

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

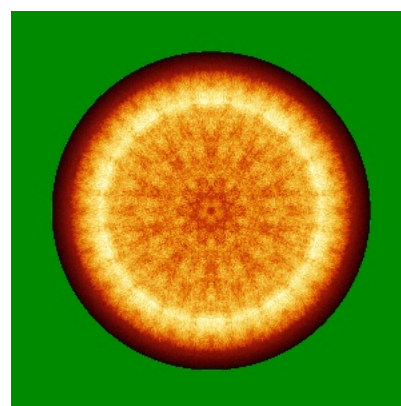
### 6.4.1 Primary map



X



Y

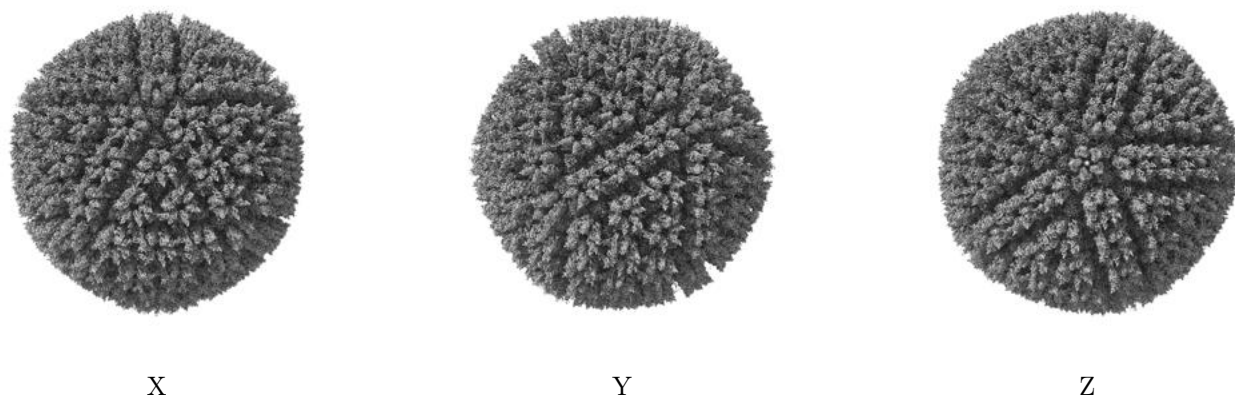


Z

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

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

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 4.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

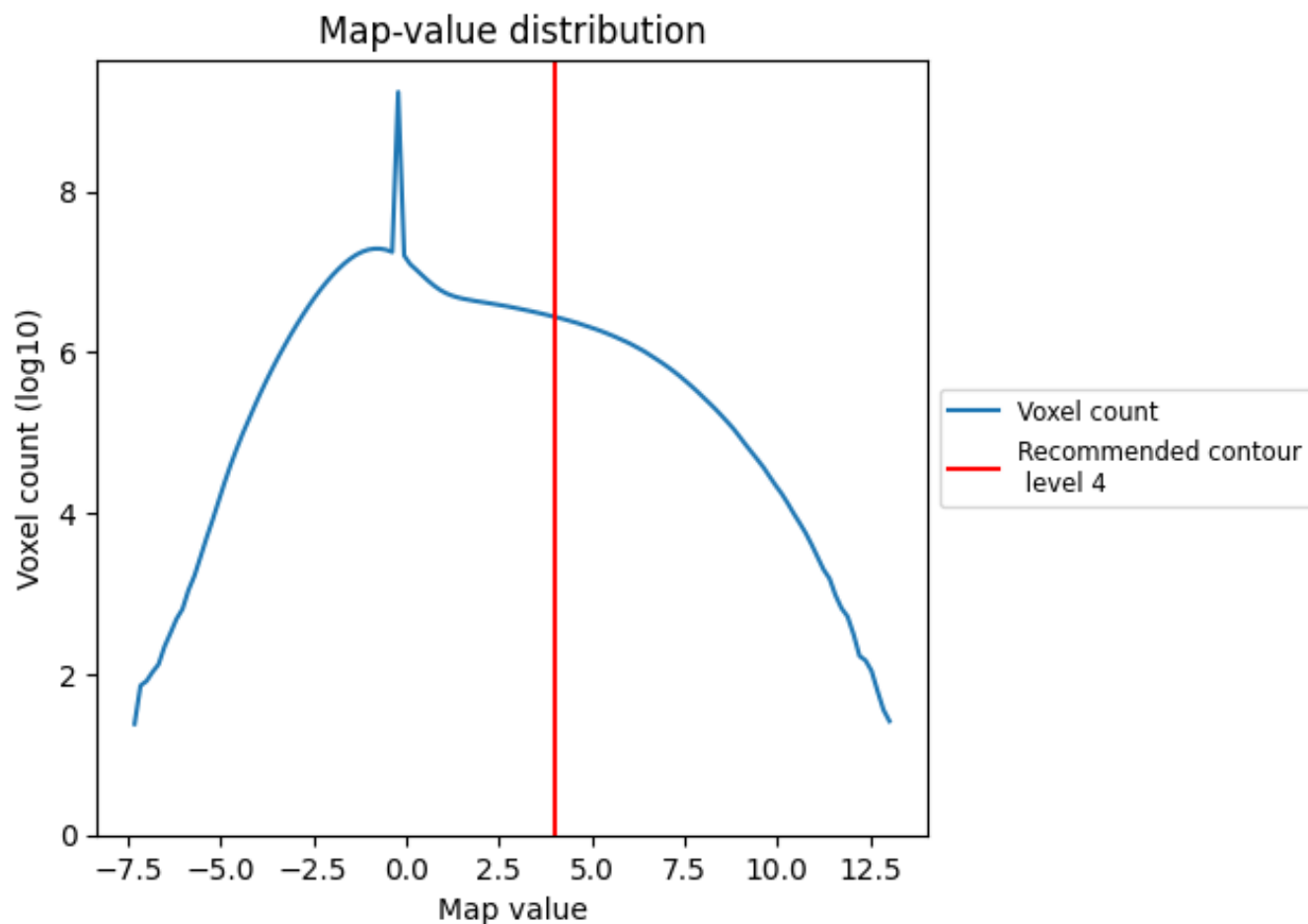
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

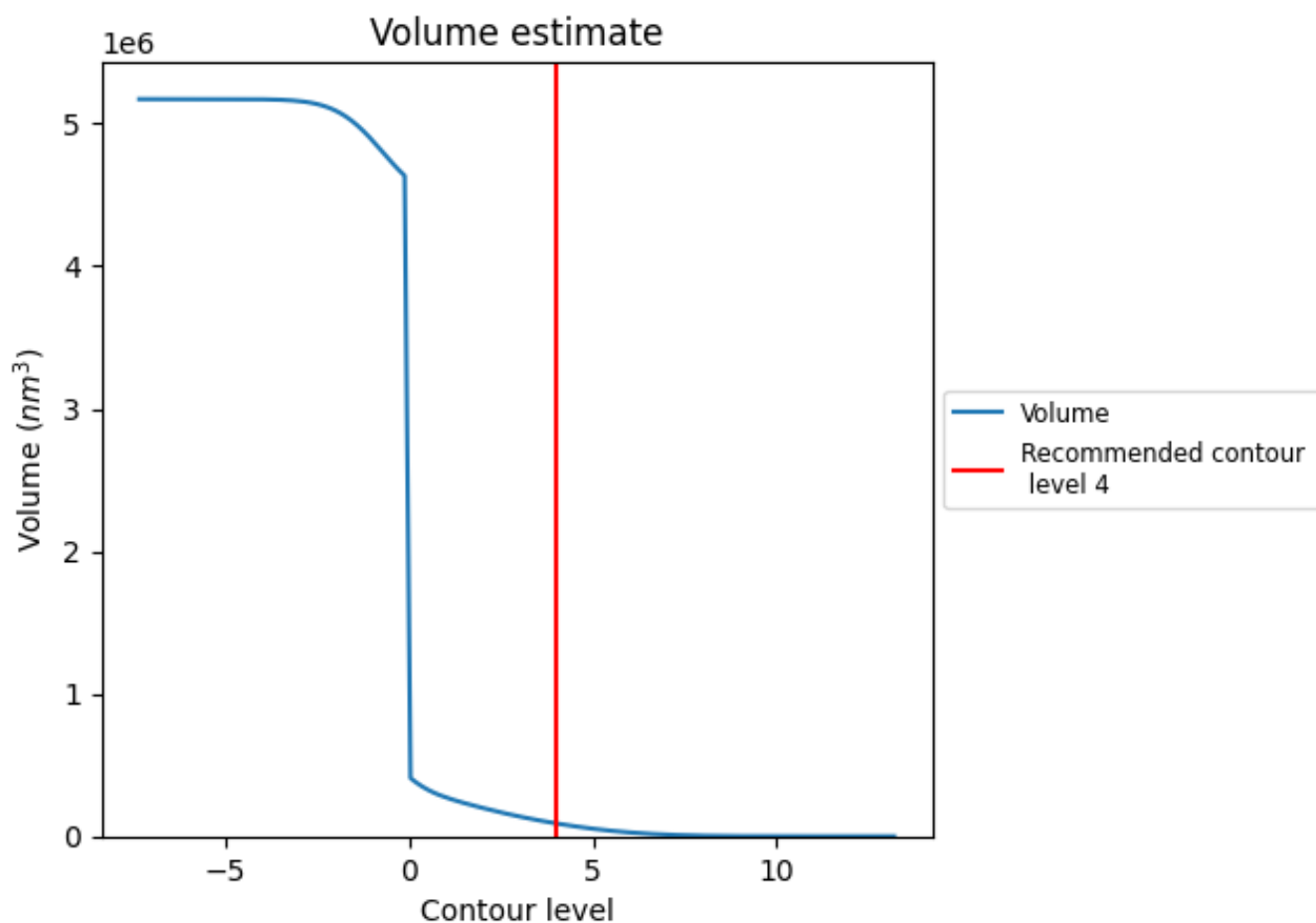
This section contains the results of statistical analysis of the map.

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



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

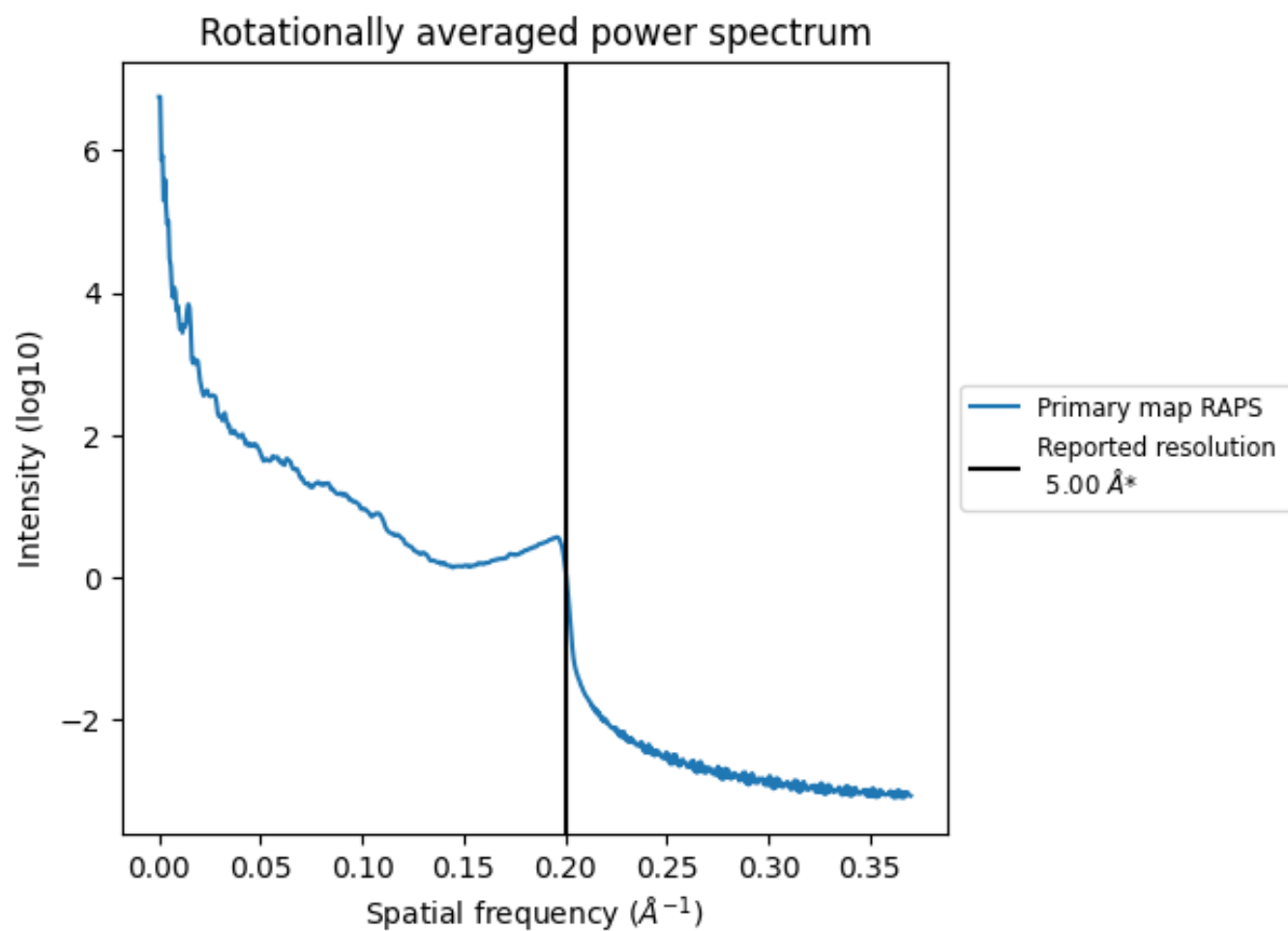
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 90561 nm<sup>3</sup>; this corresponds to an approximate mass of 81806 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 0.200 Å<sup>-1</sup>

## 8 Fourier-Shell correlation

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

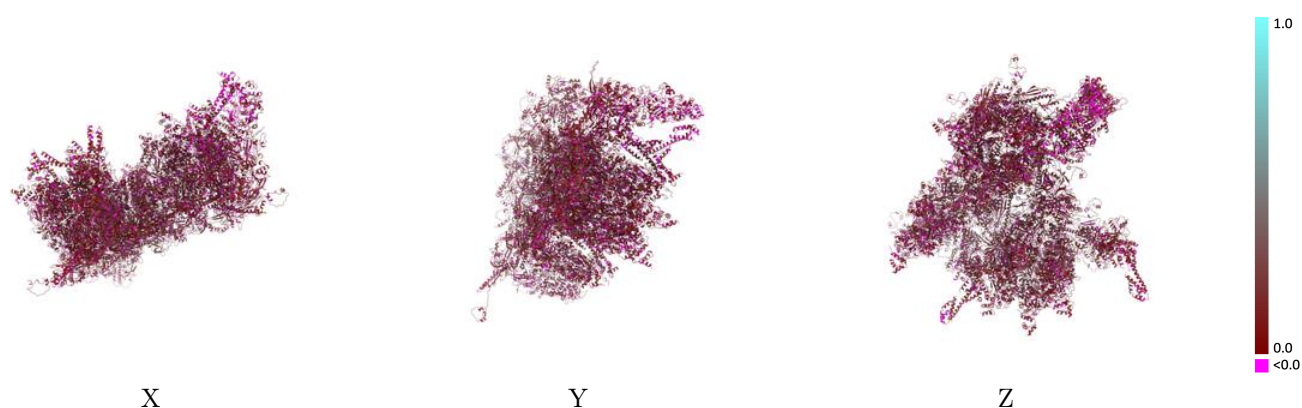
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-9366 and PDB model 6NHJ. Per-residue inclusion information can be found in section 3 on page 10.

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

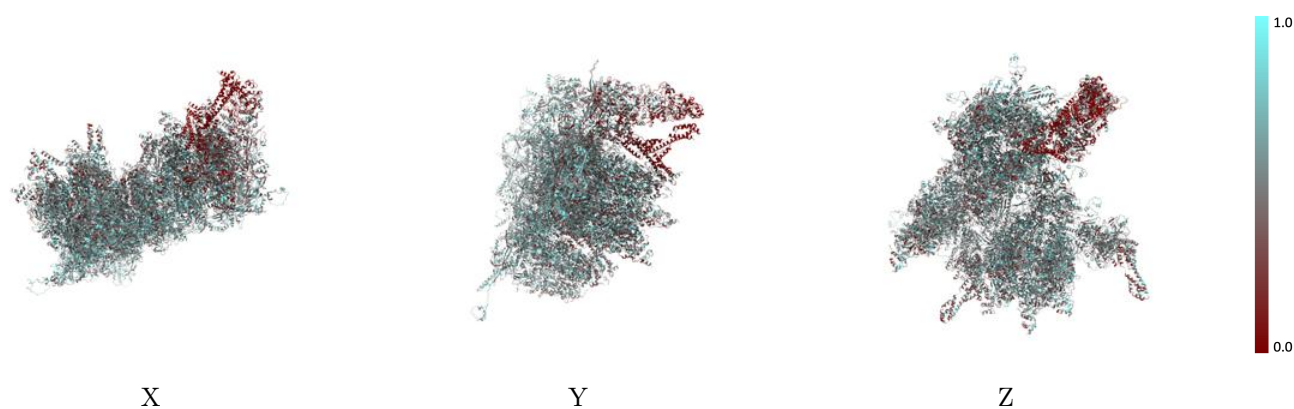
This section was not generated.

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



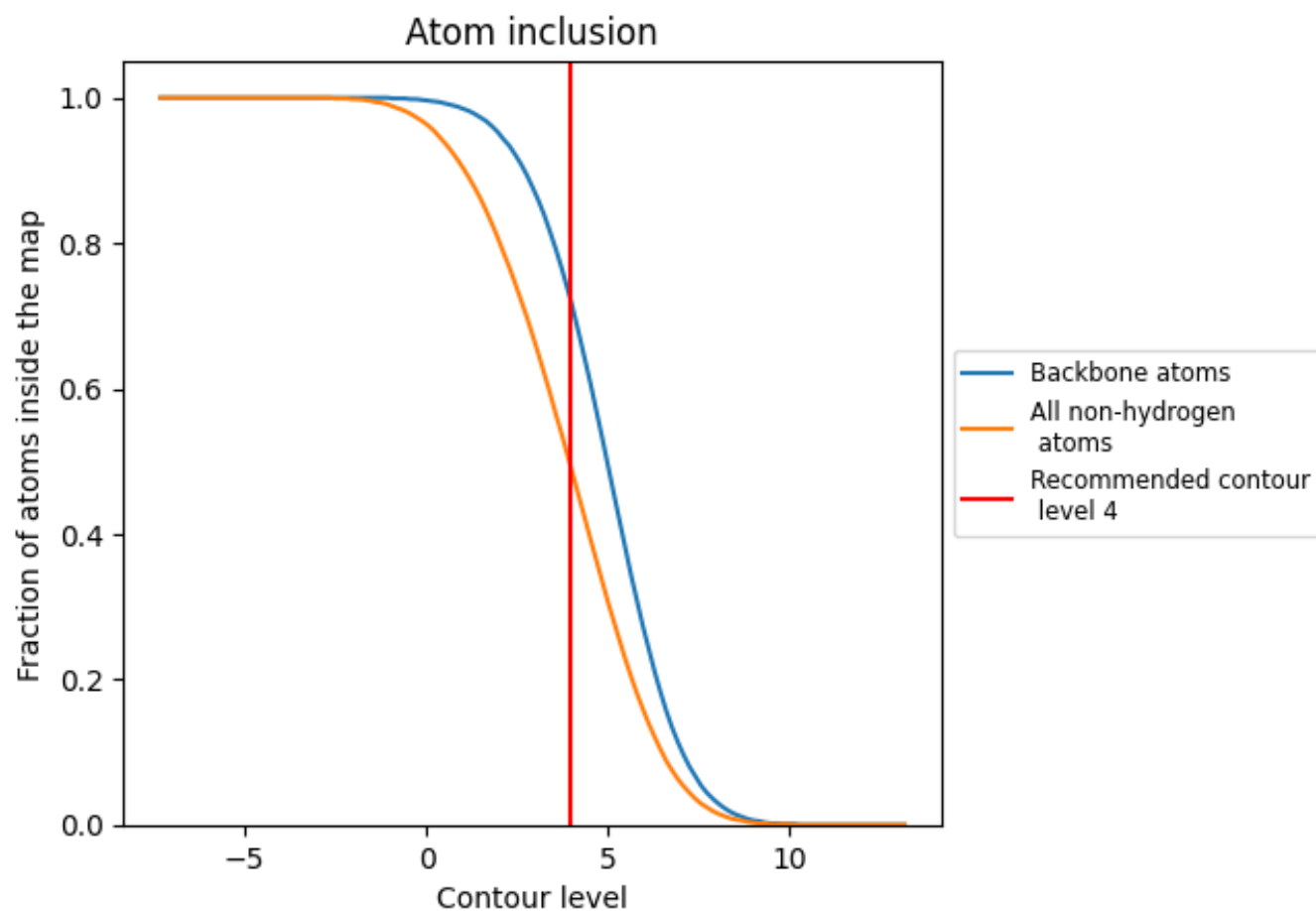
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (4).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 72% of all backbone atoms, 49% 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 (4) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion | Q-score |
|-------|----------------|---------|
| All   | 0.4900         | 0.1390  |
| 1     | 0.2890         | 0.1150  |
| 2     | 0.0080         | 0.0720  |
| 3     | 0.0220         | 0.0940  |
| A     | 0.5450         | 0.1570  |
| B     | 0.5470         | 0.1490  |
| C     | 0.5370         | 0.1410  |
| D     | 0.5280         | 0.1390  |
| E     | 0.5370         | 0.1490  |
| F     | 0.5400         | 0.1530  |
| G     | 0.5260         | 0.1470  |
| H     | 0.5170         | 0.1340  |
| I     | 0.5190         | 0.1270  |
| J     | 0.4730         | 0.1410  |
| K     | 0.4540         | 0.1350  |
| L     | 0.4360         | 0.1300  |
| M     | 0.4120         | 0.1250  |
| N     | 0.4520         | 0.1270  |
| O     | 0.4340         | 0.1210  |
| P     | 0.4470         | 0.1160  |
| Q     | 0.4540         | 0.1730  |
| R     | 0.4410         | 0.0880  |
| S     | 0.4790         | 0.1310  |
| T     | 0.4810         | 0.1380  |
| U     | 0.5040         | 0.1500  |
| V     | 0.4940         | 0.1260  |
| W     | 0.4890         | 0.1610  |
| X     | 0.4740         | 0.1550  |
| Y     | 0.4990         | 0.1580  |
| Z     | 0.4640         | 0.1350  |
| a     | 0.4880         | 0.1430  |
| b     | 0.4740         | 0.1530  |
| c     | 0.4670         | 0.1350  |
| d     | 0.4430         | 0.1250  |
| e     | 0.4230         | 0.1290  |



*Continued on next page...*

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| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| f     |  0.3670   |  0.1160   |
| g     |  0.3650   |  0.1090   |
| h     |  0.4260   |  0.1230   |
| i     |  0.4090   |  0.1310   |
| j     |  0.4000   |  0.1230   |
| k     |  0.5010   |  0.1470   |
| l     |  0.5270   |  0.1480   |
| m     |  0.5250   |  0.1390   |
| n     |  0.5140   |  0.1360   |
| o     |  0.5220   |  0.1370   |
| p     |  0.5090   |  0.1490   |
| q     |  0.3280   |  0.1180   |
| r     |  0.4080   |  0.1110   |
| s     |  0.4340   |  0.1440   |
| t     |  0.4340   |  0.1220   |
| u     |  0.3970   |  0.1250   |
| v     |  0.4470   |  0.1270   |
| w     |  0.4170  |  0.1250  |
| x     |  0.0570 |  0.0410 |
| y     |  0.3460 |  0.1190 |
| z     |  0.3360 |  0.1290 |