



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:29 AM GMT

PDB ID : 3LVG
Title : Crystal structure of a clathrin heavy chain and clathrin light chain complex
Authors : Wilbur, J.D.; Hwang, P.K.; Ybe, J.A.; Lane, M.; Sellers, B.D.; Jacobson, M.P.; Fletterick, R.J.; Brodsky, F.M.
Deposited on : 2010-02-20
Resolution : 7.94 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

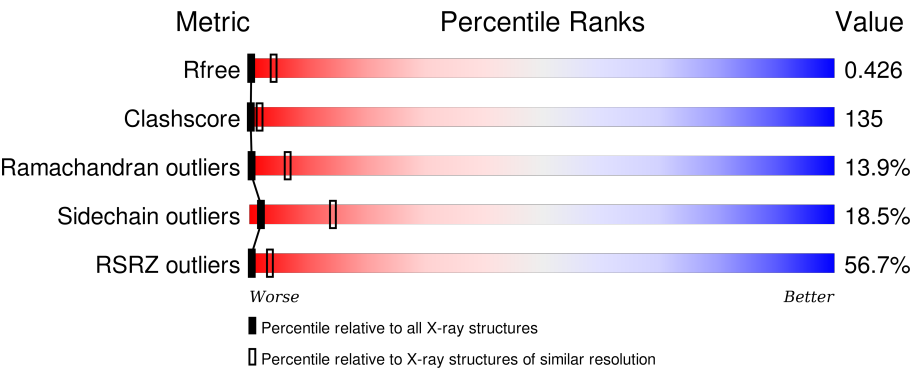
MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 7.94 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 (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| R _{free} | 91344 | 1015 (11.50-3.66) |
| Clashscore | 102246 | 1064 (11.50-3.70) |
| Ramachandran outliers | 100387 | 1036 (11.50-3.66) |
| Sidechain outliers | 100360 | 1006 (11.50-3.66) |
| RSRZ outliers | 91569 | 1014 (11.50-3.66) |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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 electron density. The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|---|
| 1 | A | 624 | <div><div>55%</div><div><div>14%</div><div>49%</div><div>21%</div><div>6%</div><div>11%</div></div></div> |
| 1 | B | 624 | <div><div>59%</div><div><div>12%</div><div>52%</div><div>20%</div><div>5%</div><div>11%</div></div></div> |
| 1 | C | 624 | <div><div>38%</div><div><div>13%</div><div>50%</div><div>20%</div><div>6%</div><div>11%</div></div></div> |
| 2 | D | 190 | <div><div>33%</div><div><div>35%</div><div>46%</div><div>12%</div><div>• 5%</div></div></div> |
| 2 | E | 190 | <div><div>14%</div><div><div>16%</div><div>32%</div><div>9%</div><div>•</div><div>39%</div></div></div> |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--------------------------------|
| 2 | F | 190 | <p>17% 18% 36% 13% 31%</p> |

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 16504 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 Clathrin heavy chain 1.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1 | A | 553 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 4543 | 2896 | 767 | 855 | 25 | | | |
| 1 | B | 553 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 4543 | 2896 | 767 | 855 | 25 | | | |
| 1 | C | 553 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 4543 | 2896 | 767 | 855 | 25 | | | |

There are 66 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------------|------------|
| A | 1052 | MET | - | EXPRESSION TAG | UNP P49951 |
| A | 1053 | GLY | - | EXPRESSION TAG | UNP P49951 |
| A | 1054 | SER | - | EXPRESSION TAG | UNP P49951 |
| A | 1055 | SER | - | EXPRESSION TAG | UNP P49951 |
| A | 1056 | HIS | - | EXPRESSION TAG | UNP P49951 |
| A | 1057 | HIS | - | EXPRESSION TAG | UNP P49951 |
| A | 1058 | HIS | - | EXPRESSION TAG | UNP P49951 |
| A | 1059 | HIS | - | EXPRESSION TAG | UNP P49951 |
| A | 1060 | HIS | - | EXPRESSION TAG | UNP P49951 |
| A | 1061 | HIS | - | EXPRESSION TAG | UNP P49951 |
| A | 1062 | SER | - | EXPRESSION TAG | UNP P49951 |
| A | 1063 | SER | - | EXPRESSION TAG | UNP P49951 |
| A | 1064 | GLY | - | EXPRESSION TAG | UNP P49951 |
| A | 1065 | LEU | - | EXPRESSION TAG | UNP P49951 |
| A | 1066 | VAL | - | EXPRESSION TAG | UNP P49951 |
| A | 1067 | PRO | - | EXPRESSION TAG | UNP P49951 |
| A | 1068 | ARG | - | EXPRESSION TAG | UNP P49951 |
| A | 1069 | GLY | - | EXPRESSION TAG | UNP P49951 |
| A | 1070 | SER | - | EXPRESSION TAG | UNP P49951 |
| A | 1071 | HIS | - | EXPRESSION TAG | UNP P49951 |
| A | 1072 | MET | - | EXPRESSION TAG | UNP P49951 |
| A | 1073 | LEU | - | EXPRESSION TAG | UNP P49951 |
| B | 1052 | MET | - | EXPRESSION TAG | UNP P49951 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------------|------------|
| B | 1053 | GLY | - | EXPRESSION TAG | UNP P49951 |
| B | 1054 | SER | - | EXPRESSION TAG | UNP P49951 |
| B | 1055 | SER | - | EXPRESSION TAG | UNP P49951 |
| B | 1056 | HIS | - | EXPRESSION TAG | UNP P49951 |
| B | 1057 | HIS | - | EXPRESSION TAG | UNP P49951 |
| B | 1058 | HIS | - | EXPRESSION TAG | UNP P49951 |
| B | 1059 | HIS | - | EXPRESSION TAG | UNP P49951 |
| B | 1060 | HIS | - | EXPRESSION TAG | UNP P49951 |
| B | 1061 | HIS | - | EXPRESSION TAG | UNP P49951 |
| B | 1062 | SER | - | EXPRESSION TAG | UNP P49951 |
| B | 1063 | SER | - | EXPRESSION TAG | UNP P49951 |
| B | 1064 | GLY | - | EXPRESSION TAG | UNP P49951 |
| B | 1065 | LEU | - | EXPRESSION TAG | UNP P49951 |
| B | 1066 | VAL | - | EXPRESSION TAG | UNP P49951 |
| B | 1067 | PRO | - | EXPRESSION TAG | UNP P49951 |
| B | 1068 | ARG | - | EXPRESSION TAG | UNP P49951 |
| B | 1069 | GLY | - | EXPRESSION TAG | UNP P49951 |
| B | 1070 | SER | - | EXPRESSION TAG | UNP P49951 |
| B | 1071 | HIS | - | EXPRESSION TAG | UNP P49951 |
| B | 1072 | MET | - | EXPRESSION TAG | UNP P49951 |
| B | 1073 | LEU | - | EXPRESSION TAG | UNP P49951 |
| C | 1052 | MET | - | EXPRESSION TAG | UNP P49951 |
| C | 1053 | GLY | - | EXPRESSION TAG | UNP P49951 |
| C | 1054 | SER | - | EXPRESSION TAG | UNP P49951 |
| C | 1055 | SER | - | EXPRESSION TAG | UNP P49951 |
| C | 1056 | HIS | - | EXPRESSION TAG | UNP P49951 |
| C | 1057 | HIS | - | EXPRESSION TAG | UNP P49951 |
| C | 1058 | HIS | - | EXPRESSION TAG | UNP P49951 |
| C | 1059 | HIS | - | EXPRESSION TAG | UNP P49951 |
| C | 1060 | HIS | - | EXPRESSION TAG | UNP P49951 |
| C | 1061 | HIS | - | EXPRESSION TAG | UNP P49951 |
| C | 1062 | SER | - | EXPRESSION TAG | UNP P49951 |
| C | 1063 | SER | - | EXPRESSION TAG | UNP P49951 |
| C | 1064 | GLY | - | EXPRESSION TAG | UNP P49951 |
| C | 1065 | LEU | - | EXPRESSION TAG | UNP P49951 |
| C | 1066 | VAL | - | EXPRESSION TAG | UNP P49951 |
| C | 1067 | PRO | - | EXPRESSION TAG | UNP P49951 |
| C | 1068 | ARG | - | EXPRESSION TAG | UNP P49951 |
| C | 1069 | GLY | - | EXPRESSION TAG | UNP P49951 |
| C | 1070 | SER | - | EXPRESSION TAG | UNP P49951 |
| C | 1071 | HIS | - | EXPRESSION TAG | UNP P49951 |
| C | 1072 | MET | - | EXPRESSION TAG | UNP P49951 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------------|------------|
| C | 1073 | LEU | - | EXPRESSION TAG | UNP P49951 |

- Molecule 2 is a protein called Clathrin light chain B.

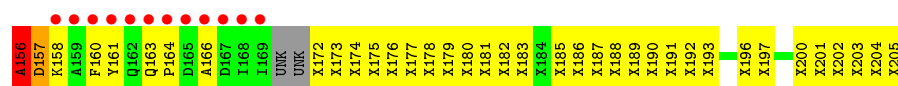
| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 2 | D | 180 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1146 | 690 | 227 | 228 | 1 | | | |
| 2 | E | 116 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 823 | 497 | 163 | 162 | 1 | | | |
| 2 | F | 132 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 906 | 546 | 179 | 180 | 1 | | | |

- Molecule 2: Clathrin light chain B

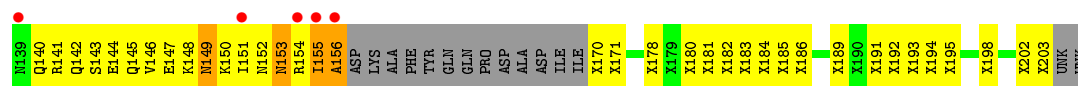
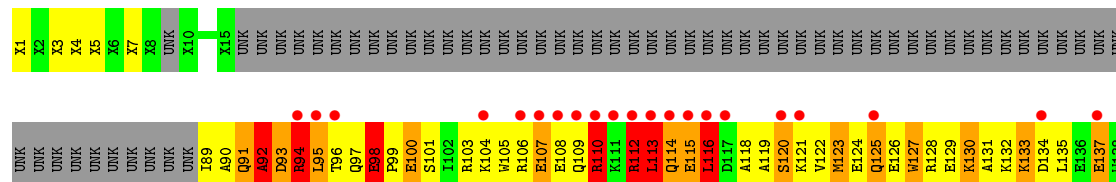
Chain D:



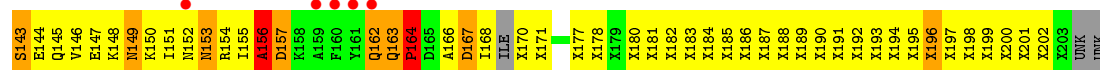
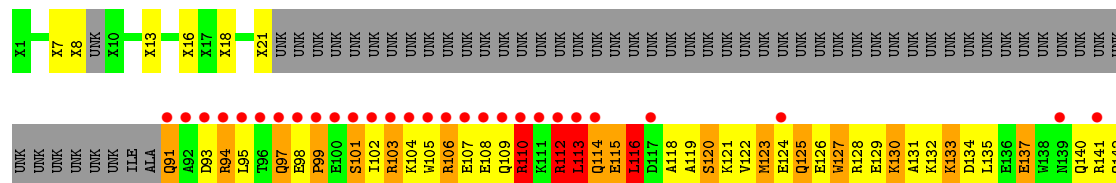
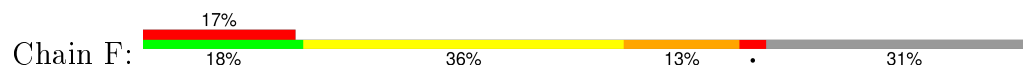
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| T96 | X1 | T97 | X5 | T98 | X10 | T99 | UNK | X11 | T100 | X12 | T101 | X13 | T102 | X14 | T103 | X15 | T104 | X16 | T105 | X19 | T106 | X23 | T107 | UNK | X25 | T108 | X26 | T109 | X27 | T110 | X28 | T111 | X29 | T112 | X36 | T113 | UNK | X38 | T114 | X45 | T115 | UNK | X47 | T116 | X48 | T117 | X49 | T118 | X50 | T119 | X51 | T120 | X52 | T121 | X53 | T122 | X54 | T123 | X55 | T124 | X58 | T125 | UNK | X60 | T126 | X61 | T127 | X62 | T128 | X63 | T129 | X64 | T130 | X65 | T131 | X66 | T132 | X69 | T133 | X70 | T134 | X71 | T135 | X72 | T136 | UNK | T137 | X77 | T138 | UNK | T139 | UNK | T140 | UNK | T141 | UNK | T142 | UNK | T143 | UNK | T144 | UNK | T145 | UNK | T146 | UNK | T147 | UNK | T148 | UNK | T149 | UNK | T150 | UNK | T151 | UNK | T152 | UNK | T153 | UNK | T154 | UNK | T155 | UNK | T156 | UNK | T157 | UNK | T158 | UNK | T159 | UNK | T160 | UNK | T161 | UNK | T162 | UNK | T163 | UNK | T164 | UNK | T165 | UNK | T166 | UNK | T167 | UNK | T168 | UNK | T169 | UNK | T170 | UNK | T171 | UNK | T172 | UNK | T173 | UNK | T174 | UNK | T175 | UNK | T176 | UNK | T177 | UNK | T178 | UNK | T179 | UNK | T180 | UNK | T181 | UNK | T182 | UNK | T183 | UNK | T184 | UNK | T185 | UNK | T186 | UNK | T187 | UNK | T188 | UNK | T189 | UNK | T190 | UNK | T191 | UNK | T192 | UNK | T193 | UNK | T194 | UNK | T195 | UNK | T196 | UNK | T197 | UNK | T198 | UNK | T199 | UNK | T200 | UNK | T201 | UNK | T202 | UNK | T203 | UNK | T204 | UNK | T205 | UNK | T206 | UNK | T207 | UNK | T208 | UNK | T209 | UNK | T210 | UNK | T211 | UNK | T212 | UNK | T213 | UNK | T214 | UNK | T215 | UNK | T216 | UNK | T217 | UNK | T218 | UNK | T219 | UNK | T220 | UNK | T221 | UNK | T222 | UNK | T223 | UNK | T224 | UNK | T225 | UNK | T226 | UNK | T227 | UNK | T228 | UNK | T229 | UNK | T230 | UNK | T231 | UNK | T232 | UNK | T233 | UNK | T234 | UNK | T235 | UNK | T236 | UNK | T237 | UNK | T238 | UNK | T239 | UNK | T240 | UNK | T241 | UNK | T242 | UNK | T243 | UNK | T244 | UNK | T245 | UNK | T246 | UNK | T247 | UNK | T248 | UNK | T249 | UNK | T250 | UNK | T251 | UNK | T252 | UNK | T253 | UNK | T254 | UNK | T255 | UNK | T256 | UNK | T257 | UNK | T258 | UNK | T259 | UNK | T260 | UNK | T261 | UNK | T262 | UNK | T263 | UNK | T264 | UNK | T265 | UNK | T266 | UNK | T267 | UNK | T268 | UNK | T269 | UNK | T270 | UNK | T271 | UNK | T272 | UNK | T273 | UNK | T274 | UNK | T275 | UNK | T276 | UNK | T277 | UNK | T278 | UNK | T279 | UNK | T280 | UNK | T281 | UNK | T282 | UNK | T283 | UNK | T284 | UNK | T285 | UNK | T286 | UNK | T287 | UNK | T288 | UNK | T289 | UNK | T290 | UNK | T291 | UNK | T292 | UNK | T293 | UNK | T294 | UNK | T295 | UNK | T296 | UNK | T297 | UNK | T298 | UNK | T299 | UNK | T300 | UNK | T301 | UNK | T302 | UNK | T303 | UNK | T304 | UNK | T305 | UNK | T306 | UNK | T307 | UNK | T308 | UNK | T309 | UNK | T310 | UNK | T311 | UNK | T312 | UNK | T313 | UNK | T314 | UNK | T315 | UNK | T316 | UNK | T317 | UNK | T318 | UNK | T319 | UNK | T320 | UNK | T321 | UNK | T322 | UNK | T323 | UNK | T324 | UNK | T325 | UNK | T326 | UNK | T327 | UNK | T328 | UNK | T329 | UNK | T330 | UNK | T331 | UNK | T332 | UNK | T333 | UNK | T334 | UNK | T335 | UNK | T336 | UNK | T337 | UNK | T338 | UNK | T339 | UNK | T340 | UNK | T341 | UNK | T342 | UNK | T343 | UNK | T344 | UNK | T345 | UNK | T346 | UNK | T347 | UNK | T348 | UNK | T349 | UNK | T350 | UNK | T351 | UNK | T352 | UNK | T353 | UNK | T354 | UNK | T355 | UNK | T356 | UNK | T357 | UNK | T358 | UNK | T359 | UNK | T360 | UNK | T361 | UNK | T362 | UNK | T363 | UNK | T364 | UNK | T365 | UNK | T366 | UNK | T367 | UNK | T368 | UNK | T369 | UNK | T370 | UNK | T371 | UNK | T372 | UNK | T373 | UNK | T374 | UNK | T375 | UNK | T376 | UNK | T377 | UNK | T378 | UNK | T379 | UNK | T380 | UNK | T381 | UNK | T382 | UNK | T383 | UNK | T384 | UNK | T385 | UNK | T386 | UNK | T387 | UNK | T388 | UNK | T389 | UNK | T390 | UNK | T391 | UNK | T392 | UNK | T393 | UNK | T394 | UNK | T395 | UNK | T396 | UNK | T397 | UNK | T398 | UNK | T399 | UNK | T400 | UNK | T401 | UNK | T402 | UNK | T403 | UNK | T404 | UNK | T405 | UNK | T406 | UNK | T407 | UNK | T408 | UNK | T409 | UNK | T410 | UNK | T411 | UNK | T412 | UNK | T413 | UNK | T414 | UNK | T415 | UNK | T416 | UNK | T417 | UNK | T418 | UNK | T419 | UNK | T420 | UNK | T421 | UNK | T422 | UNK | T423 | UNK | T424 | UNK | T425 | UNK | T426 | UNK | T427 | UNK | T428 | UNK | T429 | UNK | T430 | UNK | T431 | UNK | T432 | UNK | T433 | UNK | T434 | UNK | T435 | UNK | T436 | UNK | T437 | UNK | T438 | UNK | T439 | UNK | T440 | UNK | T441 | UNK | T442 | UNK | T443 | UNK | T444 | UNK | T445 | UNK | T446 | UNK | T447 | UNK | T448 | UNK | T449 | UNK | T450 | UNK | T451 | UNK | T452 | UNK | T453 | UNK | T454 | UNK | T455 | UNK | T456 | UNK | T457 | UNK | T458 | UNK | T459 | UNK | T460 | UNK | T461 | UNK | T462 | UNK | T463 | UNK | T464 | UNK | T465 | UNK | T466 | UNK | T467 | UNK | T468 | UNK | T469 | UNK | T470 | UNK | T471 | UNK | T472 | UNK | T473 | UNK | T474 | UNK | T475 | UNK | T476 | UNK | T477 | UNK | T478 | UNK | T479 | UNK | T480 | UNK | T481 | UNK | T482 | UNK | T483 | UNK | T484 | UNK | T485 | UNK | T486 | UNK | T487 | UNK | T488 | UNK | T489 | UNK | T490 | UNK | T491 | UNK | T492 | UNK | T493 | UNK | T494 | UNK | T495 | UNK | T496 | UNK | T497 | UNK | T498 | UNK | T499 | UNK | T500 | UNK | T501 | UNK | T502 | UNK | T503 | UNK | T504 | UNK | T505 | UNK | T506 | UNK | T507 | UNK | T508 | UNK | T509 | UNK | T510 | UNK | T511 | UNK | T512 | UNK | T513 | UNK | T514 | UNK | T515 | UNK | T516 | UNK | T517 | UNK | T518 | UNK | T519 | UNK | T520 | UNK | T521 | UNK | T522 | UNK | T523 | UNK | T524 | UNK | T525 | UNK | T526 | UNK | T527 | UNK | T528 | UNK | T529 | UNK | T530 | UNK | T531 | UNK | T532 | UNK | T533 | UNK | T534 | UNK | T535 | UNK | T536 | UNK | T537 | UNK | T538 | UNK | T539 | UNK | T540 | UNK | T541 | UNK | T542 | UNK | T543 | UNK | T544 | UNK | T545 | UNK | T546 | UNK | T547 | UNK | T548 | UNK | T549 | UNK | T550 | UNK | T551 | UNK | T552 | UNK | T553 | UNK | T554 | UNK | T555 | UNK | T556 | UNK | T557 | UNK | T558 | UNK | T559 | UNK | T560 | UNK | T561 | UNK | T562 | UNK | T563 | UNK | T564 | UNK | T565 | UNK | T566 | UNK | T567 | UNK | T568 | UNK | T569 | UNK | T570 | UNK | T571 | UNK | T572 | UNK | T573 | UNK | T574 | UNK | T575 | UNK | T576 | UNK | T577 | UNK | T578 | UNK | T579 | UNK | T580 | UNK | T581 | UNK | T582 | UNK | T583 | UNK | T584 | UNK | T585 | UNK | T586 | UNK | T587 | UNK | T588 | UNK | T589 | UNK | T590 | UNK | T591 | UNK | T592 | UNK | T593 | UNK | T594 | UNK | T595 | UNK | T596 | UNK | T597 | UNK | T598 | UNK | T599 | UNK | T600 | UNK | T601 | UNK | T602 | UNK | T603 | UNK | T604 | UNK | T605 | UNK | T606 | UNK | T607 | UNK | T608 | UNK | T609 | UNK | T610 | UNK | T611 | UNK | T612 | UNK | T613 | UNK | T614 | UNK | T615 | UNK | T616 | UNK | T617 | UNK | T618 | UNK | T619 | UNK | T620 | UNK | T621 | UNK | T622 | UNK | T623 | UNK | T624 | UNK | T625 | UNK | T626 | UNK | T627 | UNK | T628 | UNK | T629 | UNK | T630 | UNK | T631 | UNK | T632 | UNK | T633 | UNK | T634 | UNK | T635 | UNK | T636 | UNK | T637 | UNK | T638 | UNK | T639 | UNK | T640 | UNK | T641 | UNK | T642 | UNK | T643 | UNK | T644 | UNK | T645 | UNK | T646 | UNK | T647 | UNK | T648 | UNK | T649 | UNK | T650 | UNK | T651 | UNK | T652 | UNK | T653 | UNK | T654 | UNK | T655 | UNK | T656 | UNK | T657 | UNK | T658 | UNK | T659 | UNK | T660 | UNK | T661 | UNK | T662 | UNK | T663 | UNK | T664 | UNK | T665 | UNK | T666 | UNK | T667 | UNK | T668 | UNK | T669 | UNK | T670 | UNK | T671 | UNK | T672 | UNK | T673 | UNK | T674 | UNK | T675 | UNK | T676 | UNK | T677 | UNK | T678 | UNK | T679 | UNK | T680 | UNK | T681 | UNK | T682 | UNK | T683 | UNK | T684 | UNK | T685 | UNK | T686 | UNK | T687 | UNK | T688 | UNK | T689 | UNK | T690 | UNK | T691 | UNK | T692 | UNK | T693 | UNK | T694 | UNK | T695 | UNK | T696 | UNK | T697 | UNK | T698 | UNK | T699 | UNK | T700 | UNK | T701 | UNK | T702 | UNK | T703 | UNK | T704 | UNK | T705 | UNK | T706 | UNK | T707 | UNK | T708 | UNK | T709 | UNK | T710 | UNK | T711 | UNK | T712 | UNK | T713 | UNK | T714 | UNK | T715 | UNK | T716 | UNK | T717 | UNK | T718 | UNK | T719 | UNK | T720 | UNK | T721 | UNK | T722 | UNK | T723 | UNK | T724 | UNK | T725 | UNK | T726 | UNK | T727 | UNK | T728 | UNK | T729 | UNK | T730 | UNK | T731 | UNK | T732 | UNK | T733 | UNK | T734 | UNK | T735 | UNK | T736 | UNK | T737 | UNK | T738 | UNK | T739 | UNK | T740 | UNK | T741 | UNK | T742 | UNK | T743 | UNK | T744 | UNK | T745 | UNK | T746 | UNK | T747 | UNK | T748 | UNK | T749 | UNK | T750 | UNK | T751 | UNK | T752 | UNK | T753 | UNK | T754 | UNK | T755 | UNK | T756 | UNK | T757 | UNK | T758 | UNK | T759 | UNK | T760 | UNK | T761 | UNK | T762 | UNK | T763 | UNK | T764 | UNK | T765 | UNK | T766 | UNK | T767 | UNK | T768 | UNK | T769 | UNK | T770 | UNK | T771 | UNK | T772 | UNK | T773 | UNK | T774 | UNK | T775 | UNK | T776 | UNK | T777 | UNK | T778 | UNK | T779 | UNK | T780 | UNK | T781 | UNK | T782 | UNK | T783 | UNK | T784 | UNK | T785 | UNK | T786 | UNK | T787 | UNK | T788 | UNK | T789 | UNK | T790 | UNK | T791 | UNK | T792 | UNK | T793 | UNK | T794 | UNK | T795 | UNK | T796 | UNK | T797 | UNK | T798 | UNK | T799 | UNK | T800 | UNK | T801 | UNK | T802 | UNK | T803 | UNK | T804 | UNK | T805 | UNK | T806 | UNK | T807 | UNK | T808 | UNK | T809 | UNK | T810 | UNK | T811 | UNK | T812 | UNK | T813 | UNK | T814 | UNK | T815 | UNK | T816 | UNK | T817 | UNK | T818 | UNK | T819 | UNK | T820 | UNK | T821 | UNK | T822 | UNK | T823 | UNK | T824 | UNK | T825 | UNK | T826 | UNK | T827 | UNK | T828 | UNK | T829 | UNK | T830 | UNK | T831 | UNK | T832 | UNK | T833 | UNK | T834 | UNK | T835 | UNK | T836 | UNK | T837 | UNK | T838 | UNK | T839 | UNK | T840 | UNK | T841 | UNK | T842 | UNK | T843 | UNK | T844 | UNK | T845 | UNK | T846 | UNK | T847 | UNK | T848 | UNK | T849 | UNK | T850 | UNK | T851 | UNK | T852 | UNK | T853 | UNK | T854 | UNK | T855 | UNK | T856 | UNK | T857 | UNK | T858 | UNK | T859 | UNK | T860 | UNK | T861 | UNK | T862 | UNK | T863 | UNK | T864 | UNK | T865 | UNK | T866 | UNK | T867 | UNK | T868 | UNK | T869 | UNK | T870 | UNK | T871 | UNK | T872 | UNK | T873 | UNK | T874 | UNK | T875 | UNK | T876 | UNK | T877 | UNK | T878 | UNK | T879 | UNK | T880 | UNK | T881 | UNK | T882 | UNK | T883 | UNK | T884 | UNK | T885 | UNK | T886 | UNK | T887 | UNK | T888 | UNK | T889 | UNK | T890 | UNK | T891 | UNK | T892 | UNK | T893 | UNK | T894 | UNK | T895 | UNK | T896 | UNK | T897 | UNK | T898 | UNK | T899 | UNK | T900 | UNK | T901 | UNK | T902 | UNK | T903 | UNK | T904 | UNK | T905 | UNK | T906 | UNK | T907 | UNK | T908 | UNK | T909 | UNK | T910 | UNK | T911 | UNK | T912 | UNK | T913 | UNK | T914 | UNK | T915 | UNK | T916 | UNK | T917 | UNK | T918 | UNK | T919 | UNK | T920 | UNK | T921 | UNK | T922 | UNK | T923 | UNK | T924 | UNK | T925 | UNK | T926 | UNK | T927 | UNK | T928 | UNK | T929 | UNK | T930 | UNK | T931 | UNK | T932 | UNK | T933 | UNK | T934 | UNK | T935 | UNK | T936 | UNK | T937 | UNK | T938 | UNK | T939 | UNK | T940 | UNK | T941 | UNK | T942 | UNK | T943 | UNK | T944 | UNK | T945 | UNK | T946 | UNK | T947 | UNK | T948 | UNK | T949 | UNK | T950 | UNK | T951 | UNK | T952 | UNK | T953 | UNK | T954 | UNK | T955 | UNK | T956 | UNK | T957 | UNK | T958 | UNK | T959 | UNK | T960 | UNK | T961 | UNK | T962 | UNK | T963 | UNK | T964 | UNK | T965 | UNK | T966 | UNK | T967 | UNK | T968 | UNK | T969 | UNK | T970 | UNK | T971 | UNK | T972 | UNK | T973 | UNK | T974 | UNK | T975 |
|-----|----|-----|----|-----|-----|-----|-----|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|-----|------|-----|------|-----|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|-----|------|--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• Molecule 2: Clathrin light chain B



• Molecule 2: Clathrin light chain B



4 Data and refinement statistics

| Property | Value | Source |
|---|---|------------------|
| Space group | I 41 2 2 | Depositor |
| Cell constants a, b, c, α , β , γ | 228.56 Å 228.56 Å 710.32 Å 90.00° 90.00° 90.00° | Depositor |
| Resolution (Å) | 100.00 – 7.94 82.22 – 4.99 | Depositor EDS |
| % Data completeness (in resolution range) | 99.6 (100.00-7.94) 63.0 (82.22-4.99) | Depositor EDS |
| R_{merge} | (Not available) | Depositor |
| R_{sym} | 0.07 | Depositor |
| $\langle I/\sigma(I) \rangle$ ¹ | 0.97 (at 5.12 Å) | Xtriage |
| Refinement program | CNS | Depositor |
| R, R_{free} | 0.419 , 0.425 0.423 , 0.426 | Depositor DCC |
| R_{free} test set | No test flags present. | DCC |
| Wilson B-factor (Å ²) | 310.7 | Xtriage |
| Anisotropy | 0.082 | Xtriage |
| Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²) | 0.41 , 471.4 | EDS |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| L-test for twinning ² | $\langle L \rangle = 0.30$, $\langle L^2 \rangle = 0.15$ | Xtriage |
| Outliers | 0 of 26103 reflections | Xtriage |
| F_o, F_c correlation | 0.83 | EDS |
| Total number of atoms | 16504 | wwPDB-VP |
| Average B, all atoms (Å ²) | 295.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.39% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

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 | 0.83 | 20/4638 (0.4%) | 1.27 | 83/6266 (1.3%) |
| 1 | B | 0.80 | 17/4638 (0.4%) | 1.26 | 83/6266 (1.3%) |
| 1 | C | 0.77 | 13/4638 (0.3%) | 1.20 | 73/6266 (1.2%) |
| 2 | D | 0.75 | 0/647 | 1.15 | 8/866 (0.9%) |
| 2 | E | 0.69 | 0/589 | 1.24 | 5/785 (0.6%) |
| 2 | F | 0.77 | 0/642 | 1.20 | 8/859 (0.9%) |
| All | All | 0.79 | 50/15792 (0.3%) | 1.24 | 260/21308 (1.2%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1 | A | 1 | 8 |
| 1 | B | 0 | 3 |
| 1 | C | 2 | 3 |
| 2 | F | 0 | 1 |
| All | All | 3 | 15 |

All (50) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|--------|-------------|----------|
| 1 | B | 1162 | LYS | C-O | -19.68 | 0.85 | 1.23 |
| 1 | A | 1222 | SER | C-O | 18.12 | 1.57 | 1.23 |
| 1 | C | 1182 | ARG | C-O | 17.19 | 1.56 | 1.23 |
| 1 | C | 1136 | SER | C-O | -17.10 | 0.90 | 1.23 |
| 1 | C | 1248 | ASN | N-CA | 17.04 | 1.80 | 1.46 |
| 1 | B | 1280 | ALA | C-O | 16.13 | 1.54 | 1.23 |
| 1 | C | 1247 | ALA | CA-C | 15.76 | 1.94 | 1.52 |
| 1 | B | 1279 | HIS | C-O | -14.82 | 0.95 | 1.23 |
| 1 | B | 1222 | SER | C-O | 13.06 | 1.48 | 1.23 |
| 1 | A | 1162 | LYS | CA-C | 12.83 | 1.86 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|--------|-------------|----------|
| 1 | A | 1162 | LYS | C-O | -12.35 | 0.99 | 1.23 |
| 1 | A | 1223 | ASN | N-CA | 11.85 | 1.70 | 1.46 |
| 1 | A | 1103 | ASN | C-O | 11.51 | 1.45 | 1.23 |
| 1 | A | 1281 | ASP | N-CA | 11.32 | 1.69 | 1.46 |
| 1 | B | 1280 | ALA | N-CA | 10.12 | 1.66 | 1.46 |
| 1 | B | 1223 | ASN | N-CA | 9.84 | 1.66 | 1.46 |
| 1 | B | 1281 | ASP | N-CA | 9.80 | 1.66 | 1.46 |
| 1 | C | 1247 | ALA | C-O | -9.61 | 1.05 | 1.23 |
| 1 | A | 1163 | LYS | N-CA | 8.97 | 1.64 | 1.46 |
| 1 | A | 1222 | SER | C-N | 8.76 | 1.54 | 1.34 |
| 1 | A | 1280 | ALA | CA-C | 8.58 | 1.75 | 1.52 |
| 1 | B | 1279 | HIS | CA-C | 8.50 | 1.75 | 1.52 |
| 1 | A | 1575 | ASP | N-CA | 8.40 | 1.63 | 1.46 |
| 1 | C | 1136 | SER | CA-C | 8.29 | 1.74 | 1.52 |
| 1 | B | 1592 | MET | C-O | -8.01 | 1.08 | 1.23 |
| 1 | C | 1118 | LYS | C-O | 8.00 | 1.38 | 1.23 |
| 1 | C | 1592 | MET | C-O | -7.84 | 1.08 | 1.23 |
| 1 | A | 1148 | GLY | N-CA | -7.73 | 1.34 | 1.46 |
| 1 | A | 1592 | MET | C-O | -7.72 | 1.08 | 1.23 |
| 1 | B | 1280 | ALA | C-N | 7.61 | 1.51 | 1.34 |
| 1 | A | 1574 | TYR | CA-C | 7.59 | 1.72 | 1.52 |
| 1 | A | 1104 | GLU | C-N | 7.19 | 1.48 | 1.34 |
| 1 | B | 1197 | HIS | C-O | 7.06 | 1.36 | 1.23 |
| 1 | B | 1221 | VAL | C-O | 6.98 | 1.36 | 1.23 |
| 1 | B | 1134 | PRO | N-CD | -6.69 | 1.38 | 1.47 |
| 1 | A | 1104 | GLU | N-CA | -6.67 | 1.33 | 1.46 |
| 1 | B | 1222 | SER | C-N | 6.65 | 1.49 | 1.34 |
| 1 | A | 1134 | PRO | N-CD | -6.54 | 1.38 | 1.47 |
| 1 | A | 1222 | SER | CA-C | 6.30 | 1.69 | 1.52 |
| 1 | C | 1137 | TYR | CA-CB | -6.21 | 1.40 | 1.53 |
| 1 | A | 1223 | ASN | CA-CB | -6.14 | 1.37 | 1.53 |
| 1 | C | 1136 | SER | C-N | 6.11 | 1.48 | 1.34 |
| 1 | B | 1592 | MET | CA-CB | -5.79 | 1.41 | 1.53 |
| 1 | B | 1223 | ASN | CA-CB | -5.76 | 1.38 | 1.53 |
| 1 | B | 1280 | ALA | CA-C | 5.74 | 1.67 | 1.52 |
| 1 | A | 1103 | ASN | CA-C | -5.54 | 1.38 | 1.52 |
| 1 | C | 1592 | MET | CA-CB | -5.46 | 1.42 | 1.53 |
| 1 | C | 1223 | ASN | CA-CB | -5.42 | 1.39 | 1.53 |
| 1 | A | 1592 | MET | CA-CB | -5.42 | 1.42 | 1.53 |
| 1 | C | 1132 | ASP | N-CA | -5.11 | 1.36 | 1.46 |

All (260) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|---------|--------|-------------|----------|
| 1 | B | 1162 | LYS | CA-C-O | 22.12 | 166.55 | 120.10 |
| 1 | B | 1279 | HIS | O-C-N | -22.04 | 87.43 | 122.70 |
| 1 | C | 1223 | ASN | N-CA-C | 18.52 | 161.00 | 111.00 |
| 1 | A | 1103 | ASN | C-N-CA | -17.51 | 77.93 | 121.70 |
| 1 | A | 1162 | LYS | O-C-N | -16.77 | 95.87 | 122.70 |
| 1 | A | 1103 | ASN | CA-C-N | -16.07 | 81.83 | 117.20 |
| 1 | C | 1137 | TYR | N-CA-CB | 15.54 | 138.57 | 110.60 |
| 1 | C | 1247 | ALA | CA-C-N | 15.38 | 151.02 | 117.20 |
| 1 | C | 1131 | ALA | CA-C-N | -15.29 | 83.57 | 117.20 |
| 1 | B | 1429 | ARG | CB-CA-C | -14.96 | 80.47 | 110.40 |
| 1 | A | 1429 | ARG | CB-CA-C | -14.94 | 80.53 | 110.40 |
| 1 | C | 1429 | ARG | CB-CA-C | -14.93 | 80.53 | 110.40 |
| 1 | B | 1162 | LYS | CA-C-N | -14.30 | 85.73 | 117.20 |
| 1 | B | 1091 | ASN | CB-CA-C | -14.29 | 81.83 | 110.40 |
| 1 | A | 1091 | ASN | CB-CA-C | -14.23 | 81.94 | 110.40 |
| 1 | B | 1162 | LYS | C-N-CA | -14.04 | 86.60 | 121.70 |
| 1 | C | 1182 | ARG | O-C-N | 13.92 | 144.97 | 122.70 |
| 1 | B | 1121 | VAL | CB-CA-C | -13.18 | 86.35 | 111.40 |
| 1 | C | 1131 | ALA | C-N-CA | -12.97 | 89.28 | 121.70 |
| 1 | B | 1223 | ASN | N-CA-C | 12.96 | 145.99 | 111.00 |
| 1 | C | 1223 | ASN | CB-CA-C | -12.88 | 84.64 | 110.40 |
| 1 | A | 1103 | ASN | O-C-N | 12.77 | 143.12 | 122.70 |
| 1 | B | 1223 | ASN | CB-CA-C | -12.42 | 85.57 | 110.40 |
| 1 | A | 1223 | ASN | CB-CA-C | -12.35 | 85.70 | 110.40 |
| 1 | A | 1104 | GLU | C-N-CA | -12.32 | 70.27 | 122.00 |
| 1 | A | 1147 | SER | CA-C-N | -12.18 | 91.84 | 116.20 |
| 1 | A | 1593 | ASP | N-CA-CB | 12.13 | 132.44 | 110.60 |
| 1 | C | 1247 | ALA | C-N-CA | 12.13 | 152.03 | 121.70 |
| 1 | A | 1223 | ASN | N-CA-C | 12.10 | 143.67 | 111.00 |
| 1 | C | 1593 | ASP | N-CA-CB | 12.04 | 132.27 | 110.60 |
| 1 | B | 1593 | ASP | N-CA-CB | 11.98 | 132.17 | 110.60 |
| 1 | A | 1222 | SER | CA-C-O | -11.96 | 94.98 | 120.10 |
| 1 | C | 1222 | SER | C-N-CA | -11.49 | 92.97 | 121.70 |
| 1 | A | 1222 | SER | O-C-N | 11.40 | 140.94 | 122.70 |
| 1 | B | 1280 | ALA | CA-C-O | -11.33 | 96.31 | 120.10 |
| 1 | B | 1280 | ALA | CB-CA-C | -11.26 | 93.20 | 110.10 |
| 1 | A | 1598 | TYR | CB-CA-C | 11.14 | 132.69 | 110.40 |
| 1 | B | 1598 | TYR | CB-CA-C | 11.14 | 132.69 | 110.40 |
| 1 | C | 1598 | TYR | CB-CA-C | 11.08 | 132.55 | 110.40 |
| 1 | B | 1456 | GLN | CB-CA-C | -11.05 | 88.31 | 110.40 |
| 1 | A | 1592 | MET | CB-CA-C | -11.01 | 88.39 | 110.40 |
| 1 | A | 1456 | GLN | CB-CA-C | -10.98 | 88.44 | 110.40 |
| 1 | C | 1456 | GLN | CB-CA-C | -10.98 | 88.45 | 110.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 1 | C | 1592 | MET | CB-CA-C | -10.84 | 88.72 | 110.40 |
| 1 | B | 1418 | LEU | CB-CA-C | -10.68 | 89.90 | 110.20 |
| 1 | A | 1418 | LEU | CB-CA-C | -10.65 | 89.96 | 110.20 |
| 1 | C | 1418 | LEU | CB-CA-C | -10.63 | 90.01 | 110.20 |
| 1 | B | 1592 | MET | CB-CA-C | -10.60 | 89.20 | 110.40 |
| 1 | C | 1247 | ALA | O-C-N | -10.32 | 106.19 | 122.70 |
| 1 | A | 1104 | GLU | N-CA-C | 10.20 | 138.54 | 111.00 |
| 1 | B | 1532 | SER | N-CA-C | -10.14 | 83.62 | 111.00 |
| 1 | C | 1532 | SER | N-CA-C | -10.13 | 83.64 | 111.00 |
| 1 | A | 1532 | SER | N-CA-C | -10.07 | 83.82 | 111.00 |
| 1 | B | 1528 | CYS | CB-CA-C | 9.91 | 130.21 | 110.40 |
| 1 | B | 1162 | LYS | O-C-N | -9.89 | 106.88 | 122.70 |
| 1 | C | 1183 | LEU | N-CA-C | 9.78 | 137.40 | 111.00 |
| 1 | C | 1086 | ILE | N-CA-C | -9.67 | 84.88 | 111.00 |
| 1 | A | 1147 | SER | C-N-CA | -9.57 | 102.19 | 122.30 |
| 1 | B | 1280 | ALA | O-C-N | 9.49 | 137.89 | 122.70 |
| 1 | B | 1281 | ASP | N-CA-CB | 9.38 | 127.48 | 110.60 |
| 1 | C | 1136 | SER | CA-C-N | -9.30 | 96.73 | 117.20 |
| 2 | E | 113 | LEU | CA-CB-CG | 9.28 | 136.65 | 115.30 |
| 1 | B | 1251 | ARG | CB-CA-C | -9.28 | 91.85 | 110.40 |
| 1 | B | 1222 | SER | O-C-N | 9.27 | 137.53 | 122.70 |
| 1 | C | 1355 | ALA | N-CA-C | -9.26 | 86.00 | 111.00 |
| 1 | C | 1251 | ARG | CB-CA-C | -9.23 | 91.94 | 110.40 |
| 2 | F | 113 | LEU | CA-CB-CG | 9.23 | 136.52 | 115.30 |
| 1 | A | 1251 | ARG | CB-CA-C | -9.22 | 91.96 | 110.40 |
| 1 | A | 1355 | ALA | N-CA-C | -9.22 | 86.11 | 111.00 |
| 1 | B | 1355 | ALA | N-CA-C | -9.19 | 86.17 | 111.00 |
| 2 | D | 113 | LEU | CA-CB-CG | 9.11 | 136.26 | 115.30 |
| 1 | B | 1222 | SER | CA-C-O | -9.00 | 101.20 | 120.10 |
| 1 | A | 1231 | LEU | CB-CA-C | 8.95 | 127.20 | 110.20 |
| 1 | B | 1231 | LEU | CB-CA-C | 8.92 | 127.15 | 110.20 |
| 1 | B | 1210 | MET | N-CA-C | -8.84 | 87.15 | 111.00 |
| 1 | A | 1210 | MET | N-CA-C | -8.73 | 87.44 | 111.00 |
| 1 | C | 1598 | TYR | N-CA-C | -8.72 | 87.45 | 111.00 |
| 1 | A | 1598 | TYR | N-CA-C | -8.71 | 87.48 | 111.00 |
| 1 | B | 1598 | TYR | N-CA-C | -8.69 | 87.53 | 111.00 |
| 1 | C | 1247 | ALA | CA-C-O | -8.56 | 102.13 | 120.10 |
| 1 | C | 1223 | ASN | O-C-N | 8.43 | 136.19 | 122.70 |
| 1 | A | 1223 | ASN | O-C-N | 8.42 | 136.17 | 122.70 |
| 1 | C | 1131 | ALA | O-C-N | 8.38 | 136.11 | 122.70 |
| 1 | B | 1223 | ASN | O-C-N | 8.35 | 136.06 | 122.70 |
| 2 | E | 92 | ALA | N-CA-C | 8.35 | 133.54 | 111.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1 | A | 1325 | SER | N-CA-C | 8.33 | 133.50 | 111.00 |
| 1 | C | 1528 | CYS | CB-CA-C | 8.27 | 126.95 | 110.40 |
| 1 | A | 1528 | CYS | CB-CA-C | 8.26 | 126.92 | 110.40 |
| 1 | B | 1325 | SER | N-CA-C | 8.26 | 133.30 | 111.00 |
| 1 | C | 1325 | SER | N-CA-C | 8.26 | 133.30 | 111.00 |
| 1 | A | 1134 | PRO | N-CA-C | 8.24 | 133.53 | 112.10 |
| 1 | B | 1134 | PRO | N-CA-C | 8.06 | 133.06 | 112.10 |
| 1 | A | 1326 | LYS | N-CA-C | -7.90 | 89.67 | 111.00 |
| 1 | C | 1326 | LYS | N-CA-C | -7.90 | 89.67 | 111.00 |
| 1 | C | 1222 | SER | O-C-N | -7.89 | 110.08 | 122.70 |
| 1 | B | 1326 | LYS | N-CA-C | -7.87 | 89.76 | 111.00 |
| 1 | A | 1590 | ASN | N-CA-C | 7.74 | 131.91 | 111.00 |
| 1 | C | 1136 | SER | CB-CA-C | 7.71 | 124.74 | 110.10 |
| 1 | A | 1181 | ASN | CB-CA-C | -7.67 | 95.07 | 110.40 |
| 1 | A | 1222 | SER | CB-CA-C | -7.66 | 95.54 | 110.10 |
| 1 | A | 1574 | TYR | CA-C-O | -7.63 | 104.07 | 120.10 |
| 1 | B | 1256 | VAL | N-CA-C | 7.58 | 131.46 | 111.00 |
| 1 | A | 1162 | LYS | CA-C-N | 7.57 | 133.85 | 117.20 |
| 1 | C | 1256 | VAL | N-CA-C | 7.56 | 131.41 | 111.00 |
| 1 | A | 1256 | VAL | N-CA-C | 7.56 | 131.40 | 111.00 |
| 1 | C | 1182 | ARG | CA-C-N | -7.53 | 100.64 | 117.20 |
| 1 | B | 1576 | LEU | N-CA-C | -7.52 | 90.69 | 111.00 |
| 1 | C | 1576 | LEU | N-CA-C | -7.51 | 90.73 | 111.00 |
| 1 | A | 1576 | LEU | N-CA-C | -7.45 | 90.88 | 111.00 |
| 1 | B | 1590 | ASN | CB-CA-C | -7.38 | 95.64 | 110.40 |
| 1 | C | 1592 | MET | O-C-N | -7.27 | 111.06 | 122.70 |
| 1 | C | 1590 | ASN | CB-CA-C | -7.26 | 95.88 | 110.40 |
| 1 | B | 1592 | MET | O-C-N | -7.23 | 111.13 | 122.70 |
| 1 | A | 1104 | GLU | O-C-N | -7.20 | 107.42 | 121.10 |
| 1 | A | 1280 | ALA | CA-C-O | -7.18 | 105.02 | 120.10 |
| 1 | C | 1424 | MET | N-CA-C | 7.18 | 130.39 | 111.00 |
| 1 | A | 1424 | MET | N-CA-C | 7.18 | 130.38 | 111.00 |
| 1 | A | 1256 | VAL | CB-CA-C | -7.14 | 97.83 | 111.40 |
| 1 | B | 1424 | MET | N-CA-C | 7.14 | 130.28 | 111.00 |
| 1 | B | 1223 | ASN | C-N-CA | 7.14 | 139.55 | 121.70 |
| 1 | A | 1590 | ASN | CB-CA-C | -7.13 | 96.13 | 110.40 |
| 1 | A | 1527 | LEU | N-CA-C | 7.08 | 130.11 | 111.00 |
| 1 | A | 1592 | MET | O-C-N | -7.07 | 111.39 | 122.70 |
| 1 | B | 1256 | VAL | CB-CA-C | -7.07 | 97.97 | 111.40 |
| 1 | A | 1223 | ASN | C-N-CA | 7.07 | 139.36 | 121.70 |
| 1 | B | 1527 | LEU | N-CA-C | 7.07 | 130.08 | 111.00 |
| 1 | C | 1256 | VAL | CB-CA-C | -7.06 | 97.99 | 111.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1 | C | 1223 | ASN | C-N-CA | 7.06 | 139.34 | 121.70 |
| 1 | C | 1527 | LEU | N-CA-C | 7.05 | 130.03 | 111.00 |
| 1 | B | 1134 | PRO | N-CA-CB | -7.01 | 94.89 | 103.30 |
| 1 | A | 1572 | THR | N-CA-C | 6.99 | 129.86 | 111.00 |
| 1 | B | 1572 | THR | N-CA-C | 6.99 | 129.86 | 111.00 |
| 1 | C | 1181 | ASN | CB-CA-C | -6.93 | 96.54 | 110.40 |
| 1 | C | 1572 | THR | N-CA-C | 6.92 | 129.70 | 111.00 |
| 1 | C | 1182 | ARG | CA-C-O | -6.90 | 105.61 | 120.10 |
| 1 | A | 1134 | PRO | N-CA-CB | -6.85 | 95.07 | 102.60 |
| 1 | B | 1457 | ASN | N-CA-C | -6.78 | 92.69 | 111.00 |
| 1 | C | 1457 | ASN | N-CA-C | -6.75 | 92.77 | 111.00 |
| 1 | A | 1457 | ASN | N-CA-C | -6.74 | 92.80 | 111.00 |
| 1 | B | 1197 | HIS | O-C-N | 6.72 | 133.45 | 122.70 |
| 1 | B | 1590 | ASN | N-CA-C | 6.71 | 129.11 | 111.00 |
| 1 | C | 1222 | SER | CA-C-N | -6.70 | 102.45 | 117.20 |
| 1 | C | 1520 | ARG | CB-CA-C | -6.68 | 97.04 | 110.40 |
| 1 | B | 1520 | ARG | CB-CA-C | -6.61 | 97.18 | 110.40 |
| 1 | A | 1520 | ARG | CB-CA-C | -6.60 | 97.21 | 110.40 |
| 1 | A | 1133 | ASP | N-CA-C | -6.58 | 93.24 | 111.00 |
| 1 | C | 1358 | TRP | CB-CA-C | -6.56 | 97.28 | 110.40 |
| 1 | A | 1358 | TRP | CB-CA-C | -6.56 | 97.29 | 110.40 |
| 1 | B | 1358 | TRP | CB-CA-C | -6.50 | 97.39 | 110.40 |
| 1 | A | 1231 | LEU | N-CA-C | -6.35 | 93.86 | 111.00 |
| 1 | B | 1231 | LEU | N-CA-C | -6.35 | 93.87 | 111.00 |
| 1 | B | 1163 | LYS | N-CA-CB | 6.32 | 121.97 | 110.60 |
| 1 | B | 1133 | ASP | N-CA-C | -6.31 | 93.95 | 111.00 |
| 2 | D | 113 | LEU | N-CA-CB | -6.27 | 97.85 | 110.40 |
| 1 | A | 1197 | HIS | N-CA-C | -6.26 | 94.11 | 111.00 |
| 2 | F | 164 | PRO | N-CA-CB | 6.20 | 110.75 | 103.30 |
| 2 | E | 112 | ARG | N-CA-C | -6.19 | 94.30 | 111.00 |
| 1 | C | 1465 | GLU | CB-CA-C | -6.18 | 98.04 | 110.40 |
| 2 | F | 112 | ARG | N-CA-C | -6.18 | 94.32 | 111.00 |
| 2 | F | 110 | ARG | NE-CZ-NH2 | -6.16 | 117.22 | 120.30 |
| 1 | B | 1465 | GLU | CB-CA-C | -6.14 | 98.12 | 110.40 |
| 1 | A | 1465 | GLU | CB-CA-C | -6.14 | 98.13 | 110.40 |
| 1 | C | 1248 | ASN | N-CA-CB | -6.08 | 99.66 | 110.60 |
| 1 | B | 1233 | HIS | N-CA-C | -6.07 | 94.62 | 111.00 |
| 1 | C | 1167 | SER | N-CA-C | 6.06 | 127.36 | 111.00 |
| 1 | A | 1233 | HIS | N-CA-C | -6.03 | 94.72 | 111.00 |
| 1 | C | 1531 | ASP | CB-CA-C | -6.00 | 98.40 | 110.40 |
| 1 | B | 1531 | ASP | CB-CA-C | -5.97 | 98.46 | 110.40 |
| 1 | A | 1531 | ASP | CB-CA-C | -5.96 | 98.48 | 110.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1 | B | 1151 | GLU | CB-CA-C | -5.95 | 98.50 | 110.40 |
| 1 | A | 1261 | VAL | CB-CA-C | -5.95 | 100.10 | 111.40 |
| 1 | B | 1222 | SER | CB-CA-C | -5.93 | 98.83 | 110.10 |
| 1 | C | 1130 | LYS | N-CA-C | -5.93 | 95.00 | 111.00 |
| 1 | C | 1261 | VAL | CB-CA-C | -5.91 | 100.17 | 111.40 |
| 1 | A | 1235 | GLY | N-CA-C | -5.91 | 98.33 | 113.10 |
| 1 | B | 1235 | GLY | N-CA-C | -5.90 | 98.36 | 113.10 |
| 1 | B | 1261 | VAL | CB-CA-C | -5.88 | 100.23 | 111.40 |
| 2 | E | 110 | ARG | NE-CZ-NH2 | -5.87 | 117.36 | 120.30 |
| 2 | D | 110 | ARG | NE-CZ-NH2 | -5.86 | 117.37 | 120.30 |
| 1 | B | 1162 | LYS | N-CA-C | -5.86 | 95.17 | 111.00 |
| 1 | C | 1151 | GLU | CB-CA-C | -5.86 | 98.69 | 110.40 |
| 1 | A | 1151 | GLU | CB-CA-C | -5.85 | 98.70 | 110.40 |
| 2 | D | 164 | PRO | N-CA-CB | 5.84 | 110.31 | 103.30 |
| 1 | C | 1118 | LYS | O-C-N | 5.78 | 133.03 | 123.20 |
| 1 | B | 1589 | HIS | N-CA-C | 5.75 | 126.51 | 111.00 |
| 1 | A | 1183 | LEU | N-CA-C | 5.74 | 126.49 | 111.00 |
| 1 | A | 1465 | GLU | N-CA-C | 5.73 | 126.46 | 111.00 |
| 1 | B | 1465 | GLU | N-CA-C | 5.70 | 126.38 | 111.00 |
| 1 | B | 1529 | LYS | N-CA-CB | -5.69 | 100.35 | 110.60 |
| 1 | A | 1529 | LYS | N-CA-CB | -5.68 | 100.37 | 110.60 |
| 1 | C | 1465 | GLU | N-CA-C | 5.67 | 126.30 | 111.00 |
| 1 | A | 1455 | VAL | CB-CA-C | -5.66 | 100.64 | 111.40 |
| 1 | B | 1576 | LEU | CB-CA-C | 5.64 | 120.92 | 110.20 |
| 1 | C | 1455 | VAL | CB-CA-C | -5.62 | 100.73 | 111.40 |
| 1 | C | 1529 | LYS | N-CA-CB | -5.62 | 100.49 | 110.60 |
| 1 | B | 1455 | VAL | CB-CA-C | -5.60 | 100.77 | 111.40 |
| 1 | A | 1572 | THR | CB-CA-C | -5.56 | 96.59 | 111.60 |
| 1 | A | 1576 | LEU | CB-CA-C | 5.55 | 120.74 | 110.20 |
| 1 | B | 1572 | THR | CB-CA-C | -5.55 | 96.63 | 111.60 |
| 1 | A | 1574 | TYR | CA-C-N | 5.54 | 129.38 | 117.20 |
| 1 | C | 1535 | LYS | N-CA-C | 5.53 | 125.94 | 111.00 |
| 1 | A | 1325 | SER | CB-CA-C | -5.51 | 99.64 | 110.10 |
| 1 | C | 1572 | THR | CB-CA-C | -5.50 | 96.74 | 111.60 |
| 1 | C | 1355 | ALA | CB-CA-C | 5.50 | 118.36 | 110.10 |
| 1 | C | 1576 | LEU | CB-CA-C | 5.49 | 120.64 | 110.20 |
| 1 | A | 1535 | LYS | N-CA-C | 5.49 | 125.81 | 111.00 |
| 1 | B | 1355 | ALA | CB-CA-C | 5.49 | 118.33 | 110.10 |
| 1 | C | 1325 | SER | CB-CA-C | -5.47 | 99.70 | 110.10 |
| 1 | C | 1590 | ASN | N-CA-C | 5.47 | 125.77 | 111.00 |
| 1 | B | 1325 | SER | CB-CA-C | -5.46 | 99.73 | 110.10 |
| 1 | B | 1535 | LYS | N-CA-C | 5.46 | 125.74 | 111.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1 | B | 1192 | GLY | C-N-CD | -5.45 | 108.61 | 120.60 |
| 2 | F | 157 | ASP | N-CA-C | 5.43 | 125.67 | 111.00 |
| 2 | D | 157 | ASP | N-CA-C | 5.43 | 125.67 | 111.00 |
| 1 | A | 1192 | GLY | C-N-CD | -5.41 | 108.70 | 120.60 |
| 1 | A | 1463 | VAL | CB-CA-C | -5.40 | 101.13 | 111.40 |
| 2 | F | 156 | ALA | N-CA-C | -5.40 | 96.41 | 111.00 |
| 1 | A | 1355 | ALA | CB-CA-C | 5.40 | 118.20 | 110.10 |
| 2 | D | 156 | ALA | N-CA-C | -5.39 | 96.45 | 111.00 |
| 1 | B | 1463 | VAL | CB-CA-C | -5.37 | 101.20 | 111.40 |
| 1 | A | 1223 | ASN | CA-C-O | -5.36 | 108.85 | 120.10 |
| 1 | C | 1463 | VAL | CB-CA-C | -5.35 | 101.23 | 111.40 |
| 1 | A | 1107 | VAL | N-CA-C | 5.34 | 125.42 | 111.00 |
| 1 | B | 1107 | VAL | N-CA-C | 5.33 | 125.39 | 111.00 |
| 1 | C | 1593 | ASP | CB-CA-C | -5.28 | 99.84 | 110.40 |
| 1 | A | 1593 | ASP | CB-CA-C | -5.24 | 99.92 | 110.40 |
| 1 | B | 1133 | ASP | CB-CA-C | 5.22 | 120.85 | 110.40 |
| 1 | A | 1426 | LEU | CB-CA-C | -5.22 | 100.28 | 110.20 |
| 1 | C | 1426 | LEU | CB-CA-C | -5.21 | 100.30 | 110.20 |
| 1 | B | 1221 | VAL | O-C-N | 5.21 | 131.03 | 122.70 |
| 2 | F | 143 | SER | N-CA-C | 5.20 | 125.05 | 111.00 |
| 2 | D | 143 | SER | N-CA-C | 5.20 | 125.05 | 111.00 |
| 1 | B | 1593 | ASP | CB-CA-C | -5.20 | 100.01 | 110.40 |
| 1 | A | 1425 | VAL | CB-CA-C | -5.19 | 101.54 | 111.40 |
| 2 | E | 156 | ALA | N-CA-C | -5.19 | 96.99 | 111.00 |
| 2 | F | 156 | ALA | C-N-CA | 5.18 | 134.64 | 121.70 |
| 1 | B | 1223 | ASN | CA-C-O | -5.17 | 109.24 | 120.10 |
| 1 | C | 1169 | VAL | CB-CA-C | -5.17 | 101.58 | 111.40 |
| 1 | A | 1371 | TYR | CB-CA-C | -5.16 | 100.07 | 110.40 |
| 1 | C | 1371 | TYR | CB-CA-C | -5.16 | 100.08 | 110.40 |
| 2 | D | 156 | ALA | C-N-CA | 5.16 | 134.59 | 121.70 |
| 1 | A | 1133 | ASP | CB-CA-C | 5.15 | 120.71 | 110.40 |
| 1 | B | 1426 | LEU | CB-CA-C | -5.15 | 100.42 | 110.20 |
| 1 | C | 1182 | ARG | CB-CA-C | 5.14 | 120.69 | 110.40 |
| 1 | B | 1371 | TYR | CB-CA-C | -5.14 | 100.11 | 110.40 |
| 1 | C | 1425 | VAL | CB-CA-C | -5.13 | 101.66 | 111.40 |
| 1 | B | 1425 | VAL | CB-CA-C | -5.11 | 101.69 | 111.40 |
| 1 | B | 1169 | VAL | CB-CA-C | -5.11 | 101.69 | 111.40 |
| 1 | A | 1104 | GLU | CA-C-O | -5.08 | 109.43 | 120.10 |
| 1 | B | 1134 | PRO | CA-C-N | 5.08 | 128.38 | 117.20 |
| 1 | C | 1180 | THR | N-CA-C | 5.08 | 124.70 | 111.00 |
| 1 | A | 1169 | VAL | CB-CA-C | -5.04 | 101.82 | 111.40 |
| 1 | B | 1122 | LYS | CB-CA-C | -5.03 | 100.34 | 110.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1 | B | 1129 | ILE | C-N-CA | -5.03 | 109.13 | 121.70 |
| 1 | A | 1129 | ILE | C-N-CA | -5.03 | 109.14 | 121.70 |
| 1 | B | 1358 | TRP | N-CA-C | 5.02 | 124.56 | 111.00 |
| 1 | B | 1195 | ASN | CB-CA-C | -5.02 | 100.37 | 110.40 |
| 1 | A | 1195 | ASN | CB-CA-C | -5.01 | 100.38 | 110.40 |
| 1 | A | 1573 | CYS | CB-CA-C | -5.01 | 100.39 | 110.40 |
| 1 | C | 1573 | CYS | CB-CA-C | -5.00 | 100.39 | 110.40 |

All (3) chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|-----|-------|------|------|------|
| 1 | A | 1104 | GLU | CA |
| 1 | C | 1137 | TYR | CA |
| 1 | C | 1223 | ASN | CA |

All (15) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|------|------|-----------|
| 1 | A | 1103 | ASN | Mainchain |
| 1 | A | 1104 | GLU | Mainchain |
| 1 | A | 1133 | ASP | Mainchain |
| 1 | A | 1147 | SER | Mainchain |
| 1 | A | 1162 | LYS | Mainchain |
| 1 | A | 1197 | HIS | Mainchain |
| 1 | A | 1247 | ALA | Mainchain |
| 1 | A | 1280 | ALA | Mainchain |
| 1 | B | 1133 | ASP | Mainchain |
| 1 | B | 1279 | HIS | Mainchain |
| 1 | B | 1280 | ALA | Mainchain |
| 1 | C | 1131 | ALA | Mainchain |
| 1 | C | 1182 | ARG | Mainchain |
| 1 | C | 1222 | SER | Mainchain |
| 2 | F | 196 | UNK | 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 | 4543 | 0 | 4454 | 1296 | 1 |
| 1 | B | 4543 | 0 | 4456 | 1248 | 3 |
| 1 | C | 4543 | 0 | 4455 | 1291 | 4 |
| 2 | D | 1146 | 0 | 735 | 252 | 0 |
| 2 | E | 823 | 0 | 633 | 246 | 0 |
| 2 | F | 906 | 0 | 669 | 239 | 0 |
| All | All | 16504 | 0 | 15402 | 4313 | 5 |

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 135.

All (4313) 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) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:1258:PHE:HB2 | 1:A:1289:TYR:CD2 | 1.19 | 1.69 |
| 1:A:1253:TRP:CZ3 | 1:A:1276:ILE:HG22 | 1.25 | 1.64 |
| 1:C:1253:TRP:CZ3 | 1:C:1276:ILE:HG22 | 1.25 | 1.64 |
| 1:A:1258:PHE:CB | 1:A:1289:TYR:CE2 | 1.75 | 1.63 |
| 1:B:1253:TRP:CZ3 | 1:B:1276:ILE:HG22 | 1.25 | 1.63 |
| 1:A:1258:PHE:HB3 | 1:A:1289:TYR:CE2 | 1.28 | 1.61 |
| 2:E:203:UNK:C | 2:E:203:UNK:CA | 1.76 | 1.60 |
| 1:B:1264:LYS:CE | 1:B:1268:LEU:HD12 | 1.17 | 1.58 |
| 1:C:1211:TYR:CD1 | 1:C:1231:LEU:HD22 | 1.29 | 1.58 |
| 1:C:1264:LYS:CE | 1:C:1268:LEU:HD12 | 1.17 | 1.57 |
| 1:A:1264:LYS:CE | 1:A:1268:LEU:HD12 | 1.17 | 1.56 |
| 1:A:1223:ASN:CA | 1:A:1223:ASN:N | 1.70 | 1.55 |
| 1:C:1136:SER:CA | 1:C:1136:SER:C | 1.74 | 1.54 |
| 1:A:1281:ASP:CA | 1:A:1281:ASP:N | 1.69 | 1.54 |
| 1:A:1280:ALA:C | 1:A:1280:ALA:CA | 1.75 | 1.53 |
| 1:B:1279:HIS:C | 1:B:1279:HIS:CA | 1.75 | 1.51 |
| 1:B:1358:TRP:CH2 | 1:B:1381:HIS:CE1 | 1.98 | 1.50 |
| 1:C:1358:TRP:CH2 | 1:C:1381:HIS:CE1 | 1.98 | 1.50 |
| 1:C:1409:GLN:CG | 1:C:1413:GLU:HG3 | 1.41 | 1.50 |
| 1:A:1409:GLN:CG | 1:A:1413:GLU:HG3 | 1.41 | 1.49 |
| 1:A:1358:TRP:CH2 | 1:A:1381:HIS:CE1 | 1.98 | 1.48 |
| 1:B:1290:TYR:CD2 | 1:B:1299:LEU:HD13 | 1.46 | 1.47 |
| 1:B:1409:GLN:CG | 1:B:1413:GLU:HG3 | 1.41 | 1.46 |
| 1:A:1258:PHE:N | 1:A:1289:TYR:CZ | 1.77 | 1.44 |
| 1:C:1248:ASN:N | 1:C:1248:ASN:CA | 1.80 | 1.43 |
| 1:A:1244:ALA:HB3 | 1:A:1275:HIS:ND1 | 1.13 | 1.43 |
| 1:C:1211:TYR:CD1 | 1:C:1231:LEU:CD2 | 2.01 | 1.43 |
| 1:B:1244:ALA:HB3 | 1:B:1275:HIS:ND1 | 1.20 | 1.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:1244:ALA:HB3 | 1:B:1275:HIS:CE1 | 1.53 | 1.42 |
| 1:A:1244:ALA:HB3 | 1:A:1275:HIS:CE1 | 1.55 | 1.42 |
| 1:A:1162:LYS:C | 1:A:1162:LYS:CA | 1.86 | 1.42 |
| 1:B:1253:TRP:CE3 | 1:B:1276:ILE:CG2 | 2.04 | 1.40 |
| 2:F:21:UNK:C | 2:F:21:UNK:CA | 1.97 | 1.40 |
| 1:C:1253:TRP:CE3 | 1:C:1276:ILE:CG2 | 2.04 | 1.39 |
| 1:C:1602:VAL:HG13 | 2:E:203:UNK:C | 1.50 | 1.39 |
| 1:A:1253:TRP:CE3 | 1:A:1276:ILE:CG2 | 2.04 | 1.38 |
| 1:C:1247:ALA:CA | 1:C:1247:ALA:C | 1.93 | 1.37 |
| 1:C:1092:LEU:O | 1:C:1094:ARG:N | 1.59 | 1.35 |
| 1:B:1601:GLN:NE2 | 1:C:1587:TRP:CZ3 | 1.91 | 1.35 |
| 1:C:1504:LEU:HD11 | 2:E:149:ASN:ND2 | 1.06 | 1.35 |
| 1:A:1264:LYS:CE | 1:A:1268:LEU:CD1 | 2.05 | 1.35 |
| 1:A:1414:PHE:O | 1:A:1416:PRO:HD3 | 1.27 | 1.35 |
| 1:B:1264:LYS:CE | 1:B:1268:LEU:CD1 | 2.04 | 1.34 |
| 1:A:1279:HIS:NE2 | 1:A:1283:LEU:CD1 | 1.89 | 1.34 |
| 1:A:1279:HIS:NE2 | 1:A:1283:LEU:HD13 | 1.40 | 1.34 |
| 1:A:1258:PHE:CB | 1:A:1289:TYR:CD2 | 2.01 | 1.33 |
| 1:C:1264:LYS:CE | 1:C:1268:LEU:CD1 | 2.05 | 1.33 |
| 1:B:1250:THR:O | 1:B:1251:ARG:HG2 | 1.25 | 1.33 |
| 1:C:1167:SER:O | 1:C:1171:THR:HB | 1.26 | 1.33 |
| 1:B:1414:PHE:O | 1:B:1416:PRO:HD3 | 1.27 | 1.33 |
| 1:C:1253:TRP:CZ3 | 1:C:1276:ILE:CG2 | 2.13 | 1.31 |
| 1:B:1253:TRP:CZ3 | 1:B:1276:ILE:CG2 | 2.13 | 1.31 |
| 1:B:1371:TYR:CD1 | 1:B:1394:ILE:HG23 | 1.66 | 1.31 |
| 1:C:1290:TYR:CE2 | 1:C:1299:LEU:HD13 | 1.65 | 1.30 |
| 1:C:1222:SER:O | 1:C:1223:ASN:CB | 1.65 | 1.30 |
| 1:A:1371:TYR:CD1 | 1:A:1394:ILE:HG23 | 1.66 | 1.30 |
| 1:C:1371:TYR:HD1 | 1:C:1394:ILE:CG2 | 1.45 | 1.30 |
| 1:C:1414:PHE:O | 1:C:1416:PRO:HD3 | 1.27 | 1.30 |
| 1:A:1244:ALA:CB | 1:A:1275:HIS:ND1 | 1.94 | 1.29 |
| 1:C:1409:GLN:HG3 | 1:C:1413:GLU:CG | 1.62 | 1.29 |
| 2:E:104:LYS:O | 2:E:108:GLU:CG | 1.79 | 1.29 |
| 1:B:1409:GLN:HG3 | 1:B:1413:GLU:CG | 1.63 | 1.29 |
| 1:A:1371:TYR:HD1 | 1:A:1394:ILE:CG2 | 1.45 | 1.28 |
| 1:C:1371:TYR:CD1 | 1:C:1394:ILE:HG23 | 1.66 | 1.28 |
| 1:A:1253:TRP:CZ3 | 1:A:1276:ILE:CG2 | 2.13 | 1.28 |
| 1:A:1409:GLN:HG3 | 1:A:1413:GLU:CG | 1.62 | 1.28 |
| 1:B:1371:TYR:HD1 | 1:B:1394:ILE:CG2 | 1.45 | 1.28 |
| 2:D:112:ARG:C | 2:D:112:ARG:HD3 | 1.50 | 1.28 |
| 1:A:1250:THR:O | 1:A:1251:ARG:HG2 | 1.24 | 1.28 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:1395:ILE:HG13 | 1:C:1404:TYR:CE2 | 1.68 | 1.28 |
| 1:C:1250:THR:O | 1:C:1251:ARG:HG2 | 1.24 | 1.28 |
| 1:B:1137:TYR:CB | 1:B:1138:MET:HB2 | 1.65 | 1.27 |
| 1:B:1598:TYR:HE2 | 2:D:201:UNK:N | 1.31 | 1.27 |
| 1:C:1588:ARG:HH22 | 2:D:193:UNK:C | 1.48 | 1.27 |
| 1:A:1475:GLU:OE1 | 2:F:145:GLN:HB3 | 1.21 | 1.27 |
| 2:E:119:ALA:O | 2:E:123:MET:HG2 | 1.28 | 1.26 |
| 1:A:1253:TRP:CE3 | 1:A:1276:ILE:HG22 | 1.66 | 1.26 |
| 1:A:1395:ILE:HG13 | 1:A:1404:TYR:CE2 | 1.68 | 1.26 |
| 2:D:119:ALA:O | 2:D:123:MET:HG2 | 1.28 | 1.26 |
| 1:B:1395:ILE:HG13 | 1:B:1404:TYR:CE2 | 1.68 | 1.26 |
| 1:B:1244:ALA:CB | 1:B:1275:HIS:ND1 | 1.98 | 1.25 |
| 1:C:1409:GLN:HA | 1:C:1413:GLU:CG | 1.65 | 1.25 |
| 1:C:1409:GLN:CA | 1:C:1413:GLU:HG2 | 1.66 | 1.25 |
| 1:B:1409:GLN:HA | 1:B:1413:GLU:CG | 1.66 | 1.25 |
| 2:D:112:ARG:HD3 | 2:D:112:ARG:O | 1.35 | 1.25 |
| 1:C:1504:LEU:CD1 | 2:E:149:ASN:ND2 | 1.99 | 1.25 |
| 1:B:1419:LEU:O | 1:B:1422:LEU:HB3 | 1.36 | 1.25 |
| 1:C:1107:VAL:CG1 | 1:C:1111:LEU:HB2 | 1.67 | 1.24 |
| 1:B:1279:HIS:CD2 | 1:B:1280:ALA:H | 1.54 | 1.24 |
| 1:C:1434:ARG:NE | 2:E:5:UNK:HA | 1.53 | 1.24 |
| 1:A:1409:GLN:CA | 1:A:1413:GLU:HG2 | 1.65 | 1.24 |
| 1:B:1409:GLN:CA | 1:B:1413:GLU:HG2 | 1.65 | 1.24 |
| 1:A:1258:PHE:N | 1:A:1289:TYR:CE1 | 2.06 | 1.24 |
| 1:B:1463:VAL:O | 1:B:1467:LEU:HB2 | 1.06 | 1.24 |
| 1:C:1419:LEU:O | 1:C:1422:LEU:HB3 | 1.36 | 1.23 |
| 1:A:1409:GLN:HA | 1:A:1413:GLU:CG | 1.65 | 1.23 |
| 1:C:1270:GLN:CD | 1:C:1298:GLU:HG3 | 1.57 | 1.22 |
| 1:C:1412:LEU:CD1 | 1:C:1419:LEU:HD21 | 1.70 | 1.22 |
| 1:C:1429:ARG:O | 1:C:1429:ARG:CG | 1.78 | 1.21 |
| 2:F:119:ALA:O | 2:F:123:MET:HG2 | 1.36 | 1.21 |
| 2:F:114:GLN:CG | 2:F:115:GLU:H | 1.48 | 1.21 |
| 2:F:162:GLN:HA | 2:F:166:ALA:CB | 1.70 | 1.21 |
| 1:B:1587:TRP:O | 1:B:1589:HIS:N | 1.71 | 1.21 |
| 1:B:1395:ILE:CG1 | 1:B:1404:TYR:CE2 | 2.24 | 1.21 |
| 1:A:1412:LEU:CD1 | 1:A:1419:LEU:HD21 | 1.70 | 1.21 |
| 1:B:1412:LEU:CD1 | 1:B:1419:LEU:HD21 | 1.70 | 1.21 |
| 1:B:1475:GLU:OE1 | 2:D:145:GLN:HB3 | 1.05 | 1.21 |
| 1:A:1137:TYR:CB | 1:A:1138:MET:HB2 | 1.71 | 1.21 |
| 1:A:1254:LYS:O | 1:A:1289:TYR:CD2 | 1.94 | 1.20 |
| 1:A:1279:HIS:CE1 | 1:A:1283:LEU:CD1 | 2.23 | 1.20 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:1463:VAL:O | 1:C:1467:LEU:HB2 | 1.06 | 1.20 |
| 2:E:114:GLN:CG | 2:E:115:GLU:H | 1.48 | 1.20 |
| 1:A:1395:ILE:CG1 | 1:A:1404:TYR:CE2 | 2.23 | 1.20 |
| 1:B:1588:ARG:CZ | 2:F:192:UNK:HA | 1.69 | 1.20 |
| 1:B:1358:TRP:CZ2 | 1:B:1381:HIS:CE1 | 2.30 | 1.20 |
| 1:A:1463:VAL:O | 1:A:1467:LEU:HB2 | 1.06 | 1.20 |
| 1:A:1258:PHE:HB2 | 1:A:1289:TYR:CG | 1.76 | 1.19 |
| 1:A:1419:LEU:O | 1:A:1422:LEU:HB3 | 1.36 | 1.19 |
| 1:A:1254:LYS:CG | 1:A:1285:GLU:OE2 | 1.86 | 1.19 |
| 1:C:1253:TRP:CE3 | 1:C:1276:ILE:HG22 | 1.66 | 1.19 |
| 1:C:1198:ILE:HB | 1:C:1221:VAL:CG2 | 1.71 | 1.19 |
| 1:C:1358:TRP:CZ2 | 1:C:1381:HIS:CE1 | 2.30 | 1.19 |
| 1:C:1395:ILE:CG1 | 1:C:1404:TYR:CE2 | 2.24 | 1.19 |
| 1:A:1358:TRP:CZ2 | 1:A:1381:HIS:CE1 | 2.30 | 1.19 |
| 2:D:114:GLN:CG | 2:D:115:GLU:H | 1.48 | 1.19 |
| 1:B:1253:TRP:CE3 | 1:B:1276:ILE:HG22 | 1.66 | 1.19 |
| 1:C:1434:ARG:HE | 2:E:5:UNK:CA | 1.56 | 1.18 |
| 1:A:1409:GLN:O | 1:A:1413:GLU:HB2 | 1.42 | 1.18 |
| 2:E:114:GLN:HG3 | 2:E:115:GLU:N | 1.46 | 1.18 |
| 1:B:1598:TYR:CE2 | 2:D:201:UNK:N | 2.11 | 1.18 |
| 1:B:1409:GLN:O | 1:B:1413:GLU:HB2 | 1.41 | 1.18 |
| 2:D:174:UNK:HA | 2:D:176:UNK:N | 1.58 | 1.18 |
| 1:C:1408:ILE:HG22 | 1:C:1412:LEU:HB3 | 1.20 | 1.18 |
| 1:B:1429:ARG:CG | 1:B:1429:ARG:O | 1.78 | 1.18 |
| 1:B:1245:ARG:O | 1:B:1246:LYS:HG3 | 1.39 | 1.17 |
| 1:C:1221:VAL:HG13 | 1:C:1222:SER:N | 1.59 | 1.17 |
| 1:A:1411:TYR:O | 1:A:1415:LYS:O | 1.62 | 1.17 |
| 1:B:1551:GLU:CG | 1:B:1582:VAL:HG22 | 1.76 | 1.16 |
| 1:C:1409:GLN:O | 1:C:1413:GLU:HB2 | 1.41 | 1.16 |
| 1:A:1326:LYS:O | 1:A:1326:LYS:CG | 1.93 | 1.16 |
| 1:B:1408:ILE:HG22 | 1:B:1412:LEU:HB3 | 1.20 | 1.16 |
| 1:B:1361:LEU:CD2 | 1:B:1365:TYR:CE2 | 2.28 | 1.16 |
| 1:B:1427:SER:HB2 | 1:B:1428:PRO:HD3 | 1.22 | 1.16 |
| 1:B:1509:ARG:HH22 | 2:D:163:GLN:HA | 1.08 | 1.16 |
| 1:C:1326:LYS:CG | 1:C:1326:LYS:O | 1.93 | 1.15 |
| 1:B:1358:TRP:HE3 | 1:B:1377:THR:CG2 | 1.60 | 1.15 |
| 1:C:1277:VAL:O | 1:C:1279:HIS:N | 1.80 | 1.15 |
| 1:A:1427:SER:CB | 1:A:1428:PRO:HD3 | 1.77 | 1.15 |
| 1:B:1605:GLU:HA | 1:B:1608:THR:HB | 1.29 | 1.15 |
| 2:F:183:UNK:HA | 2:F:188:UNK:N | 1.61 | 1.15 |
| 1:C:1427:SER:CB | 1:C:1428:PRO:HD3 | 1.77 | 1.15 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1361:LEU:CD2 | 1:A:1365:TYR:CE2 | 2.29 | 1.15 |
| 1:B:1427:SER:CB | 1:B:1428:PRO:HD3 | 1.76 | 1.15 |
| 1:C:1361:LEU:CD2 | 1:C:1365:TYR:CE2 | 2.28 | 1.14 |
| 1:C:1222:SER:C | 1:C:1223:ASN:OD1 | 1.85 | 1.14 |
| 1:A:1429:ARG:CG | 1:A:1429:ARG:O | 1.78 | 1.14 |
| 1:C:1188:GLU:OE2 | 1:C:1191:ASN:HB2 | 1.44 | 1.14 |
| 1:C:1358:TRP:HE3 | 1:C:1377:THR:CG2 | 1.60 | 1.14 |
| 1:B:1327:PHE:HD1 | 2:D:104:LYS:HE2 | 0.99 | 1.14 |
| 1:C:1492:ASN:O | 1:C:1493:ILE:HG12 | 1.45 | 1.14 |
| 1:B:1588:ARG:NH1 | 2:F:192:UNK:HA | 1.62 | 1.14 |
| 1:A:1258:PHE:CB | 1:A:1289:TYR:CZ | 2.30 | 1.13 |
| 1:C:1602:VAL:HG13 | 2:E:203:UNK:O | 1.45 | 1.13 |
| 1:C:1490:PHE:CE1 | 1:C:1492:ASN:OD1 | 2.01 | 1.13 |
| 1:A:1492:ASN:O | 1:A:1493:ILE:HG13 | 1.47 | 1.13 |
| 1:B:1492:ASN:O | 1:B:1493:ILE:HG13 | 1.47 | 1.13 |
| 1:B:1551:GLU:HG2 | 1:B:1582:VAL:HG22 | 1.20 | 1.13 |
| 1:A:1258:PHE:CA | 1:A:1289:TYR:CZ | 2.31 | 1.13 |
| 1:B:1326:LYS:CG | 1:B:1326:LYS:O | 1.93 | 1.13 |
| 2:F:114:GLN:HG3 | 2:F:115:GLU:N | 1.46 | 1.12 |
| 1:B:1490:PHE:CE1 | 1:B:1492:ASN:OD1 | 2.01 | 1.12 |
| 1:C:1198:ILE:HA | 1:C:1201:VAL:HG21 | 1.29 | 1.12 |
| 1:A:1358:TRP:HE3 | 1:A:1377:THR:CG2 | 1.60 | 1.12 |
| 1:C:1411:TYR:HA | 1:C:1415:LYS:HB3 | 1.31 | 1.12 |
| 1:C:1107:VAL:HG12 | 1:C:1111:LEU:CB | 1.79 | 1.12 |
| 1:B:1412:LEU:HD13 | 1:B:1419:LEU:HD21 | 1.12 | 1.12 |
| 1:B:1601:GLN:NE2 | 1:C:1587:TRP:CH2 | 2.15 | 1.12 |
| 1:B:1588:ARG:NH2 | 2:F:192:UNK:HA | 1.64 | 1.12 |
| 1:B:1137:TYR:HB2 | 1:B:1138:MET:CB | 1.78 | 1.12 |
| 1:A:1490:PHE:CE1 | 1:A:1492:ASN:OD1 | 2.01 | 1.12 |
| 1:A:1326:LYS:O | 1:A:1326:LYS:HG2 | 1.33 | 1.12 |
| 1:A:1221:VAL:HG13 | 1:A:1222:SER:N | 1.59 | 1.12 |
| 1:C:1463:VAL:O | 1:C:1467:LEU:CB | 1.98 | 1.11 |
| 1:C:1253:TRP:CE3 | 1:C:1276:ILE:HG21 | 1.81 | 1.11 |
| 1:A:1427:SER:HB2 | 1:A:1428:PRO:HD3 | 1.22 | 1.11 |
| 1:C:1326:LYS:HG2 | 1:C:1326:LYS:O | 1.33 | 1.11 |
| 1:B:1463:VAL:O | 1:B:1467:LEU:CB | 1.98 | 1.11 |
| 2:F:162:GLN:C | 2:F:166:ALA:HB3 | 1.70 | 1.11 |
| 1:C:1427:SER:HB2 | 1:C:1428:PRO:CD | 1.81 | 1.10 |
| 1:A:1427:SER:HB2 | 1:A:1428:PRO:CD | 1.81 | 1.10 |
| 1:A:1578:ARG:CZ | 1:A:1583:LEU:HD23 | 1.81 | 1.10 |
| 1:B:1326:LYS:HG2 | 1:B:1326:LYS:O | 1.33 | 1.10 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:F:195:UNK:CA | 2:F:197:UNK:CB | 2.29 | 1.10 |
| 1:B:1221:VAL:HG13 | 1:B:1222:SER:N | 1.53 | 1.10 |
| 1:A:1358:TRP:CH2 | 1:A:1381:HIS:NE2 | 2.20 | 1.10 |
| 1:B:1427:SER:HB2 | 1:B:1428:PRO:CD | 1.81 | 1.10 |
| 1:B:1455:VAL:HG12 | 1:B:1456:GLN:H | 1.14 | 1.10 |
| 1:A:1264:LYS:HE2 | 1:A:1268:LEU:HD12 | 1.13 | 1.10 |
| 1:B:1358:TRP:CZ3 | 1:B:1381:HIS:NE2 | 2.20 | 1.10 |
| 1:C:1358:TRP:CZ3 | 1:C:1381:HIS:NE2 | 2.20 | 1.10 |
| 1:A:1463:VAL:O | 1:A:1467:LEU:CB | 1.98 | 1.10 |
| 1:B:1475:GLU:OE1 | 2:D:145:GLN:CB | 2.00 | 1.10 |
| 2:D:114:GLN:HG3 | 2:D:115:GLU:N | 1.46 | 1.10 |
| 1:A:1221:VAL:HG13 | 1:A:1222:SER:H | 1.14 | 1.09 |
| 1:C:1361:LEU:HD21 | 1:C:1365:TYR:CE2 | 1.85 | 1.09 |
| 1:C:1427:SER:HB2 | 1:C:1428:PRO:HD3 | 1.22 | 1.09 |
| 1:A:1258:PHE:HB2 | 1:A:1289:TYR:CE2 | 1.58 | 1.09 |
| 1:C:1578:ARG:CZ | 1:C:1583:LEU:HD23 | 1.81 | 1.09 |
| 1:B:1358:TRP:O | 1:B:1362:VAL:HG23 | 1.52 | 1.09 |
| 1:C:1358:TRP:CH2 | 1:C:1381:HIS:NE2 | 2.20 | 1.09 |
| 1:C:1504:LEU:HG | 2:E:149:ASN:OD1 | 1.51 | 1.09 |
| 1:C:1190:ILE:HD13 | 1:C:1216:LEU:HG | 1.34 | 1.09 |
| 1:B:1588:ARG:NH2 | 2:F:192:UNK:CA | 2.15 | 1.09 |
| 1:B:1411:TYR:CA | 1:B:1415:LYS:HB3 | 1.81 | 1.09 |
| 1:A:1279:HIS:CE1 | 1:A:1283:LEU:HD11 | 1.88 | 1.09 |
| 1:C:1230:THR:O | 1:C:1231:LEU:HD23 | 1.53 | 1.09 |
| 1:C:1270:GLN:OE1 | 1:C:1298:GLU:HB3 | 1.51 | 1.09 |
| 2:D:181:UNK:CA | 2:D:183:UNK:CB | 2.30 | 1.09 |
| 1:B:1578:ARG:CZ | 1:B:1583:LEU:HD23 | 1.81 | 1.09 |
| 1:C:1174:ILE:HG13 | 1:C:1196:ALA:HA | 1.29 | 1.09 |
| 1:B:1358:TRP:CH2 | 1:B:1381:HIS:NE2 | 2.20 | 1.09 |
| 1:A:1416:PRO:CD | 2:F:130:LYS:HD3 | 1.83 | 1.09 |
| 1:B:1327:PHE:CD1 | 2:D:104:LYS:HE2 | 1.87 | 1.09 |
| 1:B:1411:TYR:HA | 1:B:1415:LYS:HB3 | 1.31 | 1.09 |
| 1:A:1408:ILE:HG22 | 1:A:1412:LEU:HB3 | 1.21 | 1.08 |
| 1:B:1414:PHE:O | 2:D:130:LYS:HD3 | 1.52 | 1.08 |
| 1:A:1137:TYR:HB2 | 1:A:1138:MET:CB | 1.84 | 1.08 |
| 1:B:1107:VAL:HG12 | 1:B:1107:VAL:O | 1.28 | 1.08 |
| 1:A:1295:TYR:CD2 | 1:A:1299:LEU:HB2 | 1.89 | 1.08 |
| 1:A:1411:TYR:CA | 1:A:1415:LYS:HB3 | 1.82 | 1.08 |
| 1:C:1504:LEU:CD1 | 2:E:149:ASN:HD21 | 1.58 | 1.08 |
| 1:A:1358:TRP:CZ3 | 1:A:1381:HIS:NE2 | 2.20 | 1.08 |
| 1:C:1411:TYR:CA | 1:C:1415:LYS:HB3 | 1.82 | 1.08 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1416:PRO:HG2 | 2:F:130:LYS:HG2 | 1.08 | 1.08 |
| 1:A:1416:PRO:HG2 | 2:F:130:LYS:CG | 1.82 | 1.08 |
| 2:D:119:ALA:O | 2:D:123:MET:CG | 2.02 | 1.08 |
| 1:B:1279:HIS:CD2 | 1:B:1282:GLU:HB3 | 1.88 | 1.07 |
| 1:B:1361:LEU:HD21 | 1:B:1365:TYR:CE2 | 1.86 | 1.07 |
| 1:C:1412:LEU:HD13 | 1:C:1419:LEU:HD21 | 1.12 | 1.07 |
| 2:E:119:ALA:O | 2:E:123:MET:CG | 2.01 | 1.07 |
| 2:E:104:LYS:O | 2:E:108:GLU:HG3 | 1.51 | 1.07 |
| 1:B:1144:ALA:HB1 | 1:B:1149:ASN:HB3 | 1.36 | 1.07 |
| 1:C:1234:LEU:HD23 | 1:C:1264:LYS:NZ | 1.68 | 1.07 |
| 1:C:1264:LYS:HE2 | 1:C:1268:LEU:HD12 | 1.13 | 1.07 |
| 1:A:1358:TRP:O | 1:A:1362:VAL:HG23 | 1.52 | 1.07 |
| 1:B:1416:PRO:HD3 | 2:D:130:LYS:HD3 | 1.34 | 1.07 |
| 1:B:1122:LYS:HA | 1:B:1125:ILE:HG22 | 1.36 | 1.07 |
| 1:C:1270:GLN:OE1 | 1:C:1298:GLU:CB | 2.02 | 1.07 |
| 1:A:1605:GLU:HA | 1:A:1608:THR:HB | 1.29 | 1.07 |
| 1:C:1177:LEU:HD13 | 1:C:1189:PHE:HZ | 1.07 | 1.07 |
| 1:A:1253:TRP:CE3 | 1:A:1276:ILE:HG21 | 1.82 | 1.07 |
| 1:A:1412:LEU:HD13 | 1:A:1419:LEU:HD21 | 1.12 | 1.07 |
| 1:A:1361:LEU:HD21 | 1:A:1365:TYR:CE2 | 1.86 | 1.07 |
| 2:F:162:GLN:CA | 2:F:166:ALA:CB | 2.33 | 1.07 |
| 1:B:1490:PHE:CZ | 1:B:1492:ASN:OD1 | 2.08 | 1.07 |
| 2:D:137:GLU:O | 2:D:141:ARG:NH2 | 1.88 | 1.07 |
| 1:B:1253:TRP:CE3 | 1:B:1276:ILE:HG21 | 1.82 | 1.06 |
| 1:C:1198:ILE:O | 1:C:1201:VAL:HB | 1.54 | 1.06 |
| 1:C:1221:VAL:HG13 | 1:C:1222:SER:H | 1.13 | 1.06 |
| 2:D:174:UNK:CB | 2:D:177:UNK:CB | 2.33 | 1.06 |
| 1:A:1490:PHE:CZ | 1:A:1492:ASN:OD1 | 2.09 | 1.06 |
| 1:C:1290:TYR:CD2 | 1:C:1299:LEU:HD22 | 1.90 | 1.06 |
| 2:F:195:UNK:HA | 2:F:197:UNK:CB | 1.84 | 1.06 |
| 1:C:1358:TRP:O | 1:C:1362:VAL:HG23 | 1.53 | 1.06 |
| 1:C:1455:VAL:HG12 | 1:C:1456:GLN:H | 1.14 | 1.06 |
| 1:A:1455:VAL:HG12 | 1:A:1456:GLN:H | 1.14 | 1.06 |
| 1:C:1167:SER:O | 1:C:1171:THR:CB | 2.02 | 1.06 |
| 1:B:1416:PRO:HG2 | 2:D:130:LYS:HG2 | 1.30 | 1.06 |
| 1:B:1264:LYS:HE2 | 1:B:1268:LEU:HD12 | 1.12 | 1.06 |
| 1:C:1082:VAL:HG22 | 1:C:1107:VAL:HG21 | 1.38 | 1.06 |
| 2:F:163:GLN:N | 2:F:166:ALA:HB3 | 1.70 | 1.06 |
| 1:A:1283:LEU:HD22 | 1:A:1313:HIS:NE2 | 1.70 | 1.05 |
| 1:C:1605:GLU:HA | 1:C:1608:THR:HB | 1.29 | 1.05 |
| 1:C:1167:SER:C | 1:C:1171:THR:HB | 1.75 | 1.05 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:1588:ARG:NH2 | 2:D:193:UNK:CA | 2.19 | 1.05 |
| 1:B:1264:LYS:HE2 | 1:B:1268:LEU:CD1 | 1.77 | 1.05 |
| 1:B:1588:ARG:HH22 | 2:F:192:UNK:CA | 1.67 | 1.05 |
| 1:B:1417:LEU:O | 1:B:1418:LEU:HB2 | 1.53 | 1.05 |
| 1:B:1509:ARG:HH22 | 2:D:163:GLN:CA | 1.68 | 1.05 |
| 1:C:1414:PHE:HE1 | 2:E:127:TRP:CZ3 | 1.74 | 1.05 |
| 2:E:155:ILE:H | 2:E:155:ILE:HD12 | 1.19 | 1.05 |
| 1:C:1382:PRO:HD2 | 2:E:115:GLU:OE2 | 1.56 | 1.04 |
| 1:A:1411:TYR:HA | 1:A:1415:LYS:HB3 | 1.35 | 1.04 |
| 1:C:1387:LYS:HB2 | 1:C:1390:GLN:CB | 1.88 | 1.04 |
| 1:C:1264:LYS:HE3 | 1:C:1268:LEU:CD1 | 1.80 | 1.04 |
| 1:B:1416:PRO:HG2 | 2:D:130:LYS:CG | 1.86 | 1.04 |
| 1:B:1387:LYS:HB2 | 1:B:1390:GLN:CB | 1.87 | 1.04 |
| 1:A:1111:LEU:HD11 | 1:A:1125:ILE:CG1 | 1.87 | 1.04 |
| 2:D:181:UNK:HA | 2:D:183:UNK:CB | 1.85 | 1.04 |
| 1:C:1115:GLN:HB3 | 1:C:1125:ILE:HG12 | 1.35 | 1.04 |
| 1:A:1250:THR:O | 1:A:1251:ARG:CG | 2.06 | 1.04 |
| 1:A:1588:ARG:NH2 | 2:E:192:UNK:HA | 1.72 | 1.04 |
| 2:E:189:UNK:O | 2:E:195:UNK:CB | 2.06 | 1.04 |
| 1:C:1122:LYS:HA | 1:C:1125:ILE:HG22 | 1.40 | 1.04 |
| 1:A:1361:LEU:CD2 | 1:A:1365:TYR:HE2 | 1.70 | 1.04 |
| 1:B:1290:TYR:CD2 | 1:B:1299:LEU:CD1 | 2.39 | 1.04 |
| 1:A:1411:TYR:O | 1:A:1415:LYS:HB3 | 1.56 | 1.04 |
| 1:C:1490:PHE:CZ | 1:C:1492:ASN:OD1 | 2.09 | 1.04 |
| 1:C:1456:GLN:CG | 1:C:1456:GLN:O | 1.97 | 1.03 |
| 1:A:1408:ILE:HG22 | 1:A:1412:LEU:CB | 1.87 | 1.03 |
| 1:B:1408:ILE:HG22 | 1:B:1412:LEU:CB | 1.87 | 1.03 |
| 1:A:1107:VAL:HG12 | 1:A:1107:VAL:O | 1.28 | 1.03 |
| 1:A:1387:LYS:HB2 | 1:A:1390:GLN:CB | 1.88 | 1.03 |
| 1:A:1563:ARG:HH22 | 2:F:181:UNK:HA | 1.19 | 1.03 |
| 2:D:174:UNK:H | 2:D:175:UNK:CB | 1.70 | 1.03 |
| 1:B:1279:HIS:NE2 | 1:B:1283:LEU:HD12 | 1.73 | 1.03 |
| 1:C:1429:ARG:O | 1:C:1429:ARG:HG2 | 1.22 | 1.03 |
| 1:B:1416:PRO:CD | 2:D:130:LYS:HD3 | 1.88 | 1.03 |
| 1:B:1279:HIS:NE2 | 1:B:1283:LEU:CD1 | 2.21 | 1.03 |
| 1:C:1408:ILE:HG22 | 1:C:1412:LEU:CB | 1.87 | 1.03 |
| 1:A:1300:ILE:HG22 | 1:A:1323:LEU:HD13 | 1.39 | 1.02 |
| 1:C:1199:GLN:O | 1:C:1201:VAL:N | 1.92 | 1.02 |
| 1:B:1250:THR:O | 1:B:1251:ARG:CG | 2.07 | 1.02 |
| 1:C:1417:LEU:O | 1:C:1418:LEU:HB2 | 1.53 | 1.02 |
| 2:D:98:GLU:HB3 | 2:D:99:PRO:HD3 | 1.40 | 1.02 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:1521:TRP:CE3 | 1:B:1522:LYS:HD2 | 1.95 | 1.02 |
| 1:C:1234:LEU:HD23 | 1:C:1264:LYS:HZ2 | 1.25 | 1.02 |
| 1:A:1417:LEU:O | 1:A:1418:LEU:HB2 | 1.53 | 1.02 |
| 1:B:1300:ILE:HG22 | 1:B:1323:LEU:HD13 | 1.40 | 1.02 |
| 1:B:1411:TYR:O | 1:B:1415:LYS:HB3 | 1.60 | 1.02 |
| 1:C:1596:MET:H | 1:C:1597:PRO:HD2 | 1.23 | 1.02 |
| 1:C:1198:ILE:HA | 1:C:1201:VAL:CG2 | 1.88 | 1.02 |
| 1:A:1429:ARG:O | 1:A:1429:ARG:HG2 | 1.22 | 1.02 |
| 1:A:1122:LYS:HA | 1:A:1125:ILE:HG22 | 1.40 | 1.02 |
| 1:C:1211:TYR:CG | 1:C:1231:LEU:HD22 | 1.94 | 1.01 |
| 1:B:1509:ARG:NH2 | 2:D:163:GLN:HA | 1.72 | 1.01 |
| 1:B:1261:VAL:HG13 | 1:B:1295:TYR:CZ | 1.95 | 1.01 |
| 1:C:1521:TRP:CE3 | 1:C:1522:LYS:HD2 | 1.95 | 1.01 |
| 1:C:1300:ILE:HG22 | 1:C:1323:LEU:HD13 | 1.39 | 1.01 |
| 1:C:1250:THR:O | 1:C:1251:ARG:CG | 2.06 | 1.01 |
| 1:A:1408:ILE:O | 1:A:1412:LEU:N | 1.94 | 1.01 |
| 1:A:1107:VAL:CG1 | 1:A:1107:VAL:O | 2.04 | 1.01 |
| 1:A:1596:MET:H | 1:A:1597:PRO:HD2 | 1.26 | 1.01 |
| 1:A:1456:GLN:O | 1:A:1456:GLN:HG2 | 1.60 | 1.01 |
| 1:B:1429:ARG:HG2 | 1:B:1429:ARG:O | 1.22 | 1.01 |
| 1:C:1358:TRP:CE3 | 1:C:1377:THR:HG23 | 1.96 | 1.01 |
| 1:A:1358:TRP:CE3 | 1:A:1377:THR:HG23 | 1.96 | 1.01 |
| 1:A:1521:TRP:CE3 | 1:A:1522:LYS:HD2 | 1.95 | 1.01 |
| 1:B:1361:LEU:O | 1:B:1361:LEU:HD23 | 1.61 | 1.00 |
| 1:B:1358:TRP:CE3 | 1:B:1377:THR:HG23 | 1.96 | 1.00 |
| 1:C:1361:LEU:HD23 | 1:C:1361:LEU:O | 1.61 | 1.00 |
| 1:C:1620:ARG:HB2 | 1:C:1620:ARG:HH11 | 1.25 | 1.00 |
| 1:A:1620:ARG:CB | 1:A:1620:ARG:HH11 | 1.74 | 1.00 |
| 1:C:1414:PHE:CE1 | 2:E:123:MET:HB3 | 1.97 | 1.00 |
| 2:F:119:ALA:O | 2:F:123:MET:CG | 2.08 | 1.00 |
| 1:A:1167:SER:C | 1:A:1168:TYR:CD1 | 2.34 | 1.00 |
| 1:B:1107:VAL:CG1 | 1:B:1107:VAL:O | 2.04 | 1.00 |
| 1:A:1253:TRP:HE3 | 1:A:1276:ILE:HG21 | 1.26 | 1.00 |
| 1:A:1280:ALA:HB2 | 1:A:1311:ARG:NE | 1.75 | 1.00 |
| 1:C:1411:TYR:O | 1:C:1415:LYS:HB3 | 1.60 | 1.00 |
| 1:C:1361:LEU:CD2 | 1:C:1365:TYR:HE2 | 1.70 | 1.00 |
| 1:B:1129:ILE:O | 1:B:1131:ALA:N | 1.95 | 1.00 |
| 1:B:1244:ALA:CB | 1:B:1275:HIS:CE1 | 2.41 | 1.00 |
| 2:F:162:GLN:HA | 2:F:166:ALA:HB2 | 1.03 | 1.00 |
| 1:B:1620:ARG:HH11 | 1:B:1620:ARG:CB | 1.74 | 1.00 |
| 1:A:1361:LEU:HD23 | 1:A:1361:LEU:O | 1.61 | 0.99 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1411:TYR:C | 1:A:1415:LYS:HB3 | 1.81 | 0.99 |
| 1:C:1296:PHE:O | 1:C:1299:LEU:N | 1.95 | 0.99 |
| 1:C:1326:LYS:O | 1:C:1327:PHE:CD1 | 2.15 | 0.99 |
| 1:A:1579:PRO:HB3 | 1:C:1605:GLU:OE2 | 1.62 | 0.99 |
| 1:B:1296:PHE:O | 1:B:1299:LEU:N | 1.95 | 0.99 |
| 1:B:1150:TRP:CE3 | 2:D:5:UNK:HA | 1.95 | 0.99 |
| 1:A:1129:ILE:O | 1:A:1131:ALA:N | 1.94 | 0.99 |
| 1:B:1620:ARG:HH11 | 1:B:1620:ARG:HB2 | 1.25 | 0.99 |
| 1:C:1408:ILE:O | 1:C:1412:LEU:N | 1.95 | 0.99 |
| 1:A:1358:TRP:HE3 | 1:A:1377:THR:HG23 | 1.28 | 0.99 |
| 1:C:1264:LYS:HE2 | 1:C:1268:LEU:CD1 | 1.77 | 0.99 |
| 1:A:1620:ARG:HB2 | 1:A:1620:ARG:HH11 | 1.24 | 0.99 |
| 1:A:1326:LYS:O | 1:A:1327:PHE:CD1 | 2.15 | 0.99 |
| 1:A:1358:TRP:CZ3 | 1:A:1381:HIS:CD2 | 2.51 | 0.99 |
| 1:C:1620:ARG:CB | 1:C:1620:ARG:HH11 | 1.75 | 0.99 |
| 1:C:1358:TRP:CZ3 | 1:C:1381:HIS:CD2 | 2.51 | 0.99 |
| 1:C:1198:ILE:HB | 1:C:1221:VAL:HG22 | 1.42 | 0.99 |
| 1:A:1296:PHE:O | 1:A:1299:LEU:N | 1.95 | 0.98 |
| 1:B:1563:ARG:NH2 | 2:D:183:UNK:O | 1.96 | 0.98 |
| 1:C:1358:TRP:CE3 | 1:C:1377:THR:CG2 | 2.46 | 0.98 |
| 1:B:1326:LYS:O | 1:B:1327:PHE:CD1 | 2.15 | 0.98 |
| 1:B:1586:ALA:O | 1:B:1590:ASN:OD1 | 1.80 | 0.98 |
| 1:B:1596:MET:H | 1:B:1597:PRO:HD2 | 1.27 | 0.98 |
| 1:B:1358:TRP:CE3 | 1:B:1377:THR:CG2 | 2.46 | 0.98 |
| 1:C:1602:VAL:CG1 | 2:E:203:UNK:C | 2.41 | 0.98 |
| 1:C:1198:ILE:O | 1:C:1199:GLN:O | 1.81 | 0.98 |
| 1:C:1358:TRP:HE3 | 1:C:1377:THR:HG23 | 1.28 | 0.98 |
| 1:B:1456:GLN:CG | 1:B:1456:GLN:O | 1.97 | 0.98 |
| 1:B:1411:TYR:HA | 1:B:1415:LYS:CB | 1.93 | 0.98 |
| 1:A:1264:LYS:HE2 | 1:A:1268:LEU:CD1 | 1.77 | 0.98 |
| 1:A:1358:TRP:CE3 | 1:A:1377:THR:CG2 | 2.46 | 0.98 |
| 1:B:1408:ILE:O | 1:B:1412:LEU:N | 1.95 | 0.98 |
| 1:B:1456:GLN:O | 1:B:1456:GLN:HG2 | 1.60 | 0.98 |
| 1:C:1411:TYR:HA | 1:C:1415:LYS:CB | 1.93 | 0.98 |
| 1:A:1280:ALA:HB2 | 1:A:1311:ARG:HE | 1.27 | 0.98 |
| 1:A:1371:TYR:CD1 | 1:A:1394:ILE:CG2 | 2.36 | 0.98 |
| 1:A:1588:ARG:HD3 | 2:E:195:UNK:CB | 1.94 | 0.97 |
| 1:A:1371:TYR:HD1 | 1:A:1394:ILE:HG23 | 0.81 | 0.97 |
| 1:C:1177:LEU:HD13 | 1:C:1189:PHE:CZ | 1.98 | 0.97 |
| 1:B:1358:TRP:CZ3 | 1:B:1381:HIS:CD2 | 2.51 | 0.97 |
| 1:A:1223:ASN:N | 1:A:1223:ASN:HA | 1.77 | 0.97 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:1597:PRO:HG3 | 1:B:1600:ILE:HD12 | 1.43 | 0.97 |
| 2:D:181:UNK:C | 2:D:183:UNK:CB | 2.41 | 0.97 |
| 1:A:1456:GLN:CG | 1:A:1456:GLN:O | 1.97 | 0.97 |
| 1:B:1232:VAL:HG22 | 1:B:1233:HIS:H | 1.27 | 0.97 |
| 1:B:1358:TRP:CZ2 | 1:B:1381:HIS:ND1 | 2.33 | 0.97 |
| 1:C:1456:GLN:O | 1:C:1456:GLN:HG2 | 1.60 | 0.97 |
| 1:A:1372:ASP:O | 1:A:1376:ILE:HG13 | 1.65 | 0.97 |
| 2:E:108:GLU:OE2 | 2:E:109:GLN:HG2 | 1.62 | 0.97 |
| 1:C:1371:TYR:HD1 | 1:C:1394:ILE:HG23 | 0.81 | 0.97 |
| 2:F:162:GLN:CA | 2:F:166:ALA:HB2 | 1.92 | 0.97 |
| 1:C:1382:PRO:HD2 | 2:E:115:GLU:CD | 1.84 | 0.97 |
| 1:B:1395:ILE:HG12 | 1:B:1404:TYR:CE2 | 1.99 | 0.97 |
| 1:C:1411:TYR:C | 1:C:1415:LYS:HB3 | 1.84 | 0.97 |
| 1:B:1264:LYS:HE3 | 1:B:1268:LEU:CD1 | 1.80 | 0.96 |
| 2:F:151:ILE:O | 2:F:154:ARG:HB2 | 1.65 | 0.96 |
| 1:C:1244:ALA:N | 1:C:1275:HIS:CE1 | 2.31 | 0.96 |
| 2:F:195:UNK:C | 2:F:197:UNK:CB | 2.42 | 0.96 |
| 1:A:1254:LYS:O | 1:A:1289:TYR:HD2 | 1.45 | 0.96 |
| 1:A:1395:ILE:HG12 | 1:A:1404:TYR:CE2 | 1.99 | 0.96 |
| 1:B:1301:THR:HA | 1:B:1304:GLU:HG3 | 1.47 | 0.96 |
| 1:B:1587:TRP:C | 1:B:1589:HIS:H | 1.66 | 0.96 |
| 1:C:1588:ARG:NH2 | 2:D:193:UNK:N | 2.13 | 0.96 |
| 2:D:174:UNK:HA | 2:D:177:UNK:N | 1.80 | 0.96 |
| 2:D:151:ILE:O | 2:D:154:ARG:HB2 | 1.65 | 0.96 |
| 1:C:1301:THR:HA | 1:C:1304:GLU:HG3 | 1.47 | 0.96 |
| 1:A:1597:PRO:HG3 | 1:A:1600:ILE:HD12 | 1.43 | 0.96 |
| 2:E:202:UNK:O | 2:E:203:UNK:C | 2.14 | 0.96 |
| 1:A:1409:GLN:CA | 1:A:1413:GLU:CG | 2.35 | 0.96 |
| 1:A:1111:LEU:HD11 | 1:A:1125:ILE:HG12 | 1.47 | 0.96 |
| 1:A:1282:GLU:HG3 | 1:A:1283:LEU:H | 1.30 | 0.96 |
| 1:A:1358:TRP:CZ2 | 1:A:1381:HIS:ND1 | 2.33 | 0.96 |
| 1:B:1371:TYR:HD1 | 1:B:1394:ILE:HG23 | 0.81 | 0.96 |
| 1:B:1290:TYR:HB3 | 1:B:1299:LEU:HD22 | 1.47 | 0.96 |
| 1:B:1411:TYR:C | 1:B:1415:LYS:HB3 | 1.84 | 0.96 |
| 1:B:1221:VAL:HG13 | 1:B:1222:SER:H | 1.29 | 0.96 |
| 2:E:151:ILE:O | 2:E:154:ARG:HB2 | 1.65 | 0.96 |
| 1:B:1372:ASP:O | 1:B:1376:ILE:HG13 | 1.65 | 0.96 |
| 1:A:1232:VAL:HG22 | 1:A:1233:HIS:H | 1.26 | 0.96 |
| 1:A:1111:LEU:HD22 | 1:A:1111:LEU:O | 1.65 | 0.96 |
| 1:C:1597:PRO:HG3 | 1:C:1600:ILE:HD12 | 1.44 | 0.95 |
| 1:C:1368:TYR:CD1 | 1:C:1370:GLU:HG2 | 2.01 | 0.95 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1264:LYS:HE3 | 1:A:1268:LEU:CD1 | 1.80 | 0.95 |
| 1:A:1174:ILE:HG21 | 1:A:1201:VAL:HG22 | 1.47 | 0.95 |
| 1:B:1267:ARG:NH2 | 1:B:1298:GLU:OE2 | 1.99 | 0.95 |
| 1:B:1111:LEU:HD22 | 1:B:1111:LEU:O | 1.66 | 0.95 |
| 1:B:1174:ILE:HG21 | 1:B:1201:VAL:HG22 | 1.48 | 0.95 |
| 1:B:1282:GLU:HG3 | 1:B:1283:LEU:H | 1.30 | 0.95 |
| 1:C:1358:TRP:CZ2 | 1:C:1381:HIS:ND1 | 2.33 | 0.95 |
| 1:B:1167:SER:C | 1:B:1168:TYR:CD1 | 2.40 | 0.95 |
| 1:C:1234:LEU:CD2 | 1:C:1264:LYS:NZ | 2.29 | 0.95 |
| 1:B:1414:PHE:O | 2:D:130:LYS:CD | 2.14 | 0.95 |
| 1:A:1279:HIS:CD2 | 1:A:1282:GLU:H | 1.84 | 0.95 |
| 1:C:1111:LEU:HD22 | 1:C:1111:LEU:O | 1.65 | 0.95 |
| 1:B:1358:TRP:HE3 | 1:B:1377:THR:HG23 | 1.28 | 0.95 |
| 1:A:1258:PHE:N | 1:A:1289:TYR:OH | 1.76 | 0.95 |
| 1:A:1282:GLU:O | 1:A:1283:LEU:HB2 | 1.67 | 0.95 |
| 1:C:1395:ILE:HG12 | 1:C:1404:TYR:CE2 | 1.99 | 0.95 |
| 1:A:1368:TYR:CD1 | 1:A:1370:GLU:HG2 | 2.02 | 0.95 |
| 1:C:1254:LYS:HD2 | 1:C:1285:GLU:CG | 1.96 | 0.94 |
| 2:E:133:LYS:HA | 2:E:133:LYS:NZ | 1.82 | 0.94 |
| 2:F:133:LYS:HA | 2:F:133:LYS:NZ | 1.82 | 0.94 |
| 1:B:1368:TYR:CD1 | 1:B:1370:GLU:HG2 | 2.02 | 0.94 |
| 1:B:1472:ILE:HA | 1:B:1507:PHE:HE1 | 1.32 | 0.94 |
| 2:E:198:UNK:O | 2:E:202:UNK:CB | 2.15 | 0.94 |
| 1:A:1411:TYR:HA | 1:A:1415:LYS:CB | 1.97 | 0.94 |
| 1:B:1361:LEU:CD2 | 1:B:1365:TYR:HE2 | 1.70 | 0.94 |
| 1:B:1412:LEU:HB2 | 1:B:1419:LEU:CD1 | 1.97 | 0.94 |
| 2:D:133:LYS:HA | 2:D:133:LYS:NZ | 1.82 | 0.94 |
| 2:E:104:LYS:O | 2:E:108:GLU:HG2 | 1.66 | 0.94 |
| 1:A:1116:LEU:CD1 | 1:A:1122:LYS:HD3 | 1.98 | 0.94 |
| 1:C:1588:ARG:NH2 | 2:D:193:UNK:C | 2.30 | 0.94 |
| 1:A:1412:LEU:HB2 | 1:A:1419:LEU:CD1 | 1.97 | 0.94 |
| 1:A:1472:ILE:HA | 1:A:1507:PHE:HE1 | 1.32 | 0.94 |
| 1:C:1253:TRP:HE3 | 1:C:1276:ILE:HG21 | 1.25 | 0.94 |
| 1:B:1551:GLU:HG2 | 1:B:1582:VAL:CG2 | 1.96 | 0.94 |
| 2:D:185:UNK:HA | 2:D:189:UNK:O | 1.68 | 0.94 |
| 2:D:174:UNK:CA | 2:D:177:UNK:N | 2.31 | 0.94 |
| 2:E:189:UNK:HA | 2:E:195:UNK:N | 1.83 | 0.94 |
| 1:C:1434:ARG:HE | 2:E:5:UNK:HA | 0.79 | 0.93 |
| 1:A:1290:TYR:CD2 | 1:A:1299:LEU:HD13 | 2.04 | 0.93 |
| 1:B:1253:TRP:HE3 | 1:B:1276:ILE:HG21 | 1.26 | 0.93 |
| 1:C:1107:VAL:HG12 | 1:C:1111:LEU:HB2 | 0.94 | 0.93 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1409:GLN:CG | 1:A:1413:GLU:CG | 2.34 | 0.93 |
| 1:C:1186:LEU:HD22 | 1:C:1213:ALA:CB | 1.99 | 0.93 |
| 1:A:1301:THR:HA | 1:A:1304:GLU:HG3 | 1.48 | 0.93 |
| 1:A:1244:ALA:CB | 1:A:1275:HIS:CE1 | 2.42 | 0.93 |
| 1:A:1258:PHE:CA | 1:A:1289:TYR:CE1 | 2.50 | 0.93 |
| 1:C:1412:LEU:HB2 | 1:C:1419:LEU:CD1 | 1.97 | 0.93 |
| 1:B:1408:ILE:CG2 | 1:B:1412:LEU:CB | 2.46 | 0.93 |
| 1:B:1280:ALA:O | 1:B:1313:HIS:CE1 | 2.22 | 0.93 |
| 2:D:181:UNK:C | 2:D:183:UNK:N | 2.20 | 0.93 |
| 1:B:1362:VAL:HG22 | 1:B:1377:THR:CB | 1.99 | 0.93 |
| 1:A:1257:CYS:N | 1:A:1289:TYR:OH | 2.02 | 0.93 |
| 1:B:1412:LEU:CD1 | 1:B:1419:LEU:CD2 | 2.47 | 0.93 |
| 1:B:1405:TYR:CD2 | 1:B:1434:ARG:NH1 | 2.37 | 0.93 |
| 1:A:1254:LYS:C | 1:A:1289:TYR:CE2 | 2.41 | 0.93 |
| 1:C:1412:LEU:CD1 | 1:C:1419:LEU:CD2 | 2.47 | 0.93 |
| 1:A:1408:ILE:CG2 | 1:A:1412:LEU:CB | 2.46 | 0.93 |
| 1:A:1258:PHE:H | 1:A:1289:TYR:HH | 1.03 | 0.93 |
| 1:C:1450:PRO:HA | 1:C:1453:ARG:HG2 | 1.51 | 0.93 |
| 2:F:162:GLN:CA | 2:F:166:ALA:HB3 | 1.95 | 0.93 |
| 1:B:1408:ILE:CG2 | 1:B:1412:LEU:CD2 | 2.47 | 0.93 |
| 1:B:1409:GLN:CA | 1:B:1413:GLU:CG | 2.35 | 0.93 |
| 1:B:1587:TRP:C | 1:B:1589:HIS:N | 2.17 | 0.92 |
| 1:C:1221:VAL:CG1 | 1:C:1222:SER:N | 2.31 | 0.92 |
| 1:A:1412:LEU:CD1 | 1:A:1419:LEU:CD2 | 2.47 | 0.92 |
| 2:F:195:UNK:C | 2:F:197:UNK:N | 2.19 | 0.92 |
| 1:C:1405:TYR:CD2 | 1:C:1434:ARG:NH1 | 2.37 | 0.92 |
| 1:A:1362:VAL:HG22 | 1:A:1377:THR:CB | 1.99 | 0.92 |
| 1:C:1620:ARG:CG | 1:C:1620:ARG:HH11 | 1.83 | 0.92 |
| 1:A:1264:LYS:HE3 | 1:A:1268:LEU:HD12 | 0.92 | 0.92 |
| 1:A:1408:ILE:CG2 | 1:A:1412:LEU:CD2 | 2.47 | 0.92 |
| 2:D:112:ARG:O | 2:D:113:LEU:O | 1.86 | 0.92 |
| 1:B:1222:SER:OG | 1:B:1223:ASN:N | 1.96 | 0.92 |
| 1:B:1264:LYS:HE3 | 1:B:1268:LEU:HD12 | 0.92 | 0.92 |
| 1:B:1279:HIS:HD2 | 1:B:1280:ALA:H | 1.16 | 0.92 |
| 1:A:1405:TYR:CD2 | 1:A:1434:ARG:NH1 | 2.37 | 0.92 |
| 1:C:1362:VAL:HG22 | 1:C:1377:THR:CB | 1.99 | 0.92 |
| 1:C:1408:ILE:CG2 | 1:C:1412:LEU:CD2 | 2.47 | 0.92 |
| 1:C:1408:ILE:CG2 | 1:C:1412:LEU:CB | 2.46 | 0.92 |
| 1:C:1409:GLN:CA | 1:C:1413:GLU:CG | 2.35 | 0.92 |
| 1:C:1472:ILE:HA | 1:C:1507:PHE:HE1 | 1.32 | 0.92 |
| 1:A:1258:PHE:HB3 | 1:A:1289:TYR:HE2 | 1.27 | 0.92 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:D:174:UNK:N | 2:D:175:UNK:CB | 2.32 | 0.92 |
| 1:B:1282:GLU:O | 1:B:1283:LEU:HB2 | 1.67 | 0.91 |
| 1:C:1190:ILE:CD1 | 1:C:1216:LEU:HG | 2.00 | 0.91 |
| 1:C:1256:VAL:O | 1:C:1260:CYS:SG | 2.28 | 0.91 |
| 1:B:1333:ARG:HB2 | 1:B:1360:GLU:OE2 | 1.70 | 0.91 |
| 1:B:1416:PRO:CG | 2:D:130:LYS:HG2 | 1.99 | 0.91 |
| 1:A:1116:LEU:HD11 | 1:A:1122:LYS:HD3 | 1.50 | 0.91 |
| 1:A:1333:ARG:HB2 | 1:A:1360:GLU:OE2 | 1.70 | 0.91 |
| 1:B:1279:HIS:CD2 | 1:B:1280:ALA:N | 2.38 | 0.91 |
| 1:B:1409:GLN:CG | 1:B:1413:GLU:CG | 2.34 | 0.91 |
| 1:B:1371:TYR:CD1 | 1:B:1394:ILE:CG2 | 2.35 | 0.91 |
| 2:E:98:GLU:HA | 2:E:101:SER:HB3 | 1.52 | 0.91 |
| 1:A:1136:SER:N | 1:A:1141:VAL:HG21 | 1.85 | 0.91 |
| 1:C:1115:GLN:CB | 1:C:1125:ILE:HG12 | 2.01 | 0.91 |
| 1:A:1303:LEU:HD12 | 1:A:1320:LEU:HD13 | 1.52 | 0.91 |
| 1:A:1416:PRO:CG | 2:F:130:LYS:HG2 | 1.99 | 0.91 |
| 1:A:1256:VAL:O | 1:A:1260:CYS:SG | 2.29 | 0.91 |
| 1:C:1224:PHE:CZ | 1:C:1246:LYS:NZ | 2.39 | 0.91 |
| 1:C:1253:TRP:HZ3 | 1:C:1276:ILE:HG22 | 1.34 | 0.91 |
| 1:B:1290:TYR:HD2 | 1:B:1299:LEU:CD1 | 1.80 | 0.91 |
| 1:C:1586:ALA:HB1 | 1:C:1590:ASN:HD21 | 1.34 | 0.91 |
| 1:A:1395:ILE:HG13 | 1:A:1404:TYR:CZ | 2.06 | 0.91 |
| 2:D:174:UNK:HA | 2:D:175:UNK:C | 2.00 | 0.91 |
| 1:B:1395:ILE:HG13 | 1:B:1404:TYR:CZ | 2.05 | 0.91 |
| 2:D:174:UNK:CB | 2:D:177:UNK:N | 2.33 | 0.91 |
| 1:A:1450:PRO:HA | 1:A:1453:ARG:HG2 | 1.51 | 0.90 |
| 1:A:1261:VAL:HG11 | 1:A:1295:TYR:CD1 | 2.05 | 0.90 |
| 1:B:1256:VAL:O | 1:B:1260:CYS:SG | 2.28 | 0.90 |
| 1:A:1620:ARG:CG | 1:A:1620:ARG:HH11 | 1.83 | 0.90 |
| 1:B:1620:ARG:NH1 | 1:B:1620:ARG:HB2 | 1.86 | 0.90 |
| 1:A:1408:ILE:CG2 | 1:A:1412:LEU:HB3 | 2.01 | 0.90 |
| 1:B:1620:ARG:CG | 1:B:1620:ARG:HH11 | 1.83 | 0.90 |
| 1:B:1412:LEU:HB2 | 1:B:1419:LEU:HD11 | 1.54 | 0.90 |
| 1:C:1620:ARG:HB2 | 1:C:1620:ARG:NH1 | 1.87 | 0.90 |
| 1:C:1264:LYS:HE3 | 1:C:1268:LEU:HD12 | 0.92 | 0.90 |
| 1:C:1333:ARG:HB2 | 1:C:1360:GLU:OE2 | 1.70 | 0.90 |
| 1:C:1154:VAL:HG21 | 1:C:1180:THR:HG23 | 1.52 | 0.90 |
| 1:C:1395:ILE:HG13 | 1:C:1404:TYR:CZ | 2.06 | 0.90 |
| 1:C:1290:TYR:HE2 | 1:C:1299:LEU:HD13 | 1.05 | 0.90 |
| 1:C:1412:LEU:HA | 1:C:1419:LEU:HD22 | 1.54 | 0.90 |
| 1:B:1391:PHE:CG | 1:B:1411:TYR:OH | 2.24 | 0.90 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:1391:PHE:CG | 1:C:1411:TYR:OH | 2.24 | 0.90 |
| 1:C:1408:ILE:CG2 | 1:C:1412:LEU:HB3 | 2.00 | 0.90 |
| 1:B:1601:GLN:HG2 | 1:C:1587:TRP:HH2 | 1.37 | 0.90 |
| 1:B:1450:PRO:HA | 1:B:1453:ARG:HG2 | 1.51 | 0.90 |
| 1:A:1391:PHE:CG | 1:A:1411:TYR:OH | 2.24 | 0.90 |
| 1:C:1290:TYR:CD2 | 1:C:1299:LEU:HD13 | 2.07 | 0.89 |
| 1:B:1596:MET:SD | 1:B:1597:PRO:HD3 | 2.12 | 0.89 |
| 1:A:1412:LEU:HB2 | 1:A:1419:LEU:HD11 | 1.54 | 0.89 |
| 1:A:1171:THR:HA | 1:A:1174:ILE:HD12 | 1.54 | 0.89 |
| 1:C:1270:GLN:CD | 1:C:1298:GLU:CG | 2.40 | 0.89 |
| 1:A:1224:PHE:O | 1:A:1227:LEU:HB3 | 1.72 | 0.89 |
| 2:D:112:ARG:C | 2:D:112:ARG:CD | 2.38 | 0.89 |
| 1:B:1303:LEU:HD12 | 1:B:1320:LEU:HD13 | 1.52 | 0.89 |
| 1:C:1154:VAL:HG21 | 1:C:1180:THR:CG2 | 2.02 | 0.89 |
| 1:C:1409:GLN:CB | 1:C:1413:GLU:HG3 | 2.02 | 0.89 |
| 1:B:1224:PHE:O | 1:B:1227:LEU:HB3 | 1.72 | 0.89 |
| 1:A:1620:ARG:NH1 | 1:A:1620:ARG:HB2 | 1.86 | 0.89 |
| 1:C:1224:PHE:O | 1:C:1227:LEU:HB3 | 1.73 | 0.89 |
| 2:E:202:UNK:C | 2:E:203:UNK:C | 2.50 | 0.89 |
| 1:C:1218:TYR:HA | 1:C:1221:VAL:HG12 | 1.55 | 0.89 |
| 1:B:1150:TRP:CZ3 | 2:D:5:UNK:HA | 2.07 | 0.89 |
| 1:A:1258:PHE:HB3 | 1:A:1289:TYR:CZ | 1.99 | 0.89 |
| 1:A:1264:LYS:HE2 | 1:A:1268:LEU:HB2 | 1.54 | 0.89 |
| 1:A:1584:GLU:HG3 | 1:A:1587:TRP:CE3 | 2.08 | 0.89 |
| 1:B:1584:GLU:HG3 | 1:B:1587:TRP:CE3 | 2.08 | 0.89 |
| 1:B:1588:ARG:NH2 | 2:F:192:UNK:N | 2.21 | 0.89 |
| 1:C:1198:ILE:O | 1:C:1201:VAL:CB | 2.20 | 0.89 |
| 1:C:1412:LEU:HB2 | 1:C:1419:LEU:HD11 | 1.53 | 0.89 |
| 1:B:1218:TYR:HA | 1:B:1221:VAL:HG12 | 1.54 | 0.89 |
| 1:C:1521:TRP:HE3 | 1:C:1522:LYS:HD2 | 1.32 | 0.89 |
| 1:A:1521:TRP:HE3 | 1:A:1522:LYS:HD2 | 1.32 | 0.89 |
| 1:C:1409:GLN:CG | 1:C:1413:GLU:CG | 2.34 | 0.89 |
| 1:C:1411:TYR:O | 1:C:1415:LYS:CA | 2.21 | 0.89 |
| 2:E:114:GLN:HG3 | 2:E:115:GLU:H | 0.72 | 0.89 |
| 1:B:1408:ILE:CG2 | 1:B:1412:LEU:HB3 | 2.00 | 0.88 |
| 1:C:1270:GLN:CG | 1:C:1298:GLU:HG3 | 2.02 | 0.88 |
| 1:C:1427:SER:CB | 1:C:1428:PRO:CD | 2.44 | 0.88 |
| 1:A:1412:LEU:HA | 1:A:1419:LEU:HD22 | 1.54 | 0.88 |
| 1:B:1412:LEU:HA | 1:B:1419:LEU:HD22 | 1.55 | 0.88 |
| 1:C:1303:LEU:HD12 | 1:C:1320:LEU:HD13 | 1.52 | 0.88 |
| 1:B:1253:TRP:HZ3 | 1:B:1276:ILE:HG22 | 1.33 | 0.88 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:1584:GLU:HG3 | 1:C:1587:TRP:CE3 | 2.08 | 0.88 |
| 2:D:155:ILE:HG12 | 2:D:161:TYR:CB | 2.02 | 0.88 |
| 1:B:1409:GLN:CB | 1:B:1413:GLU:HG3 | 2.03 | 0.88 |
| 2:D:112:ARG:O | 2:D:112:ARG:CD | 2.21 | 0.88 |
| 1:A:1188:GLU:OE2 | 1:A:1191:ASN:O | 1.92 | 0.88 |
| 1:C:1211:TYR:HD1 | 1:C:1231:LEU:CD2 | 1.56 | 0.88 |
| 1:B:1601:GLN:CG | 1:C:1587:TRP:HH2 | 1.87 | 0.88 |
| 1:B:1171:THR:HA | 1:B:1174:ILE:HD12 | 1.54 | 0.88 |
| 1:B:1521:TRP:HE3 | 1:B:1522:LYS:HD2 | 1.32 | 0.88 |
| 1:C:1192:GLY:H | 1:C:1193:PRO:HD3 | 1.37 | 0.88 |
| 1:C:1222:SER:O | 1:C:1223:ASN:CG | 2.12 | 0.88 |
| 1:C:1505:ILE:HA | 1:C:1508:ARG:HB2 | 1.55 | 0.88 |
| 1:A:1108:TRP:NE1 | 1:A:1131:ALA:HB3 | 1.89 | 0.88 |
| 1:C:1234:LEU:CD2 | 1:C:1264:LYS:HZ3 | 1.86 | 0.88 |
| 1:C:1211:TYR:CD1 | 1:C:1231:LEU:HD21 | 2.05 | 0.88 |
| 2:F:198:UNK:HA | 2:F:201:UNK:CB | 2.01 | 0.88 |
| 1:C:1222:SER:O | 1:C:1223:ASN:HB2 | 1.07 | 0.88 |
| 1:B:1411:TYR:O | 1:B:1415:LYS:CA | 2.21 | 0.88 |
| 1:B:1221:VAL:CG1 | 1:B:1222:SER:N | 2.31 | 0.88 |
| 1:A:1221:VAL:CG1 | 1:A:1222:SER:N | 2.31 | 0.88 |
| 1:C:1372:ASP:O | 1:C:1376:ILE:HG12 | 1.73 | 0.88 |
| 1:A:1409:GLN:CB | 1:A:1413:GLU:HG3 | 2.03 | 0.88 |
| 2:D:65:UNK:O | 2:D:69:UNK:CB | 2.22 | 0.88 |
| 1:B:1333:ARG:HB2 | 1:B:1360:GLU:CG | 2.04 | 0.87 |
| 1:C:1254:LYS:NZ | 1:C:1285:GLU:O | 2.05 | 0.87 |
| 1:B:1264:LYS:HE2 | 1:B:1268:LEU:HB2 | 1.54 | 0.87 |
| 1:B:1572:THR:HG21 | 1:B:1599:PHE:CD2 | 2.10 | 0.87 |
| 1:B:1425:VAL:HG23 | 1:B:1426:LEU:H | 1.38 | 0.87 |
| 2:F:114:GLN:HG3 | 2:F:115:GLU:H | 0.72 | 0.87 |
| 1:C:1371:TYR:CD1 | 1:C:1394:ILE:CG2 | 2.36 | 0.87 |
| 1:C:1521:TRP:HZ3 | 1:C:1522:LYS:HZ2 | 0.90 | 0.87 |
| 1:C:1264:LYS:HE2 | 1:C:1268:LEU:HB2 | 1.54 | 0.87 |
| 1:C:1181:ASN:O | 1:C:1182:ARG:HD3 | 1.73 | 0.87 |
| 1:C:1425:VAL:HG23 | 1:C:1426:LEU:H | 1.38 | 0.87 |
| 1:A:1333:ARG:HB2 | 1:A:1360:GLU:CG | 2.05 | 0.87 |
| 1:C:1270:GLN:OE1 | 1:C:1298:GLU:CG | 2.23 | 0.87 |
| 2:D:185:UNK:HA | 2:D:189:UNK:C | 2.03 | 0.87 |
| 1:B:1198:ILE:HG23 | 1:B:1201:VAL:HB | 1.57 | 0.87 |
| 1:B:1505:ILE:HA | 1:B:1508:ARG:HB2 | 1.56 | 0.87 |
| 1:A:1218:TYR:HA | 1:A:1221:VAL:HG12 | 1.55 | 0.87 |
| 1:A:1505:ILE:HA | 1:A:1508:ARG:HB2 | 1.56 | 0.87 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:1232:VAL:C | 1:B:1234:LEU:H | 1.78 | 0.87 |
| 1:C:1127:SER:HA | 1:C:1156:TYR:OH | 1.75 | 0.87 |
| 1:B:1149:ASN:O | 1:B:1153:LEU:HB2 | 1.74 | 0.87 |
| 2:E:126:GLU:HG3 | 2:E:130:LYS:NZ | 1.90 | 0.86 |
| 1:A:1472:ILE:HG21 | 1:A:1498:ARG:HE | 1.40 | 0.86 |
| 1:A:1254:LYS:HG3 | 1:A:1285:GLU:OE2 | 1.04 | 0.86 |
| 1:A:1425:VAL:HG23 | 1:A:1426:LEU:H | 1.38 | 0.86 |
| 1:B:1411:TYR:O | 1:B:1415:LYS:CB | 2.22 | 0.86 |
| 1:C:1082:VAL:HG13 | 1:C:1083:GLN:H | 1.41 | 0.86 |
| 1:C:1412:LEU:HD13 | 1:C:1419:LEU:CD2 | 2.03 | 0.86 |
| 2:D:114:GLN:HG3 | 2:D:115:GLU:H | 0.72 | 0.86 |
| 1:C:1333:ARG:HB2 | 1:C:1360:GLU:CG | 2.05 | 0.86 |
| 1:C:1472:ILE:HG21 | 1:C:1498:ARG:HE | 1.40 | 0.86 |
| 1:A:1408:ILE:CG2 | 1:A:1412:LEU:HD23 | 2.06 | 0.86 |
| 2:D:126:GLU:HG3 | 2:D:130:LYS:NZ | 1.90 | 0.86 |
| 1:C:1411:TYR:O | 1:C:1415:LYS:CB | 2.23 | 0.86 |
| 1:A:1253:TRP:HZ3 | 1:A:1276:ILE:HG22 | 1.33 | 0.86 |
| 1:B:1588:ARG:HG3 | 1:B:1588:ARG:HH11 | 1.38 | 0.86 |
| 1:C:1588:ARG:HH22 | 2:D:193:UNK:CA | 1.82 | 0.86 |
| 1:A:1475:GLU:OE1 | 2:F:145:GLN:CB | 2.17 | 0.86 |
| 1:C:1244:ALA:C | 1:C:1275:HIS:CE1 | 2.46 | 0.86 |
| 2:F:126:GLU:HG3 | 2:F:130:LYS:NZ | 1.90 | 0.86 |
| 1:B:1508:ARG:NH2 | 1:B:1530:LYS:HD3 | 1.91 | 0.86 |
| 1:A:1232:VAL:C | 1:A:1234:LEU:H | 1.78 | 0.86 |
| 1:C:1317:PHE:H | 1:C:1317:PHE:HD2 | 1.24 | 0.86 |
| 1:A:1551:GLU:HG2 | 1:A:1582:VAL:HG22 | 1.55 | 0.86 |
| 1:C:1508:ARG:NH2 | 1:C:1530:LYS:HD3 | 1.91 | 0.86 |
| 1:A:1137:TYR:HB2 | 1:A:1138:MET:HB2 | 0.87 | 0.86 |
| 1:C:1188:GLU:HA | 1:C:1191:ASN:ND2 | 1.90 | 0.86 |
| 1:C:1190:ILE:HD13 | 1:C:1216:LEU:O | 1.75 | 0.86 |
| 1:B:1596:MET:N | 1:B:1597:PRO:HD2 | 1.91 | 0.86 |
| 1:B:1362:VAL:HG22 | 1:B:1377:THR:HB | 1.57 | 0.86 |
| 1:A:1401:VAL:HG22 | 1:A:1429:ARG:HE | 1.41 | 0.86 |
| 1:B:1601:GLN:HG2 | 1:C:1587:TRP:CH2 | 2.09 | 0.85 |
| 1:B:1082:VAL:HG13 | 1:B:1083:GLN:H | 1.40 | 0.85 |
| 1:A:1254:LYS:O | 1:A:1289:TYR:CE2 | 2.28 | 0.85 |
| 1:A:1535:LYS:HZ1 | 1:A:1563:ARG:HH12 | 1.18 | 0.85 |
| 1:B:1588:ARG:HH22 | 2:F:192:UNK:CB | 1.89 | 0.85 |
| 1:A:1521:TRP:HZ3 | 1:A:1522:LYS:HZ2 | 0.90 | 0.85 |
| 1:C:1401:VAL:HG22 | 1:C:1429:ARG:HE | 1.41 | 0.85 |
| 1:B:1408:ILE:CG2 | 1:B:1412:LEU:HD23 | 2.06 | 0.85 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1252:THR:O | 1:A:1256:VAL:HG23 | 1.76 | 0.85 |
| 1:C:1198:ILE:HB | 1:C:1221:VAL:HG21 | 1.56 | 0.85 |
| 1:C:1408:ILE:CG2 | 1:C:1412:LEU:HD23 | 2.06 | 0.85 |
| 1:A:1345:ILE:H | 1:A:1346:PRO:HD2 | 1.40 | 0.85 |
| 1:C:1260:CYS:O | 1:C:1263:GLY:O | 1.95 | 0.85 |
| 2:F:194:UNK:O | 2:F:197:UNK:CB | 2.24 | 0.85 |
| 2:F:142:GLN:O | 2:F:146:VAL:HG13 | 1.76 | 0.85 |
| 1:B:1427:SER:CB | 1:B:1428:PRO:CD | 2.44 | 0.85 |
| 2:D:148:LYS:O | 2:D:151:ILE:HG12 | 1.77 | 0.85 |
| 1:A:1260:CYS:O | 1:A:1263:GLY:O | 1.94 | 0.85 |
| 1:A:1274:LEU:HD12 | 1:A:1274:LEU:H | 1.41 | 0.85 |
| 1:A:1596:MET:N | 1:A:1597:PRO:HD2 | 1.90 | 0.85 |
| 1:B:1129:ILE:O | 1:B:1130:LYS:C | 2.12 | 0.85 |
| 1:C:1252:THR:O | 1:C:1256:VAL:HG23 | 1.76 | 0.85 |
| 1:A:1572:THR:HG21 | 1:A:1599:PHE:CD2 | 2.11 | 0.85 |
| 1:B:1472:ILE:HG21 | 1:B:1498:ARG:HE | 1.40 | 0.85 |
| 1:A:1082:VAL:HG13 | 1:A:1083:GLN:H | 1.41 | 0.85 |
| 1:B:1345:ILE:H | 1:B:1346:PRO:HD2 | 1.40 | 0.85 |
| 1:B:1375:ILE:HD11 | 1:B:1394:ILE:HB | 1.59 | 0.85 |
| 1:B:1283:LEU:HD22 | 1:B:1313:HIS:NE2 | 1.91 | 0.85 |
| 2:D:180:UNK:O | 2:D:183:UNK:CB | 2.25 | 0.85 |
| 1:C:1362:VAL:HG22 | 1:C:1377:THR:HB | 1.57 | 0.85 |
| 1:A:1408:ILE:HG21 | 1:A:1412:LEU:CD2 | 2.07 | 0.85 |
| 2:D:142:GLN:O | 2:D:146:VAL:HG13 | 1.76 | 0.85 |
| 1:B:1085:LEU:HB3 | 1:B:1095:ALA:HB1 | 1.58 | 0.85 |
| 1:A:1206:TYR:O | 1:A:1230:THR:HG21 | 1.76 | 0.85 |
| 1:A:1264:LYS:HE2 | 1:A:1268:LEU:CB | 2.07 | 0.84 |
| 1:C:1274:LEU:H | 1:C:1274:LEU:HD12 | 1.41 | 0.84 |
| 1:A:1439:PHE:O | 1:A:1442:VAL:HB | 1.77 | 0.84 |
| 1:A:1361:LEU:HD23 | 1:A:1365:TYR:CE2 | 2.13 | 0.84 |
| 1:B:1290:TYR:HD2 | 1:B:1299:LEU:HD13 | 1.09 | 0.84 |
| 1:B:1521:TRP:HZ3 | 1:B:1522:LYS:NZ | 1.75 | 0.84 |
| 2:F:148:LYS:O | 2:F:151:ILE:HG12 | 1.76 | 0.84 |
| 2:E:148:LYS:O | 2:E:151:ILE:HG12 | 1.77 | 0.84 |
| 1:A:1412:LEU:HD13 | 1:A:1419:LEU:CD2 | 2.03 | 0.84 |
| 1:A:1427:SER:CB | 1:A:1428:PRO:CD | 2.44 | 0.84 |
| 1:A:1475:GLU:OE2 | 2:F:149:ASN:OD1 | 1.94 | 0.84 |
| 1:C:1345:ILE:H | 1:C:1346:PRO:HD2 | 1.41 | 0.84 |
| 1:A:1598:TYR:CE1 | 1:B:1584:GLU:OE2 | 2.31 | 0.84 |
| 1:A:1411:TYR:O | 1:A:1415:LYS:CB | 2.25 | 0.84 |
| 1:A:1387:LYS:HB2 | 1:A:1390:GLN:HB2 | 1.59 | 0.84 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1317:PHE:HD2 | 1:A:1317:PHE:H | 1.24 | 0.84 |
| 1:B:1264:LYS:HE2 | 1:B:1268:LEU:CB | 2.07 | 0.84 |
| 1:B:1401:VAL:HG22 | 1:B:1429:ARG:HE | 1.41 | 0.84 |
| 1:A:1508:ARG:NH2 | 1:A:1530:LYS:HD3 | 1.91 | 0.84 |
| 1:A:1080:SER:O | 1:A:1084:VAL:HG23 | 1.78 | 0.84 |
| 1:A:1129:ILE:O | 1:A:1130:LYS:C | 2.12 | 0.84 |
| 1:B:1601:GLN:NE2 | 1:C:1587:TRP:HZ3 | 1.49 | 0.84 |
| 1:B:1387:LYS:HB2 | 1:B:1390:GLN:HB2 | 1.59 | 0.84 |
| 1:A:1282:GLU:HG3 | 1:A:1283:LEU:N | 1.93 | 0.84 |
| 1:B:1332:MET:SD | 1:B:1360:GLU:HG2 | 2.18 | 0.84 |
| 1:C:1264:LYS:HE2 | 1:C:1268:LEU:CB | 2.07 | 0.84 |
| 1:B:1282:GLU:HG3 | 1:B:1283:LEU:N | 1.93 | 0.84 |
| 1:A:1472:ILE:HB | 1:A:1498:ARG:HH21 | 1.43 | 0.84 |
| 1:B:1136:SER:HB3 | 1:B:1141:VAL:HG11 | 1.57 | 0.84 |
| 2:D:174:UNK:CA | 2:D:176:UNK:N | 2.39 | 0.84 |
| 1:B:1317:PHE:HD2 | 1:B:1317:PHE:H | 1.24 | 0.84 |
| 1:C:1107:VAL:O | 1:C:1108:TRP:CE3 | 2.31 | 0.84 |
| 1:C:1504:LEU:HD11 | 2:E:149:ASN:CG | 1.96 | 0.84 |
| 1:A:1108:TRP:CD1 | 1:A:1131:ALA:HB3 | 2.13 | 0.84 |
| 1:B:1430:LEU:HG | 1:B:1432:HIS:H | 1.43 | 0.84 |
| 1:B:1408:ILE:HG21 | 1:B:1412:LEU:CD2 | 2.07 | 0.83 |
| 1:B:1439:PHE:O | 1:B:1442:VAL:HB | 1.78 | 0.83 |
| 1:A:1492:ASN:O | 1:A:1493:ILE:CG1 | 2.26 | 0.83 |
| 1:C:1465:GLU:CD | 1:C:1465:GLU:O | 2.16 | 0.83 |
| 1:A:1430:LEU:HG | 1:A:1432:HIS:H | 1.42 | 0.83 |
| 1:B:1551:GLU:CG | 1:B:1582:VAL:CG2 | 2.56 | 0.83 |
| 1:A:1416:PRO:HD3 | 2:F:130:LYS:HD3 | 1.60 | 0.83 |
| 1:B:1465:GLU:CD | 1:B:1465:GLU:O | 2.16 | 0.83 |
| 1:B:1260:CYS:O | 1:B:1263:GLY:O | 1.95 | 0.83 |
| 1:C:1439:PHE:O | 1:C:1442:VAL:HB | 1.77 | 0.83 |
| 1:B:1409:GLN:CB | 1:B:1413:GLU:CG | 2.56 | 0.83 |
| 1:A:1375:ILE:HD11 | 1:A:1394:ILE:HB | 1.59 | 0.83 |
| 1:B:1521:TRP:HZ3 | 1:B:1522:LYS:HZ2 | 0.90 | 0.83 |
| 2:F:195:UNK:O | 2:F:197:UNK:CB | 2.27 | 0.83 |
| 1:C:1409:GLN:CB | 1:C:1413:GLU:CG | 2.56 | 0.83 |
| 2:E:142:GLN:O | 2:E:146:VAL:HG13 | 1.77 | 0.83 |
| 1:B:1167:SER:HB3 | 1:B:1168:TYR:CD1 | 2.14 | 0.83 |
| 1:A:1295:TYR:CE2 | 1:A:1299:LEU:HB2 | 2.12 | 0.83 |
| 1:C:1361:LEU:HD23 | 1:C:1365:TYR:CE2 | 2.12 | 0.83 |
| 1:C:1191:ASN:N | 1:C:1191:ASN:HD22 | 1.75 | 0.83 |
| 1:B:1085:LEU:HD13 | 1:B:1125:ILE:HD11 | 1.61 | 0.83 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1448:VAL:HB | 1:A:1451:TYR:CD2 | 2.14 | 0.83 |
| 2:E:104:LYS:O | 2:E:108:GLU:CB | 2.25 | 0.83 |
| 1:A:1465:GLU:CD | 1:A:1465:GLU:O | 2.17 | 0.83 |
| 1:A:1587:TRP:HH2 | 1:C:1601:GLN:HG2 | 1.43 | 0.83 |
| 1:B:1290:TYR:CE2 | 1:B:1299:LEU:HD13 | 2.13 | 0.83 |
| 1:A:1332:MET:SD | 1:A:1360:GLU:HG2 | 2.18 | 0.83 |
| 1:B:1252:THR:O | 1:B:1256:VAL:HG23 | 1.76 | 0.83 |
| 1:C:1122:LYS:HZ3 | 1:C:1147:SER:CB | 1.92 | 0.83 |
| 1:A:1362:VAL:HG22 | 1:A:1377:THR:HB | 1.57 | 0.83 |
| 1:C:1387:LYS:HB2 | 1:C:1390:GLN:HB2 | 1.59 | 0.83 |
| 1:A:1521:TRP:HZ3 | 1:A:1522:LYS:NZ | 1.75 | 0.83 |
| 1:C:1332:MET:SD | 1:C:1360:GLU:HG2 | 2.17 | 0.82 |
| 1:A:1611:ASP:OD2 | 1:B:1607:LEU:HD22 | 1.79 | 0.82 |
| 1:A:1605:GLU:OE2 | 1:B:1579:PRO:HA | 1.79 | 0.82 |
| 1:C:1420:ASN:OD1 | 1:C:1447:LEU:HD22 | 1.78 | 0.82 |
| 1:B:1420:ASN:OD1 | 1:B:1447:LEU:HD22 | 1.78 | 0.82 |
| 1:C:1375:ILE:HD11 | 1:C:1394:ILE:HB | 1.59 | 0.82 |
| 1:B:1136:SER:CA | 1:B:1141:VAL:HG21 | 2.09 | 0.82 |
| 1:C:1136:SER:CA | 1:C:1137:TYR:N | 2.41 | 0.82 |
| 1:C:1408:ILE:HG21 | 1:C:1412:LEU:CD2 | 2.07 | 0.82 |
| 1:A:1167:SER:O | 1:A:1168:TYR:CD1 | 2.31 | 0.82 |
| 2:E:105:TRP:O | 2:E:108:GLU:HG3 | 1.79 | 0.82 |
| 1:C:1259:ALA:HA | 1:C:1293:ARG:HH12 | 1.44 | 0.82 |
| 1:B:1448:VAL:HB | 1:B:1451:TYR:CD2 | 2.13 | 0.82 |
| 2:E:90:ALA:H | 2:E:91:GLN:CB | 1.92 | 0.82 |
| 1:A:1258:PHE:N | 1:A:1289:TYR:HH | 1.66 | 0.82 |
| 2:D:181:UNK:O | 2:D:183:UNK:CB | 2.26 | 0.82 |
| 1:A:1420:ASN:OD1 | 1:A:1447:LEU:HD22 | 1.78 | 0.82 |
| 1:B:1408:ILE:HG21 | 1:B:1412:LEU:HD23 | 1.61 | 0.82 |
| 1:C:1596:MET:N | 1:C:1597:PRO:HD2 | 1.90 | 0.82 |
| 2:D:180:UNK:C | 2:D:183:UNK:CA | 2.57 | 0.82 |
| 1:C:1419:LEU:O | 1:C:1422:LEU:CB | 2.25 | 0.82 |
| 1:C:1448:VAL:HB | 1:C:1451:TYR:CD2 | 2.13 | 0.82 |
| 1:B:1274:LEU:HD12 | 1:B:1274:LEU:H | 1.41 | 0.82 |
| 2:D:180:UNK:O | 2:D:183:UNK:CA | 2.27 | 0.82 |
| 1:B:1325:SER:O | 1:B:1355:ALA:HB1 | 1.79 | 0.82 |
| 1:C:1290:TYR:CE2 | 1:C:1299:LEU:CD1 | 2.59 | 0.82 |
| 1:C:1577:LEU:O | 1:C:1579:PRO:HD3 | 1.80 | 0.82 |
| 2:D:66:UNK:O | 2:D:70:UNK:CB | 2.28 | 0.82 |
| 1:B:1245:ARG:O | 1:B:1246:LYS:CG | 2.24 | 0.82 |
| 1:B:1472:ILE:HB | 1:B:1498:ARG:HH21 | 1.43 | 0.82 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:F:21:UNK:O | 2:F:21:UNK:C | 0.52 | 0.82 |
| 1:A:1596:MET:SD | 1:A:1597:PRO:HD3 | 2.20 | 0.82 |
| 2:F:190:UNK:O | 2:F:192:UNK:N | 2.13 | 0.82 |
| 1:C:1395:ILE:HG12 | 1:C:1404:TYR:CD2 | 2.14 | 0.82 |
| 1:C:1472:ILE:HB | 1:C:1498:ARG:HH21 | 1.42 | 0.82 |
| 2:D:180:UNK:C | 2:D:183:UNK:HA | 2.09 | 0.82 |
| 1:B:1588:ARG:HH12 | 2:F:192:UNK:HA | 1.40 | 0.82 |
| 1:C:1115:GLN:HG3 | 1:C:1125:ILE:HD11 | 1.61 | 0.82 |
| 1:B:1361:LEU:HD23 | 1:B:1365:TYR:CE2 | 2.12 | 0.82 |
| 1:B:1419:LEU:O | 1:B:1422:LEU:CB | 2.26 | 0.82 |
| 1:C:1521:TRP:HZ3 | 1:C:1522:LYS:NZ | 1.75 | 0.82 |
| 1:C:1108:TRP:CZ3 | 1:C:1129:ILE:HG22 | 2.15 | 0.81 |
| 1:A:1401:VAL:HG22 | 1:A:1429:ARG:NE | 1.94 | 0.81 |
| 1:B:1598:TYR:HA | 1:C:1584:GLU:OE2 | 1.80 | 0.81 |
| 1:C:1198:ILE:CA | 1:C:1201:VAL:CG2 | 2.58 | 0.81 |
| 1:B:1438:TYR:O | 1:B:1442:VAL:HG23 | 1.80 | 0.81 |
| 1:A:1325:SER:O | 1:A:1355:ALA:HB1 | 1.79 | 0.81 |
| 1:C:1244:ALA:N | 1:C:1275:HIS:HE1 | 1.77 | 0.81 |
| 1:B:1535:LYS:HE2 | 1:B:1535:LYS:HA | 1.63 | 0.81 |
| 1:B:1598:TYR:CD1 | 1:C:1584:GLU:OE2 | 2.33 | 0.81 |
| 2:F:194:UNK:O | 2:F:197:UNK:CA | 2.29 | 0.81 |
| 1:C:1198:ILE:CB | 1:C:1221:VAL:CG2 | 2.58 | 0.81 |
| 1:C:1414:PHE:CE1 | 2:E:127:TRP:CZ3 | 2.65 | 0.81 |
| 1:A:1404:TYR:O | 1:A:1407:ALA:HB3 | 1.79 | 0.81 |
| 1:A:1122:LYS:O | 1:A:1126:ASP:HB2 | 1.80 | 0.81 |
| 1:C:1230:THR:O | 1:C:1231:LEU:CD2 | 2.28 | 0.81 |
| 1:C:1404:TYR:O | 1:C:1407:ALA:HB3 | 1.80 | 0.81 |
| 1:A:1438:TYR:O | 1:A:1442:VAL:HG23 | 1.80 | 0.81 |
| 1:B:1404:TYR:O | 1:B:1407:ALA:HB3 | 1.79 | 0.81 |
| 1:A:1177:LEU:HA | 1:A:1180:THR:OG1 | 1.81 | 0.81 |
| 1:B:1492:ASN:O | 1:B:1493:ILE:CG1 | 2.26 | 0.81 |
| 1:B:1206:TYR:O | 1:B:1230:THR:HG21 | 1.80 | 0.81 |
| 1:A:1395:ILE:HG12 | 1:A:1404:TYR:CD2 | 2.14 | 0.81 |
| 1:A:1408:ILE:HG21 | 1:A:1412:LEU:HD23 | 1.61 | 0.81 |
| 1:B:1245:ARG:O | 1:B:1245:ARG:HG2 | 1.81 | 0.81 |
| 1:A:1222:SER:OG | 1:A:1223:ASN:N | 2.13 | 0.81 |
| 1:A:1412:LEU:HD12 | 1:A:1419:LEU:CD2 | 2.11 | 0.81 |
| 1:B:1395:ILE:HG12 | 1:B:1404:TYR:CD2 | 2.14 | 0.81 |
| 1:B:1401:VAL:HG22 | 1:B:1429:ARG:NE | 1.94 | 0.81 |
| 1:A:1326:LYS:O | 1:A:1327:PHE:CG | 2.34 | 0.81 |
| 1:C:1325:SER:O | 1:C:1355:ALA:HB1 | 1.79 | 0.81 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:E:203:UNK:C | 2:E:203:UNK:N | 2.42 | 0.81 |
| 1:C:1180:THR:HB | 1:C:1185:GLU:OE2 | 1.79 | 0.81 |
| 1:C:1401:VAL:HG22 | 1:C:1429:ARG:NE | 1.94 | 0.81 |
| 1:C:1411:TYR:O | 1:C:1415:LYS:N | 2.14 | 0.81 |
| 1:C:1492:ASN:O | 1:C:1493:ILE:CG1 | 2.25 | 0.81 |
| 1:B:1149:ASN:O | 1:B:1153:LEU:CB | 2.29 | 0.81 |
| 2:D:155:ILE:H | 2:D:155:ILE:HD13 | 1.45 | 0.81 |
| 1:C:1430:LEU:HG | 1:C:1432:HIS:H | 1.43 | 0.81 |
| 1:B:1279:HIS:C | 1:B:1279:HIS:CB | 2.48 | 0.81 |
| 1:C:1405:TYR:CG | 1:C:1434:ARG:NH1 | 2.49 | 0.81 |
| 1:B:1332:MET:HE2 | 1:B:1357:LEU:HD13 | 1.60 | 0.81 |
| 1:A:1387:LYS:CB | 1:A:1390:GLN:HB2 | 2.11 | 0.81 |
| 1:C:1605:GLU:HA | 1:C:1608:THR:CB | 2.10 | 0.81 |
| 1:C:1412:LEU:HD12 | 1:C:1419:LEU:CD2 | 2.10 | 0.81 |
| 1:C:1438:TYR:O | 1:C:1442:VAL:HG23 | 1.80 | 0.81 |
| 1:A:1296:PHE:HE2 | 2:F:101:SER:HG | 1.25 | 0.81 |
| 1:A:1577:LEU:O | 1:A:1579:PRO:HD3 | 1.80 | 0.81 |
| 1:C:1122:LYS:O | 1:C:1126:ASP:HB2 | 1.80 | 0.81 |
| 1:A:1566:PHE:HE2 | 2:F:180:UNK:CB | 1.94 | 0.80 |
| 1:A:1409:GLN:CB | 1:A:1413:GLU:CG | 2.56 | 0.80 |
| 1:B:1412:LEU:HD12 | 1:B:1419:LEU:CD2 | 2.10 | 0.80 |
| 1:C:1387:LYS:CB | 1:C:1390:GLN:HB2 | 2.11 | 0.80 |
| 2:E:90:ALA:H | 2:E:91:GLN:CA | 1.94 | 0.80 |
| 2:E:126:GLU:O | 2:E:129:GLU:HG2 | 1.81 | 0.80 |
| 1:C:1191:ASN:HD22 | 1:C:1191:ASN:H | 1.27 | 0.80 |
| 1:A:1264:LYS:HE2 | 1:A:1268:LEU:CG | 2.12 | 0.80 |
| 1:C:1161:ARG:NH2 | 1:C:1174:ILE:HD11 | 1.97 | 0.80 |
| 1:C:1408:ILE:HG21 | 1:C:1412:LEU:HD23 | 1.61 | 0.80 |
| 1:B:1412:LEU:HD13 | 1:B:1419:LEU:CD2 | 2.03 | 0.80 |
| 1:B:1405:TYR:CG | 1:B:1434:ARG:NH1 | 2.49 | 0.80 |
| 1:A:1254:LYS:C | 1:A:1289:TYR:CD2 | 2.54 | 0.80 |
| 1:A:1122:LYS:HG3 | 1:A:1123:GLU:H | 1.46 | 0.80 |
| 1:C:1282:GLU:OE2 | 1:C:1285:GLU:HB3 | 1.80 | 0.80 |
| 1:C:1326:LYS:O | 1:C:1327:PHE:CG | 2.34 | 0.80 |
| 2:D:126:GLU:O | 2:D:129:GLU:HG2 | 1.81 | 0.80 |
| 1:C:1278:VAL:HG12 | 1:C:1278:VAL:O | 1.81 | 0.80 |
| 1:C:1122:LYS:HG3 | 1:C:1123:GLU:H | 1.46 | 0.80 |
| 1:C:1382:PRO:CD | 2:E:115:GLU:OE2 | 2.30 | 0.80 |
| 1:B:1336:LEU:HD13 | 1:B:1364:LEU:HD21 | 1.63 | 0.80 |
| 1:C:1186:LEU:HD22 | 1:C:1213:ALA:HB3 | 1.63 | 0.80 |
| 2:E:155:ILE:H | 2:E:155:ILE:CD1 | 1.95 | 0.80 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:1264:LYS:HE2 | 1:C:1268:LEU:CG | 2.12 | 0.80 |
| 1:C:1438:TYR:O | 1:C:1442:VAL:CG2 | 2.29 | 0.80 |
| 1:B:1577:LEU:O | 1:B:1579:PRO:HD3 | 1.80 | 0.80 |
| 1:B:1605:GLU:HG3 | 1:C:1580:ASP:OD2 | 1.80 | 0.80 |
| 2:F:180:UNK:O | 2:F:182:UNK:N | 2.15 | 0.80 |
| 1:C:1504:LEU:CG | 2:E:149:ASN:OD1 | 2.30 | 0.80 |
| 1:B:1086:ILE:HB | 1:B:1089:ILE:HD13 | 1.64 | 0.80 |
| 1:B:1598:TYR:HE2 | 2:D:200:UNK:C | 1.94 | 0.80 |
| 1:B:1601:GLN:HE21 | 1:C:1587:TRP:HZ3 | 0.80 | 0.80 |
| 1:C:1596:MET:SD | 1:C:1597:PRO:HD3 | 2.21 | 0.80 |
| 1:B:1326:LYS:O | 1:B:1327:PHE:CG | 2.34 | 0.80 |
| 1:A:1292:ASP:O | 2:F:97:GLN:HG2 | 1.82 | 0.80 |
| 1:C:1336:LEU:HD13 | 1:C:1364:LEU:HD21 | 1.63 | 0.80 |
| 1:A:1583:LEU:O | 1:A:1587:TRP:NE1 | 2.15 | 0.80 |
| 1:C:1504:LEU:CG | 2:E:149:ASN:CG | 2.49 | 0.80 |
| 2:F:133:LYS:HA | 2:F:133:LYS:HZ1 | 1.43 | 0.80 |
| 1:B:1136:SER:N | 1:B:1141:VAL:HG21 | 1.97 | 0.80 |
| 1:B:1122:LYS:O | 1:B:1126:ASP:HB2 | 1.80 | 0.80 |
| 1:A:1431:ASP:O | 1:A:1433:THR:N | 2.15 | 0.80 |
| 1:A:1535:LYS:HA | 1:A:1535:LYS:HE2 | 1.63 | 0.79 |
| 1:A:1358:TRP:O | 1:A:1362:VAL:CG2 | 2.30 | 0.79 |
| 1:A:1336:LEU:HD13 | 1:A:1364:LEU:HD21 | 1.63 | 0.79 |
| 1:B:1583:LEU:O | 1:B:1587:TRP:NE1 | 2.15 | 0.79 |
| 1:C:1588:ARG:NH2 | 2:D:192:UNK:C | 2.45 | 0.79 |
| 1:B:1362:VAL:HG22 | 1:B:1377:THR:CG2 | 2.12 | 0.79 |
| 1:B:1438:TYR:O | 1:B:1442:VAL:CG2 | 2.29 | 0.79 |
| 1:A:1509:ARG:HH22 | 2:F:162:GLN:CB | 1.96 | 0.79 |
| 1:A:1580:ASP:CG | 1:C:1605:GLU:HG3 | 2.02 | 0.79 |
| 1:C:1362:VAL:HG22 | 1:C:1377:THR:CG2 | 2.12 | 0.79 |
| 1:A:1405:TYR:CG | 1:A:1434:ARG:NH1 | 2.49 | 0.79 |
| 1:B:1494:SER:HA | 1:B:1497:GLN:CD | 2.03 | 0.79 |
| 1:A:1551:GLU:CG | 1:A:1582:VAL:HG22 | 2.13 | 0.79 |
| 1:A:1605:GLU:HA | 1:A:1608:THR:CB | 2.10 | 0.79 |
| 1:A:1605:GLU:CA | 1:A:1608:THR:HB | 2.12 | 0.79 |
| 1:C:1445:LEU:N | 1:C:1446:PRO:HD2 | 1.97 | 0.79 |
| 1:A:1438:TYR:O | 1:A:1442:VAL:CG2 | 2.29 | 0.79 |
| 1:B:1538:MET:HE3 | 1:B:1566:PHE:HB3 | 1.65 | 0.79 |
| 1:C:1154:VAL:HG11 | 1:C:1180:THR:OG1 | 1.80 | 0.79 |
| 1:A:1361:LEU:HD21 | 1:A:1365:TYR:CZ | 2.18 | 0.79 |
| 1:B:1411:TYR:O | 1:B:1415:LYS:N | 2.14 | 0.79 |
| 1:B:1264:LYS:HE2 | 1:B:1268:LEU:CG | 2.11 | 0.79 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:1167:SER:O | 1:C:1171:THR:CA | 2.31 | 0.79 |
| 1:B:1358:TRP:O | 1:B:1362:VAL:CG2 | 2.31 | 0.79 |
| 1:C:1494:SER:HA | 1:C:1497:GLN:CD | 2.03 | 0.79 |
| 1:B:1122:LYS:HG3 | 1:B:1123:GLU:H | 1.47 | 0.79 |
| 1:B:1387:LYS:CB | 1:B:1390:GLN:HB2 | 2.11 | 0.79 |
| 2:E:127:TRP:HA | 2:E:130:LYS:HE3 | 1.65 | 0.79 |
| 2:F:126:GLU:O | 2:F:129:GLU:HG2 | 1.81 | 0.79 |
| 1:A:1234:LEU:HG | 1:A:1235:GLY:H | 1.48 | 0.79 |
| 1:C:1583:LEU:O | 1:C:1587:TRP:NE1 | 2.15 | 0.79 |
| 1:A:1445:LEU:N | 1:A:1446:PRO:HD2 | 1.98 | 0.79 |
| 1:A:1082:VAL:HG11 | 1:A:1105:PRO:HB2 | 1.63 | 0.79 |
| 1:C:1082:VAL:HG13 | 1:C:1083:GLN:N | 1.98 | 0.79 |
| 1:A:1514:LEU:O | 1:A:1514:LEU:HD23 | 1.83 | 0.79 |
| 1:C:1514:LEU:HD23 | 1:C:1514:LEU:O | 1.83 | 0.79 |
| 2:F:194:UNK:C | 2:F:197:UNK:CA | 2.61 | 0.78 |
| 1:C:1455:VAL:HG12 | 1:C:1456:GLN:N | 1.95 | 0.78 |
| 1:C:1414:PHE:CD1 | 2:E:123:MET:HB3 | 2.18 | 0.78 |
| 2:E:133:LYS:HA | 2:E:133:LYS:HZ1 | 1.44 | 0.78 |
| 1:B:1514:LEU:O | 1:B:1514:LEU:HD23 | 1.83 | 0.78 |
| 1:A:1494:SER:HA | 1:A:1497:GLN:CD | 2.03 | 0.78 |
| 1:B:1108:TRP:NE1 | 1:B:1131:ALA:HB3 | 1.98 | 0.78 |
| 1:B:1455:VAL:HG12 | 1:B:1456:GLN:N | 1.95 | 0.78 |
| 1:C:1481:ARG:NH1 | 1:C:1510:ILE:HG12 | 1.97 | 0.78 |
| 1:B:1079:THR:HG22 | 1:B:1079:THR:O | 1.83 | 0.78 |
| 2:D:181:UNK:O | 2:D:182:UNK:C | 2.28 | 0.78 |
| 1:B:1082:VAL:HG13 | 1:B:1083:GLN:N | 1.98 | 0.78 |
| 1:A:1253:TRP:C | 1:A:1255:GLU:H | 1.87 | 0.78 |
| 1:B:1277:VAL:HG23 | 1:B:1278:VAL:H | 1.48 | 0.78 |
| 1:C:1535:LYS:HA | 1:C:1535:LYS:HE2 | 1.63 | 0.78 |
| 1:C:1108:TRP:CE3 | 1:C:1108:TRP:HA | 2.19 | 0.78 |
| 1:B:1361:LEU:HD21 | 1:B:1365:TYR:CZ | 2.18 | 0.78 |
| 1:A:1412:LEU:CA | 1:A:1419:LEU:HD13 | 2.14 | 0.78 |
| 1:B:1234:LEU:HG | 1:B:1235:GLY:H | 1.48 | 0.78 |
| 2:F:150:LYS:O | 2:F:152:ASN:O | 2.02 | 0.78 |
| 1:A:1271:MET:O | 1:A:1275:HIS:HB2 | 1.84 | 0.78 |
| 1:A:1358:TRP:CE3 | 1:A:1381:HIS:CD2 | 2.72 | 0.78 |
| 1:A:1136:SER:CA | 1:A:1141:VAL:HG21 | 2.13 | 0.78 |
| 1:A:1279:HIS:CE1 | 1:A:1283:LEU:HD12 | 2.18 | 0.78 |
| 1:C:1244:ALA:C | 1:C:1275:HIS:HE1 | 1.86 | 0.78 |
| 1:B:1445:LEU:N | 1:B:1446:PRO:HD2 | 1.98 | 0.78 |
| 2:D:172:UNK:O | 2:D:175:UNK:CB | 2.31 | 0.78 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1079:THR:O | 1:A:1079:THR:HG22 | 1.84 | 0.78 |
| 1:C:1079:THR:O | 1:C:1079:THR:HG22 | 1.83 | 0.78 |
| 2:E:202:UNK:O | 2:E:203:UNK:O | 2.01 | 0.78 |
| 1:C:1149:ASN:O | 1:C:1153:LEU:HB2 | 1.84 | 0.78 |
| 1:B:1469:ASN:HA | 1:B:1472:ILE:HD12 | 1.66 | 0.78 |
| 1:C:1621:LYS:O | 1:C:1625:GLN:HG3 | 1.83 | 0.78 |
| 1:A:1621:LYS:O | 1:A:1625:GLN:HG3 | 1.83 | 0.78 |
| 2:D:150:LYS:O | 2:D:152:ASN:O | 2.02 | 0.78 |
| 1:B:1431:ASP:O | 1:B:1433:THR:N | 2.15 | 0.78 |
| 1:C:1206:TYR:CD1 | 1:C:1226:ARG:HD2 | 2.19 | 0.78 |
| 1:B:1271:MET:O | 1:B:1275:HIS:HB2 | 1.83 | 0.78 |
| 1:A:1455:VAL:HG12 | 1:A:1456:GLN:N | 1.96 | 0.78 |
| 1:B:1409:GLN:HA | 1:B:1413:GLU:HG2 | 0.81 | 0.78 |
| 1:B:1412:LEU:HD12 | 1:B:1419:LEU:HD21 | 1.66 | 0.78 |
| 1:C:1270:GLN:OE1 | 1:C:1298:GLU:HG3 | 1.84 | 0.78 |
| 1:B:1246:LYS:O | 1:B:1247:ALA:CB | 2.32 | 0.78 |
| 1:A:1214:ALA:O | 1:A:1218:TYR:HB2 | 1.84 | 0.78 |
| 1:C:1175:PHE:CE1 | 1:C:1200:GLN:HB3 | 2.18 | 0.78 |
| 1:C:1358:TRP:O | 1:C:1362:VAL:CG2 | 2.31 | 0.78 |
| 1:B:1167:SER:HB3 | 1:B:1168:TYR:CE1 | 2.19 | 0.78 |
| 1:C:1499:LEU:HB2 | 1:C:1511:ALA:HB2 | 1.66 | 0.78 |
| 1:C:1264:LYS:HZ1 | 1:C:1268:LEU:HD13 | 1.47 | 0.78 |
| 1:C:1605:GLU:CA | 1:C:1608:THR:HB | 2.12 | 0.78 |
| 2:D:180:UNK:O | 2:D:183:UNK:HA | 1.84 | 0.78 |
| 1:A:1279:HIS:HD2 | 1:A:1282:GLU:H | 1.28 | 0.77 |
| 1:B:1605:GLU:HA | 1:B:1608:THR:CB | 2.10 | 0.77 |
| 1:C:1586:ALA:CB | 1:C:1594:PHE:CE1 | 2.67 | 0.77 |
| 1:C:1168:TYR:H | 1:C:1168:TYR:HD1 | 1.32 | 0.77 |
| 1:C:1198:ILE:HG12 | 1:C:1199:GLN:N | 1.99 | 0.77 |
| 1:C:1361:LEU:C | 1:C:1361:LEU:HD23 | 2.04 | 0.77 |
| 1:C:1361:LEU:HD21 | 1:C:1365:TYR:CZ | 2.17 | 0.77 |
| 1:A:1362:VAL:HG22 | 1:A:1377:THR:CG2 | 2.12 | 0.77 |
| 2:E:108:GLU:OE2 | 2:E:109:GLN:CG | 2.32 | 0.77 |
| 1:A:1082:VAL:HG13 | 1:A:1083:GLN:N | 1.98 | 0.77 |
| 1:B:1499:LEU:HB2 | 1:B:1511:ALA:HB2 | 1.66 | 0.77 |
| 1:A:1149:ASN:O | 1:A:1153:LEU:HB2 | 1.84 | 0.77 |
| 1:B:1412:LEU:CA | 1:B:1419:LEU:HD13 | 2.14 | 0.77 |
| 1:A:1107:VAL:HG12 | 1:A:1111:LEU:HB2 | 1.67 | 0.77 |
| 1:A:1116:LEU:HD11 | 1:A:1122:LYS:CD | 2.13 | 0.77 |
| 2:E:151:ILE:HA | 2:E:154:ARG:HD3 | 1.66 | 0.77 |
| 2:D:126:GLU:HG3 | 2:D:130:LYS:HZ3 | 1.49 | 0.77 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:1144:ALA:O | 1:B:1153:LEU:HD13 | 1.83 | 0.77 |
| 2:E:150:LYS:O | 2:E:152:ASN:O | 2.02 | 0.77 |
| 1:A:1538:MET:HE3 | 1:A:1566:PHE:HB3 | 1.65 | 0.77 |
| 1:C:1161:ARG:HE | 1:C:1170:GLU:HB2 | 1.48 | 0.77 |
| 2:E:146:VAL:HA | 2:E:149:ASN:OD1 | 1.85 | 0.77 |
| 1:A:1471:PHE:HB3 | 1:A:1480:LEU:HB2 | 1.66 | 0.77 |
| 1:B:1471:PHE:HA | 1:B:1474:GLU:HG2 | 1.67 | 0.77 |
| 1:B:1525:VAL:HG13 | 1:B:1526:GLU:OE2 | 1.85 | 0.77 |
| 1:A:1277:VAL:HG23 | 1:A:1278:VAL:H | 1.48 | 0.77 |
| 1:A:1469:ASN:HA | 1:A:1472:ILE:HD12 | 1.66 | 0.77 |
| 1:B:1135:SER:OG | 1:B:1160:ALA:HA | 1.84 | 0.77 |
| 1:C:1271:MET:O | 1:C:1275:HIS:HB2 | 1.83 | 0.77 |
| 1:C:1245:ARG:N | 1:C:1275:HIS:HE1 | 1.82 | 0.77 |
| 1:B:1253:TRP:C | 1:B:1255:GLU:H | 1.87 | 0.77 |
| 1:A:1161:ARG:HG2 | 1:A:1173:LEU:CD2 | 2.14 | 0.77 |
| 1:B:1180:THR:O | 1:B:1181:ASN:HB3 | 1.82 | 0.77 |
| 1:B:1605:GLU:CA | 1:B:1608:THR:HB | 2.12 | 0.77 |
| 1:B:1358:TRP:CE3 | 1:B:1381:HIS:CD2 | 2.72 | 0.77 |
| 1:C:1472:ILE:HA | 1:C:1507:PHE:CE1 | 2.19 | 0.77 |
| 1:A:1174:ILE:CG2 | 1:A:1201:VAL:HG22 | 2.15 | 0.77 |
| 2:F:151:ILE:HA | 2:F:154:ARG:HD3 | 1.66 | 0.77 |
| 1:A:1279:HIS:CD2 | 1:A:1282:GLU:HB3 | 2.20 | 0.77 |
| 1:B:1214:ALA:O | 1:B:1218:TYR:HB2 | 1.84 | 0.77 |
| 1:C:1609:LYS:HG2 | 1:C:1612:LYS:HD2 | 1.66 | 0.77 |
| 2:F:194:UNK:O | 2:F:197:UNK:HA | 1.85 | 0.77 |
| 1:C:1412:LEU:CA | 1:C:1419:LEU:HD13 | 2.14 | 0.77 |
| 1:C:1471:PHE:HB3 | 1:C:1480:LEU:HB2 | 1.67 | 0.77 |
| 2:F:127:TRP:HA | 2:F:130:LYS:HE3 | 1.66 | 0.77 |
| 1:C:1513:TYR:O | 1:C:1516:LYS:HG2 | 1.85 | 0.77 |
| 1:A:1332:MET:HE2 | 1:A:1357:LEU:HD13 | 1.66 | 0.77 |
| 1:C:1277:VAL:HG23 | 1:C:1278:VAL:H | 1.49 | 0.77 |
| 1:B:1471:PHE:HB3 | 1:B:1480:LEU:HB2 | 1.67 | 0.77 |
| 2:D:127:TRP:HA | 2:D:130:LYS:HE3 | 1.65 | 0.77 |
| 1:A:1492:ASN:C | 1:A:1493:ILE:HG13 | 2.05 | 0.77 |
| 1:B:1387:LYS:HB2 | 1:B:1390:GLN:HB3 | 1.65 | 0.77 |
| 1:A:1232:VAL:C | 1:A:1234:LEU:N | 2.38 | 0.77 |
| 1:C:1113:LYS:HG3 | 1:C:1139:GLU:OE1 | 1.84 | 0.77 |
| 1:A:1535:LYS:NZ | 2:F:181:UNK:CB | 2.48 | 0.76 |
| 1:C:1358:TRP:CE3 | 1:C:1381:HIS:CD2 | 2.72 | 0.76 |
| 1:C:1525:VAL:HG13 | 1:C:1526:GLU:OE2 | 1.85 | 0.76 |
| 1:B:1361:LEU:C | 1:B:1361:LEU:HD23 | 2.05 | 0.76 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:F:118:ALA:HA | 2:F:121:LYS:CE | 2.15 | 0.76 |
| 1:B:1408:ILE:HG23 | 1:B:1412:LEU:HB2 | 1.68 | 0.76 |
| 1:A:1499:LEU:HB2 | 1:A:1511:ALA:HB2 | 1.66 | 0.76 |
| 1:A:1609:LYS:HG2 | 1:A:1612:LYS:HD2 | 1.66 | 0.76 |
| 1:C:1108:TRP:HE3 | 1:C:1108:TRP:HA | 1.51 | 0.76 |
| 1:A:1409:GLN:HA | 1:A:1413:GLU:HG2 | 0.81 | 0.76 |
| 2:D:118:ALA:HA | 2:D:121:LYS:CE | 2.15 | 0.76 |
| 1:A:1122:LYS:HG3 | 1:A:1123:GLU:N | 2.01 | 0.76 |
| 1:A:1525:VAL:HG13 | 1:A:1526:GLU:OE2 | 1.85 | 0.76 |
| 1:C:1211:TYR:CE1 | 1:C:1231:LEU:HD21 | 2.20 | 0.76 |
| 2:F:190:UNK:O | 2:F:191:UNK:C | 2.33 | 0.76 |
| 1:C:1427:SER:HB3 | 1:C:1428:PRO:HD3 | 1.67 | 0.76 |
| 2:F:146:VAL:HA | 2:F:149:ASN:OD1 | 1.85 | 0.76 |
| 1:C:1492:ASN:C | 1:C:1493:ILE:HG12 | 2.04 | 0.76 |
| 1:B:1513:TYR:O | 1:B:1516:LYS:HG2 | 1.85 | 0.76 |
| 1:B:1277:VAL:HG23 | 1:B:1278:VAL:N | 2.01 | 0.76 |
| 1:C:1596:MET:O | 1:C:1598:TYR:CE2 | 2.38 | 0.76 |
| 1:C:1572:THR:HG21 | 1:C:1599:PHE:CD2 | 2.20 | 0.76 |
| 1:A:1403:LEU:HD13 | 1:A:1403:LEU:O | 1.86 | 0.76 |
| 1:A:1116:LEU:CD1 | 1:A:1122:LYS:HB3 | 2.15 | 0.76 |
| 2:D:151:ILE:HA | 2:D:154:ARG:HD3 | 1.66 | 0.76 |
| 1:A:1403:LEU:C | 1:A:1403:LEU:HD13 | 2.06 | 0.76 |
| 2:D:146:VAL:HA | 2:D:149:ASN:OD1 | 1.85 | 0.76 |
| 1:A:1086:ILE:HD12 | 1:A:1089:ILE:HG12 | 1.67 | 0.76 |
| 1:C:1504:LEU:HD21 | 2:E:149:ASN:CB | 2.15 | 0.76 |
| 2:F:118:ALA:HA | 2:F:121:LYS:HE3 | 1.68 | 0.76 |
| 1:B:1107:VAL:HG12 | 1:B:1111:LEU:HB2 | 1.67 | 0.76 |
| 1:C:1387:LYS:HB2 | 1:C:1390:GLN:HB3 | 1.65 | 0.76 |
| 1:B:1232:VAL:C | 1:B:1234:LEU:N | 2.38 | 0.76 |
| 1:A:1257:CYS:HA | 1:A:1260:CYS:SG | 2.26 | 0.76 |
| 1:C:1253:TRP:C | 1:C:1255:GLU:H | 1.86 | 0.76 |
| 1:C:1214:ALA:O | 1:C:1218:TYR:HB2 | 1.84 | 0.76 |
| 1:A:1419:LEU:O | 1:A:1422:LEU:CB | 2.25 | 0.76 |
| 1:B:1403:LEU:O | 1:B:1403:LEU:HD13 | 1.86 | 0.76 |
| 1:B:1492:ASN:C | 1:B:1493:ILE:HG13 | 2.04 | 0.76 |
| 1:C:1277:VAL:HG23 | 1:C:1278:VAL:N | 2.01 | 0.76 |
| 1:C:1082:VAL:CG2 | 1:C:1107:VAL:HG21 | 2.14 | 0.76 |
| 1:C:1222:SER:C | 1:C:1223:ASN:CG | 2.23 | 0.76 |
| 1:B:1358:TRP:HE3 | 1:B:1377:THR:HG22 | 1.50 | 0.76 |
| 1:C:1403:LEU:HD13 | 1:C:1403:LEU:O | 1.86 | 0.76 |
| 1:C:1469:ASN:HA | 1:C:1472:ILE:HD12 | 1.67 | 0.76 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1361:LEU:HD23 | 1:A:1361:LEU:C | 2.05 | 0.76 |
| 1:C:1617:GLU:HA | 1:C:1620:ARG:NH1 | 2.01 | 0.76 |
| 1:C:1211:TYR:HD1 | 1:C:1231:LEU:HD22 | 0.95 | 0.76 |
| 1:C:1601:GLN:HG3 | 1:C:1604:LYS:HD2 | 1.69 | 0.76 |
| 1:B:1137:TYR:HB2 | 1:B:1138:MET:HB2 | 0.81 | 0.76 |
| 1:C:1431:ASP:O | 1:C:1433:THR:N | 2.15 | 0.76 |
| 1:A:1513:TYR:O | 1:A:1516:LYS:HG2 | 1.85 | 0.76 |
| 1:C:1414:PHE:HE1 | 2:E:127:TRP:CE3 | 2.04 | 0.75 |
| 1:C:1471:PHE:HA | 1:C:1474:GLU:HG2 | 1.67 | 0.75 |
| 1:B:1161:ARG:HH11 | 1:B:1194:ASN:HB2 | 1.50 | 0.75 |
| 1:A:1277:VAL:HG23 | 1:A:1278:VAL:N | 2.01 | 0.75 |
| 1:C:1290:TYR:HD2 | 1:C:1299:LEU:HD22 | 1.50 | 0.75 |
| 1:A:1601:GLN:HG3 | 1:A:1604:LYS:HD2 | 1.68 | 0.75 |
| 1:C:1475:GLU:HB2 | 2:E:145:GLN:HG3 | 1.69 | 0.75 |
| 1:B:1472:ILE:HA | 1:B:1507:PHE:CE1 | 2.19 | 0.75 |
| 1:B:1136:SER:CB | 1:B:1141:VAL:HG11 | 2.15 | 0.75 |
| 2:F:91:GLN:NE2 | 2:F:94:ARG:HG2 | 2.01 | 0.75 |
| 1:C:1257:CYS:HA | 1:C:1260:CYS:SG | 2.26 | 0.75 |
| 1:B:1609:LYS:HG2 | 1:B:1612:LYS:HD2 | 1.66 | 0.75 |
| 2:E:118:ALA:O | 2:E:122:VAL:HG22 | 1.87 | 0.75 |
| 1:A:1471:PHE:HA | 1:A:1474:GLU:HG2 | 1.67 | 0.75 |
| 1:B:1144:ALA:HB1 | 1:B:1149:ASN:CB | 2.14 | 0.75 |
| 1:C:1538:MET:HE3 | 1:C:1566:PHE:HB3 | 1.67 | 0.75 |
| 1:C:1198:ILE:CA | 1:C:1201:VAL:HG21 | 2.14 | 0.75 |
| 1:C:1475:GLU:OE1 | 2:E:145:GLN:HG3 | 1.85 | 0.75 |
| 1:B:1082:VAL:HG11 | 1:B:1105:PRO:CB | 2.16 | 0.75 |
| 1:B:1584:GLU:HA | 1:B:1587:TRP:CD2 | 2.21 | 0.75 |
| 2:E:118:ALA:HA | 2:E:121:LYS:CE | 2.15 | 0.75 |
| 1:A:1358:TRP:HE3 | 1:A:1377:THR:HG22 | 1.50 | 0.75 |
| 1:B:1617:GLU:HA | 1:B:1620:ARG:NH1 | 2.01 | 0.75 |
| 1:A:1584:GLU:HA | 1:A:1587:TRP:CD2 | 2.21 | 0.75 |
| 1:B:1535:LYS:NZ | 1:B:1563:ARG:HH12 | 1.85 | 0.75 |
| 1:C:1198:ILE:O | 1:C:1199:GLN:C | 2.23 | 0.75 |
| 1:A:1387:LYS:HB2 | 1:A:1390:GLN:HB3 | 1.65 | 0.75 |
| 1:C:1261:VAL:HG13 | 1:C:1295:TYR:CE1 | 2.22 | 0.75 |
| 1:A:1535:LYS:NZ | 1:A:1563:ARG:HH12 | 1.85 | 0.75 |
| 1:C:1584:GLU:HA | 1:C:1587:TRP:CD2 | 2.21 | 0.75 |
| 1:C:1591:ILE:HG23 | 1:C:1592:MET:H | 1.52 | 0.75 |
| 1:B:1218:TYR:HE2 | 1:B:1227:LEU:HB2 | 1.52 | 0.75 |
| 1:A:1144:ALA:O | 1:A:1153:LEU:HD13 | 1.87 | 0.75 |
| 1:C:1403:LEU:HD13 | 1:C:1403:LEU:C | 2.06 | 0.75 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1445:LEU:O | 1:A:1448:VAL:HG22 | 1.87 | 0.75 |
| 2:F:118:ALA:O | 2:F:122:VAL:HG22 | 1.87 | 0.75 |
| 1:B:1122:LYS:HG3 | 1:B:1123:GLU:N | 2.01 | 0.75 |
| 1:A:1274:LEU:C | 1:A:1277:VAL:HG22 | 2.08 | 0.74 |
| 1:C:1408:ILE:HG23 | 1:C:1412:LEU:HB2 | 1.69 | 0.74 |
| 1:C:1444:GLN:C | 1:C:1446:PRO:HD2 | 2.07 | 0.74 |
| 1:C:1190:ILE:CD1 | 1:C:1216:LEU:O | 2.35 | 0.74 |
| 1:B:1598:TYR:CE2 | 2:D:201:UNK:CA | 2.69 | 0.74 |
| 1:A:1427:SER:HB3 | 1:A:1428:PRO:HD3 | 1.67 | 0.74 |
| 1:B:1403:LEU:C | 1:B:1403:LEU:HD13 | 2.06 | 0.74 |
| 2:F:21:UNK:N | 2:F:21:UNK:C | 2.49 | 0.74 |
| 1:B:1192:GLY:N | 1:B:1193:PRO:HD3 | 2.01 | 0.74 |
| 1:C:1521:TRP:O | 1:C:1525:VAL:HG12 | 1.87 | 0.74 |
| 1:B:1274:LEU:HA | 1:B:1277:VAL:CG2 | 2.17 | 0.74 |
| 1:A:1602:VAL:O | 1:A:1606:TYR:HB2 | 1.87 | 0.74 |
| 1:B:1566:PHE:HE2 | 2:D:182:UNK:CB | 1.99 | 0.74 |
| 1:A:1535:LYS:HZ3 | 2:F:181:UNK:CB | 1.99 | 0.74 |
| 1:C:1412:LEU:HD21 | 1:C:1439:PHE:CE1 | 2.22 | 0.74 |
| 1:C:1504:LEU:HD21 | 2:E:149:ASN:CG | 2.07 | 0.74 |
| 1:A:1161:ARG:CZ | 1:A:1170:GLU:HB2 | 2.17 | 0.74 |
| 1:B:1521:TRP:O | 1:B:1525:VAL:HG12 | 1.87 | 0.74 |
| 1:A:1617:GLU:HA | 1:A:1620:ARG:NH1 | 2.01 | 0.74 |
| 1:C:1274:LEU:HA | 1:C:1277:VAL:CG2 | 2.18 | 0.74 |
| 1:B:1605:GLU:HB2 | 1:C:1580:ASP:OD1 | 1.86 | 0.74 |
| 1:A:1416:PRO:HD2 | 2:F:130:LYS:HD3 | 1.69 | 0.74 |
| 1:B:1412:LEU:HD21 | 1:B:1439:PHE:CE1 | 2.23 | 0.74 |
| 1:C:1602:VAL:O | 1:C:1606:TYR:HB2 | 1.88 | 0.74 |
| 1:C:1412:LEU:HB2 | 1:C:1419:LEU:HD13 | 1.70 | 0.74 |
| 1:C:1412:LEU:HD12 | 1:C:1419:LEU:HD21 | 1.66 | 0.74 |
| 2:E:118:ALA:HA | 2:E:121:LYS:HE3 | 1.68 | 0.74 |
| 1:A:1412:LEU:HD21 | 1:A:1439:PHE:CE1 | 2.23 | 0.74 |
| 1:A:1444:GLN:C | 1:A:1446:PRO:HD2 | 2.08 | 0.74 |
| 1:B:1444:GLN:C | 1:B:1446:PRO:HD2 | 2.08 | 0.74 |
| 1:A:1116:LEU:CD2 | 1:A:1122:LYS:HB3 | 2.17 | 0.74 |
| 1:C:1617:GLU:HG2 | 1:C:1621:LYS:HZ3 | 1.51 | 0.74 |
| 1:A:1274:LEU:HA | 1:A:1277:VAL:CG2 | 2.18 | 0.74 |
| 1:A:1332:MET:CE | 1:A:1357:LEU:HD13 | 2.18 | 0.74 |
| 1:B:1588:ARG:NH1 | 1:B:1588:ARG:HG3 | 2.00 | 0.74 |
| 1:A:1611:ASP:OD2 | 1:B:1607:LEU:CD2 | 2.36 | 0.74 |
| 1:C:1362:VAL:HG22 | 1:C:1377:THR:HG21 | 1.70 | 0.74 |
| 1:C:1409:GLN:HA | 1:C:1413:GLU:HG2 | 0.81 | 0.74 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:1445:LEU:O | 1:C:1448:VAL:HG22 | 1.88 | 0.74 |
| 1:B:1257:CYS:HA | 1:B:1260:CYS:SG | 2.27 | 0.74 |
| 1:B:1274:LEU:C | 1:B:1277:VAL:HG22 | 2.07 | 0.74 |
| 1:C:1597:PRO:HB3 | 1:C:1601:GLN:HE22 | 1.53 | 0.74 |
| 1:A:1579:PRO:CB | 1:C:1605:GLU:OE2 | 2.36 | 0.74 |
| 1:C:1177:LEU:HA | 1:C:1180:THR:OG1 | 1.87 | 0.74 |
| 2:E:146:VAL:O | 2:E:149:ASN:HB2 | 1.87 | 0.74 |
| 1:A:1521:TRP:O | 1:A:1525:VAL:HG12 | 1.87 | 0.74 |
| 1:A:1554:LEU:HA | 1:A:1557:PHE:HD2 | 1.53 | 0.74 |
| 2:F:146:VAL:O | 2:F:149:ASN:HB2 | 1.87 | 0.74 |
| 1:B:1445:LEU:O | 1:B:1448:VAL:HG22 | 1.88 | 0.74 |
| 1:B:1554:LEU:HA | 1:B:1557:PHE:HD2 | 1.53 | 0.74 |
| 1:C:1296:PHE:O | 1:C:1297:GLU:C | 2.26 | 0.74 |
| 1:A:1587:TRP:O | 1:A:1588:ARG:C | 2.26 | 0.74 |
| 1:B:1601:GLN:HG3 | 1:B:1604:LYS:HD2 | 1.68 | 0.74 |
| 1:C:1122:LYS:HG3 | 1:C:1123:GLU:N | 2.01 | 0.74 |
| 1:C:1115:GLN:HG3 | 1:C:1125:ILE:CD1 | 2.17 | 0.74 |
| 1:B:1209:LYS:HB3 | 1:B:1230:THR:HG22 | 1.69 | 0.74 |
| 1:A:1513:TYR:HD1 | 1:A:1516:LYS:HE2 | 1.53 | 0.74 |
| 1:A:1282:GLU:CG | 1:A:1283:LEU:H | 2.00 | 0.73 |
| 2:E:192:UNK:O | 2:E:193:UNK:C | 2.35 | 0.73 |
| 1:C:1198:ILE:HG12 | 1:C:1199:GLN:H | 1.52 | 0.73 |
| 1:A:1408:ILE:HG23 | 1:A:1412:LEU:HB2 | 1.68 | 0.73 |
| 1:B:1455:VAL:CG1 | 1:B:1456:GLN:H | 1.95 | 0.73 |
| 2:F:152:ASN:O | 2:F:153:ASN:HB2 | 1.88 | 0.73 |
| 1:A:1255:GLU:CA | 1:A:1289:TYR:HE2 | 2.01 | 0.73 |
| 1:C:1332:MET:CE | 1:C:1357:LEU:HD13 | 2.17 | 0.73 |
| 1:B:1597:PRO:HB3 | 1:B:1601:GLN:HE22 | 1.53 | 0.73 |
| 1:C:1535:LYS:NZ | 1:C:1563:ARG:HH12 | 1.85 | 0.73 |
| 1:C:1177:LEU:CD1 | 1:C:1189:PHE:HZ | 1.96 | 0.73 |
| 1:A:1412:LEU:HB2 | 1:A:1419:LEU:HD13 | 1.69 | 0.73 |
| 1:B:1427:SER:HB3 | 1:B:1428:PRO:HD3 | 1.67 | 0.73 |
| 1:C:1261:VAL:HG13 | 1:C:1295:TYR:CZ | 2.23 | 0.73 |
| 1:B:1282:GLU:CG | 1:B:1283:LEU:H | 2.00 | 0.73 |
| 1:B:1602:VAL:O | 1:B:1606:TYR:HB2 | 1.88 | 0.73 |
| 2:D:118:ALA:O | 2:D:122:VAL:HG22 | 1.87 | 0.73 |
| 2:D:129:GLU:HB2 | 2:D:132:LYS:HZ2 | 1.53 | 0.73 |
| 1:B:1162:LYS:O | 1:B:1163:LYS:HB2 | 1.88 | 0.73 |
| 1:B:1509:ARG:CZ | 2:D:163:GLN:HA | 2.17 | 0.73 |
| 1:B:1513:TYR:HD1 | 1:B:1516:LYS:HE2 | 1.54 | 0.73 |
| 1:B:1279:HIS:NE2 | 1:B:1283:LEU:HD11 | 2.02 | 0.73 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:E:129:GLU:HB2 | 2:E:132:LYS:HZ2 | 1.54 | 0.73 |
| 2:D:146:VAL:O | 2:D:149:ASN:HB2 | 1.87 | 0.73 |
| 1:A:1371:TYR:HB3 | 1:A:1394:ILE:HG22 | 1.69 | 0.73 |
| 1:C:1332:MET:HE2 | 1:C:1357:LEU:HD13 | 1.69 | 0.73 |
| 1:B:1264:LYS:NZ | 1:B:1268:LEU:CD1 | 2.51 | 0.73 |
| 1:C:1428:PRO:O | 1:C:1429:ARG:CB | 2.33 | 0.73 |
| 2:F:162:GLN:C | 2:F:166:ALA:CB | 2.51 | 0.73 |
| 1:B:1134:PRO:HD2 | 1:B:1156:TYR:HE1 | 1.54 | 0.73 |
| 1:C:1264:LYS:NZ | 1:C:1268:LEU:CD1 | 2.51 | 0.73 |
| 1:C:1290:TYR:CD2 | 1:C:1299:LEU:CD2 | 2.71 | 0.73 |
| 1:C:1198:ILE:CG1 | 1:C:1199:GLN:N | 2.51 | 0.73 |
| 1:B:1362:VAL:HG22 | 1:B:1377:THR:HG21 | 1.70 | 0.73 |
| 1:A:1472:ILE:HA | 1:A:1507:PHE:CE1 | 2.19 | 0.73 |
| 1:B:1167:SER:O | 1:B:1169:VAL:N | 2.20 | 0.73 |
| 2:F:183:UNK:O | 2:F:187:UNK:N | 2.21 | 0.73 |
| 1:B:1332:MET:CE | 1:B:1357:LEU:HD13 | 2.18 | 0.73 |
| 1:B:1084:VAL:HG13 | 1:B:1089:ILE:HG22 | 1.70 | 0.73 |
| 1:A:1332:MET:HG3 | 1:A:1357:LEU:CD1 | 2.19 | 0.73 |
| 1:A:1586:ALA:O | 1:A:1590:ASN:OD1 | 2.06 | 0.73 |
| 1:C:1554:LEU:HA | 1:C:1557:PHE:HD2 | 1.53 | 0.73 |
| 2:D:118:ALA:HA | 2:D:121:LYS:HE3 | 1.68 | 0.73 |
| 1:B:1371:TYR:HB3 | 1:B:1394:ILE:HG22 | 1.69 | 0.73 |
| 2:D:152:ASN:O | 2:D:153:ASN:HB2 | 1.88 | 0.73 |
| 1:A:1597:PRO:HB3 | 1:A:1601:GLN:HE22 | 1.53 | 0.73 |
| 1:C:1414:PHE:HE1 | 2:E:127:TRP:HZ3 | 1.34 | 0.73 |
| 1:B:1296:PHE:O | 1:B:1297:GLU:C | 2.26 | 0.73 |
| 2:E:155:ILE:HD12 | 2:E:155:ILE:N | 2.02 | 0.73 |
| 2:E:152:ASN:O | 2:E:153:ASN:HB2 | 1.89 | 0.73 |
| 1:A:1264:LYS:NZ | 1:A:1268:LEU:CD1 | 2.51 | 0.73 |
| 1:B:1292:ASP:O | 2:D:97:GLN:HA | 1.87 | 0.73 |
| 1:C:1414:PHE:O | 1:C:1416:PRO:CD | 2.23 | 0.73 |
| 1:C:1513:TYR:HD1 | 1:C:1516:LYS:HE2 | 1.54 | 0.73 |
| 1:C:1257:CYS:HB3 | 1:C:1289:TYR:OH | 1.89 | 0.72 |
| 1:C:1254:LYS:HA | 1:C:1289:TYR:CD2 | 2.24 | 0.72 |
| 1:B:1274:LEU:HA | 1:B:1277:VAL:HG21 | 1.71 | 0.72 |
| 1:B:1293:ARG:HG2 | 2:D:97:GLN:HE22 | 1.54 | 0.72 |
| 1:C:1122:LYS:HZ3 | 1:C:1147:SER:HB3 | 1.52 | 0.72 |
| 1:C:1434:ARG:HG3 | 2:E:4:UNK:O | 1.89 | 0.72 |
| 1:B:1428:PRO:O | 1:B:1429:ARG:CB | 2.34 | 0.72 |
| 1:A:1159:MET:SD | 1:A:1162:LYS:HB3 | 2.29 | 0.72 |
| 1:A:1198:ILE:HG23 | 1:A:1201:VAL:HG21 | 1.71 | 0.72 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:1261:VAL:HG13 | 1:B:1295:TYR:CE2 | 2.24 | 0.72 |
| 1:C:1387:LYS:CB | 1:C:1390:GLN:CB | 2.67 | 0.72 |
| 1:B:1206:TYR:CD1 | 1:B:1226:ARG:O | 2.42 | 0.72 |
| 1:C:1496:ALA:HB2 | 1:C:1514:LEU:HD22 | 1.70 | 0.72 |
| 1:C:1274:LEU:C | 1:C:1277:VAL:HG22 | 2.08 | 0.72 |
| 2:E:134:ASP:O | 2:E:137:GLU:HB2 | 1.89 | 0.72 |
| 1:B:1412:LEU:HB2 | 1:B:1419:LEU:HD13 | 1.70 | 0.72 |
| 1:C:1332:MET:HG3 | 1:C:1357:LEU:CD1 | 2.19 | 0.72 |
| 1:A:1588:ARG:HG3 | 1:A:1588:ARG:HH11 | 1.54 | 0.72 |
| 1:C:1358:TRP:HE3 | 1:C:1377:THR:HG22 | 1.51 | 0.72 |
| 1:C:1444:GLN:NE2 | 2:E:130:LYS:HD2 | 2.03 | 0.72 |
| 1:B:1330:GLN:HG3 | 1:B:1331:LYS:H | 1.55 | 0.72 |
| 1:B:1419:LEU:C | 1:B:1422:LEU:HB3 | 2.09 | 0.72 |
| 1:C:1371:TYR:HB3 | 1:C:1394:ILE:HG22 | 1.69 | 0.72 |
| 1:C:1215:LYS:O | 1:C:1217:LEU:N | 2.22 | 0.72 |
| 1:A:1296:PHE:O | 1:A:1297:GLU:C | 2.27 | 0.72 |
| 1:C:1274:LEU:HA | 1:C:1277:VAL:HG21 | 1.71 | 0.72 |
| 1:B:1592:MET:HG2 | 1:B:1593:ASP:H | 1.53 | 0.72 |
| 1:C:1588:ARG:NH1 | 2:D:197:UNK:CB | 2.53 | 0.72 |
| 1:B:1496:ALA:HB2 | 1:B:1514:LEU:HD22 | 1.70 | 0.72 |
| 1:A:1324:TYR:HD2 | 1:A:1332:MET:HA | 1.55 | 0.72 |
| 1:B:1167:SER:C | 1:B:1169:VAL:H | 1.93 | 0.72 |
| 1:B:1215:LYS:O | 1:B:1217:LEU:N | 2.23 | 0.72 |
| 1:C:1330:GLN:HG3 | 1:C:1331:LYS:H | 1.55 | 0.72 |
| 1:C:1358:TRP:CE3 | 1:C:1377:THR:HG22 | 2.24 | 0.72 |
| 2:D:127:TRP:CD1 | 2:D:128:ARG:HG3 | 2.24 | 0.72 |
| 1:A:1282:GLU:O | 1:A:1283:LEU:CB | 2.38 | 0.72 |
| 1:C:1253:TRP:O | 1:C:1289:TYR:CE2 | 2.41 | 0.72 |
| 2:D:106:ARG:HH21 | 2:D:106:ARG:HA | 1.55 | 0.72 |
| 2:F:200:UNK:C | 2:F:202:UNK:H | 2.00 | 0.72 |
| 1:C:1175:PHE:HE1 | 1:C:1200:GLN:HB3 | 1.52 | 0.72 |
| 2:E:127:TRP:CD1 | 2:E:128:ARG:HG3 | 2.25 | 0.72 |
| 1:A:1411:TYR:O | 1:A:1415:LYS:C | 2.27 | 0.72 |
| 1:A:1215:LYS:O | 1:A:1217:LEU:N | 2.22 | 0.72 |
| 1:A:1258:PHE:HE1 | 1:A:1293:ARG:HG3 | 1.55 | 0.71 |
| 2:F:194:UNK:C | 2:F:197:UNK:CB | 2.68 | 0.71 |
| 1:C:1119:GLY:O | 1:C:1120:MET:SD | 2.48 | 0.71 |
| 1:C:1149:ASN:O | 1:C:1153:LEU:CB | 2.38 | 0.71 |
| 1:B:1332:MET:HG3 | 1:B:1357:LEU:CD1 | 2.18 | 0.71 |
| 1:A:1209:LYS:HB2 | 1:A:1231:LEU:HB3 | 1.71 | 0.71 |
| 2:F:106:ARG:HH21 | 2:F:106:ARG:HA | 1.55 | 0.71 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:1588:ARG:HH21 | 2:D:192:UNK:C | 2.03 | 0.71 |
| 1:B:1598:TYR:OH | 2:D:197:UNK:O | 2.06 | 0.71 |
| 1:A:1419:LEU:C | 1:A:1422:LEU:HB3 | 2.09 | 0.71 |
| 1:A:1161:ARG:NE | 1:A:1173:LEU:HD23 | 2.05 | 0.71 |
| 1:A:1496:ALA:HB2 | 1:A:1514:LEU:HD22 | 1.70 | 0.71 |
| 1:B:1587:TRP:O | 1:B:1588:ARG:C | 2.29 | 0.71 |
| 1:B:1409:GLN:O | 1:B:1413:GLU:CB | 2.31 | 0.71 |
| 2:E:105:TRP:C | 2:E:108:GLU:HG3 | 2.10 | 0.71 |
| 1:B:1282:GLU:O | 1:B:1283:LEU:CB | 2.38 | 0.71 |
| 1:C:1586:ALA:HB3 | 1:C:1594:PHE:CZ | 2.24 | 0.71 |
| 2:F:126:GLU:HG3 | 2:F:130:LYS:HZ1 | 1.53 | 0.71 |
| 1:B:1112:ALA:HB1 | 1:B:1140:VAL:HG21 | 1.72 | 0.71 |
| 2:E:90:ALA:H | 2:E:91:GLN:HA | 1.55 | 0.71 |
| 1:C:1324:TYR:HD2 | 1:C:1332:MET:HA | 1.55 | 0.71 |
| 1:B:1572:THR:HG21 | 1:B:1599:PHE:HD2 | 1.55 | 0.71 |
| 1:C:1136:SER:CB | 1:C:1140:VAL:HG23 | 2.21 | 0.71 |
| 1:C:1122:LYS:NZ | 1:C:1147:SER:HB3 | 2.05 | 0.71 |
| 1:C:1130:LYS:HD2 | 1:C:1156:TYR:CD1 | 2.26 | 0.71 |
| 2:F:127:TRP:CD1 | 2:F:128:ARG:HG3 | 2.25 | 0.71 |
| 1:A:1362:VAL:CG2 | 1:A:1377:THR:HG21 | 2.21 | 0.71 |
| 1:A:1159:MET:CE | 1:A:1162:LYS:HD2 | 2.20 | 0.71 |
| 1:A:1180:THR:HG22 | 1:A:1181:ASN:ND2 | 2.05 | 0.71 |
| 1:A:1149:ASN:O | 1:A:1153:LEU:CB | 2.39 | 0.71 |
| 1:A:1150:TRP:O | 1:A:1153:LEU:N | 2.24 | 0.71 |
| 1:C:1244:ALA:H | 1:C:1275:HIS:CE1 | 2.07 | 0.71 |
| 1:B:1279:HIS:HD2 | 1:B:1282:GLU:HB3 | 1.55 | 0.71 |
| 1:C:1554:LEU:HD11 | 1:C:1568:ALA:HB2 | 1.73 | 0.71 |
| 1:A:1358:TRP:CE3 | 1:A:1377:THR:HG22 | 2.24 | 0.71 |
| 1:B:1411:TYR:O | 1:B:1415:LYS:O | 2.09 | 0.71 |
| 1:B:1266:PHE:HB2 | 1:B:1268:LEU:HG | 1.72 | 0.71 |
| 2:E:118:ALA:HA | 2:E:121:LYS:NZ | 2.06 | 0.71 |
| 1:A:1463:VAL:HG12 | 1:A:1467:LEU:HD22 | 1.73 | 0.71 |
| 1:B:1333:ARG:HB2 | 1:B:1360:GLU:CD | 2.11 | 0.71 |
| 1:A:1136:SER:CB | 1:A:1141:VAL:HG11 | 2.21 | 0.71 |
| 1:C:1247:ALA:O | 1:C:1247:ALA:CA | 2.39 | 0.71 |
| 1:B:1116:LEU:HD11 | 1:B:1122:LYS:HD3 | 1.71 | 0.71 |
| 1:A:1266:PHE:HB2 | 1:A:1268:LEU:HG | 1.72 | 0.71 |
| 1:C:1259:ALA:HA | 1:C:1293:ARG:NH1 | 2.05 | 0.71 |
| 1:A:1554:LEU:HD11 | 1:A:1568:ALA:HB2 | 1.73 | 0.71 |
| 1:C:1411:TYR:O | 1:C:1415:LYS:O | 2.09 | 0.71 |
| 1:B:1554:LEU:HD11 | 1:B:1568:ALA:HB2 | 1.73 | 0.71 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:1168:TYR:CD1 | 1:C:1168:TYR:N | 2.55 | 0.71 |
| 2:F:118:ALA:HA | 2:F:121:LYS:NZ | 2.06 | 0.71 |
| 1:A:1362:VAL:HG22 | 1:A:1377:THR:HG21 | 1.70 | 0.71 |
| 1:B:1161:ARG:NE | 1:B:1173:LEU:HD23 | 2.06 | 0.71 |
| 1:A:1274:LEU:HA | 1:A:1277:VAL:HG21 | 1.71 | 0.70 |
| 1:A:1598:TYR:CZ | 1:B:1584:GLU:OE2 | 2.44 | 0.70 |
| 1:C:1150:TRP:O | 1:C:1153:LEU:N | 2.24 | 0.70 |
| 1:A:1086:ILE:HB | 1:A:1089:ILE:HB | 1.73 | 0.70 |
| 1:A:1116:LEU:HD11 | 1:A:1122:LYS:HB3 | 1.73 | 0.70 |
| 1:A:1368:TYR:CD1 | 1:A:1370:GLU:CG | 2.75 | 0.70 |
| 2:F:134:ASP:O | 2:F:137:GLU:HB2 | 1.90 | 0.70 |
| 1:B:1358:TRP:CE3 | 1:B:1377:THR:HG22 | 2.24 | 0.70 |
| 1:C:1425:VAL:HG23 | 1:C:1426:LEU:N | 2.06 | 0.70 |
| 1:B:1324:TYR:HD2 | 1:B:1332:MET:HA | 1.55 | 0.70 |
| 1:A:1161:ARG:HE | 1:A:1173:LEU:HD23 | 1.55 | 0.70 |
| 1:B:1084:VAL:HB | 1:B:1098:PHE:CZ | 2.26 | 0.70 |
| 1:C:1266:PHE:HB2 | 1:C:1268:LEU:HG | 1.72 | 0.70 |
| 1:C:1295:TYR:O | 1:C:1296:PHE:CG | 2.44 | 0.70 |
| 1:A:1218:TYR:HE2 | 1:A:1227:LEU:HB2 | 1.56 | 0.70 |
| 1:B:1475:GLU:CD | 2:D:145:GLN:HB3 | 2.06 | 0.70 |
| 1:C:1620:ARG:HG3 | 1:C:1620:ARG:HH11 | 1.57 | 0.70 |
| 1:B:1358:TRP:HH2 | 1:B:1381:HIS:CE1 | 2.05 | 0.70 |
| 1:C:1419:LEU:C | 1:C:1422:LEU:HB3 | 2.09 | 0.70 |
| 1:B:1463:VAL:HG12 | 1:B:1467:LEU:HD22 | 1.73 | 0.70 |
| 2:D:118:ALA:HA | 2:D:121:LYS:NZ | 2.06 | 0.70 |
| 1:C:1481:ARG:HH11 | 1:C:1510:ILE:HG12 | 1.55 | 0.70 |
| 1:A:1588:ARG:NH1 | 1:A:1588:ARG:HG3 | 2.07 | 0.70 |
| 2:F:129:GLU:HB2 | 2:F:132:LYS:HZ2 | 1.56 | 0.70 |
| 1:C:1368:TYR:CD1 | 1:C:1370:GLU:CG | 2.74 | 0.70 |
| 1:B:1368:TYR:CD1 | 1:B:1370:GLU:CG | 2.75 | 0.70 |
| 1:B:1206:TYR:CD2 | 1:B:1226:ARG:HG3 | 2.26 | 0.70 |
| 1:B:1598:TYR:CE2 | 2:D:200:UNK:CB | 2.74 | 0.70 |
| 1:A:1428:PRO:O | 1:A:1429:ARG:CB | 2.34 | 0.70 |
| 1:A:1608:THR:HG23 | 1:B:1607:LEU:CD1 | 2.22 | 0.70 |
| 1:C:1594:PHE:O | 1:C:1596:MET:HG3 | 1.91 | 0.70 |
| 2:F:191:UNK:O | 2:F:192:UNK:C | 2.39 | 0.70 |
| 1:B:1362:VAL:CG2 | 1:B:1377:THR:HG21 | 2.21 | 0.70 |
| 1:C:1479:ALA:O | 1:C:1483:SER:N | 2.23 | 0.70 |
| 1:A:1466:SER:O | 1:A:1470:LEU:HG | 1.92 | 0.70 |
| 1:A:1588:ARG:NH2 | 2:E:192:UNK:CA | 2.51 | 0.70 |
| 1:C:1253:TRP:CE3 | 1:C:1276:ILE:CB | 2.75 | 0.70 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:1253:TRP:CE3 | 1:B:1276:ILE:CB | 2.75 | 0.70 |
| 2:F:194:UNK:C | 2:F:197:UNK:HA | 2.20 | 0.70 |
| 1:B:1425:VAL:HG23 | 1:B:1426:LEU:N | 2.06 | 0.70 |
| 1:B:1466:SER:O | 1:B:1470:LEU:HG | 1.92 | 0.70 |
| 1:A:1333:ARG:HB2 | 1:A:1360:GLU:CD | 2.12 | 0.70 |
| 2:D:180:UNK:C | 2:D:183:UNK:CB | 2.69 | 0.70 |
| 2:E:189:UNK:CA | 2:E:195:UNK:N | 2.55 | 0.70 |
| 1:C:1192:GLY:H | 1:C:1193:PRO:CD | 2.03 | 0.70 |
| 1:A:1281:ASP:CB | 1:A:1281:ASP:N | 2.54 | 0.70 |
| 1:A:1425:VAL:HG23 | 1:A:1426:LEU:N | 2.05 | 0.70 |
| 1:B:1116:LEU:CD1 | 1:B:1122:LYS:HD3 | 2.21 | 0.70 |
| 1:A:1587:TRP:CH2 | 1:C:1601:GLN:HG2 | 2.27 | 0.69 |
| 1:C:1362:VAL:CG2 | 1:C:1377:THR:HG21 | 2.21 | 0.69 |
| 1:C:1290:TYR:HE2 | 1:C:1299:LEU:CD1 | 1.96 | 0.69 |
| 1:C:1412:LEU:N | 1:C:1419:LEU:HD13 | 2.07 | 0.69 |
| 1:A:1157:LEU:HD13 | 1:A:1177:LEU:HD23 | 1.73 | 0.69 |
| 1:A:1496:ALA:HB3 | 1:A:1515:PHE:CZ | 2.28 | 0.69 |
| 2:F:98:GLU:HB2 | 2:F:99:PRO:HD3 | 1.74 | 0.69 |
| 1:A:1330:GLN:HG3 | 1:A:1331:LYS:H | 1.55 | 0.69 |
| 1:A:1382:PRO:HG3 | 1:A:1410:PHE:HE1 | 1.57 | 0.69 |
| 1:B:1496:ALA:HB3 | 1:B:1515:PHE:CZ | 2.28 | 0.69 |
| 1:C:1615:ALA:O | 1:C:1619:LEU:HD23 | 1.93 | 0.69 |
| 2:E:180:UNK:O | 2:E:181:UNK:C | 2.40 | 0.69 |
| 1:A:1258:PHE:CE1 | 1:A:1293:ARG:HG3 | 2.27 | 0.69 |
| 1:C:1182:ARG:H | 1:C:1183:LEU:HG | 1.57 | 0.69 |
| 1:C:1215:LYS:C | 1:C:1217:LEU:H | 1.96 | 0.69 |
| 1:A:1232:VAL:HG22 | 1:A:1233:HIS:N | 2.06 | 0.69 |
| 1:C:1333:ARG:HB2 | 1:C:1360:GLU:CD | 2.12 | 0.69 |
| 1:C:1377:THR:HA | 1:C:1381:HIS:HD2 | 1.56 | 0.69 |
| 1:A:1448:VAL:HB | 1:A:1451:TYR:HD2 | 1.58 | 0.69 |
| 1:A:1111:LEU:HD11 | 1:A:1125:ILE:HG13 | 1.72 | 0.69 |
| 1:B:1303:LEU:O | 1:B:1307:LEU:HD13 | 1.92 | 0.69 |
| 1:A:1566:PHE:CE2 | 2:F:180:UNK:CB | 2.74 | 0.69 |
| 2:F:195:UNK:C | 2:F:197:UNK:H2 | 2.06 | 0.69 |
| 1:C:1382:PRO:HG3 | 1:C:1410:PHE:HE1 | 1.57 | 0.69 |
| 1:B:1448:VAL:HB | 1:B:1451:TYR:HD2 | 1.57 | 0.69 |
| 2:D:189:UNK:O | 2:D:190:UNK:C | 2.40 | 0.69 |
| 1:B:1190:ILE:HD13 | 1:B:1216:LEU:HD11 | 1.73 | 0.69 |
| 1:A:1253:TRP:CE3 | 1:A:1276:ILE:CB | 2.75 | 0.69 |
| 1:C:1409:GLN:O | 1:C:1413:GLU:CB | 2.31 | 0.69 |
| 1:B:1168:TYR:CD1 | 1:B:1168:TYR:N | 2.59 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:1494:SER:HA | 1:C:1497:GLN:CG | 2.22 | 0.69 |
| 1:A:1103:ASN:O | 1:A:1105:PRO:HD3 | 1.91 | 0.69 |
| 1:C:1317:PHE:HD2 | 1:C:1317:PHE:N | 1.91 | 0.69 |
| 1:A:1290:TYR:CD2 | 1:A:1295:TYR:HE2 | 2.10 | 0.69 |
| 1:C:1596:MET:CE | 1:C:1597:PRO:HD3 | 2.23 | 0.69 |
| 1:B:1588:ARG:CZ | 2:F:190:UNK:O | 2.40 | 0.69 |
| 1:C:1167:SER:O | 1:C:1171:THR:N | 2.26 | 0.69 |
| 1:B:1377:THR:HA | 1:B:1381:HIS:HD2 | 1.57 | 0.69 |
| 1:C:1463:VAL:HG12 | 1:C:1467:LEU:HD22 | 1.73 | 0.69 |
| 1:B:1412:LEU:N | 1:B:1419:LEU:HD13 | 2.08 | 0.69 |
| 1:B:1416:PRO:CG | 2:D:130:LYS:CG | 2.63 | 0.69 |
| 2:E:108:GLU:OE1 | 2:E:108:GLU:C | 2.31 | 0.69 |
| 2:D:174:UNK:N | 2:D:176:UNK:N | 2.41 | 0.69 |
| 1:B:1509:ARG:NH1 | 2:D:163:GLN:HA | 2.08 | 0.69 |
| 1:B:1085:LEU:HD22 | 1:B:1125:ILE:HD11 | 1.73 | 0.69 |
| 1:A:1386:TRP:CZ2 | 1:A:1388:GLU:HA | 2.28 | 0.69 |
| 1:A:1387:LYS:CB | 1:A:1390:GLN:CB | 2.67 | 0.69 |
| 1:B:1521:TRP:CZ3 | 1:B:1522:LYS:HD2 | 2.28 | 0.69 |
| 1:A:1615:ALA:O | 1:A:1619:LEU:HD23 | 1.92 | 0.69 |
| 1:A:1620:ARG:HG3 | 1:A:1620:ARG:HH11 | 1.57 | 0.69 |
| 1:C:1113:LYS:HG3 | 1:C:1139:GLU:CD | 2.13 | 0.69 |
| 1:C:1098:PHE:O | 1:C:1102:CYS:HB3 | 1.91 | 0.69 |
| 1:C:1482:THR:HA | 1:C:1485:ASP:OD2 | 1.93 | 0.69 |
| 1:A:1409:GLN:O | 1:A:1413:GLU:CB | 2.31 | 0.69 |
| 1:A:1303:LEU:O | 1:A:1307:LEU:HD13 | 1.92 | 0.69 |
| 1:A:1279:HIS:NE2 | 1:A:1283:LEU:HD11 | 1.87 | 0.69 |
| 1:C:1279:HIS:NE2 | 1:C:1283:LEU:CD1 | 2.56 | 0.69 |
| 1:A:1586:ALA:O | 1:A:1590:ASN:CG | 2.31 | 0.69 |
| 1:A:1402:GLU:OE1 | 1:A:1402:GLU:C | 2.32 | 0.69 |
| 1:C:1303:LEU:O | 1:C:1307:LEU:HD13 | 1.92 | 0.69 |
| 1:A:1209:LYS:HB3 | 1:A:1230:THR:HG22 | 1.73 | 0.69 |
| 1:C:1496:ALA:HB3 | 1:C:1515:PHE:CZ | 2.28 | 0.69 |
| 1:B:1615:ALA:O | 1:B:1619:LEU:HD23 | 1.92 | 0.69 |
| 1:A:1482:THR:HA | 1:A:1485:ASP:OD2 | 1.93 | 0.69 |
| 1:C:1234:LEU:HD21 | 1:C:1264:LYS:HZ3 | 1.58 | 0.68 |
| 1:A:1605:GLU:HB2 | 1:B:1580:ASP:OD1 | 1.93 | 0.68 |
| 1:C:1120:MET:O | 1:C:1121:VAL:HG13 | 1.93 | 0.68 |
| 1:C:1466:SER:O | 1:C:1470:LEU:HG | 1.92 | 0.68 |
| 1:B:1327:PHE:HE1 | 2:D:104:LYS:HG3 | 1.58 | 0.68 |
| 1:B:1414:PHE:HD1 | 2:D:127:TRP:CB | 2.06 | 0.68 |
| 2:D:127:TRP:HA | 2:D:130:LYS:CE | 2.23 | 0.68 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1159:MET:HE1 | 1:A:1162:LYS:HD2 | 1.73 | 0.68 |
| 1:A:1494:SER:HA | 1:A:1497:GLN:CG | 2.23 | 0.68 |
| 1:B:1085:LEU:O | 1:B:1085:LEU:HD12 | 1.93 | 0.68 |
| 1:B:1122:LYS:O | 1:B:1126:ASP:CB | 2.41 | 0.68 |
| 1:A:1130:LYS:HZ3 | 1:A:1155:LYS:HB3 | 1.57 | 0.68 |
| 1:A:1521:TRP:CZ3 | 1:A:1522:LYS:HD2 | 2.28 | 0.68 |
| 1:C:1465:GLU:CD | 1:C:1465:GLU:C | 2.52 | 0.68 |
| 1:B:1382:PRO:HG3 | 1:B:1410:PHE:HE1 | 1.57 | 0.68 |
| 1:C:1349:LEU:HA | 1:C:1352:ALA:HB3 | 1.76 | 0.68 |
| 1:A:1168:TYR:N | 1:A:1168:TYR:CD1 | 2.60 | 0.68 |
| 1:A:1157:LEU:HD13 | 1:A:1177:LEU:CD2 | 2.23 | 0.68 |
| 1:B:1174:ILE:CG2 | 1:B:1201:VAL:HG22 | 2.23 | 0.68 |
| 1:B:1617:GLU:HG2 | 1:B:1621:LYS:HZ3 | 1.58 | 0.68 |
| 1:C:1113:LYS:HG3 | 1:C:1139:GLU:OE2 | 1.94 | 0.68 |
| 1:A:1290:TYR:CD2 | 1:A:1295:TYR:CE2 | 2.80 | 0.68 |
| 1:C:1402:GLU:OE1 | 1:C:1402:GLU:C | 2.31 | 0.68 |
| 1:B:1494:SER:HA | 1:B:1497:GLN:CG | 2.23 | 0.68 |
| 1:B:1386:TRP:CZ2 | 1:B:1388:GLU:HA | 2.28 | 0.68 |
| 1:C:1142:GLN:C | 1:C:1142:GLN:OE1 | 2.31 | 0.68 |
| 1:C:1270:GLN:HG3 | 1:C:1298:GLU:HG3 | 1.75 | 0.68 |
| 2:E:127:TRP:HA | 2:E:130:LYS:CE | 2.23 | 0.68 |
| 1:A:1192:GLY:N | 1:A:1193:PRO:HD3 | 2.07 | 0.68 |
| 1:B:1170:GLU:CD | 1:B:1196:ALA:HB2 | 2.14 | 0.68 |
| 1:B:1209:LYS:HB2 | 1:B:1231:LEU:HB3 | 1.75 | 0.68 |
| 1:A:1263:GLY:O | 1:A:1264:LYS:HB3 | 1.94 | 0.68 |
| 1:C:1191:ASN:N | 1:C:1191:ASN:ND2 | 2.42 | 0.68 |
| 1:B:1537:ALA:HA | 1:B:1540:TYR:CZ | 2.28 | 0.68 |
| 2:E:110:ARG:HB2 | 2:E:110:ARG:CZ | 2.24 | 0.68 |
| 1:A:1142:GLN:C | 1:A:1142:GLN:OE1 | 2.32 | 0.68 |
| 2:F:195:UNK:O | 2:F:196:UNK:C | 2.38 | 0.68 |
| 1:C:1122:LYS:O | 1:C:1126:ASP:CB | 2.41 | 0.68 |
| 1:C:1157:LEU:HB2 | 1:C:1173:LEU:HD13 | 1.75 | 0.68 |
| 1:A:1377:THR:HA | 1:A:1381:HIS:HD2 | 1.57 | 0.68 |
| 1:B:1327:PHE:CE1 | 2:D:104:LYS:HG3 | 2.28 | 0.68 |
| 1:B:1408:ILE:CG2 | 1:B:1412:LEU:HB2 | 2.23 | 0.68 |
| 2:E:104:LYS:O | 2:E:108:GLU:HB3 | 1.92 | 0.68 |
| 1:B:1384:ASP:OD1 | 2:D:115:GLU:OE1 | 2.11 | 0.68 |
| 1:B:1509:ARG:HH12 | 2:D:163:GLN:HA | 1.58 | 0.68 |
| 1:C:1386:TRP:CZ2 | 1:C:1388:GLU:HA | 2.28 | 0.68 |
| 1:C:1537:ALA:HA | 1:C:1540:TYR:CZ | 2.28 | 0.68 |
| 1:B:1317:PHE:HD2 | 1:B:1317:PHE:N | 1.91 | 0.68 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:1087:GLU:O | 1:C:1088:HIS:HB2 | 1.93 | 0.68 |
| 2:E:100:GLU:OE2 | 2:E:103:ARG:HD2 | 1.94 | 0.68 |
| 1:B:1594:PHE:O | 1:B:1596:MET:HG3 | 1.94 | 0.68 |
| 1:B:1566:PHE:CE2 | 2:D:182:UNK:CB | 2.77 | 0.68 |
| 1:C:1588:ARG:HH21 | 2:D:193:UNK:CA | 2.03 | 0.68 |
| 1:C:1168:TYR:HA | 1:C:1172:GLU:OE2 | 1.93 | 0.68 |
| 1:B:1349:LEU:HA | 1:B:1352:ALA:HB3 | 1.76 | 0.68 |
| 1:A:1082:VAL:HG21 | 1:A:1105:PRO:HG3 | 1.76 | 0.68 |
| 1:B:1620:ARG:HG3 | 1:B:1620:ARG:HH11 | 1.57 | 0.68 |
| 1:C:1566:PHE:CE2 | 2:E:181:UNK:HA | 2.28 | 0.68 |
| 2:E:110:ARG:NH2 | 2:E:110:ARG:HB2 | 2.09 | 0.68 |
| 2:D:110:ARG:HB2 | 2:D:110:ARG:CZ | 2.23 | 0.68 |
| 1:C:1136:SER:HB2 | 1:C:1140:VAL:HG23 | 1.76 | 0.68 |
| 1:C:1455:VAL:CG1 | 1:C:1456:GLN:H | 1.95 | 0.68 |
| 1:A:1349:LEU:HA | 1:A:1352:ALA:HB3 | 1.76 | 0.68 |
| 1:B:1420:ASN:HA | 1:B:1423:LEU:HG | 1.76 | 0.68 |
| 1:A:1197:HIS:C | 1:A:1199:GLN:H | 1.96 | 0.68 |
| 1:A:1327:PHE:O | 1:A:1329:PRO:HD3 | 1.94 | 0.68 |
| 1:B:1263:GLY:O | 1:B:1264:LYS:HB3 | 1.93 | 0.68 |
| 1:B:1568:ALA:HB1 | 1:B:1578:ARG:NH2 | 2.09 | 0.68 |
| 1:B:1218:TYR:CD2 | 1:B:1227:LEU:HD12 | 2.29 | 0.68 |
| 1:B:1122:LYS:HA | 1:B:1125:ILE:CG2 | 2.20 | 0.68 |
| 2:E:90:ALA:HB3 | 2:E:91:GLN:HA | 1.75 | 0.68 |
| 1:A:1588:ARG:CD | 2:E:195:UNK:CB | 2.70 | 0.68 |
| 1:C:1199:GLN:OE1 | 1:C:1199:GLN:HA | 1.92 | 0.68 |
| 1:C:1376:ILE:HD13 | 1:C:1379:MET:SD | 2.34 | 0.68 |
| 1:A:1617:GLU:HG2 | 1:A:1621:LYS:HZ3 | 1.59 | 0.68 |
| 2:F:110:ARG:CZ | 2:F:110:ARG:HB2 | 2.24 | 0.68 |
| 1:A:1246:LYS:O | 1:A:1247:ALA:HB3 | 1.92 | 0.68 |
| 1:A:1279:HIS:CG | 1:A:1282:GLU:HB3 | 2.29 | 0.67 |
| 1:C:1161:ARG:HH22 | 1:C:1174:ILE:HD11 | 1.58 | 0.67 |
| 1:B:1402:GLU:OE1 | 1:B:1402:GLU:C | 2.32 | 0.67 |
| 1:A:1223:ASN:CB | 1:A:1223:ASN:N | 2.55 | 0.67 |
| 1:B:1107:VAL:CG1 | 1:B:1111:LEU:HB2 | 2.24 | 0.67 |
| 1:A:1122:LYS:O | 1:A:1126:ASP:CB | 2.41 | 0.67 |
| 1:A:1326:LYS:HZ3 | 1:A:1354:GLN:HG2 | 1.59 | 0.67 |
| 1:B:1475:GLU:OE2 | 2:D:149:ASN:OD1 | 2.12 | 0.67 |
| 1:A:1174:ILE:HG21 | 1:A:1201:VAL:CG2 | 2.24 | 0.67 |
| 1:A:1279:HIS:CD2 | 1:A:1282:GLU:N | 2.60 | 0.67 |
| 1:C:1584:GLU:HA | 1:C:1587:TRP:CE2 | 2.30 | 0.67 |
| 1:B:1327:PHE:O | 1:B:1329:PRO:HD3 | 1.94 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1167:SER:C | 1:A:1169:VAL:H | 1.97 | 0.67 |
| 1:C:1527:LEU:HD21 | 1:C:1540:TYR:OH | 1.95 | 0.67 |
| 1:A:1317:PHE:N | 1:A:1317:PHE:HD2 | 1.91 | 0.67 |
| 1:B:1482:THR:HA | 1:B:1485:ASP:OD2 | 1.93 | 0.67 |
| 1:C:1211:TYR:CE1 | 1:C:1231:LEU:CD2 | 2.72 | 0.67 |
| 1:C:1420:ASN:HA | 1:C:1423:LEU:HG | 1.76 | 0.67 |
| 1:C:1188:GLU:OE2 | 1:C:1191:ASN:CB | 2.34 | 0.67 |
| 1:B:1082:VAL:HG11 | 1:B:1105:PRO:HB2 | 1.77 | 0.67 |
| 1:A:1537:ALA:HA | 1:A:1540:TYR:CZ | 2.29 | 0.67 |
| 1:B:1215:LYS:C | 1:B:1217:LEU:H | 1.96 | 0.67 |
| 2:F:110:ARG:NH2 | 2:F:110:ARG:HB2 | 2.09 | 0.67 |
| 1:C:1263:GLY:O | 1:C:1264:LYS:HB3 | 1.94 | 0.67 |
| 1:C:1296:PHE:CD2 | 1:C:1297:GLU:HG2 | 2.29 | 0.67 |
| 1:A:1107:VAL:CG1 | 1:A:1111:LEU:HB2 | 2.24 | 0.67 |
| 1:A:1465:GLU:C | 1:A:1465:GLU:CD | 2.52 | 0.67 |
| 1:B:1142:GLN:C | 1:B:1142:GLN:OE1 | 2.31 | 0.67 |
| 1:A:1257:CYS:SG | 1:A:1269:ALA:HB1 | 2.35 | 0.67 |
| 1:B:1257:CYS:SG | 1:B:1269:ALA:HB1 | 2.35 | 0.67 |
| 1:B:1584:GLU:HA | 1:B:1587:TRP:CE2 | 2.30 | 0.67 |
| 1:C:1448:VAL:HB | 1:C:1451:TYR:HD2 | 1.57 | 0.67 |
| 1:B:1465:GLU:C | 1:B:1465:GLU:CD | 2.52 | 0.67 |
| 1:B:1596:MET:CE | 1:B:1597:PRO:HD3 | 2.23 | 0.67 |
| 1:C:1414:PHE:CE1 | 2:E:127:TRP:CE3 | 2.83 | 0.67 |
| 1:B:1333:ARG:CB | 1:B:1360:GLU:CG | 2.73 | 0.67 |
| 2:D:133:LYS:HA | 2:D:133:LYS:HZ2 | 1.59 | 0.67 |
| 1:A:1572:THR:HG21 | 1:A:1599:PHE:HD2 | 1.59 | 0.67 |
| 1:B:1551:GLU:CD | 1:B:1582:VAL:HG22 | 2.15 | 0.67 |
| 2:E:119:ALA:C | 2:E:123:MET:HG2 | 2.15 | 0.67 |
| 1:A:1167:SER:O | 1:A:1168:TYR:CG | 2.47 | 0.67 |
| 1:B:1232:VAL:HG22 | 1:B:1233:HIS:N | 2.06 | 0.67 |
| 2:D:110:ARG:HB2 | 2:D:110:ARG:NH2 | 2.09 | 0.67 |
| 1:C:1199:GLN:C | 1:C:1201:VAL:H | 1.97 | 0.67 |
| 2:F:127:TRP:HA | 2:F:130:LYS:CE | 2.23 | 0.67 |
| 1:A:1083:GLN:NE2 | 1:A:1107:VAL:HG23 | 2.09 | 0.67 |
| 1:C:1327:PHE:O | 1:C:1329:PRO:HD3 | 1.94 | 0.66 |
| 1:C:1372:ASP:OD1 | 1:C:1373:ASN:N | 2.28 | 0.66 |
| 1:C:1474:GLU:O | 2:E:141:ARG:HD3 | 1.95 | 0.66 |
| 2:E:181:UNK:O | 2:E:183:UNK:N | 2.28 | 0.66 |
| 1:A:1420:ASN:HA | 1:A:1423:LEU:HG | 1.76 | 0.66 |
| 1:A:1479:ALA:O | 1:A:1483:SER:N | 2.23 | 0.66 |
| 1:B:1479:ALA:O | 1:B:1483:SER:N | 2.23 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1136:SER:HA | 1:A:1141:VAL:HG21 | 1.78 | 0.66 |
| 1:B:1527:LEU:HD21 | 1:B:1540:TYR:OH | 1.95 | 0.66 |
| 1:C:1521:TRP:CZ3 | 1:C:1522:LYS:HD2 | 2.29 | 0.66 |
| 1:C:1594:PHE:O | 1:C:1596:MET:HE3 | 1.95 | 0.66 |
| 2:D:133:LYS:HA | 2:D:133:LYS:HZ1 | 1.59 | 0.66 |
| 1:B:1180:THR:HG22 | 1:B:1181:ASN:OD1 | 1.95 | 0.66 |
| 1:A:1215:LYS:C | 1:A:1217:LEU:H | 1.96 | 0.66 |
| 1:C:1257:CYS:SG | 1:C:1269:ALA:HB1 | 2.35 | 0.66 |
| 1:B:1600:ILE:O | 1:B:1604:LYS:HG3 | 1.95 | 0.66 |
| 1:C:1379:MET:HE1 | 1:C:1406:ARG:HD3 | 1.77 | 0.66 |
| 1:B:1372:ASP:OD1 | 1:B:1373:ASN:N | 2.28 | 0.66 |
| 1:C:1092:LEU:C | 1:C:1094:ARG:N | 2.46 | 0.66 |
| 1:A:1384:ASP:OD1 | 2:F:115:GLU:CD | 2.32 | 0.66 |
| 1:B:1083:GLN:NE2 | 1:B:1106:ALA:HB3 | 2.10 | 0.66 |
| 2:E:112:ARG:O | 2:E:113:LEU:C | 2.32 | 0.66 |
| 1:C:1199:GLN:C | 1:C:1201:VAL:N | 2.46 | 0.66 |
| 1:A:1362:VAL:CG2 | 1:A:1377:THR:CG2 | 2.74 | 0.66 |
| 1:C:1091:ASN:O | 1:C:1092:LEU:HD12 | 1.95 | 0.66 |
| 1:C:1215:LYS:HD3 | 1:C:1216:LEU:N | 2.11 | 0.66 |
| 2:D:103:ARG:NH1 | 2:D:106:ARG:HG3 | 2.11 | 0.66 |
| 2:E:89:ILE:N | 2:E:90:ALA:HA | 2.08 | 0.66 |
| 1:A:1333:ARG:CB | 1:A:1360:GLU:CG | 2.73 | 0.66 |
| 1:B:1253:TRP:C | 1:B:1255:GLU:N | 2.47 | 0.66 |
| 1:A:1584:GLU:HA | 1:A:1587:TRP:CE2 | 2.30 | 0.66 |
| 1:B:1547:THR:HG23 | 1:B:1577:LEU:HB2 | 1.78 | 0.66 |
| 1:B:1387:LYS:CB | 1:B:1390:GLN:CB | 2.67 | 0.66 |
| 2:F:154:ARG:HB3 | 2:F:154:ARG:NH1 | 2.11 | 0.66 |
| 1:A:1206:TYR:CD1 | 1:A:1226:ARG:O | 2.48 | 0.66 |
| 1:A:1253:TRP:C | 1:A:1255:GLU:N | 2.48 | 0.66 |
| 1:C:1277:VAL:O | 1:C:1278:VAL:C | 2.34 | 0.66 |
| 1:B:1572:THR:HG21 | 1:B:1599:PHE:CE2 | 2.31 | 0.66 |
| 1:B:1601:GLN:CD | 1:C:1587:TRP:CH2 | 2.69 | 0.66 |
| 1:A:1280:ALA:CA | 1:A:1280:ALA:O | 2.40 | 0.66 |
| 2:E:134:ASP:O | 2:E:137:GLU:CB | 2.43 | 0.66 |
| 1:A:1447:LEU:O | 1:A:1450:PRO:HD2 | 1.96 | 0.66 |
| 1:A:1161:ARG:NH2 | 1:A:1174:ILE:HG13 | 2.11 | 0.66 |
| 1:C:1371:TYR:CD1 | 1:C:1394:ILE:HG22 | 2.30 | 0.66 |
| 1:B:1198:ILE:O | 1:B:1198:ILE:CG2 | 2.44 | 0.66 |
| 2:D:154:ARG:HB3 | 2:D:154:ARG:NH1 | 2.11 | 0.66 |
| 1:A:1234:LEU:CG | 1:A:1235:GLY:H | 2.09 | 0.66 |
| 1:A:1332:MET:SD | 1:A:1360:GLU:CG | 2.84 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:1230:THR:O | 1:C:1231:LEU:CB | 2.44 | 0.66 |
| 1:C:1332:MET:SD | 1:C:1360:GLU:CG | 2.83 | 0.66 |
| 1:C:1333:ARG:CB | 1:C:1360:GLU:CG | 2.74 | 0.66 |
| 1:C:1336:LEU:HD12 | 1:C:1360:GLU:HB3 | 1.78 | 0.66 |
| 1:C:1600:ILE:O | 1:C:1604:LYS:HG3 | 1.95 | 0.66 |
| 1:B:1588:ARG:NH2 | 2:F:192:UNK:H2 | 1.93 | 0.66 |
| 1:B:1447:LEU:O | 1:B:1450:PRO:HD2 | 1.96 | 0.66 |
| 1:B:1371:TYR:CD1 | 1:B:1394:ILE:HG22 | 2.30 | 0.66 |
| 1:B:1122:LYS:CA | 1:B:1125:ILE:HG22 | 2.21 | 0.66 |
| 1:B:1624:GLU:C | 1:B:1626:ALA:H | 1.98 | 0.66 |
| 2:F:112:ARG:O | 2:F:113:LEU:C | 2.32 | 0.66 |
| 1:A:1336:LEU:HD12 | 1:A:1360:GLU:HB3 | 1.78 | 0.66 |
| 1:A:1578:ARG:HD3 | 1:A:1582:VAL:HB | 1.78 | 0.66 |
| 1:C:1406:ARG:O | 1:C:1409:GLN:HB3 | 1.95 | 0.66 |
| 1:A:1358:TRP:CE2 | 1:A:1381:HIS:ND1 | 2.64 | 0.66 |
| 1:A:1136:SER:HB3 | 1:A:1141:VAL:HG11 | 1.76 | 0.66 |
| 1:B:1168:TYR:HA | 1:B:1172:GLU:OE2 | 1.95 | 0.66 |
| 1:B:1192:GLY:N | 1:B:1193:PRO:CD | 2.59 | 0.66 |
| 1:A:1116:LEU:HD21 | 1:A:1122:LYS:HB3 | 1.77 | 0.66 |
| 1:A:1130:LYS:HG2 | 1:A:1156:TYR:CZ | 2.31 | 0.66 |
| 1:A:1527:LEU:HD21 | 1:A:1540:TYR:OH | 1.95 | 0.66 |
| 1:A:1596:MET:CE | 1:A:1597:PRO:HD3 | 2.26 | 0.66 |
| 1:C:1588:ARG:NH2 | 2:D:193:UNK:O | 2.27 | 0.66 |
| 1:C:1082:VAL:HG22 | 1:C:1107:VAL:CG2 | 2.20 | 0.66 |
| 1:A:1372:ASP:OD1 | 1:A:1373:ASN:N | 2.28 | 0.66 |
| 1:A:1406:ARG:O | 1:A:1409:GLN:HB3 | 1.95 | 0.66 |
| 1:B:1167:SER:O | 1:B:1168:TYR:CD1 | 2.49 | 0.66 |
| 1:A:1539:GLN:NE2 | 2:F:177:UNK:CB | 2.59 | 0.66 |
| 1:A:1255:GLU:N | 1:A:1289:TYR:CE2 | 2.65 | 0.65 |
| 1:C:1279:HIS:NE2 | 1:C:1283:LEU:HD11 | 2.10 | 0.65 |
| 1:C:1258:PHE:CE1 | 1:C:1293:ARG:CZ | 2.80 | 0.65 |
| 1:C:1362:VAL:CG2 | 1:C:1377:THR:CG2 | 2.74 | 0.65 |
| 1:C:1358:TRP:CZ3 | 1:C:1381:HIS:CE1 | 2.70 | 0.65 |
| 1:B:1414:PHE:HD1 | 2:D:127:TRP:HB2 | 1.61 | 0.65 |
| 2:D:98:GLU:HB3 | 2:D:99:PRO:CD | 2.23 | 0.65 |
| 2:F:134:ASP:O | 2:F:137:GLU:CB | 2.44 | 0.65 |
| 2:E:93:ASP:OD2 | 2:E:97:GLN:HG2 | 1.95 | 0.65 |
| 1:C:1362:VAL:CG2 | 1:C:1377:THR:HB | 2.26 | 0.65 |
| 1:A:1160:ALA:O | 1:A:1164:ALA:HB3 | 1.95 | 0.65 |
| 1:A:1121:VAL:O | 1:A:1123:GLU:N | 2.29 | 0.65 |
| 1:B:1234:LEU:CG | 1:B:1235:GLY:H | 2.09 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:1514:LEU:HD23 | 1:C:1514:LEU:C | 2.16 | 0.65 |
| 1:B:1165:ARG:O | 1:B:1165:ARG:HG3 | 1.96 | 0.65 |
| 1:A:1290:TYR:CE2 | 1:A:1295:TYR:HE2 | 2.14 | 0.65 |
| 1:C:1253:TRP:C | 1:C:1255:GLU:N | 2.47 | 0.65 |
| 1:C:1326:LYS:HZ3 | 1:C:1354:GLN:HG2 | 1.59 | 0.65 |
| 1:A:1600:ILE:O | 1:A:1604:LYS:HG3 | 1.95 | 0.65 |
| 1:C:1161:ARG:NH2 | 1:C:1195:ASN:HB3 | 2.11 | 0.65 |
| 1:B:1336:LEU:HD12 | 1:B:1360:GLU:HB3 | 1.79 | 0.65 |
| 1:B:1277:VAL:O | 1:B:1278:VAL:C | 2.34 | 0.65 |
| 1:A:1605:GLU:HG3 | 1:B:1580:ASP:OD2 | 1.96 | 0.65 |
| 1:C:1578:ARG:HD3 | 1:C:1582:VAL:HB | 1.78 | 0.65 |
| 1:C:1428:PRO:O | 1:C:1429:ARG:HB3 | 1.96 | 0.65 |
| 1:B:1332:MET:SD | 1:B:1360:GLU:CG | 2.84 | 0.65 |
| 1:A:1598:TYR:CD2 | 2:F:198:UNK:CB | 2.80 | 0.65 |
| 1:A:1409:GLN:CB | 1:A:1413:GLU:HG2 | 2.25 | 0.65 |
| 1:B:1157:LEU:HD13 | 1:B:1177:LEU:HD23 | 1.77 | 0.65 |
| 1:A:1257:CYS:SG | 1:A:1290:TYR:CE1 | 2.89 | 0.65 |
| 1:B:1578:ARG:HD3 | 1:B:1582:VAL:HB | 1.78 | 0.65 |
| 1:B:1588:ARG:NH2 | 2:F:190:UNK:O | 2.28 | 0.65 |
| 1:C:1198:ILE:CB | 1:C:1221:VAL:HG22 | 2.25 | 0.65 |
| 1:B:1358:TRP:CE2 | 1:B:1381:HIS:ND1 | 2.64 | 0.65 |
| 1:C:1447:LEU:O | 1:C:1450:PRO:HD2 | 1.95 | 0.65 |
| 1:B:1406:ARG:O | 1:B:1409:GLN:HB3 | 1.95 | 0.65 |
| 2:D:155:ILE:N | 2:D:155:ILE:HD13 | 2.12 | 0.65 |
| 1:C:1112:ALA:O | 1:C:1116:LEU:HB2 | 1.97 | 0.65 |
| 1:A:1295:TYR:CE1 | 1:A:1298:GLU:HB2 | 2.31 | 0.65 |
| 1:B:1362:VAL:CG2 | 1:B:1377:THR:CG2 | 2.74 | 0.65 |
| 1:C:1358:TRP:CE2 | 1:C:1381:HIS:ND1 | 2.65 | 0.65 |
| 2:F:162:GLN:O | 2:F:164:PRO:N | 2.30 | 0.65 |
| 1:B:1215:LYS:HD3 | 1:B:1216:LEU:N | 2.11 | 0.65 |
| 2:D:60:UNK:O | 2:D:61:UNK:C | 2.44 | 0.65 |
| 1:B:1379:MET:HE1 | 1:B:1406:ARG:HD3 | 1.79 | 0.65 |
| 1:A:1162:LYS:O | 1:A:1163:LYS:HE2 | 1.97 | 0.65 |
| 1:B:1514:LEU:C | 1:B:1514:LEU:HD23 | 2.17 | 0.65 |
| 1:A:1112:ALA:O | 1:A:1116:LEU:HB2 | 1.97 | 0.65 |
| 2:F:109:GLN:O | 2:F:112:ARG:HB3 | 1.97 | 0.65 |
| 1:C:1232:VAL:HG13 | 1:C:1233:HIS:N | 2.11 | 0.65 |
| 1:A:1572:THR:HG21 | 1:A:1599:PHE:CE2 | 2.31 | 0.65 |
| 1:B:1475:GLU:CD | 2:D:149:ASN:HD21 | 2.00 | 0.65 |
| 1:A:1108:TRP:NE1 | 1:A:1131:ALA:CB | 2.59 | 0.65 |
| 2:F:184:UNK:O | 2:F:185:UNK:C | 2.44 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:1409:GLN:HG3 | 1:C:1413:GLU:HG3 | 0.67 | 0.65 |
| 1:C:1504:LEU:CD2 | 2:E:149:ASN:CG | 2.66 | 0.65 |
| 1:A:1379:MET:HE1 | 1:A:1406:ARG:HD3 | 1.78 | 0.65 |
| 2:D:109:GLN:O | 2:D:112:ARG:HB3 | 1.96 | 0.65 |
| 1:A:1086:ILE:HB | 1:A:1089:ILE:HD13 | 1.79 | 0.65 |
| 2:F:143:SER:O | 2:F:147:GLU:HB2 | 1.97 | 0.65 |
| 1:A:1578:ARG:CZ | 1:A:1583:LEU:CD2 | 2.69 | 0.64 |
| 1:C:1588:ARG:NH2 | 2:D:193:UNK:HA | 2.12 | 0.64 |
| 1:B:1409:GLN:HG3 | 1:B:1413:GLU:HG3 | 0.68 | 0.64 |
| 1:A:1085:LEU:CD1 | 1:A:1111:LEU:HG | 2.28 | 0.64 |
| 1:C:1295:TYR:C | 1:C:1296:PHE:CG | 2.71 | 0.64 |
| 1:B:1277:VAL:O | 1:B:1279:HIS:ND1 | 2.31 | 0.64 |
| 1:C:1174:ILE:CG1 | 1:C:1196:ALA:HA | 2.18 | 0.64 |
| 1:C:1358:TRP:HH2 | 1:C:1381:HIS:CE1 | 2.05 | 0.64 |
| 1:C:1412:LEU:CB | 1:C:1419:LEU:HD13 | 2.27 | 0.64 |
| 1:C:1248:ASN:N | 1:C:1248:ASN:CB | 2.59 | 0.64 |
| 1:B:1082:VAL:HG11 | 1:B:1105:PRO:HB3 | 1.78 | 0.64 |
| 2:E:154:ARG:NH1 | 2:E:154:ARG:HB3 | 2.11 | 0.64 |
| 1:A:1215:LYS:HD3 | 1:A:1216:LEU:N | 2.11 | 0.64 |
| 1:A:1277:VAL:O | 1:A:1278:VAL:C | 2.34 | 0.64 |
| 1:B:1245:ARG:O | 1:B:1245:ARG:CG | 2.45 | 0.64 |
| 1:A:1218:TYR:CD2 | 1:A:1227:LEU:HD12 | 2.32 | 0.64 |
| 1:C:1504:LEU:HD11 | 2:E:149:ASN:HD21 | 0.81 | 0.64 |
| 1:B:1112:ALA:O | 1:B:1116:LEU:HB2 | 1.97 | 0.64 |
| 1:B:1620:ARG:NH1 | 1:B:1620:ARG:CG | 2.53 | 0.64 |
| 1:C:1295:TYR:C | 1:C:1296:PHE:CD1 | 2.71 | 0.64 |
| 2:F:191:UNK:O | 2:F:193:UNK:N | 2.30 | 0.64 |
| 1:B:1347:LYS:HD3 | 1:B:1348:VAL:N | 2.12 | 0.64 |
| 2:E:116:LEU:O | 2:E:119:ALA:HB3 | 1.98 | 0.64 |
| 1:A:1168:TYR:HA | 1:A:1172:GLU:OE2 | 1.97 | 0.64 |
| 1:A:1514:LEU:C | 1:A:1514:LEU:HD23 | 2.17 | 0.64 |
| 1:A:1296:PHE:O | 1:A:1298:GLU:N | 2.30 | 0.64 |
| 1:B:1554:LEU:HD23 | 1:B:1582:VAL:CG1 | 2.28 | 0.64 |
| 1:C:1402:GLU:OE1 | 1:C:1403:LEU:N | 2.31 | 0.64 |
| 1:C:1417:LEU:O | 1:C:1418:LEU:CB | 2.35 | 0.64 |
| 1:A:1409:GLN:C | 1:A:1413:GLU:HB2 | 2.18 | 0.64 |
| 1:A:1412:LEU:N | 1:A:1419:LEU:HD13 | 2.12 | 0.64 |
| 1:A:1443:LYS:O | 1:A:1443:LYS:HG2 | 1.97 | 0.64 |
| 1:A:1347:LYS:HD3 | 1:A:1348:VAL:N | 2.12 | 0.64 |
| 1:B:1136:SER:HA | 1:B:1141:VAL:HG21 | 1.79 | 0.64 |
| 2:E:112:ARG:O | 2:E:113:LEU:O | 2.16 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:1254:LYS:HD2 | 1:C:1285:GLU:CD | 2.17 | 0.64 |
| 1:B:1264:LYS:HG3 | 1:B:1266:PHE:CD2 | 2.32 | 0.64 |
| 1:C:1401:VAL:HA | 1:C:1404:TYR:CD1 | 2.32 | 0.64 |
| 1:C:1408:ILE:HG22 | 1:C:1412:LEU:HD23 | 1.80 | 0.64 |
| 1:C:1414:PHE:CE1 | 2:E:127:TRP:HZ3 | 2.12 | 0.64 |
| 1:A:1428:PRO:O | 1:A:1429:ARG:HB3 | 1.97 | 0.64 |
| 1:B:1409:GLN:C | 1:B:1413:GLU:HB2 | 2.18 | 0.64 |
| 1:B:1080:SER:O | 1:B:1084:VAL:HG23 | 1.97 | 0.64 |
| 1:C:1360:GLU:N | 1:C:1360:GLU:OE1 | 2.31 | 0.64 |
| 1:B:1601:GLN:CD | 1:C:1587:TRP:HH2 | 2.01 | 0.64 |
| 1:C:1122:LYS:HA | 1:C:1125:ILE:CG2 | 2.24 | 0.64 |
| 1:B:1350:ARG:HH21 | 1:B:1353:GLU:HB3 | 1.62 | 0.64 |
| 1:B:1362:VAL:CG2 | 1:B:1377:THR:HB | 2.26 | 0.64 |
| 1:B:1360:GLU:OE1 | 1:B:1360:GLU:N | 2.31 | 0.64 |
| 1:B:1401:VAL:HA | 1:B:1404:TYR:CD1 | 2.32 | 0.64 |
| 1:B:1402:GLU:OE1 | 1:B:1403:LEU:N | 2.31 | 0.64 |
| 1:B:1408:ILE:HG22 | 1:B:1412:LEU:CD2 | 2.28 | 0.64 |
| 2:E:108:GLU:OE2 | 2:E:109:GLN:NE2 | 2.31 | 0.64 |
| 1:B:1135:SER:HB3 | 1:B:1159:MET:O | 1.97 | 0.64 |
| 1:A:1108:TRP:CE3 | 1:A:1108:TRP:HA | 2.33 | 0.64 |
| 1:A:1108:TRP:HA | 1:A:1108:TRP:HE3 | 1.63 | 0.64 |
| 2:D:66:UNK:O | 2:D:70:UNK:N | 2.31 | 0.64 |
| 2:D:143:SER:O | 2:D:147:GLU:HB2 | 1.97 | 0.64 |
| 2:F:16:UNK:C | 2:F:18:UNK:H | 2.09 | 0.64 |
| 1:C:1264:LYS:HG3 | 1:C:1266:PHE:CD2 | 2.32 | 0.64 |
| 1:C:1401:VAL:HA | 1:C:1404:TYR:CE1 | 2.33 | 0.64 |
| 1:C:1408:ILE:HG22 | 1:C:1412:LEU:CD2 | 2.28 | 0.64 |
| 1:C:1443:LYS:O | 1:C:1443:LYS:HG2 | 1.97 | 0.64 |
| 1:A:1401:VAL:HA | 1:A:1404:TYR:CD1 | 2.32 | 0.64 |
| 2:D:116:LEU:O | 2:D:119:ALA:HB3 | 1.98 | 0.64 |
| 1:A:1264:LYS:HG3 | 1:A:1266:PHE:CD2 | 2.33 | 0.64 |
| 1:A:1350:ARG:HH21 | 1:A:1353:GLU:HB3 | 1.62 | 0.64 |
| 1:B:1401:VAL:HA | 1:B:1404:TYR:CE1 | 2.33 | 0.64 |
| 1:B:1471:PHE:HB2 | 1:B:1480:LEU:HD13 | 1.80 | 0.64 |
| 1:B:1142:GLN:OE1 | 1:B:1143:ALA:N | 2.31 | 0.64 |
| 1:A:1091:ASN:ND2 | 1:A:1092:LEU:HG | 2.12 | 0.64 |
| 1:C:1296:PHE:O | 1:C:1298:GLU:N | 2.31 | 0.63 |
| 1:C:1350:ARG:HH21 | 1:C:1353:GLU:HB3 | 1.62 | 0.63 |
| 1:C:1468:ASN:O | 1:C:1472:ILE:HG13 | 1.98 | 0.63 |
| 1:B:1296:PHE:O | 1:B:1298:GLU:N | 2.30 | 0.63 |
| 2:D:124:GLU:HG3 | 2:D:125:GLN:N | 2.12 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:E:98:GLU:CA | 2:E:101:SER:HB3 | 2.27 | 0.63 |
| 1:C:1142:GLN:OE1 | 1:C:1143:ALA:N | 2.31 | 0.63 |
| 2:F:112:ARG:O | 2:F:113:LEU:O | 2.16 | 0.63 |
| 1:A:1360:GLU:OE1 | 1:A:1360:GLU:N | 2.31 | 0.63 |
| 1:C:1145:ASN:O | 1:C:1150:TRP:NE1 | 2.31 | 0.63 |
| 1:C:1175:PHE:CE2 | 1:C:1204:ARG:NH2 | 2.66 | 0.63 |
| 1:C:1349:LEU:HB3 | 1:C:1353:GLU:OE1 | 1.99 | 0.63 |
| 1:A:1408:ILE:HG22 | 1:A:1412:LEU:HD23 | 1.80 | 0.63 |
| 1:B:1412:LEU:CB | 1:B:1419:LEU:HD13 | 2.27 | 0.63 |
| 1:B:1428:PRO:O | 1:B:1429:ARG:HB3 | 1.97 | 0.63 |
| 1:C:1516:LYS:HB3 | 1:C:1523:GLN:HB2 | 1.80 | 0.63 |
| 1:A:1142:GLN:OE1 | 1:A:1143:ALA:N | 2.31 | 0.63 |
| 1:A:1279:HIS:HE1 | 1:A:1283:LEU:HD11 | 1.60 | 0.63 |
| 1:A:1412:LEU:CB | 1:A:1419:LEU:CD1 | 2.76 | 0.63 |
| 2:F:124:GLU:HG3 | 2:F:125:GLN:N | 2.12 | 0.63 |
| 1:B:1443:LYS:HG2 | 1:B:1443:LYS:O | 1.97 | 0.63 |
| 1:B:1468:ASN:O | 1:B:1472:ILE:HG13 | 1.99 | 0.63 |
| 2:D:204:UNK:O | 2:D:205:UNK:C | 2.47 | 0.63 |
| 1:C:1475:GLU:OE1 | 2:E:145:GLN:CG | 2.46 | 0.63 |
| 1:A:1412:LEU:CB | 1:A:1419:LEU:HD13 | 2.27 | 0.63 |
| 2:F:119:ALA:C | 2:F:123:MET:HG2 | 2.17 | 0.63 |
| 1:B:1326:LYS:HZ3 | 1:B:1354:GLN:HG2 | 1.62 | 0.63 |
| 1:B:1412:LEU:CB | 1:B:1419:LEU:CD1 | 2.76 | 0.63 |
| 1:B:1419:LEU:HD12 | 1:B:1422:LEU:HD12 | 1.81 | 0.63 |
| 1:B:1161:ARG:HH12 | 1:B:1193:PRO:C | 2.02 | 0.63 |
| 1:A:1130:LYS:NZ | 1:A:1155:LYS:HG2 | 2.13 | 0.63 |
| 1:B:1092:LEU:O | 1:B:1094:ARG:N | 2.29 | 0.63 |
| 1:C:1258:PHE:CZ | 1:C:1293:ARG:NH2 | 2.67 | 0.63 |
| 1:B:1293:ARG:HA | 2:D:97:GLN:OE1 | 1.99 | 0.63 |
| 1:B:1414:PHE:CD1 | 2:D:127:TRP:CB | 2.81 | 0.63 |
| 2:D:129:GLU:O | 2:D:132:LYS:HG2 | 1.99 | 0.63 |
| 1:C:1188:GLU:C | 1:C:1190:ILE:H | 2.02 | 0.63 |
| 1:B:1626:ALA:O | 1:B:1630:GLN:HB2 | 1.98 | 0.63 |
| 1:B:1264:LYS:NZ | 1:B:1268:LEU:HD13 | 2.13 | 0.63 |
| 1:A:1547:THR:HG23 | 1:A:1577:LEU:HB2 | 1.79 | 0.63 |
| 1:C:1594:PHE:O | 1:C:1596:MET:CE | 2.46 | 0.63 |
| 1:C:1181:ASN:C | 1:C:1182:ARG:HD3 | 2.19 | 0.63 |
| 2:E:89:ILE:CB | 2:E:90:ALA:HA | 2.27 | 0.63 |
| 1:A:1264:LYS:NZ | 1:A:1268:LEU:HD13 | 2.14 | 0.63 |
| 1:B:1258:PHE:HB2 | 1:B:1289:TYR:CE2 | 2.34 | 0.63 |
| 1:A:1605:GLU:OE2 | 1:B:1579:PRO:CA | 2.46 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:F:182:UNK:O | 2:F:184:UNK:N | 2.31 | 0.63 |
| 1:B:1349:LEU:HB3 | 1:B:1353:GLU:OE1 | 1.99 | 0.63 |
| 1:C:1347:LYS:HD3 | 1:C:1348:VAL:N | 2.12 | 0.63 |
| 1:C:1409:GLN:C | 1:C:1413:GLU:HB2 | 2.18 | 0.63 |
| 1:A:1401:VAL:HA | 1:A:1404:TYR:CE1 | 2.33 | 0.63 |
| 1:A:1416:PRO:CD | 2:F:130:LYS:CD | 2.70 | 0.63 |
| 2:F:129:GLU:O | 2:F:132:LYS:HG2 | 1.99 | 0.63 |
| 1:B:1170:GLU:OE2 | 1:B:1196:ALA:HB2 | 1.99 | 0.63 |
| 1:B:1198:ILE:O | 1:B:1198:ILE:HG22 | 1.99 | 0.63 |
| 1:B:1108:TRP:CE3 | 1:B:1108:TRP:HA | 2.33 | 0.63 |
| 1:B:1108:TRP:HE3 | 1:B:1108:TRP:HA | 1.63 | 0.63 |
| 1:B:1516:LYS:HB3 | 1:B:1523:GLN:HB2 | 1.80 | 0.63 |
| 1:C:1419:LEU:HD12 | 1:C:1422:LEU:HD12 | 1.81 | 0.63 |
| 1:C:1450:PRO:HA | 1:C:1453:ARG:CG | 2.28 | 0.63 |
| 1:C:1475:GLU:CB | 2:E:145:GLN:HG3 | 2.29 | 0.63 |
| 2:E:130:LYS:O | 2:E:133:LYS:HB2 | 1.99 | 0.63 |
| 1:A:1409:GLN:HG3 | 1:A:1413:GLU:HG3 | 0.67 | 0.63 |
| 1:A:1419:LEU:HD12 | 1:A:1422:LEU:HD12 | 1.81 | 0.63 |
| 1:A:1362:VAL:CG2 | 1:A:1377:THR:HB | 2.27 | 0.63 |
| 1:B:1434:ARG:HG2 | 1:B:1434:ARG:O | 1.99 | 0.63 |
| 1:C:1381:HIS:N | 1:C:1382:PRO:HD3 | 2.14 | 0.63 |
| 1:C:1407:ALA:O | 1:C:1409:GLN:N | 2.32 | 0.63 |
| 1:C:1412:LEU:CB | 1:C:1419:LEU:CD1 | 2.76 | 0.63 |
| 1:A:1407:ALA:O | 1:A:1409:GLN:N | 2.32 | 0.63 |
| 1:A:1471:PHE:HB2 | 1:A:1480:LEU:HD13 | 1.80 | 0.63 |
| 1:B:1408:ILE:HG22 | 1:B:1412:LEU:HD23 | 1.80 | 0.63 |
| 1:B:1198:ILE:HG23 | 1:B:1201:VAL:CB | 2.29 | 0.63 |
| 1:A:1459:ASN:ND2 | 1:A:1489:ASN:HB2 | 2.14 | 0.63 |
| 1:B:1578:ARG:CZ | 1:B:1583:LEU:CD2 | 2.70 | 0.62 |
| 2:E:129:GLU:O | 2:E:132:LYS:HG2 | 1.99 | 0.62 |
| 1:A:1468:ASN:O | 1:A:1472:ILE:HG13 | 1.99 | 0.62 |
| 1:A:1116:LEU:HD11 | 1:A:1122:LYS:CB | 2.29 | 0.62 |
| 1:B:1459:ASN:ND2 | 1:B:1489:ASN:HB2 | 2.14 | 0.62 |
| 1:C:1496:ALA:HB3 | 1:C:1515:PHE:CE1 | 2.34 | 0.62 |
| 1:A:1594:PHE:O | 1:A:1596:MET:CE | 2.47 | 0.62 |
| 1:B:1572:THR:CG2 | 1:B:1599:PHE:CD2 | 2.83 | 0.62 |
| 1:C:1584:GLU:O | 1:C:1587:TRP:N | 2.29 | 0.62 |
| 1:A:1402:GLU:OE1 | 1:A:1403:LEU:N | 2.31 | 0.62 |
| 2:F:116:LEU:O | 2:F:119:ALA:HB3 | 1.98 | 0.62 |
| 1:A:1349:LEU:HB3 | 1:A:1353:GLU:OE1 | 1.98 | 0.62 |
| 1:B:1503:GLU:HG3 | 1:B:1504:LEU:N | 2.14 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:1144:ALA:CB | 1:B:1149:ASN:HB3 | 2.23 | 0.62 |
| 1:C:1434:ARG:HG2 | 1:C:1434:ARG:O | 1.99 | 0.62 |
| 1:A:1408:ILE:CG2 | 1:A:1412:LEU:HD22 | 2.28 | 0.62 |
| 1:B:1496:ALA:HB3 | 1:B:1515:PHE:CE1 | 2.34 | 0.62 |
| 1:B:1078:ASN:HB2 | 1:B:1102:CYS:SG | 2.39 | 0.62 |
| 1:C:1078:ASN:HB2 | 1:C:1098:PHE:CZ | 2.34 | 0.62 |
| 1:C:1351:ALA:HA | 1:C:1354:GLN:HG2 | 1.81 | 0.62 |
| 1:C:1609:LYS:HA | 1:C:1612:LYS:HG3 | 1.80 | 0.62 |
| 1:C:1218:TYR:CE2 | 1:C:1223:ASN:HB3 | 2.34 | 0.62 |
| 1:B:1407:ALA:O | 1:B:1409:GLN:N | 2.32 | 0.62 |
| 1:B:1442:VAL:HG12 | 1:B:1444:GLN:HB2 | 1.82 | 0.62 |
| 1:A:1411:TYR:O | 1:A:1415:LYS:CA | 2.46 | 0.62 |
| 1:C:1186:LEU:HB3 | 1:C:1213:ALA:HB2 | 1.81 | 0.62 |
| 1:C:1190:ILE:CG1 | 1:C:1216:LEU:HG | 2.30 | 0.62 |
| 1:A:1280:ALA:HB2 | 1:A:1311:ARG:CZ | 2.29 | 0.62 |
| 1:C:1395:ILE:CG1 | 1:C:1404:TYR:CD2 | 2.76 | 0.62 |
| 1:C:1442:VAL:HG12 | 1:C:1444:GLN:HB2 | 1.82 | 0.62 |
| 1:A:1395:ILE:CG1 | 1:A:1404:TYR:HE2 | 2.07 | 0.62 |
| 1:B:1395:ILE:CG1 | 1:B:1404:TYR:HE2 | 2.07 | 0.62 |
| 1:B:1408:ILE:CG2 | 1:B:1412:LEU:HD22 | 2.28 | 0.62 |
| 1:C:1326:LYS:O | 1:C:1327:PHE:CE1 | 2.52 | 0.62 |
| 1:C:1408:ILE:CG2 | 1:C:1412:LEU:HD22 | 2.29 | 0.62 |
| 1:B:1450:PRO:HA | 1:B:1453:ARG:CG | 2.28 | 0.62 |
| 1:B:1085:LEU:HD22 | 1:B:1125:ILE:CD1 | 2.30 | 0.62 |
| 1:A:1083:GLN:HE21 | 1:A:1106:ALA:HB3 | 1.64 | 0.62 |
| 1:A:1594:PHE:O | 1:A:1596:MET:HG3 | 2.00 | 0.62 |
| 1:B:1594:PHE:O | 1:B:1596:MET:CE | 2.48 | 0.62 |
| 1:B:1350:ARG:HH21 | 1:B:1353:GLU:CB | 2.13 | 0.62 |
| 2:E:124:GLU:HG3 | 2:E:125:GLN:N | 2.13 | 0.62 |
| 1:B:1332:MET:SD | 1:B:1357:LEU:HD13 | 2.40 | 0.62 |
| 1:B:1414:PHE:CD1 | 2:D:127:TRP:HB3 | 2.35 | 0.62 |
| 1:C:1317:PHE:N | 1:C:1317:PHE:CD2 | 2.63 | 0.62 |
| 1:A:1296:PHE:HE2 | 2:F:101:SER:OG | 1.83 | 0.62 |
| 1:C:1290:TYR:CD2 | 1:C:1299:LEU:CD1 | 2.82 | 0.62 |
| 1:B:1279:HIS:O | 1:B:1280:ALA:HB2 | 1.97 | 0.62 |
| 1:B:1600:ILE:HG22 | 1:B:1604:LYS:HE3 | 1.82 | 0.62 |
| 1:A:1402:GLU:HA | 1:A:1405:TYR:CE2 | 2.35 | 0.62 |
| 1:A:1442:VAL:HG12 | 1:A:1444:GLN:HB2 | 1.82 | 0.62 |
| 1:B:1326:LYS:O | 1:B:1327:PHE:CE1 | 2.53 | 0.62 |
| 1:C:1344:ASN:O | 1:C:1345:ILE:HD13 | 1.99 | 0.62 |
| 1:A:1277:VAL:O | 1:A:1279:HIS:ND1 | 2.31 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:1578:ARG:CZ | 1:C:1583:LEU:CD2 | 2.69 | 0.62 |
| 1:C:1600:ILE:HG22 | 1:C:1604:LYS:HE3 | 1.82 | 0.62 |
| 1:C:1180:THR:HG22 | 1:C:1181:ASN:N | 2.14 | 0.62 |
| 1:C:1471:PHE:HB2 | 1:C:1480:LEU:HD13 | 1.80 | 0.62 |
| 1:C:1503:GLU:HG3 | 1:C:1504:LEU:N | 2.14 | 0.62 |
| 1:A:1408:ILE:HG21 | 1:A:1412:LEU:HD22 | 1.82 | 0.62 |
| 1:A:1434:ARG:O | 1:A:1434:ARG:HG2 | 1.99 | 0.62 |
| 1:B:1351:ALA:HA | 1:B:1354:GLN:HG2 | 1.81 | 0.62 |
| 1:B:1417:LEU:O | 1:B:1418:LEU:CB | 2.36 | 0.62 |
| 1:A:1496:ALA:HB3 | 1:A:1515:PHE:CE1 | 2.34 | 0.62 |
| 1:C:1459:ASN:ND2 | 1:C:1489:ASN:HB2 | 2.14 | 0.62 |
| 1:C:1174:ILE:HG13 | 1:C:1196:ALA:CA | 2.19 | 0.62 |
| 1:C:1402:GLU:HA | 1:C:1405:TYR:CE2 | 2.35 | 0.62 |
| 1:C:1234:LEU:CD2 | 1:C:1264:LYS:HZ2 | 2.00 | 0.61 |
| 1:A:1578:ARG:NH1 | 1:A:1583:LEU:HA | 2.15 | 0.61 |
| 1:C:1350:ARG:HH21 | 1:C:1353:GLU:CB | 2.13 | 0.61 |
| 2:E:146:VAL:HA | 2:E:149:ASN:CG | 2.20 | 0.61 |
| 1:A:1381:HIS:N | 1:A:1382:PRO:HD3 | 2.15 | 0.61 |
| 1:A:1159:MET:SD | 1:A:1163:LYS:NZ | 2.73 | 0.61 |
| 2:D:49:UNK:C | 2:D:51:UNK:N | 2.61 | 0.61 |
| 1:A:1250:THR:O | 1:A:1251:ARG:CB | 2.47 | 0.61 |
| 1:B:1381:HIS:N | 1:B:1382:PRO:HD3 | 2.14 | 0.61 |
| 2:E:126:GLU:HG3 | 2:E:130:LYS:HZ3 | 1.65 | 0.61 |
| 2:F:130:LYS:O | 2:F:133:LYS:HB2 | 2.00 | 0.61 |
| 1:B:1509:ARG:HB3 | 1:B:1510:ILE:HD13 | 1.82 | 0.61 |
| 1:A:1516:LYS:HB3 | 1:A:1523:GLN:HB2 | 1.80 | 0.61 |
| 1:A:1282:GLU:OE2 | 1:A:1285:GLU:HB3 | 2.00 | 0.61 |
| 1:B:1250:THR:O | 1:B:1251:ARG:CB | 2.47 | 0.61 |
| 1:A:1584:GLU:O | 1:A:1586:ALA:N | 2.33 | 0.61 |
| 1:B:1584:GLU:O | 1:B:1586:ALA:N | 2.33 | 0.61 |
| 1:A:1358:TRP:HH2 | 1:A:1381:HIS:CE1 | 2.05 | 0.61 |
| 1:B:1402:GLU:HA | 1:B:1405:TYR:CE2 | 2.35 | 0.61 |
| 1:B:1130:LYS:NZ | 1:B:1155:LYS:HG2 | 2.15 | 0.61 |
| 1:A:1122:LYS:CA | 1:A:1125:ILE:HG22 | 2.25 | 0.61 |
| 1:B:1617:GLU:HA | 1:B:1620:ARG:HB2 | 1.82 | 0.61 |
| 1:A:1290:TYR:CG | 1:A:1295:TYR:CE2 | 2.89 | 0.61 |
| 1:C:1332:MET:SD | 1:C:1357:LEU:HD13 | 2.40 | 0.61 |
| 1:A:1600:ILE:HG22 | 1:A:1604:LYS:HE3 | 1.82 | 0.61 |
| 1:B:1593:ASP:O | 1:B:1594:PHE:HB2 | 2.01 | 0.61 |
| 2:F:121:LYS:O | 2:F:124:GLU:HB3 | 2.01 | 0.61 |
| 1:A:1350:ARG:HH21 | 1:A:1353:GLU:CB | 2.13 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:1398:VAL:HG12 | 1:B:1400:ASN:H | 1.66 | 0.61 |
| 1:A:1167:SER:HB3 | 1:A:1168:TYR:CD1 | 2.35 | 0.61 |
| 1:B:1164:ALA:HB1 | 1:B:1169:VAL:HG11 | 1.83 | 0.61 |
| 1:B:1505:ILE:O | 1:B:1509:ARG:N | 2.34 | 0.61 |
| 1:A:1365:TYR:HB2 | 1:A:1374:ALA:HB2 | 1.83 | 0.61 |
| 2:E:90:ALA:N | 2:E:91:GLN:HA | 2.13 | 0.61 |
| 1:A:1092:LEU:O | 1:A:1094:ARG:N | 2.29 | 0.61 |
| 1:C:1264:LYS:NZ | 1:C:1268:LEU:HD13 | 2.13 | 0.61 |
| 1:A:1587:TRP:O | 1:A:1589:HIS:N | 2.34 | 0.61 |
| 2:D:130:LYS:O | 2:D:133:LYS:HB2 | 1.99 | 0.61 |
| 1:C:1411:TYR:O | 1:C:1415:LYS:C | 2.39 | 0.61 |
| 2:D:112:ARG:C | 2:D:113:LEU:O | 2.38 | 0.61 |
| 2:F:112:ARG:HD3 | 2:F:112:ARG:C | 2.20 | 0.61 |
| 1:A:1351:ALA:HA | 1:A:1354:GLN:HG2 | 1.81 | 0.61 |
| 1:B:1274:LEU:CA | 1:B:1277:VAL:HG22 | 2.31 | 0.61 |
| 1:C:1584:GLU:O | 1:C:1586:ALA:N | 2.34 | 0.61 |
| 1:A:1580:ASP:OD1 | 1:C:1605:GLU:HG3 | 1.99 | 0.61 |
| 1:C:1121:VAL:O | 1:C:1123:GLU:N | 2.34 | 0.61 |
| 1:C:1365:TYR:HB2 | 1:C:1374:ALA:HB2 | 1.82 | 0.61 |
| 1:C:1504:LEU:HD21 | 2:E:149:ASN:HB3 | 1.82 | 0.61 |
| 1:C:1504:LEU:HG | 2:E:149:ASN:CG | 2.12 | 0.61 |
| 1:C:1505:ILE:O | 1:C:1509:ARG:N | 2.34 | 0.61 |
| 2:E:126:GLU:HG3 | 2:E:130:LYS:HZ1 | 1.65 | 0.61 |
| 1:B:1161:ARG:NH1 | 1:B:1194:ASN:HB2 | 2.15 | 0.61 |
| 1:A:1503:GLU:HG3 | 1:A:1504:LEU:N | 2.14 | 0.61 |
| 2:D:174:UNK:HA | 2:D:176:UNK:CA | 2.30 | 0.61 |
| 2:D:102:ILE:O | 2:D:106:ARG:N | 2.34 | 0.61 |
| 2:E:90:ALA:H | 2:E:91:GLN:HB3 | 1.64 | 0.61 |
| 1:C:1158:GLN:HG2 | 1:C:1159:MET:SD | 2.40 | 0.61 |
| 1:A:1274:LEU:CA | 1:A:1277:VAL:HG22 | 2.31 | 0.61 |
| 1:A:1332:MET:SD | 1:A:1357:LEU:HD13 | 2.40 | 0.61 |
| 1:C:1274:LEU:CA | 1:C:1277:VAL:HG22 | 2.31 | 0.61 |
| 1:B:1578:ARG:NH1 | 1:B:1583:LEU:HA | 2.16 | 0.61 |
| 2:E:189:UNK:CB | 2:E:195:UNK:N | 2.63 | 0.61 |
| 1:C:1414:PHE:CD1 | 2:E:123:MET:CB | 2.84 | 0.61 |
| 1:B:1297:GLU:O | 1:B:1300:ILE:HG13 | 2.01 | 0.61 |
| 1:B:1408:ILE:HG21 | 1:B:1412:LEU:HD22 | 1.83 | 0.61 |
| 1:A:1177:LEU:HA | 1:A:1180:THR:HG1 | 1.66 | 0.61 |
| 1:A:1082:VAL:HG21 | 1:A:1105:PRO:CG | 2.30 | 0.61 |
| 1:A:1297:GLU:O | 1:A:1300:ILE:HG13 | 2.01 | 0.61 |
| 1:C:1230:THR:O | 1:C:1231:LEU:CG | 2.48 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1587:TRP:CH2 | 1:C:1601:GLN:NE2 | 2.69 | 0.61 |
| 1:C:1562:LYS:C | 1:C:1564:GLU:H | 2.04 | 0.61 |
| 1:A:1371:TYR:CD1 | 1:A:1394:ILE:HG22 | 2.30 | 0.61 |
| 1:B:1137:TYR:CB | 1:B:1138:MET:CB | 2.58 | 0.61 |
| 1:B:1163:LYS:O | 1:B:1164:ALA:HB2 | 1.99 | 0.61 |
| 1:B:1261:VAL:CG1 | 1:B:1295:TYR:CE2 | 2.84 | 0.61 |
| 1:A:1188:GLU:C | 1:A:1190:ILE:H | 2.02 | 0.61 |
| 2:E:184:UNK:O | 2:E:186:UNK:N | 2.33 | 0.61 |
| 1:B:1282:GLU:OE2 | 1:B:1285:GLU:HB3 | 2.00 | 0.61 |
| 1:B:1414:PHE:O | 1:B:1416:PRO:CD | 2.23 | 0.61 |
| 1:A:1198:ILE:HG23 | 1:A:1201:VAL:CG2 | 2.30 | 0.61 |
| 2:D:173:UNK:O | 2:D:176:UNK:CB | 2.49 | 0.61 |
| 1:B:1150:TRP:O | 1:B:1153:LEU:N | 2.34 | 0.61 |
| 1:C:1078:ASN:HB3 | 1:C:1098:PHE:CE2 | 2.35 | 0.61 |
| 1:C:1254:LYS:HD2 | 1:C:1285:GLU:HG2 | 1.80 | 0.60 |
| 1:B:1609:LYS:HA | 1:B:1612:LYS:HG3 | 1.82 | 0.60 |
| 1:B:1134:PRO:HD2 | 1:B:1156:TYR:CE1 | 2.34 | 0.60 |
| 1:B:1188:GLU:C | 1:B:1190:ILE:H | 2.02 | 0.60 |
| 2:E:143:SER:O | 2:E:147:GLU:HB2 | 2.00 | 0.60 |
| 1:B:1584:GLU:O | 1:B:1587:TRP:N | 2.29 | 0.60 |
| 1:B:1596:MET:O | 1:B:1597:PRO:O | 2.19 | 0.60 |
| 1:C:1144:ALA:HB1 | 1:C:1153:LEU:HD13 | 1.82 | 0.60 |
| 1:B:1401:VAL:CG2 | 1:B:1429:ARG:HE | 2.13 | 0.60 |
| 2:E:112:ARG:C | 2:E:112:ARG:HD3 | 2.20 | 0.60 |
| 1:A:1261:VAL:CG1 | 1:A:1295:TYR:CD1 | 2.81 | 0.60 |
| 1:A:1290:TYR:CE2 | 1:A:1295:TYR:CE2 | 2.90 | 0.60 |
| 1:A:1326:LYS:O | 1:A:1327:PHE:CE1 | 2.52 | 0.60 |
| 1:C:1596:MET:O | 1:C:1597:PRO:O | 2.19 | 0.60 |
| 1:C:1602:VAL:CG1 | 2:E:203:UNK:O | 2.36 | 0.60 |
| 1:A:1563:ARG:NH2 | 2:F:181:UNK:HA | 2.04 | 0.60 |
| 2:D:121:LYS:O | 2:D:124:GLU:HB3 | 2.00 | 0.60 |
| 1:B:1173:LEU:O | 1:B:1177:LEU:HG | 2.02 | 0.60 |
| 1:A:1596:MET:O | 1:A:1597:PRO:O | 2.19 | 0.60 |
| 1:A:1609:LYS:HA | 1:A:1612:LYS:HG3 | 1.81 | 0.60 |
| 1:B:1562:LYS:C | 1:B:1564:GLU:H | 2.04 | 0.60 |
| 1:B:1358:TRP:CZ3 | 1:B:1377:THR:HG23 | 2.37 | 0.60 |
| 1:C:1395:ILE:O | 1:C:1404:TYR:OH | 2.18 | 0.60 |
| 1:B:1333:ARG:CA | 1:B:1360:GLU:HG2 | 2.32 | 0.60 |
| 1:A:1173:LEU:O | 1:A:1177:LEU:HG | 2.01 | 0.60 |
| 2:E:95:LEU:HD13 | 2:E:95:LEU:O | 2.01 | 0.60 |
| 1:A:1509:ARG:HB3 | 1:A:1510:ILE:HD13 | 1.82 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:1279:HIS:O | 1:B:1280:ALA:CB | 2.45 | 0.60 |
| 1:B:1572:THR:OG1 | 1:B:1599:PHE:CD2 | 2.50 | 0.60 |
| 1:C:1149:ASN:N | 1:C:1149:ASN:HD22 | 1.99 | 0.60 |
| 1:C:1377:THR:HA | 1:C:1381:HIS:CD2 | 2.36 | 0.60 |
| 1:A:1451:TYR:O | 1:A:1455:VAL:CG2 | 2.49 | 0.60 |
| 1:A:1416:PRO:CG | 2:F:130:LYS:HD3 | 2.31 | 0.60 |
| 1:A:1490:PHE:CD1 | 1:A:1492:ASN:OD1 | 2.54 | 0.60 |
| 1:B:1279:HIS:CD2 | 1:B:1283:LEU:CD1 | 2.85 | 0.60 |
| 1:C:1167:SER:HA | 1:C:1171:THR:H | 1.67 | 0.60 |
| 2:F:146:VAL:HA | 2:F:149:ASN:CG | 2.21 | 0.60 |
| 1:B:1326:LYS:HG3 | 1:B:1326:LYS:O | 1.99 | 0.60 |
| 1:B:1261:VAL:CG1 | 1:B:1295:TYR:CZ | 2.81 | 0.60 |
| 1:C:1617:GLU:HA | 1:C:1620:ARG:HB2 | 1.82 | 0.60 |
| 1:A:1333:ARG:HA | 1:A:1360:GLU:HG2 | 1.84 | 0.60 |
| 1:B:1246:LYS:O | 1:B:1247:ALA:HB2 | 2.01 | 0.60 |
| 1:B:1592:MET:HG2 | 1:B:1593:ASP:N | 2.16 | 0.60 |
| 1:C:1578:ARG:NH1 | 1:C:1583:LEU:HA | 2.15 | 0.60 |
| 1:C:1173:LEU:O | 1:C:1177:LEU:HG | 2.01 | 0.60 |
| 1:C:1358:TRP:CZ3 | 1:C:1377:THR:HG23 | 2.37 | 0.60 |
| 1:B:1412:LEU:HD12 | 1:B:1419:LEU:HD22 | 1.84 | 0.60 |
| 1:B:1416:PRO:CG | 2:D:130:LYS:HD3 | 2.32 | 0.60 |
| 2:D:146:VAL:HA | 2:D:149:ASN:CG | 2.21 | 0.60 |
| 1:A:1255:GLU:C | 1:A:1289:TYR:HE2 | 2.05 | 0.60 |
| 1:C:1245:ARG:N | 1:C:1275:HIS:CE1 | 2.65 | 0.60 |
| 1:A:1280:ALA:CB | 1:A:1311:ARG:HE | 2.09 | 0.60 |
| 1:A:1398:VAL:HG12 | 1:A:1400:ASN:H | 1.66 | 0.60 |
| 1:A:1417:LEU:O | 1:A:1418:LEU:CB | 2.35 | 0.60 |
| 1:A:1472:ILE:HB | 1:A:1498:ARG:NH2 | 2.16 | 0.60 |
| 1:A:1377:THR:HA | 1:A:1381:HIS:CD2 | 2.37 | 0.60 |
| 1:B:1325:SER:O | 1:B:1355:ALA:CB | 2.50 | 0.60 |
| 1:B:1162:LYS:O | 1:B:1163:LYS:C | 2.13 | 0.60 |
| 1:A:1333:ARG:CA | 1:A:1360:GLU:HG2 | 2.32 | 0.60 |
| 1:A:1325:SER:O | 1:A:1355:ALA:CB | 2.50 | 0.60 |
| 1:C:1250:THR:O | 1:C:1251:ARG:CB | 2.47 | 0.60 |
| 1:C:1333:ARG:CA | 1:C:1360:GLU:HG2 | 2.32 | 0.60 |
| 1:C:1593:ASP:O | 1:C:1594:PHE:HB2 | 2.01 | 0.60 |
| 1:C:1572:THR:HG21 | 1:C:1599:PHE:CE2 | 2.37 | 0.60 |
| 1:B:1350:ARG:NE | 1:B:1350:ARG:HA | 2.17 | 0.60 |
| 1:B:1171:THR:OG1 | 1:B:1196:ALA:HB1 | 2.02 | 0.60 |
| 1:A:1505:ILE:O | 1:A:1509:ARG:N | 2.33 | 0.60 |
| 1:C:1620:ARG:HG3 | 1:C:1620:ARG:NH1 | 2.16 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:1290:TYR:HD2 | 1:C:1299:LEU:CD2 | 2.12 | 0.60 |
| 2:F:195:UNK:N | 2:F:197:UNK:CB | 2.65 | 0.60 |
| 1:A:1416:PRO:HG2 | 2:F:130:LYS:CD | 2.31 | 0.60 |
| 1:A:1414:PHE:O | 2:F:130:LYS:CD | 2.50 | 0.60 |
| 1:C:1082:VAL:CG1 | 1:C:1083:GLN:H | 2.15 | 0.59 |
| 1:B:1451:TYR:O | 1:B:1455:VAL:CG2 | 2.50 | 0.59 |
| 1:A:1617:GLU:HA | 1:A:1620:ARG:HB2 | 1.83 | 0.59 |
| 2:D:186:UNK:N | 2:D:190:UNK:CB | 2.65 | 0.59 |
| 1:A:1326:LYS:O | 1:A:1326:LYS:HG3 | 1.99 | 0.59 |
| 1:A:1572:THR:CG2 | 1:A:1599:PHE:CD2 | 2.85 | 0.59 |
| 1:C:1533:LEU:HG | 1:C:1535:LYS:H | 1.67 | 0.59 |
| 1:C:1168:TYR:O | 1:C:1172:GLU:HG2 | 2.02 | 0.59 |
| 1:A:1395:ILE:O | 1:A:1404:TYR:OH | 2.17 | 0.59 |
| 1:B:1180:THR:O | 1:B:1181:ASN:CB | 2.49 | 0.59 |
| 1:A:1111:LEU:CD1 | 1:A:1125:ILE:HG12 | 2.29 | 0.59 |
| 1:A:1459:ASN:HD21 | 1:A:1489:ASN:HB2 | 1.67 | 0.59 |
| 1:A:1513:TYR:CD1 | 1:A:1516:LYS:HE2 | 2.37 | 0.59 |
| 1:B:1188:GLU:OE2 | 1:B:1191:ASN:O | 2.20 | 0.59 |
| 1:C:1152:GLU:OE2 | 1:C:1152:GLU:N | 2.35 | 0.59 |
| 1:A:1152:GLU:N | 1:A:1152:GLU:OE2 | 2.35 | 0.59 |
| 1:B:1578:ARG:HD3 | 1:B:1582:VAL:CG1 | 2.32 | 0.59 |
| 2:F:188:UNK:O | 2:F:189:UNK:C | 2.50 | 0.59 |
| 1:A:1358:TRP:CZ3 | 1:A:1377:THR:HG23 | 2.37 | 0.59 |
| 1:A:1620:ARG:HG3 | 1:A:1620:ARG:NH1 | 2.16 | 0.59 |
| 1:B:1617:GLU:HG2 | 1:B:1621:LYS:NZ | 2.18 | 0.59 |
| 1:B:1152:GLU:N | 1:B:1152:GLU:OE2 | 2.35 | 0.59 |
| 1:C:1372:ASP:O | 1:C:1376:ILE:CG1 | 2.48 | 0.59 |
| 1:C:1398:VAL:HG12 | 1:C:1400:ASN:H | 1.66 | 0.59 |
| 1:A:1416:PRO:CG | 2:F:130:LYS:CD | 2.81 | 0.59 |
| 1:A:1505:ILE:O | 1:A:1509:ARG:HB2 | 2.02 | 0.59 |
| 2:D:173:UNK:O | 2:D:174:UNK:CB | 2.45 | 0.59 |
| 1:C:1459:ASN:HD21 | 1:C:1489:ASN:HB2 | 1.67 | 0.59 |
| 1:B:1365:TYR:HB2 | 1:B:1374:ALA:HB2 | 1.83 | 0.59 |
| 1:C:1451:TYR:O | 1:C:1455:VAL:CG2 | 2.49 | 0.59 |
| 1:A:1445:LEU:N | 1:A:1446:PRO:CD | 2.66 | 0.59 |
| 2:D:119:ALA:C | 2:D:123:MET:HG2 | 2.15 | 0.59 |
| 1:B:1459:ASN:HD21 | 1:B:1489:ASN:HB2 | 1.67 | 0.59 |
| 1:B:1190:ILE:CD1 | 1:B:1216:LEU:HD11 | 2.32 | 0.59 |
| 1:C:1254:LYS:HD2 | 1:C:1285:GLU:HG3 | 1.82 | 0.59 |
| 1:A:1562:LYS:C | 1:A:1564:GLU:H | 2.06 | 0.59 |
| 2:F:197:UNK:C | 2:F:199:UNK:N | 2.64 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:1409:GLN:CB | 1:C:1413:GLU:HG2 | 2.24 | 0.59 |
| 1:C:1438:TYR:HD1 | 2:E:1:UNK:H2 | 1.49 | 0.59 |
| 2:E:121:LYS:O | 2:E:124:GLU:HB3 | 2.01 | 0.59 |
| 1:B:1136:SER:H | 1:B:1141:VAL:HG21 | 1.66 | 0.59 |
| 1:A:1510:ILE:HD13 | 1:A:1510:ILE:N | 2.18 | 0.59 |
| 1:B:1089:ILE:HG12 | 2:D:19:UNK:O | 2.02 | 0.59 |
| 1:A:1277:VAL:O | 1:A:1279:HIS:N | 2.36 | 0.59 |
| 1:B:1592:MET:CG | 1:B:1593:ASP:N | 2.61 | 0.59 |
| 1:C:1472:ILE:HB | 1:C:1498:ARG:NH2 | 2.15 | 0.59 |
| 2:E:120:SER:HA | 2:E:123:MET:HB2 | 1.85 | 0.59 |
| 2:D:99:PRO:O | 2:D:102:ILE:HG12 | 2.02 | 0.59 |
| 1:A:1215:LYS:C | 1:A:1217:LEU:N | 2.55 | 0.59 |
| 2:D:60:UNK:O | 2:D:63:UNK:N | 2.36 | 0.59 |
| 1:A:1185:GLU:O | 1:A:1185:GLU:HG2 | 2.03 | 0.59 |
| 1:A:1608:THR:HG23 | 1:B:1607:LEU:HD11 | 1.85 | 0.59 |
| 1:C:1141:VAL:HG11 | 1:C:1172:GLU:HG2 | 1.84 | 0.59 |
| 1:C:1412:LEU:HD12 | 1:C:1419:LEU:HD22 | 1.84 | 0.59 |
| 1:A:1401:VAL:CG2 | 1:A:1429:ARG:HE | 2.13 | 0.59 |
| 2:E:95:LEU:O | 2:E:99:PRO:HG2 | 2.01 | 0.59 |
| 1:B:1510:ILE:N | 1:B:1510:ILE:HD13 | 2.18 | 0.59 |
| 1:A:1126:ASP:CG | 1:A:1156:TYR:OH | 2.41 | 0.59 |
| 2:D:101:SER:O | 2:D:105:TRP:HB2 | 2.03 | 0.59 |
| 1:C:1600:ILE:HA | 1:C:1603:MET:HE3 | 1.85 | 0.59 |
| 1:C:1445:LEU:N | 1:C:1446:PRO:CD | 2.65 | 0.59 |
| 1:A:1395:ILE:CG1 | 1:A:1404:TYR:CD2 | 2.75 | 0.59 |
| 1:A:1438:TYR:O | 1:A:1442:VAL:HG21 | 2.03 | 0.59 |
| 1:A:1350:ARG:HA | 1:A:1350:ARG:NE | 2.17 | 0.59 |
| 1:A:1162:LYS:HG2 | 1:A:1163:LYS:HE2 | 1.84 | 0.59 |
| 1:B:1411:TYR:O | 1:B:1415:LYS:C | 2.39 | 0.59 |
| 1:B:1166:GLU:O | 1:B:1167:SER:O | 2.21 | 0.59 |
| 1:A:1530:LYS:HG2 | 1:A:1531:ASP:OD1 | 2.03 | 0.59 |
| 2:D:174:UNK:HA | 2:D:176:UNK:C | 2.32 | 0.59 |
| 1:A:1188:GLU:OE2 | 1:A:1191:ASN:C | 2.41 | 0.59 |
| 1:C:1546:ASP:OD2 | 1:C:1549:LEU:HD23 | 2.03 | 0.59 |
| 1:A:1319:GLU:HA | 1:A:1322:ILE:HD12 | 1.85 | 0.59 |
| 1:B:1280:ALA:O | 1:B:1313:HIS:NE2 | 2.36 | 0.59 |
| 1:A:1546:ASP:OD2 | 1:A:1549:LEU:HD23 | 2.03 | 0.59 |
| 2:F:120:SER:HA | 2:F:123:MET:HB2 | 1.85 | 0.59 |
| 1:B:1333:ARG:HA | 1:B:1360:GLU:HG2 | 1.84 | 0.59 |
| 1:B:1505:ILE:O | 1:B:1509:ARG:HB2 | 2.03 | 0.59 |
| 1:B:1620:ARG:NH1 | 1:B:1620:ARG:HG3 | 2.16 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1145:ASN:OD1 | 1:A:1179:LYS:O | 2.21 | 0.59 |
| 1:C:1571:PHE:O | 1:C:1577:LEU:HD21 | 2.02 | 0.58 |
| 2:F:195:UNK:C | 2:F:197:UNK:CA | 2.81 | 0.58 |
| 1:C:1401:VAL:CG2 | 1:C:1429:ARG:HE | 2.13 | 0.58 |
| 1:A:1358:TRP:CZ3 | 1:A:1381:HIS:CE1 | 2.70 | 0.58 |
| 1:B:1445:LEU:N | 1:B:1446:PRO:CD | 2.65 | 0.58 |
| 1:B:1472:ILE:CB | 1:B:1498:ARG:HH21 | 2.14 | 0.58 |
| 1:A:1168:TYR:O | 1:A:1172:GLU:HG2 | 2.03 | 0.58 |
| 1:A:1145:ASN:ND2 | 1:A:1153:LEU:CD2 | 2.66 | 0.58 |
| 1:B:1279:HIS:CG | 1:B:1280:ALA:H | 2.16 | 0.58 |
| 2:F:182:UNK:C | 2:F:184:UNK:N | 2.64 | 0.58 |
| 1:B:1377:THR:HA | 1:B:1381:HIS:CD2 | 2.37 | 0.58 |
| 1:C:1408:ILE:HG21 | 1:C:1412:LEU:HD22 | 1.83 | 0.58 |
| 1:C:1401:VAL:HG22 | 1:C:1429:ARG:CZ | 2.33 | 0.58 |
| 1:C:1530:LYS:HG2 | 1:C:1531:ASP:OD1 | 2.03 | 0.58 |
| 1:A:1412:LEU:HD12 | 1:A:1419:LEU:HD22 | 1.85 | 0.58 |
| 1:A:1375:ILE:CD1 | 1:A:1394:ILE:HB | 2.33 | 0.58 |
| 1:B:1384:ASP:OD1 | 2:D:115:GLU:CD | 2.41 | 0.58 |
| 2:D:174:UNK:CB | 2:D:177:UNK:CA | 2.81 | 0.58 |
| 1:C:1490:PHE:CD1 | 1:C:1492:ASN:OD1 | 2.54 | 0.58 |
| 1:C:1224:PHE:CE1 | 1:C:1246:LYS:NZ | 2.69 | 0.58 |
| 1:B:1319:GLU:HA | 1:B:1322:ILE:HD12 | 1.84 | 0.58 |
| 1:A:1283:LEU:HD22 | 1:A:1313:HIS:CE1 | 2.35 | 0.58 |
| 1:A:1588:ARG:CG | 1:A:1588:ARG:HH11 | 2.16 | 0.58 |
| 1:C:1471:PHE:CB | 1:C:1480:LEU:HB2 | 2.32 | 0.58 |
| 1:B:1530:LYS:HG2 | 1:B:1531:ASP:OD1 | 2.03 | 0.58 |
| 1:A:1206:TYR:CD2 | 1:A:1226:ARG:HG3 | 2.37 | 0.58 |
| 1:A:1533:LEU:HG | 1:A:1535:LYS:HB2 | 1.85 | 0.58 |
| 1:A:1578:ARG:HD3 | 1:A:1582:VAL:CG1 | 2.33 | 0.58 |
| 1:A:1471:PHE:CB | 1:A:1480:LEU:HB2 | 2.32 | 0.58 |
| 1:A:1198:ILE:HA | 1:A:1201:VAL:HG23 | 1.85 | 0.58 |
| 1:A:1190:ILE:CD1 | 1:A:1216:LEU:HD11 | 2.33 | 0.58 |
| 1:A:1145:ASN:HA | 1:A:1153:LEU:HD22 | 1.85 | 0.58 |
| 1:A:1533:LEU:HG | 1:A:1535:LYS:H | 1.67 | 0.58 |
| 1:B:1533:LEU:HG | 1:B:1535:LYS:HB2 | 1.84 | 0.58 |
| 1:C:1578:ARG:HD3 | 1:C:1582:VAL:CG1 | 2.32 | 0.58 |
| 1:C:1185:GLU:O | 1:C:1185:GLU:HG2 | 2.03 | 0.58 |
| 1:C:1350:ARG:HA | 1:C:1350:ARG:NE | 2.17 | 0.58 |
| 1:B:1407:ALA:O | 1:B:1408:ILE:C | 2.42 | 0.58 |
| 1:A:1157:LEU:HB3 | 1:A:1173:LEU:CD1 | 2.34 | 0.58 |
| 1:B:1161:ARG:HG2 | 1:B:1173:LEU:CD2 | 2.33 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1617:GLU:HG2 | 1:A:1621:LYS:NZ | 2.18 | 0.58 |
| 1:B:1215:LYS:C | 1:B:1217:LEU:N | 2.55 | 0.58 |
| 1:C:1130:LYS:HA | 1:C:1133:ASP:O | 2.02 | 0.58 |
| 1:A:1163:LYS:O | 1:A:1164:ALA:HB2 | 2.02 | 0.58 |
| 1:A:1157:LEU:CD1 | 1:A:1177:LEU:HD23 | 2.34 | 0.58 |
| 1:C:1537:ALA:HA | 1:C:1540:TYR:CE2 | 2.39 | 0.58 |
| 2:D:186:UNK:O | 2:D:187:UNK:C | 2.51 | 0.58 |
| 1:A:1251:ARG:O | 1:A:1252:THR:OG1 | 2.20 | 0.58 |
| 1:C:1148:GLY:O | 1:C:1149:ASN:HB3 | 2.03 | 0.58 |
| 2:D:120:SER:HA | 2:D:123:MET:HB2 | 1.85 | 0.58 |
| 1:A:1162:LYS:CA | 1:A:1162:LYS:O | 2.41 | 0.58 |
| 1:A:1181:ASN:CG | 1:A:1182:ARG:H | 1.98 | 0.58 |
| 1:B:1490:PHE:CD1 | 1:B:1492:ASN:OD1 | 2.54 | 0.58 |
| 1:C:1208:GLU:HA | 1:C:1208:GLU:OE1 | 2.01 | 0.58 |
| 2:E:189:UNK:C | 2:E:195:UNK:CB | 2.82 | 0.58 |
| 1:B:1404:TYR:OH | 1:B:1429:ARG:NH1 | 2.37 | 0.58 |
| 1:B:1471:PHE:CB | 1:B:1480:LEU:HB2 | 2.32 | 0.58 |
| 2:D:119:ALA:O | 2:D:123:MET:CB | 2.52 | 0.58 |
| 1:A:1088:HIS:C | 1:A:1089:ILE:HD12 | 2.23 | 0.58 |
| 1:A:1122:LYS:HA | 1:A:1125:ILE:CG2 | 2.24 | 0.58 |
| 1:B:1277:VAL:O | 1:B:1279:HIS:N | 2.37 | 0.58 |
| 1:C:1505:ILE:O | 1:C:1509:ARG:HB2 | 2.03 | 0.58 |
| 1:B:1168:TYR:O | 1:B:1172:GLU:HG2 | 2.03 | 0.58 |
| 2:E:90:ALA:N | 2:E:91:GLN:HB3 | 2.18 | 0.58 |
| 1:B:1206:TYR:HD1 | 1:B:1226:ARG:O | 1.82 | 0.58 |
| 1:A:1258:PHE:HA | 1:A:1289:TYR:CE1 | 2.39 | 0.58 |
| 1:C:1333:ARG:HA | 1:C:1360:GLU:HG2 | 1.85 | 0.58 |
| 1:A:1608:THR:HG23 | 1:B:1607:LEU:HD13 | 1.85 | 0.58 |
| 1:C:1198:ILE:CA | 1:C:1201:VAL:HG23 | 2.34 | 0.58 |
| 1:C:1358:TRP:HA | 1:C:1361:LEU:HB3 | 1.86 | 0.58 |
| 1:A:1407:ALA:C | 1:A:1409:GLN:N | 2.56 | 0.58 |
| 1:B:1395:ILE:CG1 | 1:B:1404:TYR:CD2 | 2.76 | 0.58 |
| 1:B:1375:ILE:CD1 | 1:B:1394:ILE:HB | 2.33 | 0.58 |
| 1:C:1215:LYS:C | 1:C:1217:LEU:N | 2.55 | 0.58 |
| 2:F:150:LYS:O | 2:F:154:ARG:HG3 | 2.04 | 0.58 |
| 1:B:1185:GLU:O | 1:B:1185:GLU:HG2 | 2.03 | 0.58 |
| 1:C:1253:TRP:O | 1:C:1255:GLU:N | 2.37 | 0.57 |
| 1:A:1587:TRP:NE1 | 1:A:1594:PHE:CE2 | 2.66 | 0.57 |
| 1:B:1533:LEU:HG | 1:B:1535:LYS:H | 1.67 | 0.57 |
| 1:C:1472:ILE:CB | 1:C:1498:ARG:HH21 | 2.14 | 0.57 |
| 2:E:119:ALA:O | 2:E:123:MET:CB | 2.51 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1401:VAL:HG22 | 1:A:1429:ARG:CZ | 2.33 | 0.57 |
| 1:A:1407:ALA:O | 1:A:1408:ILE:C | 2.42 | 0.57 |
| 1:B:1150:TRP:CZ3 | 2:D:5:UNK:CA | 2.85 | 0.57 |
| 1:A:1537:ALA:HA | 1:A:1540:TYR:CE2 | 2.39 | 0.57 |
| 1:B:1513:TYR:CD1 | 1:B:1516:LYS:HE2 | 2.37 | 0.57 |
| 1:B:1528:CYS:O | 1:B:1532:SER:HB2 | 2.04 | 0.57 |
| 2:D:181:UNK:C | 2:D:183:UNK:CA | 2.82 | 0.57 |
| 2:E:191:UNK:O | 2:E:192:UNK:CB | 2.52 | 0.57 |
| 1:B:1358:TRP:HA | 1:B:1361:LEU:HB3 | 1.86 | 0.57 |
| 1:C:1395:ILE:CG1 | 1:C:1404:TYR:HE2 | 2.07 | 0.57 |
| 1:C:1404:TYR:OH | 1:C:1429:ARG:NH1 | 2.37 | 0.57 |
| 2:E:105:TRP:O | 2:E:109:GLN:HG2 | 2.04 | 0.57 |
| 1:A:1317:PHE:N | 1:A:1317:PHE:CD2 | 2.64 | 0.57 |
| 1:A:1255:GLU:O | 1:A:1258:PHE:HB3 | 2.04 | 0.57 |
| 1:A:1332:MET:CG | 1:A:1357:LEU:HD13 | 2.35 | 0.57 |
| 1:C:1161:ARG:NE | 1:C:1170:GLU:HB2 | 2.19 | 0.57 |
| 1:C:1198:ILE:O | 1:C:1201:VAL:N | 2.37 | 0.57 |
| 1:B:1382:PRO:HG3 | 1:B:1410:PHE:CE1 | 2.39 | 0.57 |
| 1:C:1382:PRO:CG | 2:E:115:GLU:OE2 | 2.52 | 0.57 |
| 1:C:1407:ALA:O | 1:C:1408:ILE:C | 2.42 | 0.57 |
| 1:A:1404:TYR:OH | 1:A:1429:ARG:NH1 | 2.37 | 0.57 |
| 1:A:1382:PRO:HG3 | 1:A:1410:PHE:CE1 | 2.38 | 0.57 |
| 1:B:1401:VAL:HG22 | 1:B:1429:ARG:CZ | 2.33 | 0.57 |
| 1:B:1391:PHE:CD2 | 1:B:1411:TYR:OH | 2.54 | 0.57 |
| 1:A:1504:LEU:HD13 | 1:A:1506:GLU:HG3 | 1.86 | 0.57 |
| 1:B:1537:ALA:HA | 1:B:1540:TYR:CE2 | 2.39 | 0.57 |
| 1:C:1617:GLU:HG2 | 1:C:1621:LYS:NZ | 2.18 | 0.57 |
| 2:F:151:ILE:HG13 | 2:F:152:ASN:N | 2.18 | 0.57 |
| 1:B:1253:TRP:O | 1:B:1255:GLU:N | 2.37 | 0.57 |
| 1:B:1546:ASP:OD2 | 1:B:1549:LEU:HD23 | 2.03 | 0.57 |
| 1:C:1504:LEU:CD1 | 2:E:149:ASN:CG | 2.57 | 0.57 |
| 1:C:1504:LEU:HD13 | 1:C:1506:GLU:HG3 | 1.85 | 0.57 |
| 1:A:1192:GLY:N | 1:A:1193:PRO:CD | 2.68 | 0.57 |
| 2:E:108:GLU:CD | 2:E:109:GLN:HG2 | 2.24 | 0.57 |
| 2:D:114:GLN:CG | 2:D:115:GLU:N | 2.26 | 0.57 |
| 1:C:1344:ASN:C | 1:C:1345:ILE:HD13 | 2.25 | 0.57 |
| 1:B:1610:VAL:O | 1:B:1614:ASP:OD1 | 2.22 | 0.57 |
| 1:C:1533:LEU:HG | 1:C:1535:LYS:HB2 | 1.85 | 0.57 |
| 1:B:1598:TYR:HD1 | 1:C:1584:GLU:OE2 | 1.85 | 0.57 |
| 1:A:1218:TYR:HD2 | 1:A:1227:LEU:HD12 | 1.68 | 0.57 |
| 1:C:1407:ALA:C | 1:C:1409:GLN:N | 2.56 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:E:141:ARG:NH2 | 2:E:141:ARG:HB2 | 2.20 | 0.57 |
| 1:B:1160:ALA:CB | 1:B:1173:LEU:HD13 | 2.34 | 0.57 |
| 1:C:1319:GLU:HA | 1:C:1322:ILE:HD12 | 1.86 | 0.57 |
| 1:A:1290:TYR:HD2 | 1:A:1299:LEU:HD13 | 1.62 | 0.57 |
| 1:C:1122:LYS:CA | 1:C:1125:ILE:HG22 | 2.25 | 0.57 |
| 1:B:1218:TYR:HD2 | 1:B:1227:LEU:HD12 | 1.68 | 0.57 |
| 1:B:1111:LEU:HD21 | 1:B:1115:GLN:CG | 2.35 | 0.57 |
| 1:A:1083:GLN:O | 1:A:1086:ILE:HG12 | 2.05 | 0.57 |
| 2:D:151:ILE:HG13 | 2:D:152:ASN:N | 2.20 | 0.57 |
| 1:C:1513:TYR:CD1 | 1:C:1516:LYS:HE2 | 2.37 | 0.57 |
| 2:F:170:UNK:O | 2:F:171:UNK:C | 2.53 | 0.57 |
| 1:C:1136:SER:C | 1:C:1136:SER:HA | 2.09 | 0.57 |
| 1:C:1192:GLY:N | 1:C:1193:PRO:HD3 | 2.12 | 0.57 |
| 1:C:1382:PRO:HG3 | 1:C:1410:PHE:CE1 | 2.38 | 0.57 |
| 1:A:1130:LYS:HD2 | 1:A:1156:TYR:HA | 1.86 | 0.57 |
| 1:B:1206:TYR:CG | 1:B:1226:ARG:HG3 | 2.39 | 0.57 |
| 1:B:1284:GLU:O | 1:B:1287:ILE:HG13 | 2.04 | 0.57 |
| 1:B:1257:CYS:HB3 | 1:B:1289:TYR:OH | 2.04 | 0.57 |
| 1:A:1594:PHE:O | 1:A:1596:MET:HE3 | 2.04 | 0.57 |
| 1:B:1586:ALA:O | 1:B:1590:ASN:CG | 2.41 | 0.57 |
| 1:C:1438:TYR:O | 1:C:1442:VAL:HG21 | 2.04 | 0.57 |
| 1:C:1434:ARG:HG3 | 2:E:4:UNK:C | 2.34 | 0.57 |
| 1:C:1434:ARG:CG | 2:E:4:UNK:O | 2.53 | 0.57 |
| 1:B:1407:ALA:C | 1:B:1409:GLN:N | 2.56 | 0.57 |
| 1:B:1438:TYR:O | 1:B:1442:VAL:HG21 | 2.03 | 0.57 |
| 2:D:141:ARG:HB2 | 2:D:141:ARG:HH21 | 1.70 | 0.57 |
| 1:A:1620:ARG:CG | 1:A:1620:ARG:NH1 | 2.53 | 0.57 |
| 2:F:141:ARG:HH21 | 2:F:141:ARG:HB2 | 1.70 | 0.57 |
| 1:C:1326:LYS:HG3 | 1:C:1326:LYS:O | 1.99 | 0.57 |
| 2:D:181:UNK:N | 2:D:183:UNK:CB | 2.67 | 0.57 |
| 1:A:1450:PRO:HA | 1:A:1453:ARG:CG | 2.28 | 0.57 |
| 2:D:127:TRP:HD1 | 2:D:128:ARG:N | 2.03 | 0.57 |
| 1:B:1167:SER:CB | 1:B:1168:TYR:CD1 | 2.87 | 0.57 |
| 1:A:1494:SER:HA | 1:A:1497:GLN:HG3 | 1.86 | 0.57 |
| 1:B:1494:SER:HA | 1:B:1497:GLN:HG3 | 1.86 | 0.57 |
| 1:A:1090:GLY:O | 1:A:1091:ASN:HB2 | 2.04 | 0.57 |
| 1:A:1253:TRP:O | 1:A:1255:GLU:N | 2.38 | 0.56 |
| 1:C:1533:LEU:C | 1:C:1535:LYS:H | 2.08 | 0.56 |
| 1:C:1456:GLN:HG2 | 1:C:1487:TYR:CE2 | 2.40 | 0.56 |
| 1:C:1414:PHE:CG | 2:E:123:MET:HG3 | 2.40 | 0.56 |
| 2:E:127:TRP:HD1 | 2:E:128:ARG:N | 2.03 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:1472:ILE:HB | 1:B:1498:ARG:NH2 | 2.16 | 0.56 |
| 2:E:108:GLU:OE2 | 2:E:109:GLN:CD | 2.42 | 0.56 |
| 2:E:151:ILE:HG13 | 2:E:152:ASN:N | 2.20 | 0.56 |
| 2:E:150:LYS:O | 2:E:154:ARG:HG3 | 2.04 | 0.56 |
| 2:E:90:ALA:N | 2:E:91:GLN:CA | 2.59 | 0.56 |
| 1:A:1602:VAL:HG13 | 2:F:202:UNK:O | 2.05 | 0.56 |
| 1:B:1601:GLN:CG | 1:C:1587:TRP:CH2 | 2.74 | 0.56 |
| 1:C:1134:PRO:O | 1:C:1135:SER:C | 2.44 | 0.56 |
| 1:C:1361:LEU:C | 1:C:1361:LEU:CD2 | 2.72 | 0.56 |
| 1:A:1358:TRP:HA | 1:A:1361:LEU:HB3 | 1.86 | 0.56 |
| 1:B:1300:ILE:O | 1:B:1300:ILE:HD12 | 2.05 | 0.56 |
| 1:A:1157:LEU:O | 1:A:1160:ALA:N | 2.38 | 0.56 |
| 1:C:1104:GLU:N | 1:C:1104:GLU:CD | 2.57 | 0.56 |
| 1:A:1277:VAL:CG2 | 1:A:1278:VAL:H | 2.17 | 0.56 |
| 1:C:1296:PHE:HD2 | 1:C:1297:GLU:HG2 | 1.67 | 0.56 |
| 1:C:1277:VAL:CG2 | 1:C:1278:VAL:H | 2.17 | 0.56 |
| 1:B:1277:VAL:CG2 | 1:B:1278:VAL:H | 2.17 | 0.56 |
| 1:B:1533:LEU:C | 1:B:1535:LYS:H | 2.08 | 0.56 |
| 1:A:1586:ALA:O | 1:A:1590:ASN:ND2 | 2.38 | 0.56 |
| 1:C:1111:LEU:HD12 | 1:C:1129:ILE:HG21 | 1.87 | 0.56 |
| 1:A:1180:THR:HG22 | 1:A:1181:ASN:CG | 2.25 | 0.56 |
| 1:B:1504:LEU:HD13 | 1:B:1506:GLU:HG3 | 1.86 | 0.56 |
| 1:B:1509:ARG:HH22 | 2:D:163:GLN:CB | 2.18 | 0.56 |
| 1:A:1111:LEU:HD21 | 1:A:1115:GLN:CG | 2.35 | 0.56 |
| 1:A:1387:LYS:HB3 | 1:A:1390:GLN:HB2 | 1.87 | 0.56 |
| 1:A:1368:TYR:HD1 | 1:A:1370:GLU:HG2 | 1.66 | 0.56 |
| 1:C:1465:GLU:OE2 | 1:C:1465:GLU:O | 2.23 | 0.56 |
| 2:F:141:ARG:NH2 | 2:F:141:ARG:HB2 | 2.20 | 0.56 |
| 2:E:184:UNK:C | 2:E:186:UNK:N | 2.68 | 0.56 |
| 1:A:1284:GLU:O | 1:A:1287:ILE:HG13 | 2.04 | 0.56 |
| 1:C:1258:PHE:CE1 | 1:C:1293:ARG:NE | 2.74 | 0.56 |
| 1:B:1594:PHE:O | 1:B:1596:MET:HE3 | 2.04 | 0.56 |
| 1:C:1107:VAL:O | 1:C:1108:TRP:HE3 | 1.86 | 0.56 |
| 1:B:1361:LEU:C | 1:B:1361:LEU:CD2 | 2.73 | 0.56 |
| 1:A:1159:MET:SD | 1:A:1162:LYS:HD2 | 2.46 | 0.56 |
| 1:B:1317:PHE:CD2 | 1:B:1317:PHE:N | 2.64 | 0.56 |
| 1:C:1510:ILE:O | 1:C:1514:LEU:N | 2.34 | 0.56 |
| 1:B:1623:GLU:O | 1:B:1626:ALA:HB3 | 2.05 | 0.56 |
| 1:A:1183:LEU:HG | 1:A:1184:ALA:H | 1.71 | 0.56 |
| 1:C:1610:VAL:O | 1:C:1614:ASP:OD1 | 2.23 | 0.56 |
| 1:A:1290:TYR:O | 1:A:1295:TYR:CB | 2.54 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:1325:SER:O | 1:C:1355:ALA:CB | 2.50 | 0.56 |
| 1:A:1596:MET:HE3 | 1:A:1597:PRO:HD3 | 1.86 | 0.56 |
| 1:C:1133:ASP:HB2 | 1:C:1134:PRO:HD2 | 1.88 | 0.56 |
| 1:C:1476:ASP:OD1 | 1:C:1479:ALA:HB3 | 2.06 | 0.56 |
| 1:A:1414:PHE:O | 2:F:130:LYS:HD2 | 2.05 | 0.56 |
| 1:A:1361:LEU:CD2 | 1:A:1361:LEU:C | 2.73 | 0.56 |
| 1:B:1404:TYR:O | 1:B:1407:ALA:CB | 2.52 | 0.56 |
| 1:B:1476:ASP:OD1 | 1:B:1479:ALA:HB3 | 2.05 | 0.56 |
| 1:C:1391:PHE:CD2 | 1:C:1411:TYR:OH | 2.54 | 0.56 |
| 1:B:1167:SER:HB3 | 1:B:1168:TYR:HD1 | 1.68 | 0.56 |
| 1:C:1387:LYS:O | 1:C:1390:GLN:N | 2.31 | 0.56 |
| 1:A:1105:PRO:HG2 | 1:A:1108:TRP:CZ2 | 2.41 | 0.56 |
| 1:C:1161:ARG:HH21 | 1:C:1170:GLU:HG3 | 1.71 | 0.56 |
| 1:C:1174:ILE:HD13 | 1:C:1174:ILE:N | 2.20 | 0.56 |
| 1:C:1179:LYS:C | 1:C:1182:ARG:HH12 | 2.08 | 0.56 |
| 1:A:1358:TRP:CD2 | 1:A:1381:HIS:CG | 2.94 | 0.56 |
| 1:B:1332:MET:CG | 1:B:1357:LEU:HD13 | 2.34 | 0.56 |
| 2:E:105:TRP:O | 2:E:108:GLU:CG | 2.51 | 0.56 |
| 1:C:1494:SER:HA | 1:C:1497:GLN:HG3 | 1.86 | 0.56 |
| 1:A:1465:GLU:OE2 | 1:A:1465:GLU:O | 2.23 | 0.56 |
| 1:A:1257:CYS:C | 1:A:1289:TYR:CE1 | 2.78 | 0.56 |
| 1:A:1533:LEU:C | 1:A:1535:LYS:H | 2.08 | 0.56 |
| 1:B:1602:VAL:HG13 | 2:D:205:UNK:O | 2.06 | 0.56 |
| 1:C:1108:TRP:NE1 | 1:C:1131:ALA:HB2 | 2.20 | 0.56 |
| 1:C:1161:ARG:CZ | 1:C:1195:ASN:HB3 | 2.36 | 0.56 |
| 1:C:1167:SER:C | 1:C:1171:THR:CB | 2.60 | 0.56 |
| 1:B:1198:ILE:HG12 | 1:B:1201:VAL:HG21 | 1.87 | 0.56 |
| 1:B:1144:ALA:HA | 1:B:1149:ASN:HB2 | 1.87 | 0.56 |
| 1:A:1524:SER:O | 1:A:1527:LEU:HD13 | 2.06 | 0.56 |
| 1:B:1188:GLU:OE2 | 1:B:1191:ASN:C | 2.43 | 0.56 |
| 1:C:1279:HIS:NE2 | 1:C:1283:LEU:HD12 | 2.21 | 0.56 |
| 1:C:1332:MET:CG | 1:C:1357:LEU:HD13 | 2.35 | 0.56 |
| 1:B:1258:PHE:CD1 | 1:B:1293:ARG:HD2 | 2.41 | 0.56 |
| 2:F:184:UNK:O | 2:F:186:UNK:N | 2.39 | 0.56 |
| 2:E:127:TRP:O | 2:E:130:LYS:HB2 | 2.06 | 0.56 |
| 1:B:1332:MET:HG3 | 1:B:1357:LEU:HD13 | 1.87 | 0.56 |
| 1:B:1395:ILE:O | 1:B:1404:TYR:OH | 2.17 | 0.56 |
| 1:B:1509:ARG:CZ | 2:D:166:ALA:HB3 | 2.36 | 0.56 |
| 1:B:1130:LYS:HZ3 | 1:B:1155:LYS:HD3 | 1.71 | 0.56 |
| 2:E:184:UNK:C | 2:E:186:UNK:H | 2.19 | 0.56 |
| 2:D:134:ASP:OD1 | 2:D:135:LEU:N | 2.39 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:1253:TRP:O | 1:C:1289:TYR:HE2 | 1.85 | 0.56 |
| 1:C:1295:TYR:O | 1:C:1296:PHE:CD2 | 2.59 | 0.56 |
| 1:A:1476:ASP:OD1 | 1:A:1479:ALA:HB3 | 2.06 | 0.56 |
| 1:A:1456:GLN:HG2 | 1:A:1487:TYR:CE2 | 2.41 | 0.56 |
| 1:A:1472:ILE:CB | 1:A:1498:ARG:HH21 | 2.14 | 0.56 |
| 1:B:1108:TRP:NE1 | 1:B:1131:ALA:CB | 2.67 | 0.56 |
| 1:B:1387:LYS:HD2 | 1:B:1390:GLN:NE2 | 2.21 | 0.56 |
| 2:D:150:LYS:O | 2:D:154:ARG:HG3 | 2.05 | 0.56 |
| 1:A:1255:GLU:C | 1:A:1289:TYR:CE2 | 2.79 | 0.56 |
| 1:A:1332:MET:HG3 | 1:A:1357:LEU:HD13 | 1.87 | 0.56 |
| 1:C:1167:SER:HA | 1:C:1171:THR:OG1 | 2.06 | 0.56 |
| 1:B:1160:ALA:HB3 | 1:B:1173:LEU:HD22 | 1.88 | 0.56 |
| 1:A:1529:LYS:O | 1:A:1532:SER:HB3 | 2.06 | 0.56 |
| 1:A:1300:ILE:O | 1:A:1300:ILE:HD12 | 2.05 | 0.55 |
| 1:C:1111:LEU:HD21 | 1:C:1115:GLN:CG | 2.35 | 0.55 |
| 1:C:1414:PHE:CD1 | 2:E:123:MET:HG3 | 2.40 | 0.55 |
| 1:B:1333:ARG:CB | 1:B:1360:GLU:HG3 | 2.36 | 0.55 |
| 1:C:1387:LYS:HD2 | 1:C:1390:GLN:NE2 | 2.21 | 0.55 |
| 1:A:1206:TYR:CE1 | 1:A:1230:THR:HB | 2.42 | 0.55 |
| 1:C:1499:LEU:CB | 1:C:1511:ALA:HB2 | 2.36 | 0.55 |
| 1:A:1610:VAL:O | 1:A:1614:ASP:OD1 | 2.23 | 0.55 |
| 1:A:1255:GLU:CA | 1:A:1289:TYR:CE2 | 2.88 | 0.55 |
| 1:C:1255:GLU:O | 1:C:1258:PHE:HB3 | 2.06 | 0.55 |
| 1:C:1254:LYS:HA | 1:C:1289:TYR:CE2 | 2.40 | 0.55 |
| 1:B:1572:THR:CB | 1:B:1599:PHE:CD2 | 2.89 | 0.55 |
| 1:C:1194:ASN:HD22 | 1:C:1195:ASN:N | 2.04 | 0.55 |
| 1:A:1193:PRO:O | 1:A:1194:ASN:C | 2.44 | 0.55 |
| 1:C:1092:LEU:O | 1:C:1093:ASP:C | 2.36 | 0.55 |
| 1:B:1387:LYS:HB3 | 1:B:1390:GLN:HB2 | 1.88 | 0.55 |
| 2:E:184:UNK:O | 2:E:185:UNK:C | 2.53 | 0.55 |
| 1:B:1244:ALA:O | 1:B:1246:LYS:N | 2.39 | 0.55 |
| 1:A:1451:TYR:O | 1:A:1455:VAL:HG21 | 2.07 | 0.55 |
| 2:F:127:TRP:HD1 | 2:F:128:ARG:N | 2.03 | 0.55 |
| 1:A:1510:ILE:O | 1:A:1514:LEU:N | 2.34 | 0.55 |
| 2:D:141:ARG:HB2 | 2:D:141:ARG:NH2 | 2.20 | 0.55 |
| 1:A:1116:LEU:HD21 | 1:A:1122:LYS:CB | 2.36 | 0.55 |
| 2:F:102:ILE:HG13 | 2:F:103:ARG:N | 2.22 | 0.55 |
| 1:A:1290:TYR:O | 1:A:1295:TYR:HB2 | 2.06 | 0.55 |
| 1:C:1333:ARG:CB | 1:C:1360:GLU:HG3 | 2.36 | 0.55 |
| 1:B:1451:TYR:O | 1:B:1455:VAL:HG21 | 2.07 | 0.55 |
| 2:E:98:GLU:HA | 2:E:101:SER:CB | 2.31 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:1510:ILE:O | 1:B:1514:LEU:N | 2.34 | 0.55 |
| 1:B:1524:SER:O | 1:B:1527:LEU:HD13 | 2.06 | 0.55 |
| 1:B:1255:GLU:O | 1:B:1258:PHE:HB3 | 2.06 | 0.55 |
| 1:B:1596:MET:HE3 | 1:B:1597:PRO:HD3 | 1.88 | 0.55 |
| 2:E:141:ARG:HH21 | 2:E:141:ARG:HB2 | 1.70 | 0.55 |
| 1:B:1395:ILE:CD1 | 1:B:1403:LEU:HD12 | 2.37 | 0.55 |
| 1:B:1456:GLN:HG2 | 1:B:1487:TYR:CE2 | 2.41 | 0.55 |
| 1:C:1375:ILE:CD1 | 1:C:1394:ILE:HB | 2.32 | 0.55 |
| 2:F:151:ILE:CA | 2:F:154:ARG:HD3 | 2.36 | 0.55 |
| 1:B:1206:TYR:CE2 | 1:B:1226:ARG:HG3 | 2.40 | 0.55 |
| 1:A:1584:GLU:O | 1:A:1587:TRP:N | 2.29 | 0.55 |
| 1:C:1179:LYS:O | 1:C:1182:ARG:NH2 | 2.40 | 0.55 |
| 1:C:1434:ARG:HG3 | 2:E:4:UNK:CB | 2.36 | 0.55 |
| 2:E:134:ASP:OD1 | 2:E:135:LEU:N | 2.39 | 0.55 |
| 2:F:127:TRP:O | 2:F:130:LYS:HB2 | 2.07 | 0.55 |
| 1:B:1426:LEU:O | 1:B:1427:SER:C | 2.45 | 0.55 |
| 2:D:118:ALA:HA | 2:D:121:LYS:HZ2 | 1.70 | 0.55 |
| 2:D:186:UNK:O | 2:D:188:UNK:N | 2.40 | 0.55 |
| 2:F:134:ASP:OD1 | 2:F:135:LEU:N | 2.39 | 0.55 |
| 1:A:1256:VAL:C | 1:A:1289:TYR:OH | 2.44 | 0.55 |
| 1:C:1108:TRP:HE1 | 1:C:1131:ALA:HB2 | 1.71 | 0.55 |
| 1:C:1130:LYS:HG3 | 1:C:1133:ASP:HA | 1.89 | 0.55 |
| 1:B:1358:TRP:CD2 | 1:B:1381:HIS:CG | 2.94 | 0.55 |
| 1:C:1451:TYR:O | 1:C:1455:VAL:HG21 | 2.07 | 0.55 |
| 1:A:1414:PHE:HD1 | 2:F:127:TRP:HB2 | 1.70 | 0.55 |
| 2:F:119:ALA:O | 2:F:123:MET:CB | 2.55 | 0.55 |
| 1:B:1481:ARG:HH11 | 1:B:1510:ILE:HG13 | 1.72 | 0.55 |
| 1:B:1587:TRP:O | 1:B:1589:HIS:CA | 2.54 | 0.55 |
| 1:C:1141:VAL:CG1 | 1:C:1172:GLU:HG2 | 2.36 | 0.55 |
| 1:C:1358:TRP:CD2 | 1:C:1381:HIS:CG | 2.94 | 0.55 |
| 1:C:1404:TYR:O | 1:C:1407:ALA:CB | 2.53 | 0.55 |
| 1:C:1412:LEU:CD2 | 1:C:1439:PHE:CE1 | 2.89 | 0.55 |
| 1:A:1409:GLN:HA | 1:A:1413:GLU:CB | 2.35 | 0.55 |
| 2:E:94:ARG:O | 2:E:96:THR:N | 2.40 | 0.55 |
| 1:A:1481:ARG:HH12 | 1:A:1510:ILE:HD12 | 1.72 | 0.55 |
| 1:B:1149:ASN:O | 1:B:1153:LEU:HB3 | 2.03 | 0.55 |
| 1:B:1600:ILE:HA | 1:B:1603:MET:HE3 | 1.88 | 0.55 |
| 1:C:1175:PHE:HE2 | 1:C:1204:ARG:NH2 | 2.05 | 0.55 |
| 1:C:1480:LEU:O | 1:C:1484:ILE:HG12 | 2.06 | 0.55 |
| 1:B:1448:VAL:O | 1:B:1452:LEU:HG | 2.07 | 0.55 |
| 2:D:127:TRP:O | 2:D:130:LYS:HB2 | 2.06 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1154:VAL:HG13 | 1:A:1180:THR:CG2 | 2.37 | 0.55 |
| 1:A:1082:VAL:CG1 | 1:A:1083:GLN:N | 2.69 | 0.55 |
| 1:B:1465:GLU:OE2 | 1:B:1465:GLU:O | 2.23 | 0.55 |
| 2:E:170:UNK:O | 2:E:171:UNK:C | 2.54 | 0.55 |
| 1:B:1277:VAL:CG2 | 1:B:1278:VAL:N | 2.70 | 0.55 |
| 1:B:1387:LYS:O | 1:B:1390:GLN:N | 2.31 | 0.55 |
| 1:A:1246:LYS:O | 1:A:1247:ALA:CB | 2.55 | 0.55 |
| 1:A:1333:ARG:CB | 1:A:1360:GLU:HG3 | 2.36 | 0.54 |
| 1:C:1395:ILE:CD1 | 1:C:1403:LEU:HD12 | 2.36 | 0.54 |
| 1:A:1426:LEU:O | 1:A:1427:SER:C | 2.45 | 0.54 |
| 1:B:1206:TYR:CE1 | 1:B:1226:ARG:HA | 2.42 | 0.54 |
| 1:B:1190:ILE:HG23 | 1:B:1191:ASN:ND2 | 2.22 | 0.54 |
| 1:C:1528:CYS:O | 1:C:1532:SER:HB2 | 2.07 | 0.54 |
| 1:A:1253:TRP:O | 1:A:1289:TYR:CZ | 2.60 | 0.54 |
| 1:C:1554:LEU:HA | 1:C:1557:PHE:CD2 | 2.41 | 0.54 |
| 1:C:1111:LEU:HD21 | 1:C:1115:GLN:HG3 | 1.89 | 0.54 |
| 1:C:1122:LYS:CG | 1:C:1123:GLU:H | 2.19 | 0.54 |
| 1:A:1448:VAL:O | 1:A:1452:LEU:HG | 2.07 | 0.54 |
| 1:A:1387:LYS:HD2 | 1:A:1390:GLN:NE2 | 2.21 | 0.54 |
| 1:C:1524:SER:O | 1:C:1527:LEU:HD13 | 2.06 | 0.54 |
| 1:A:1319:GLU:HA | 1:A:1322:ILE:CD1 | 2.38 | 0.54 |
| 1:A:1601:GLN:HA | 1:A:1604:LYS:HD2 | 1.89 | 0.54 |
| 1:B:1596:MET:N | 1:B:1597:PRO:CD | 2.69 | 0.54 |
| 1:C:1154:VAL:CG1 | 1:C:1177:LEU:HD23 | 2.38 | 0.54 |
| 1:C:1192:GLY:N | 1:C:1193:PRO:CD | 2.66 | 0.54 |
| 1:C:1448:VAL:O | 1:C:1452:LEU:HG | 2.07 | 0.54 |
| 1:A:1449:LYS:HB3 | 1:A:1450:PRO:CD | 2.37 | 0.54 |
| 1:A:1467:LEU:HG | 1:A:1471:PHE:CE2 | 2.43 | 0.54 |
| 1:A:1162:LYS:O | 1:A:1163:LYS:HB2 | 2.06 | 0.54 |
| 1:C:1389:GLY:O | 1:C:1392:LYS:N | 2.40 | 0.54 |
| 1:C:1585:THR:O | 1:C:1589:HIS:HB2 | 2.08 | 0.54 |
| 1:A:1403:LEU:C | 1:A:1403:LEU:CD1 | 2.75 | 0.54 |
| 1:A:1493:ILE:HG22 | 1:A:1494:SER:N | 2.23 | 0.54 |
| 1:B:1102:CYS:O | 1:B:1103:ASN:HB2 | 2.06 | 0.54 |
| 1:B:1130:LYS:NZ | 1:B:1155:LYS:CG | 2.70 | 0.54 |
| 1:A:1387:LYS:O | 1:A:1390:GLN:N | 2.31 | 0.54 |
| 2:D:51:UNK:C | 2:D:53:UNK:N | 2.69 | 0.54 |
| 1:A:1359:ALA:HB3 | 1:A:1360:GLU:OE1 | 2.08 | 0.54 |
| 1:C:1277:VAL:CG2 | 1:C:1278:VAL:N | 2.70 | 0.54 |
| 1:B:1535:LYS:CA | 1:B:1535:LYS:HE2 | 2.36 | 0.54 |
| 1:B:1551:GLU:OE1 | 1:B:1582:VAL:HG22 | 2.08 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:1404:TYR:O | 1:B:1407:ALA:N | 2.41 | 0.54 |
| 1:B:1414:PHE:CE1 | 2:D:127:TRP:CE3 | 2.96 | 0.54 |
| 1:B:1469:ASN:HD22 | 1:B:1498:ARG:NH2 | 2.05 | 0.54 |
| 2:E:94:ARG:C | 2:E:96:THR:H | 2.11 | 0.54 |
| 1:A:1111:LEU:HD21 | 1:A:1115:GLN:HG3 | 1.89 | 0.54 |
| 1:C:1225:GLY:C | 1:C:1227:LEU:H | 2.10 | 0.54 |
| 1:C:1227:LEU:HD23 | 1:C:1228:ALA:N | 2.23 | 0.54 |
| 1:A:1150:TRP:O | 1:A:1153:LEU:HB3 | 2.07 | 0.54 |
| 1:B:1190:ILE:HD13 | 1:B:1216:LEU:CD1 | 2.37 | 0.54 |
| 1:C:1529:LYS:O | 1:C:1532:SER:HB3 | 2.06 | 0.54 |
| 1:A:1282:GLU:O | 1:A:1283:LEU:HD13 | 2.07 | 0.54 |
| 1:C:1414:PHE:CD1 | 2:E:123:MET:CG | 2.91 | 0.54 |
| 1:C:1469:ASN:HD22 | 1:C:1498:ARG:NH2 | 2.05 | 0.54 |
| 1:A:1395:ILE:CD1 | 1:A:1403:LEU:HD12 | 2.37 | 0.54 |
| 1:B:1376:ILE:HA | 1:B:1379:MET:SD | 2.48 | 0.54 |
| 1:B:1412:LEU:CD2 | 1:B:1439:PHE:CE1 | 2.90 | 0.54 |
| 1:A:1159:MET:O | 1:A:1162:LYS:HB3 | 2.08 | 0.54 |
| 1:B:1234:LEU:HG | 1:B:1235:GLY:N | 2.20 | 0.54 |
| 1:A:1317:PHE:HD1 | 1:A:1339:PHE:HB3 | 1.71 | 0.54 |
| 1:B:1529:LYS:O | 1:B:1532:SER:HB3 | 2.07 | 0.54 |
| 1:C:1251:ARG:O | 1:C:1252:THR:OG1 | 2.20 | 0.54 |
| 1:B:1605:GLU:OE2 | 1:C:1579:PRO:HB3 | 2.07 | 0.54 |
| 1:A:1404:TYR:O | 1:A:1407:ALA:N | 2.40 | 0.54 |
| 1:B:1403:LEU:C | 1:B:1403:LEU:CD1 | 2.75 | 0.54 |
| 1:A:1162:LYS:O | 1:A:1163:LYS:CB | 2.55 | 0.54 |
| 1:B:1086:ILE:HG22 | 1:B:1087:GLU:N | 2.21 | 0.54 |
| 1:A:1122:LYS:CG | 1:A:1123:GLU:H | 2.18 | 0.54 |
| 2:D:27:UNK:C | 2:D:29:UNK:H | 2.21 | 0.54 |
| 1:A:1290:TYR:CG | 1:A:1295:TYR:CD2 | 2.96 | 0.54 |
| 1:C:1332:MET:HG3 | 1:C:1357:LEU:HD13 | 1.87 | 0.54 |
| 1:B:1274:LEU:CA | 1:B:1277:VAL:CG2 | 2.86 | 0.54 |
| 1:C:1596:MET:N | 1:C:1597:PRO:CD | 2.68 | 0.54 |
| 1:A:1376:ILE:HA | 1:A:1379:MET:SD | 2.48 | 0.54 |
| 1:A:1469:ASN:HD22 | 1:A:1498:ARG:NH2 | 2.05 | 0.54 |
| 1:B:1467:LEU:HG | 1:B:1471:PHE:CE2 | 2.43 | 0.54 |
| 1:B:1225:GLY:C | 1:B:1227:LEU:H | 2.10 | 0.54 |
| 2:E:93:ASP:HB3 | 2:E:97:GLN:CG | 2.38 | 0.54 |
| 1:A:1274:LEU:O | 1:A:1277:VAL:HG22 | 2.08 | 0.54 |
| 1:C:1359:ALA:HB3 | 1:C:1360:GLU:OE1 | 2.07 | 0.54 |
| 1:C:1596:MET:HE3 | 1:C:1597:PRO:HD3 | 1.90 | 0.54 |
| 1:C:1111:LEU:CD2 | 1:C:1115:GLN:HG2 | 2.38 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1408:ILE:HG22 | 1:A:1412:LEU:CD2 | 2.28 | 0.54 |
| 1:C:1368:TYR:HD1 | 1:C:1370:GLU:HG2 | 1.66 | 0.54 |
| 1:C:1535:LYS:HE2 | 1:C:1535:LYS:CA | 2.36 | 0.54 |
| 1:A:1227:LEU:HD23 | 1:A:1228:ALA:N | 2.23 | 0.54 |
| 2:F:127:TRP:HD1 | 2:F:128:ARG:HG3 | 1.72 | 0.54 |
| 1:A:1377:THR:CA | 1:A:1381:HIS:HD2 | 2.21 | 0.54 |
| 1:B:1227:LEU:HD23 | 1:B:1228:ALA:N | 2.22 | 0.54 |
| 1:B:1103:ASN:C | 1:B:1105:PRO:HD3 | 2.28 | 0.54 |
| 1:A:1111:LEU:CD2 | 1:A:1115:GLN:HG2 | 2.38 | 0.54 |
| 1:B:1236:GLU:C | 1:B:1238:GLN:H | 2.12 | 0.54 |
| 2:D:151:ILE:CA | 2:D:154:ARG:HD3 | 2.36 | 0.54 |
| 2:D:49:UNK:O | 2:D:51:UNK:N | 2.40 | 0.54 |
| 1:A:1283:LEU:CD2 | 1:A:1313:HIS:NE2 | 2.58 | 0.53 |
| 1:C:1277:VAL:C | 1:C:1279:HIS:N | 2.53 | 0.53 |
| 1:A:1572:THR:OG1 | 1:A:1599:PHE:CD2 | 2.56 | 0.53 |
| 1:B:1535:LYS:HZ3 | 1:B:1563:ARG:HH12 | 1.55 | 0.53 |
| 1:C:1586:ALA:CB | 1:C:1594:PHE:CZ | 2.90 | 0.53 |
| 1:A:1598:TYR:HD2 | 2:F:198:UNK:CB | 2.20 | 0.53 |
| 1:A:1225:GLY:C | 1:A:1227:LEU:H | 2.10 | 0.53 |
| 1:B:1372:ASP:O | 1:B:1376:ILE:CG1 | 2.49 | 0.53 |
| 1:B:1493:ILE:HG22 | 1:B:1494:SER:N | 2.22 | 0.53 |
| 1:B:1144:ALA:CB | 1:B:1149:ASN:CB | 2.84 | 0.53 |
| 1:A:1085:LEU:HB3 | 1:A:1095:ALA:HB1 | 1.90 | 0.53 |
| 1:A:1087:GLU:C | 1:A:1089:ILE:H | 2.10 | 0.53 |
| 1:C:1317:PHE:HD1 | 1:C:1339:PHE:HB3 | 1.71 | 0.53 |
| 2:E:93:ASP:HB3 | 2:E:97:GLN:HG3 | 1.90 | 0.53 |
| 1:A:1274:LEU:CA | 1:A:1277:VAL:CG2 | 2.86 | 0.53 |
| 1:C:1274:LEU:O | 1:C:1277:VAL:HG22 | 2.08 | 0.53 |
| 1:C:1584:GLU:O | 1:C:1585:THR:C | 2.46 | 0.53 |
| 1:C:1144:ALA:O | 1:C:1145:ASN:HB2 | 2.08 | 0.53 |
| 1:C:1376:ILE:HA | 1:C:1379:MET:SD | 2.48 | 0.53 |
| 1:C:1426:LEU:O | 1:C:1427:SER:C | 2.45 | 0.53 |
| 1:C:1449:LYS:HB3 | 1:C:1450:PRO:CD | 2.38 | 0.53 |
| 1:B:1409:GLN:CB | 1:B:1413:GLU:HG2 | 2.25 | 0.53 |
| 1:A:1167:SER:O | 1:A:1169:VAL:N | 2.37 | 0.53 |
| 1:C:1493:ILE:HG22 | 1:C:1494:SER:N | 2.23 | 0.53 |
| 1:B:1111:LEU:CD2 | 1:B:1115:GLN:HG2 | 2.38 | 0.53 |
| 1:A:1082:VAL:CG1 | 1:A:1083:GLN:H | 2.15 | 0.53 |
| 2:E:89:ILE:N | 2:E:90:ALA:CA | 2.70 | 0.53 |
| 1:B:1190:ILE:HD13 | 1:B:1216:LEU:CG | 2.38 | 0.53 |
| 1:B:1319:GLU:HA | 1:B:1322:ILE:CD1 | 2.37 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:1084:VAL:O | 1:C:1086:ILE:O | 2.25 | 0.53 |
| 1:A:1535:LYS:CA | 1:A:1535:LYS:HE2 | 2.36 | 0.53 |
| 1:C:1467:LEU:HG | 1:C:1471:PHE:CE2 | 2.43 | 0.53 |
| 1:A:1469:ASN:HD22 | 1:A:1498:ARG:HH22 | 1.55 | 0.53 |
| 1:B:1449:LYS:HB3 | 1:B:1450:PRO:CD | 2.38 | 0.53 |
| 2:F:166:ALA:O | 2:F:167:ASP:CB | 2.55 | 0.53 |
| 1:B:1111:LEU:HD21 | 1:B:1115:GLN:HG3 | 1.89 | 0.53 |
| 1:C:1387:LYS:HB3 | 1:C:1390:GLN:HB2 | 1.87 | 0.53 |
| 2:E:178:UNK:C | 2:E:180:UNK:N | 2.70 | 0.53 |
| 1:A:1360:GLU:O | 1:A:1364:LEU:HG | 2.09 | 0.53 |
| 1:B:1282:GLU:O | 1:B:1283:LEU:HD13 | 2.08 | 0.53 |
| 1:B:1572:THR:CG2 | 1:B:1599:PHE:HD2 | 2.21 | 0.53 |
| 1:C:1434:ARG:CD | 2:E:4:UNK:O | 2.57 | 0.53 |
| 1:B:1449:LYS:HB3 | 1:B:1450:PRO:HD3 | 1.90 | 0.53 |
| 1:B:1148:GLY:HA2 | 1:B:1150:TRP:CZ3 | 2.44 | 0.53 |
| 1:A:1211:TYR:HB2 | 1:A:1231:LEU:CD1 | 2.38 | 0.53 |
| 1:A:1144:ALA:O | 1:A:1145:ASN:HB2 | 2.08 | 0.53 |
| 1:A:1528:CYS:O | 1:A:1532:SER:HB2 | 2.08 | 0.53 |
| 1:B:1574:TYR:O | 1:B:1575:ASP:C | 2.46 | 0.53 |
| 1:A:1578:ARG:NH1 | 1:A:1583:LEU:HD23 | 2.21 | 0.53 |
| 1:A:1584:GLU:C | 1:A:1586:ALA:N | 2.62 | 0.53 |
| 1:B:1578:ARG:NH1 | 1:B:1583:LEU:HD23 | 2.21 | 0.53 |
| 1:C:1608:THR:O | 1:C:1612:LYS:HG3 | 2.09 | 0.53 |
| 1:A:1412:LEU:CD2 | 1:A:1439:PHE:CE1 | 2.90 | 0.53 |
| 1:A:1368:TYR:O | 1:A:1369:GLU:HB2 | 2.09 | 0.53 |
| 1:B:1317:PHE:HD1 | 1:B:1339:PHE:HB3 | 1.72 | 0.53 |
| 1:B:1251:ARG:O | 1:B:1252:THR:OG1 | 2.20 | 0.53 |
| 1:B:1596:MET:SD | 1:B:1597:PRO:CD | 2.92 | 0.53 |
| 1:C:1148:GLY:O | 1:C:1149:ASN:CB | 2.56 | 0.53 |
| 1:B:1330:GLN:CG | 1:B:1331:LYS:H | 2.22 | 0.53 |
| 1:C:1247:ALA:O | 1:C:1247:ALA:CB | 2.56 | 0.53 |
| 1:B:1161:ARG:NH2 | 1:B:1192:GLY:C | 2.62 | 0.53 |
| 1:A:1084:VAL:O | 1:A:1089:ILE:HG22 | 2.09 | 0.53 |
| 1:A:1091:ASN:HD21 | 1:A:1092:LEU:HG | 1.72 | 0.53 |
| 1:B:1092:LEU:C | 1:B:1094:ARG:H | 2.12 | 0.53 |
| 1:A:1278:VAL:HG12 | 1:A:1278:VAL:O | 2.09 | 0.53 |
| 1:C:1235:GLY:O | 1:C:1238:GLN:HB2 | 2.08 | 0.53 |
| 1:C:1254:LYS:NZ | 1:C:1285:GLU:HG2 | 2.24 | 0.53 |
| 1:B:1279:HIS:CG | 1:B:1280:ALA:N | 2.75 | 0.53 |
| 1:B:1601:GLN:HA | 1:B:1604:LYS:HD2 | 1.90 | 0.53 |
| 1:C:1150:TRP:O | 1:C:1153:LEU:HB3 | 2.07 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:1404:TYR:O | 1:C:1407:ALA:N | 2.40 | 0.53 |
| 1:A:1416:PRO:CG | 2:F:130:LYS:CG | 2.70 | 0.53 |
| 1:A:1481:ARG:HH11 | 1:A:1510:ILE:HG13 | 1.72 | 0.53 |
| 1:B:1122:LYS:CG | 1:B:1123:GLU:H | 2.19 | 0.53 |
| 1:A:1130:LYS:HZ3 | 1:A:1155:LYS:CB | 2.21 | 0.53 |
| 1:A:1236:GLU:C | 1:A:1238:GLN:H | 2.12 | 0.53 |
| 1:A:1578:ARG:HH11 | 1:A:1582:VAL:HG12 | 1.74 | 0.53 |
| 1:C:1572:THR:HG21 | 1:C:1599:PHE:HD2 | 1.69 | 0.53 |
| 1:A:1414:PHE:O | 1:A:1416:PRO:CD | 2.23 | 0.53 |
| 1:B:1409:GLN:HA | 1:B:1413:GLU:CB | 2.35 | 0.53 |
| 1:B:1469:ASN:HD22 | 1:B:1498:ARG:HH22 | 1.56 | 0.53 |
| 1:B:1481:ARG:HH12 | 1:B:1510:ILE:HD12 | 1.72 | 0.53 |
| 1:C:1230:THR:O | 1:C:1231:LEU:HB3 | 2.08 | 0.53 |
| 1:A:1572:THR:CB | 1:A:1599:PHE:CD2 | 2.92 | 0.53 |
| 1:C:1535:LYS:HZ3 | 1:C:1563:ARG:HH12 | 1.55 | 0.53 |
| 1:A:1449:LYS:HB3 | 1:A:1450:PRO:HD3 | 1.90 | 0.53 |
| 1:B:1359:ALA:HB3 | 1:B:1360:GLU:OE1 | 2.08 | 0.53 |
| 1:B:1360:GLU:O | 1:B:1364:LEU:HG | 2.09 | 0.53 |
| 1:B:1150:TRP:HE3 | 2:D:5:UNK:HA | 1.64 | 0.53 |
| 1:A:1126:ASP:OD1 | 1:A:1156:TYR:OH | 2.27 | 0.53 |
| 2:E:90:ALA:N | 2:E:91:GLN:CB | 2.67 | 0.53 |
| 1:A:1421:ASP:HA | 1:A:1424:MET:SD | 2.49 | 0.53 |
| 1:A:1596:MET:N | 1:A:1597:PRO:CD | 2.68 | 0.53 |
| 1:B:1588:ARG:CZ | 2:F:192:UNK:CA | 2.59 | 0.53 |
| 1:C:1199:GLN:O | 1:C:1200:GLN:C | 2.44 | 0.53 |
| 1:C:1471:PHE:CA | 1:C:1474:GLU:HG2 | 2.38 | 0.53 |
| 1:B:1144:ALA:O | 1:B:1145:ASN:HB2 | 2.07 | 0.53 |
| 1:C:1360:GLU:O | 1:C:1364:LEU:HG | 2.09 | 0.52 |
| 1:A:1601:GLN:CG | 1:A:1604:LYS:HD2 | 2.39 | 0.52 |
| 2:F:180:UNK:O | 2:F:181:UNK:C | 2.57 | 0.52 |
| 1:A:1535:LYS:HZ2 | 2:F:181:UNK:CB | 2.22 | 0.52 |
| 1:B:1414:PHE:O | 2:D:130:LYS:HD2 | 2.03 | 0.52 |
| 1:C:1620:ARG:CG | 1:C:1620:ARG:NH1 | 2.53 | 0.52 |
| 1:A:1584:GLU:O | 1:A:1585:THR:C | 2.46 | 0.52 |
| 1:A:1608:THR:O | 1:A:1612:LYS:HG3 | 2.09 | 0.52 |
| 1:B:1554:LEU:HA | 1:B:1557:PHE:CD2 | 2.40 | 0.52 |
| 1:C:1170:GLU:HG2 | 1:C:1171:THR:N | 2.24 | 0.52 |
| 1:A:1471:PHE:CA | 1:A:1474:GLU:HG2 | 2.38 | 0.52 |
| 1:B:1354:GLN:HG3 | 1:B:1354:GLN:O | 2.09 | 0.52 |
| 1:B:1419:LEU:HD23 | 1:B:1447:LEU:CD1 | 2.40 | 0.52 |
| 1:A:1170:GLU:HG2 | 1:A:1171:THR:N | 2.25 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:1174:ILE:HG21 | 1:B:1201:VAL:CG2 | 2.30 | 0.52 |
| 1:A:1137:TYR:CB | 1:A:1138:MET:CB | 2.64 | 0.52 |
| 1:B:1085:LEU:CD1 | 1:B:1125:ILE:HD11 | 2.35 | 0.52 |
| 2:E:155:ILE:O | 2:E:156:ALA:HB3 | 2.09 | 0.52 |
| 1:A:1085:LEU:HD12 | 1:A:1085:LEU:O | 2.08 | 0.52 |
| 1:A:1103:ASN:O | 1:A:1105:PRO:CD | 2.56 | 0.52 |
| 2:D:98:GLU:CB | 2:D:99:PRO:HD3 | 2.26 | 0.52 |
| 1:C:1301:THR:CA | 1:C:1304:GLU:HG3 | 2.32 | 0.52 |
| 2:F:155:ILE:O | 2:F:156:ALA:HB3 | 2.09 | 0.52 |
| 1:C:1354:GLN:HG3 | 1:C:1354:GLN:O | 2.09 | 0.52 |
| 1:B:1274:LEU:O | 1:B:1277:VAL:HG22 | 2.08 | 0.52 |
| 1:A:1597:PRO:HB3 | 1:A:1601:GLN:NE2 | 2.24 | 0.52 |
| 1:B:1608:THR:O | 1:B:1612:LYS:HG3 | 2.09 | 0.52 |
| 1:C:1584:GLU:C | 1:C:1586:ALA:N | 2.62 | 0.52 |
| 1:C:1127:SER:CA | 1:C:1156:TYR:OH | 2.54 | 0.52 |
| 1:C:1409:GLN:HA | 1:C:1413:GLU:CB | 2.35 | 0.52 |
| 1:B:1420:ASN:OD1 | 1:B:1447:LEU:O | 2.27 | 0.52 |
| 1:B:1445:LEU:HD23 | 1:B:1448:VAL:HG22 | 1.91 | 0.52 |
| 1:A:1136:SER:OG | 1:A:1141:VAL:HG11 | 2.09 | 0.52 |
| 1:A:1167:SER:C | 1:A:1168:TYR:CG | 2.81 | 0.52 |
| 2:E:98:GLU:H | 2:E:99:PRO:CD | 2.21 | 0.52 |
| 2:D:112:ARG:O | 2:D:112:ARG:NH1 | 2.42 | 0.52 |
| 2:E:151:ILE:CA | 2:E:154:ARG:HD3 | 2.36 | 0.52 |
| 1:C:1345:ILE:H | 1:C:1346:PRO:CD | 2.18 | 0.52 |
| 2:D:155:ILE:O | 2:D:156:ALA:HB3 | 2.09 | 0.52 |
| 1:A:1570:LEU:O | 1:A:1570:LEU:HD23 | 2.08 | 0.52 |
| 1:A:1354:GLN:HG3 | 1:A:1354:GLN:O | 2.09 | 0.52 |
| 1:C:1234:LEU:HD21 | 1:C:1264:LYS:NZ | 2.15 | 0.52 |
| 1:B:1254:LYS:NZ | 1:B:1285:GLU:HG2 | 2.25 | 0.52 |
| 1:B:1583:LEU:O | 1:B:1587:TRP:CE2 | 2.63 | 0.52 |
| 1:B:1588:ARG:HD3 | 2:F:195:UNK:CB | 2.40 | 0.52 |
| 1:C:1601:GLN:HA | 1:C:1604:LYS:HD2 | 1.90 | 0.52 |
| 1:C:1082:VAL:HG22 | 1:C:1107:VAL:HG11 | 1.90 | 0.52 |
| 1:A:1404:TYR:O | 1:A:1407:ALA:CB | 2.52 | 0.52 |
| 1:A:1420:ASN:OD1 | 1:A:1447:LEU:O | 2.27 | 0.52 |
| 1:B:1471:PHE:CA | 1:B:1474:GLU:HG2 | 2.38 | 0.52 |
| 1:B:1170:GLU:C | 1:B:1172:GLU:N | 2.63 | 0.52 |
| 2:D:102:ILE:O | 2:D:106:ARG:HB2 | 2.09 | 0.52 |
| 1:C:1525:VAL:HG22 | 1:C:1525:VAL:O | 2.09 | 0.52 |
| 1:B:1090:GLY:HA2 | 1:B:1094:ARG:NH2 | 2.24 | 0.52 |
| 1:C:1421:ASP:HA | 1:C:1424:MET:SD | 2.49 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1267:ARG:NH2 | 1:A:1298:GLU:OE1 | 2.42 | 0.52 |
| 1:A:1587:TRP:HE1 | 1:A:1594:PHE:HE2 | 1.46 | 0.52 |
| 1:B:1578:ARG:HH11 | 1:B:1582:VAL:HG12 | 1.74 | 0.52 |
| 1:B:1584:GLU:O | 1:B:1585:THR:C | 2.46 | 0.52 |
| 1:C:1449:LYS:HB3 | 1:C:1450:PRO:HD3 | 1.91 | 0.52 |
| 1:A:1164:ALA:O | 1:A:1165:ARG:HB3 | 2.10 | 0.52 |
| 1:B:1170:GLU:HG2 | 1:B:1171:THR:N | 2.24 | 0.52 |
| 1:A:1510:ILE:CD1 | 1:A:1510:ILE:N | 2.73 | 0.52 |
| 1:B:1510:ILE:N | 1:B:1510:ILE:CD1 | 2.73 | 0.52 |
| 1:A:1525:VAL:O | 1:A:1525:VAL:HG22 | 2.09 | 0.52 |
| 2:E:154:ARG:CB | 2:E:154:ARG:NH1 | 2.73 | 0.52 |
| 1:B:1624:GLU:O | 1:B:1626:ALA:N | 2.42 | 0.52 |
| 2:D:14:UNK:C | 2:D:16:UNK:H | 2.21 | 0.52 |
| 1:B:1570:LEU:HD23 | 1:B:1570:LEU:O | 2.08 | 0.52 |
| 1:C:1570:LEU:O | 1:C:1570:LEU:HD23 | 2.09 | 0.52 |
| 1:B:1278:VAL:HG12 | 1:B:1278:VAL:O | 2.09 | 0.52 |
| 1:A:1588:ARG:CZ | 2:E:192:UNK:HA | 2.38 | 0.52 |
| 2:D:154:ARG:CB | 2:D:154:ARG:NH1 | 2.73 | 0.52 |
| 1:C:1303:LEU:HD12 | 1:C:1320:LEU:CD1 | 2.34 | 0.52 |
| 1:C:1240:ALA:C | 1:C:1242:ASP:H | 2.12 | 0.52 |
| 1:C:1613:LEU:O | 1:C:1616:SER:HB2 | 2.10 | 0.52 |
| 1:B:1421:ASP:HA | 1:B:1424:MET:SD | 2.49 | 0.52 |
| 1:C:1154:VAL:HG13 | 1:C:1176:ALA:HB1 | 1.90 | 0.52 |
| 1:C:1377:THR:CA | 1:C:1381:HIS:HD2 | 2.21 | 0.52 |
| 1:C:1469:ASN:HD22 | 1:C:1498:ARG:HH22 | 1.56 | 0.52 |
| 1:A:1382:PRO:CG | 1:A:1410:PHE:HE1 | 2.23 | 0.52 |
| 1:B:1167:SER:O | 1:B:1168:TYR:CG | 2.61 | 0.52 |
| 1:A:1121:VAL:HG12 | 1:A:1125:ILE:HB | 1.91 | 0.52 |
| 1:C:1368:TYR:O | 1:C:1369:GLU:HB2 | 2.09 | 0.52 |
| 1:B:1368:TYR:HD1 | 1:B:1370:GLU:HG2 | 1.66 | 0.52 |
| 1:C:1236:GLU:C | 1:C:1238:GLN:H | 2.12 | 0.52 |
| 1:C:1297:GLU:HA | 1:C:1300:ILE:HG12 | 1.92 | 0.52 |
| 1:A:1595:ALA:C | 1:A:1596:MET:HG3 | 2.30 | 0.52 |
| 1:B:1597:PRO:HB3 | 1:B:1601:GLN:NE2 | 2.23 | 0.52 |
| 1:C:1111:LEU:HD22 | 1:C:1111:LEU:C | 2.29 | 0.52 |
| 1:C:1353:GLU:OE2 | 1:C:1361:LEU:HD11 | 2.10 | 0.52 |
| 1:A:1419:LEU:HD23 | 1:A:1447:LEU:CD1 | 2.40 | 0.52 |
| 2:D:127:TRP:HD1 | 2:D:128:ARG:HG3 | 1.72 | 0.52 |
| 1:A:1083:GLN:HG2 | 1:A:1107:VAL:HB | 1.91 | 0.52 |
| 1:A:1086:ILE:CB | 1:A:1089:ILE:HB | 2.40 | 0.52 |
| 2:F:154:ARG:CB | 2:F:154:ARG:NH1 | 2.73 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:1345:ILE:H | 1:B:1346:PRO:CD | 2.18 | 0.52 |
| 2:E:181:UNK:C | 2:E:183:UNK:N | 2.71 | 0.52 |
| 1:C:1279:HIS:CD2 | 1:C:1283:LEU:CD1 | 2.93 | 0.52 |
| 1:C:1207:ASP:CG | 1:C:1207:ASP:O | 2.48 | 0.52 |
| 1:C:1403:LEU:CD1 | 1:C:1403:LEU:C | 2.75 | 0.52 |
| 1:C:1423:LEU:HD12 | 1:C:1451:TYR:HB2 | 1.92 | 0.52 |
| 1:C:1419:LEU:HD23 | 1:C:1447:LEU:CD1 | 2.40 | 0.52 |
| 1:A:1358:TRP:CE3 | 1:A:1381:HIS:CG | 2.98 | 0.52 |
| 1:B:1136:SER:OG | 1:B:1141:VAL:HG11 | 2.09 | 0.52 |
| 1:A:1235:GLY:O | 1:A:1236:GLU:HB2 | 2.10 | 0.52 |
| 1:A:1292:ASP:O | 2:F:97:GLN:CG | 2.56 | 0.52 |
| 1:C:1206:TYR:HB2 | 1:C:1226:ARG:HG3 | 1.91 | 0.52 |
| 1:C:1319:GLU:HA | 1:C:1322:ILE:CD1 | 2.39 | 0.52 |
| 1:A:1587:TRP:HH2 | 1:C:1601:GLN:CG | 2.19 | 0.52 |
| 1:C:1129:ILE:HD12 | 1:C:1129:ILE:C | 2.31 | 0.52 |
| 1:A:1445:LEU:HD23 | 1:A:1448:VAL:HG22 | 1.91 | 0.52 |
| 1:A:1161:ARG:NE | 1:A:1170:GLU:HB2 | 2.25 | 0.52 |
| 1:A:1391:PHE:CD2 | 1:A:1411:TYR:OH | 2.54 | 0.52 |
| 1:B:1150:TRP:O | 1:B:1153:LEU:HB3 | 2.10 | 0.52 |
| 1:A:1234:LEU:HG | 1:A:1235:GLY:N | 2.20 | 0.52 |
| 1:B:1368:TYR:O | 1:B:1369:GLU:HB2 | 2.09 | 0.52 |
| 1:C:1461:LYS:HG2 | 1:C:1489:ASN:HD21 | 1.74 | 0.52 |
| 1:C:1566:PHE:HE2 | 2:E:181:UNK:HA | 1.71 | 0.52 |
| 1:C:1208:GLU:O | 1:C:1209:LYS:HG2 | 2.10 | 0.52 |
| 1:A:1363:PHE:O | 1:A:1366:ASP:HB3 | 2.10 | 0.52 |
| 1:A:1295:TYR:C | 1:A:1296:PHE:CG | 2.81 | 0.51 |
| 1:B:1588:ARG:HH12 | 2:F:192:UNK:CA | 2.17 | 0.51 |
| 1:B:1605:GLU:HG3 | 1:C:1580:ASP:CG | 2.30 | 0.51 |
| 1:C:1358:TRP:CE3 | 1:C:1381:HIS:CG | 2.98 | 0.51 |
| 1:A:1353:GLU:OE2 | 1:A:1361:LEU:HD11 | 2.10 | 0.51 |
| 1:B:1177:LEU:O | 1:B:1180:THR:OG1 | 2.24 | 0.51 |
| 1:B:1082:VAL:CG1 | 1:B:1083:GLN:H | 2.15 | 0.51 |
| 1:C:1151:GLU:O | 1:C:1151:GLU:HG2 | 2.10 | 0.51 |
| 1:A:1240:ALA:C | 1:A:1242:ASP:H | 2.12 | 0.51 |
| 1:A:1282:GLU:C | 1:A:1283:LEU:HD13 | 2.31 | 0.51 |
| 1:A:1549:LEU:O | 1:A:1552:GLU:HB2 | 2.10 | 0.51 |
| 1:A:1583:LEU:O | 1:A:1587:TRP:CE2 | 2.63 | 0.51 |
| 1:C:1578:ARG:HH11 | 1:C:1582:VAL:HG12 | 1.74 | 0.51 |
| 1:C:1122:LYS:O | 1:C:1126:ASP:N | 2.44 | 0.51 |
| 1:C:1420:ASN:OD1 | 1:C:1447:LEU:O | 2.28 | 0.51 |
| 2:E:127:TRP:HD1 | 2:E:128:ARG:HG3 | 1.72 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1445:LEU:O | 1:A:1445:LEU:HD23 | 2.10 | 0.51 |
| 1:A:1361:LEU:HD21 | 1:A:1365:TYR:OH | 2.10 | 0.51 |
| 1:B:1416:PRO:CG | 2:D:130:LYS:CD | 2.87 | 0.51 |
| 1:B:1420:ASN:HD21 | 1:B:1447:LEU:HD13 | 1.76 | 0.51 |
| 1:A:1389:GLY:O | 1:A:1392:LYS:N | 2.40 | 0.51 |
| 1:B:1079:THR:O | 1:B:1079:THR:CG2 | 2.56 | 0.51 |
| 1:B:1190:ILE:HD13 | 1:B:1216:LEU:HD21 | 1.92 | 0.51 |
| 1:C:1286:LEU:HG | 1:C:1286:LEU:O | 2.11 | 0.51 |
| 1:B:1244:ALA:HB2 | 1:B:1275:HIS:ND1 | 2.15 | 0.51 |
| 1:C:1122:LYS:HD2 | 1:C:1149:ASN:OD1 | 2.10 | 0.51 |
| 1:C:1157:LEU:HD12 | 1:C:1173:LEU:HD13 | 1.92 | 0.51 |
| 1:C:1167:SER:CA | 1:C:1171:THR:CB | 2.88 | 0.51 |
| 1:B:1361:LEU:HD21 | 1:B:1365:TYR:OH | 2.10 | 0.51 |
| 1:C:1455:VAL:O | 1:C:1456:GLN:HB3 | 2.11 | 0.51 |
| 1:A:1455:VAL:O | 1:A:1456:GLN:HB3 | 2.11 | 0.51 |
| 2:F:124:GLU:HA | 2:F:127:TRP:CE2 | 2.45 | 0.51 |
| 1:B:1170:GLU:CG | 1:B:1196:ALA:HB2 | 2.40 | 0.51 |
| 1:C:1494:SER:O | 1:C:1497:GLN:HB2 | 2.11 | 0.51 |
| 1:A:1112:ALA:O | 1:A:1116:LEU:HD23 | 2.10 | 0.51 |
| 1:B:1525:VAL:HG22 | 1:B:1525:VAL:O | 2.09 | 0.51 |
| 2:E:154:ARG:CZ | 2:E:154:ARG:HB3 | 2.40 | 0.51 |
| 2:F:103:ARG:HG3 | 2:F:103:ARG:O | 2.10 | 0.51 |
| 1:B:1377:THR:CA | 1:B:1381:HIS:HD2 | 2.21 | 0.51 |
| 1:A:1412:LEU:HA | 1:A:1419:LEU:CD2 | 2.33 | 0.51 |
| 1:A:1170:GLU:C | 1:A:1172:GLU:N | 2.63 | 0.51 |
| 1:B:1122:LYS:O | 1:B:1126:ASP:N | 2.44 | 0.51 |
| 2:D:154:ARG:HB3 | 2:D:154:ARG:CZ | 2.40 | 0.51 |
| 2:E:152:ASN:O | 2:E:153:ASN:CB | 2.59 | 0.51 |
| 2:D:53:UNK:C | 2:D:55:UNK:N | 2.72 | 0.51 |
| 1:A:1286:LEU:HG | 1:A:1286:LEU:O | 2.11 | 0.51 |
| 1:A:1274:LEU:O | 1:A:1278:VAL:HG23 | 2.10 | 0.51 |
| 1:A:1258:PHE:CG | 1:A:1289:TYR:CD2 | 2.89 | 0.51 |
| 1:C:1274:LEU:HA | 1:C:1277:VAL:HG22 | 1.90 | 0.51 |
| 1:B:1595:ALA:C | 1:B:1596:MET:HG3 | 2.30 | 0.51 |
| 1:C:1578:ARG:NH1 | 1:C:1583:LEU:HD23 | 2.21 | 0.51 |
| 2:F:188:UNK:O | 2:F:191:UNK:N | 2.43 | 0.51 |
| 1:B:1420:ASN:ND2 | 1:B:1447:LEU:HD13 | 2.26 | 0.51 |
| 1:A:1108:TRP:HE1 | 1:A:1131:ALA:CB | 2.23 | 0.51 |
| 1:A:1145:ASN:ND2 | 1:A:1153:LEU:HD21 | 2.26 | 0.51 |
| 2:D:51:UNK:O | 2:D:53:UNK:N | 2.44 | 0.51 |
| 1:A:1613:LEU:O | 1:A:1616:SER:HB2 | 2.10 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:1584:GLU:C | 1:B:1586:ALA:N | 2.62 | 0.51 |
| 1:B:1412:LEU:HA | 1:B:1419:LEU:CD2 | 2.33 | 0.51 |
| 1:B:1445:LEU:O | 1:B:1445:LEU:HD23 | 2.11 | 0.51 |
| 2:D:124:GLU:HA | 2:D:127:TRP:CE2 | 2.45 | 0.51 |
| 1:A:1159:MET:CE | 1:A:1163:LYS:HZ1 | 2.23 | 0.51 |
| 1:A:1151:GLU:HG2 | 1:A:1151:GLU:O | 2.10 | 0.51 |
| 1:A:1548:GLU:CD | 1:A:1548:GLU:H | 2.14 | 0.51 |
| 1:C:1233:HIS:O | 1:C:1234:LEU:O | 2.29 | 0.51 |
| 1:C:1586:ALA:HB2 | 1:C:1594:PHE:CE1 | 2.46 | 0.51 |
| 1:B:1598:TYR:CE2 | 2:D:200:UNK:C | 2.79 | 0.51 |
| 1:C:1130:LYS:HD2 | 1:C:1156:TYR:CE1 | 2.46 | 0.51 |
| 1:C:1401:VAL:HG22 | 1:C:1429:ARG:NH2 | 2.26 | 0.51 |
| 1:B:1401:VAL:HG22 | 1:B:1429:ARG:NH2 | 2.26 | 0.51 |
| 1:B:1494:SER:O | 1:B:1497:GLN:HB2 | 2.11 | 0.51 |
| 1:B:1083:GLN:O | 1:B:1085:LEU:N | 2.44 | 0.51 |
| 1:A:1232:VAL:CG2 | 1:A:1233:HIS:H | 2.09 | 0.51 |
| 2:D:188:UNK:C | 2:D:190:UNK:H2 | 2.24 | 0.51 |
| 1:A:1206:TYR:CE2 | 1:A:1226:ARG:HG3 | 2.46 | 0.51 |
| 1:A:1554:LEU:HA | 1:A:1557:PHE:CD2 | 2.40 | 0.51 |
| 1:B:1578:ARG:HD3 | 1:B:1582:VAL:CB | 2.40 | 0.51 |
| 1:C:1578:ARG:HD3 | 1:C:1582:VAL:CB | 2.40 | 0.51 |
| 1:C:1583:LEU:O | 1:C:1587:TRP:CE2 | 2.63 | 0.51 |
| 1:C:1082:VAL:CG1 | 1:C:1083:GLN:N | 2.69 | 0.51 |
| 1:C:1420:ASN:HD21 | 1:C:1447:LEU:HD13 | 1.76 | 0.51 |
| 1:A:1395:ILE:HD11 | 1:A:1403:LEU:HD12 | 1.93 | 0.51 |
| 1:A:1092:LEU:C | 1:A:1094:ARG:H | 2.12 | 0.51 |
| 1:B:1363:PHE:O | 1:B:1366:ASP:HB3 | 2.11 | 0.51 |
| 1:C:1231:LEU:HD12 | 1:C:1231:LEU:O | 2.11 | 0.51 |
| 1:B:1549:LEU:O | 1:B:1552:GLU:HB2 | 2.10 | 0.51 |
| 1:C:1592:MET:HG2 | 1:C:1593:ASP:H | 1.76 | 0.51 |
| 1:C:1609:LYS:O | 1:C:1612:LYS:HB2 | 2.11 | 0.51 |
| 1:C:1145:ASN:HD22 | 1:C:1150:TRP:HE1 | 1.58 | 0.51 |
| 1:C:1144:ALA:CB | 1:C:1153:LEU:HD13 | 2.39 | 0.51 |
| 1:B:1382:PRO:CG | 1:B:1410:PHE:HE1 | 2.23 | 0.51 |
| 1:C:1445:LEU:HD23 | 1:C:1448:VAL:HG22 | 1.92 | 0.51 |
| 2:F:129:GLU:HB2 | 2:F:132:LYS:NZ | 2.24 | 0.51 |
| 1:C:1411:TYR:HA | 1:C:1415:LYS:HB2 | 1.89 | 0.51 |
| 1:B:1235:GLY:O | 1:B:1236:GLU:HB2 | 2.10 | 0.51 |
| 1:A:1499:LEU:CB | 1:A:1511:ALA:HB2 | 2.36 | 0.51 |
| 2:F:98:GLU:C | 2:F:102:ILE:HG23 | 2.31 | 0.51 |
| 2:F:91:GLN:OE1 | 2:F:95:LEU:HG | 2.11 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:1549:LEU:O | 1:C:1552:GLU:HB2 | 2.10 | 0.51 |
| 1:B:1151:GLU:HG2 | 1:B:1151:GLU:O | 2.11 | 0.51 |
| 1:B:1240:ALA:C | 1:B:1242:ASP:H | 2.12 | 0.51 |
| 1:B:1272:CYS:HA | 1:B:1275:HIS:CB | 2.41 | 0.51 |
| 1:B:1274:LEU:O | 1:B:1278:VAL:HG23 | 2.10 | 0.51 |
| 2:D:203:UNK:O | 2:D:204:UNK:C | 2.59 | 0.51 |
| 1:C:1136:SER:HB2 | 1:C:1140:VAL:CG2 | 2.41 | 0.51 |
| 1:B:1353:GLU:OE2 | 1:B:1361:LEU:HD11 | 2.10 | 0.51 |
| 1:C:1434:ARG:CZ | 2:E:5:UNK:HA | 2.36 | 0.51 |
| 1:A:1420:ASN:ND2 | 1:A:1447:LEU:HD13 | 2.26 | 0.51 |
| 2:D:133:LYS:HA | 2:D:133:LYS:CE | 2.41 | 0.51 |
| 1:A:1161:ARG:HH22 | 1:A:1174:ILE:HG13 | 1.76 | 0.51 |
| 2:F:162:GLN:O | 2:F:163:GLN:C | 2.48 | 0.51 |
| 1:B:1108:TRP:CD1 | 1:B:1131:ALA:HB3 | 2.46 | 0.51 |
| 1:A:1122:LYS:O | 1:A:1126:ASP:N | 2.44 | 0.51 |
| 1:C:1343:VAL:HG22 | 1:C:1344:ASN:N | 2.26 | 0.51 |
| 1:A:1343:VAL:HG22 | 1:A:1344:ASN:N | 2.26 | 0.51 |
| 1:A:1206:TYR:HD1 | 1:A:1226:ARG:O | 1.92 | 0.51 |
| 1:B:1461:LYS:HG2 | 1:B:1489:ASN:HD21 | 1.75 | 0.51 |
| 1:A:1461:LYS:HG2 | 1:A:1489:ASN:HD21 | 1.75 | 0.51 |
| 1:B:1548:GLU:H | 1:B:1548:GLU:CD | 2.14 | 0.51 |
| 1:A:1261:VAL:CG1 | 1:A:1295:TYR:CE1 | 2.94 | 0.50 |
| 1:C:1333:ARG:HB2 | 1:C:1360:GLU:HG3 | 1.91 | 0.50 |
| 1:B:1273:GLY:C | 1:B:1275:HIS:N | 2.64 | 0.50 |
| 2:E:203:UNK:C | 2:E:203:UNK:CB | 2.79 | 0.50 |
| 1:C:1218:TYR:CE2 | 1:C:1223:ASN:O | 2.64 | 0.50 |
| 1:C:1361:LEU:HD21 | 1:C:1365:TYR:OH | 2.11 | 0.50 |
| 1:C:1395:ILE:HD11 | 1:C:1403:LEU:HD12 | 1.93 | 0.50 |
| 1:C:1412:LEU:HA | 1:C:1419:LEU:CD2 | 2.33 | 0.50 |
| 2:E:133:LYS:HA | 2:E:133:LYS:CE | 2.41 | 0.50 |
| 2:D:129:GLU:HB2 | 2:D:132:LYS:NZ | 2.24 | 0.50 |
| 1:B:1105:PRO:O | 1:B:1106:ALA:HB2 | 2.11 | 0.50 |
| 2:F:154:ARG:HB3 | 2:F:154:ARG:CZ | 2.40 | 0.50 |
| 1:B:1189:PHE:O | 1:B:1217:LEU:HD23 | 2.10 | 0.50 |
| 1:C:1272:CYS:HA | 1:C:1275:HIS:CB | 2.41 | 0.50 |
| 1:C:1332:MET:O | 1:C:1336:LEU:HG | 2.11 | 0.50 |
| 1:A:1578:ARG:HD3 | 1:A:1582:VAL:CB | 2.41 | 0.50 |
| 1:A:1578:ARG:NE | 1:A:1583:LEU:HD23 | 2.24 | 0.50 |
| 1:B:1533:LEU:C | 1:B:1535:LYS:N | 2.65 | 0.50 |
| 1:C:1597:PRO:O | 1:C:1598:TYR:CD2 | 2.64 | 0.50 |
| 1:C:1469:ASN:HD21 | 1:C:1498:ARG:HH12 | 1.59 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:1395:ILE:HD11 | 1:B:1403:LEU:HD12 | 1.93 | 0.50 |
| 1:B:1159:MET:SD | 1:B:1162:LYS:HD3 | 2.51 | 0.50 |
| 1:B:1168:TYR:O | 1:B:1172:GLU:CG | 2.60 | 0.50 |
| 1:B:1198:ILE:HA | 1:B:1201:VAL:HG23 | 1.92 | 0.50 |
| 1:A:1125:ILE:O | 1:A:1129:ILE:HD13 | 2.10 | 0.50 |
| 1:A:1234:LEU:O | 1:A:1236:GLU:OE1 | 2.29 | 0.50 |
| 1:A:1079:THR:O | 1:A:1079:THR:CG2 | 2.56 | 0.50 |
| 1:B:1499:LEU:CB | 1:B:1511:ALA:HB2 | 2.36 | 0.50 |
| 1:C:1269:ALA:HB3 | 1:C:1295:TYR:OH | 2.12 | 0.50 |
| 1:C:1167:SER:CA | 1:C:1171:THR:HB | 2.41 | 0.50 |
| 2:F:118:ALA:HA | 2:F:121:LYS:HZ2 | 1.73 | 0.50 |
| 2:D:127:TRP:CD1 | 2:D:128:ARG:N | 2.80 | 0.50 |
| 1:A:1157:LEU:HB3 | 1:A:1173:LEU:HD11 | 1.92 | 0.50 |
| 1:B:1112:ALA:O | 1:B:1116:LEU:HD23 | 2.10 | 0.50 |
| 1:A:1089:ILE:HD11 | 2:F:13:UNK:CB | 2.42 | 0.50 |
| 1:B:1343:VAL:HG22 | 1:B:1344:ASN:N | 2.26 | 0.50 |
| 1:A:1197:HIS:C | 1:A:1199:GLN:N | 2.64 | 0.50 |
| 1:C:1420:ASN:ND2 | 1:C:1447:LEU:HD13 | 2.26 | 0.50 |
| 2:E:124:GLU:HA | 2:E:127:TRP:CE2 | 2.46 | 0.50 |
| 1:B:1336:LEU:CD1 | 1:B:1360:GLU:HB3 | 2.41 | 0.50 |
| 1:B:1116:LEU:HD11 | 1:B:1122:LYS:CD | 2.41 | 0.50 |
| 1:C:1387:LYS:HB2 | 1:C:1390:GLN:CG | 2.41 | 0.50 |
| 2:F:94:ARG:NE | 2:F:98:GLU:OE2 | 2.39 | 0.50 |
| 1:A:1273:GLY:C | 1:A:1275:HIS:N | 2.65 | 0.50 |
| 1:A:1336:LEU:CD1 | 1:A:1360:GLU:HB3 | 2.41 | 0.50 |
| 1:C:1270:GLN:HG3 | 1:C:1298:GLU:CG | 2.42 | 0.50 |
| 1:B:1282:GLU:C | 1:B:1283:LEU:HD13 | 2.31 | 0.50 |
| 1:B:1358:TRP:CE3 | 1:B:1381:HIS:CG | 2.98 | 0.50 |
| 1:C:1445:LEU:HD23 | 1:C:1445:LEU:O | 2.11 | 0.50 |
| 2:E:118:ALA:HA | 2:E:121:LYS:HZ2 | 1.76 | 0.50 |
| 2:F:127:TRP:CD1 | 2:F:128:ARG:N | 2.80 | 0.50 |
| 1:B:1469:ASN:HD21 | 1:B:1498:ARG:HH12 | 1.59 | 0.50 |
| 1:B:1469:ASN:ND2 | 1:B:1498:ARG:HH22 | 2.09 | 0.50 |
| 1:C:1247:ALA:CB | 1:C:1247:ALA:C | 2.74 | 0.50 |
| 1:C:1345:ILE:N | 1:C:1346:PRO:HD2 | 2.20 | 0.50 |
| 1:A:1301:THR:CA | 1:A:1304:GLU:HG3 | 2.32 | 0.50 |
| 1:A:1189:PHE:O | 1:A:1217:LEU:HD23 | 2.11 | 0.50 |
| 1:A:1190:ILE:HD13 | 1:A:1216:LEU:HD21 | 1.94 | 0.50 |
| 1:C:1317:PHE:CD1 | 1:C:1339:PHE:HB3 | 2.47 | 0.50 |
| 1:C:1513:TYR:HA | 1:C:1516:LYS:HE2 | 1.93 | 0.50 |
| 1:B:1286:LEU:O | 1:B:1286:LEU:HG | 2.10 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:1554:LEU:HD23 | 1:B:1582:VAL:HG12 | 1.93 | 0.50 |
| 1:C:1586:ALA:O | 1:C:1590:ASN:ND2 | 2.44 | 0.50 |
| 1:C:1602:VAL:HG22 | 2:E:203:UNK:C | 2.42 | 0.50 |
| 2:F:192:UNK:O | 2:F:195:UNK:CB | 2.60 | 0.50 |
| 1:C:1414:PHE:CE1 | 2:E:123:MET:CB | 2.82 | 0.50 |
| 2:E:118:ALA:CA | 2:E:121:LYS:HE3 | 2.41 | 0.50 |
| 1:B:1402:GLU:HA | 1:B:1405:TYR:CD2 | 2.47 | 0.50 |
| 1:A:1161:ARG:HG2 | 1:A:1173:LEU:HD23 | 1.91 | 0.50 |
| 1:A:1125:ILE:O | 1:A:1129:ILE:CD1 | 2.60 | 0.50 |
| 1:B:1234:LEU:O | 1:B:1236:GLU:OE1 | 2.29 | 0.50 |
| 1:C:1514:LEU:C | 1:C:1514:LEU:CD2 | 2.80 | 0.50 |
| 1:B:1165:ARG:O | 1:B:1165:ARG:CG | 2.59 | 0.50 |
| 1:C:1112:ALA:O | 1:C:1116:LEU:HD23 | 2.10 | 0.50 |
| 1:B:1613:LEU:O | 1:B:1616:SER:HB2 | 2.11 | 0.50 |
| 1:A:1272:CYS:HA | 1:A:1275:HIS:CB | 2.41 | 0.50 |
| 1:A:1533:LEU:C | 1:A:1535:LYS:N | 2.65 | 0.50 |
| 1:C:1597:PRO:O | 1:C:1598:TYR:CG | 2.65 | 0.50 |
| 1:C:1122:LYS:NZ | 1:C:1147:SER:CB | 2.68 | 0.50 |
| 1:C:1170:GLU:C | 1:C:1172:GLU:N | 2.63 | 0.50 |
| 1:A:1420:ASN:HD21 | 1:A:1447:LEU:HD13 | 1.76 | 0.50 |
| 1:B:1332:MET:O | 1:B:1336:LEU:HG | 2.11 | 0.50 |
| 1:B:1428:PRO:O | 1:B:1429:ARG:HB2 | 2.11 | 0.50 |
| 1:A:1384:ASP:OD1 | 2:F:115:GLU:OE1 | 2.30 | 0.50 |
| 1:A:1494:SER:O | 1:A:1497:GLN:HB2 | 2.11 | 0.50 |
| 1:B:1088:HIS:N | 1:B:1089:ILE:HD12 | 2.26 | 0.50 |
| 1:B:1083:GLN:HE21 | 1:B:1106:ALA:C | 2.14 | 0.50 |
| 1:A:1130:LYS:HG2 | 1:A:1156:TYR:CE2 | 2.46 | 0.50 |
| 2:D:152:ASN:O | 2:D:153:ASN:CB | 2.58 | 0.50 |
| 1:C:1363:PHE:O | 1:C:1366:ASP:HB3 | 2.11 | 0.50 |
| 1:C:1533:LEU:C | 1:C:1535:LYS:N | 2.64 | 0.50 |
| 1:A:1214:ALA:O | 1:A:1218:TYR:CB | 2.57 | 0.50 |
| 1:C:1149:ASN:ND2 | 1:C:1149:ASN:N | 2.60 | 0.50 |
| 1:C:1382:PRO:CG | 1:C:1410:PHE:HE1 | 2.23 | 0.50 |
| 1:C:1422:LEU:O | 1:C:1422:LEU:HD22 | 2.12 | 0.50 |
| 1:C:1469:ASN:ND2 | 1:C:1498:ARG:HH22 | 2.09 | 0.50 |
| 1:A:1401:VAL:HG22 | 1:A:1429:ARG:NH2 | 2.26 | 0.50 |
| 1:A:1361:LEU:HD21 | 1:A:1365:TYR:HH | 1.76 | 0.50 |
| 1:B:1513:TYR:HA | 1:B:1516:LYS:HE2 | 1.94 | 0.50 |
| 1:C:1273:GLY:C | 1:C:1275:HIS:N | 2.65 | 0.50 |
| 1:A:1580:ASP:OD1 | 1:C:1605:GLU:HB2 | 2.12 | 0.50 |
| 1:B:1551:GLU:OE1 | 1:B:1581:VAL:HG12 | 2.11 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:1194:ASN:ND2 | 1:C:1194:ASN:N | 2.59 | 0.50 |
| 1:C:1377:THR:O | 1:C:1381:HIS:HB2 | 2.12 | 0.50 |
| 1:A:1448:VAL:CA | 1:A:1451:TYR:HB3 | 2.42 | 0.50 |
| 1:A:1469:ASN:ND2 | 1:A:1498:ARG:HH22 | 2.09 | 0.50 |
| 1:B:1414:PHE:C | 1:B:1416:PRO:HD3 | 2.21 | 0.50 |
| 1:A:1148:GLY:HA2 | 1:A:1150:TRP:CH2 | 2.47 | 0.50 |
| 1:C:1330:GLN:CG | 1:C:1331:LYS:H | 2.22 | 0.49 |
| 1:A:1587:TRP:O | 1:A:1589:HIS:O | 2.30 | 0.49 |
| 1:A:1609:LYS:O | 1:A:1612:LYS:HB2 | 2.12 | 0.49 |
| 2:D:178:UNK:O | 2:D:181:UNK:CB | 2.60 | 0.49 |
| 1:A:1227:LEU:HD23 | 1:A:1227:LEU:C | 2.33 | 0.49 |
| 1:C:1167:SER:CA | 1:C:1171:THR:OG1 | 2.60 | 0.49 |
| 1:A:1402:GLU:HA | 1:A:1405:TYR:CD2 | 2.47 | 0.49 |
| 1:A:1435:ALA:O | 1:A:1439:PHE:CD2 | 2.65 | 0.49 |
| 1:A:1423:LEU:HD12 | 1:A:1451:TYR:HB2 | 1.93 | 0.49 |
| 1:B:1455:VAL:O | 1:B:1456:GLN:HB3 | 2.11 | 0.49 |
| 1:A:1375:ILE:HA | 1:A:1378:MET:HE3 | 1.94 | 0.49 |
| 1:B:1496:ALA:HB2 | 1:B:1514:LEU:HD13 | 1.94 | 0.49 |
| 1:B:1125:ILE:O | 1:B:1129:ILE:CD1 | 2.60 | 0.49 |
| 1:B:1125:ILE:O | 1:B:1129:ILE:HD13 | 2.10 | 0.49 |
| 1:A:1130:LYS:HZ1 | 1:A:1155:LYS:HG2 | 1.77 | 0.49 |
| 1:A:1208:GLU:HA | 1:A:1208:GLU:OE1 | 2.12 | 0.49 |
| 1:A:1256:VAL:C | 1:A:1289:TYR:HH | 2.16 | 0.49 |
| 1:A:1593:ASP:O | 1:A:1594:PHE:HB2 | 2.11 | 0.49 |
| 1:C:1600:ILE:HA | 1:C:1603:MET:CE | 2.42 | 0.49 |
| 1:C:1082:VAL:CG2 | 1:C:1107:VAL:HG11 | 2.42 | 0.49 |
| 1:C:1149:ASN:O | 1:C:1153:LEU:HB3 | 2.12 | 0.49 |
| 1:B:1448:VAL:CA | 1:B:1451:TYR:HB3 | 2.42 | 0.49 |
| 1:A:1514:LEU:C | 1:A:1514:LEU:CD2 | 2.81 | 0.49 |
| 1:B:1389:GLY:O | 1:B:1392:LYS:N | 2.40 | 0.49 |
| 1:C:1301:THR:O | 1:C:1304:GLU:HB2 | 2.12 | 0.49 |
| 1:A:1317:PHE:CD1 | 1:A:1339:PHE:HB3 | 2.47 | 0.49 |
| 1:B:1211:TYR:HB2 | 1:B:1231:LEU:CD1 | 2.42 | 0.49 |
| 1:B:1513:TYR:HD1 | 1:B:1516:LYS:CE | 2.23 | 0.49 |
| 1:A:1513:TYR:HA | 1:A:1516:LYS:HE2 | 1.94 | 0.49 |
| 1:A:1258:PHE:HB2 | 1:A:1289:TYR:CD1 | 2.40 | 0.49 |
| 1:A:1295:TYR:O | 1:A:1296:PHE:CD2 | 2.65 | 0.49 |
| 1:A:1330:GLN:CG | 1:A:1331:LYS:H | 2.22 | 0.49 |
| 1:B:1246:LYS:O | 1:B:1247:ALA:HB3 | 2.09 | 0.49 |
| 1:B:1609:LYS:O | 1:B:1612:LYS:HB2 | 2.12 | 0.49 |
| 1:A:1598:TYR:CE2 | 2:F:198:UNK:CB | 2.95 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:1377:THR:O | 1:B:1381:HIS:HB2 | 2.12 | 0.49 |
| 1:A:1111:LEU:CD1 | 1:A:1125:ILE:CG1 | 2.77 | 0.49 |
| 1:A:1234:LEU:CG | 1:A:1235:GLY:N | 2.74 | 0.49 |
| 2:F:98:GLU:O | 2:F:102:ILE:N | 2.45 | 0.49 |
| 1:A:1332:MET:O | 1:A:1336:LEU:HG | 2.11 | 0.49 |
| 1:C:1578:ARG:CD | 1:C:1582:VAL:HB | 2.43 | 0.49 |
| 1:C:1197:HIS:O | 1:C:1199:GLN:N | 2.45 | 0.49 |
| 1:C:1402:GLU:HA | 1:C:1405:TYR:CD2 | 2.47 | 0.49 |
| 1:C:1435:ALA:O | 1:C:1439:PHE:CD2 | 2.65 | 0.49 |
| 2:E:127:TRP:CD1 | 2:E:128:ARG:N | 2.80 | 0.49 |
| 1:B:1408:ILE:CD1 | 1:B:1422:LEU:HD11 | 2.42 | 0.49 |
| 1:B:1416:PRO:HG2 | 2:D:130:LYS:HG3 | 1.89 | 0.49 |
| 1:B:1423:LEU:HD12 | 1:B:1451:TYR:HB2 | 1.93 | 0.49 |
| 2:F:167:ASP:O | 2:F:168:ILE:O | 2.31 | 0.49 |
| 1:C:1188:GLU:C | 1:C:1190:ILE:N | 2.66 | 0.49 |
| 1:B:1144:ALA:O | 1:B:1153:LEU:HD22 | 2.12 | 0.49 |
| 1:A:1345:ILE:N | 1:A:1346:PRO:HD2 | 2.20 | 0.49 |
| 2:D:155:ILE:O | 2:D:156:ALA:CB | 2.60 | 0.49 |
| 2:E:112:ARG:HD3 | 2:E:113:LEU:N | 2.27 | 0.49 |
| 1:A:1257:CYS:SG | 1:A:1290:TYR:CZ | 3.05 | 0.49 |
| 1:A:1263:GLY:O | 1:A:1264:LYS:CB | 2.61 | 0.49 |
| 1:C:1274:LEU:O | 1:C:1278:VAL:HG23 | 2.12 | 0.49 |
| 1:C:1336:LEU:CD1 | 1:C:1360:GLU:HB3 | 2.41 | 0.49 |
| 1:B:1263:GLY:O | 1:B:1264:LYS:CB | 2.60 | 0.49 |
| 1:A:1596:MET:H | 1:A:1597:PRO:CD | 2.12 | 0.49 |
| 1:C:1168:TYR:O | 1:C:1172:GLU:CG | 2.59 | 0.49 |
| 1:A:1358:TRP:CE2 | 1:A:1381:HIS:CG | 3.01 | 0.49 |
| 1:A:1168:TYR:O | 1:A:1172:GLU:CG | 2.60 | 0.49 |
| 1:A:1137:TYR:CA | 1:A:1138:MET:HB2 | 2.38 | 0.49 |
| 1:B:1108:TRP:HE1 | 1:B:1131:ALA:CB | 2.25 | 0.49 |
| 2:F:95:LEU:O | 2:F:99:PRO:HD2 | 2.13 | 0.49 |
| 2:F:131:ALA:HA | 2:F:134:ASP:OD2 | 2.13 | 0.49 |
| 1:A:1253:TRP:CE3 | 1:A:1276:ILE:HB | 2.48 | 0.49 |
| 1:A:1279:HIS:CD2 | 1:A:1282:GLU:CB | 2.95 | 0.49 |
| 1:C:1596:MET:O | 1:C:1598:TYR:CD2 | 2.65 | 0.49 |
| 1:C:1145:ASN:ND2 | 1:C:1150:TRP:HE1 | 2.09 | 0.49 |
| 1:C:1132:ASP:O | 1:C:1163:LYS:HE2 | 2.12 | 0.49 |
| 1:C:1358:TRP:CE2 | 1:C:1381:HIS:CG | 3.01 | 0.49 |
| 1:C:1428:PRO:O | 1:C:1429:ARG:HB2 | 2.11 | 0.49 |
| 1:A:1422:LEU:HD22 | 1:A:1422:LEU:O | 2.13 | 0.49 |
| 1:B:1170:GLU:OE2 | 1:B:1195:ASN:O | 2.30 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1496:ALA:HB2 | 1:A:1514:LEU:HD13 | 1.95 | 0.49 |
| 2:F:99:PRO:HA | 2:F:102:ILE:HG12 | 1.93 | 0.49 |
| 1:B:1208:GLU:OE1 | 1:B:1208:GLU:HA | 2.12 | 0.49 |
| 1:A:1273:GLY:O | 1:A:1277:VAL:HG13 | 2.12 | 0.49 |
| 1:A:1592:MET:CG | 1:A:1593:ASP:N | 2.75 | 0.49 |
| 1:C:1448:VAL:CA | 1:C:1451:TYR:HB3 | 2.42 | 0.49 |
| 2:E:131:ALA:HA | 2:E:134:ASP:OD2 | 2.13 | 0.49 |
| 1:A:1408:ILE:CD1 | 1:A:1422:LEU:HD11 | 2.42 | 0.49 |
| 1:B:1227:LEU:HD23 | 1:B:1227:LEU:C | 2.33 | 0.49 |
| 1:B:1081:ALA:O | 1:B:1098:PHE:CD1 | 2.65 | 0.49 |
| 1:C:1389:GLY:O | 1:C:1392:LYS:HB2 | 2.13 | 0.49 |
| 2:F:154:ARG:HH11 | 2:F:154:ARG:CB | 2.26 | 0.49 |
| 1:A:1301:THR:O | 1:A:1304:GLU:HB2 | 2.12 | 0.49 |
| 1:C:1513:TYR:HD1 | 1:C:1516:LYS:CE | 2.23 | 0.49 |
| 1:A:1513:TYR:HA | 1:A:1516:LYS:HG2 | 1.95 | 0.49 |
| 1:C:1261:VAL:HG11 | 1:C:1294:GLY:O | 2.13 | 0.49 |
| 1:A:1600:ILE:HA | 1:A:1603:MET:CE | 2.43 | 0.49 |
| 1:C:1601:GLN:CG | 1:C:1604:LYS:HD2 | 2.40 | 0.49 |
| 1:C:1361:LEU:HD22 | 1:C:1365:TYR:HE2 | 1.72 | 0.49 |
| 1:A:1372:ASP:O | 1:A:1376:ILE:CG1 | 2.49 | 0.49 |
| 1:A:1414:PHE:HD1 | 2:F:127:TRP:CB | 2.25 | 0.49 |
| 1:B:1422:LEU:O | 1:B:1422:LEU:HD22 | 2.13 | 0.49 |
| 1:B:1435:ALA:O | 1:B:1439:PHE:CD2 | 2.65 | 0.49 |
| 1:B:1137:TYR:CG | 1:B:1138:MET:HB2 | 2.42 | 0.49 |
| 1:C:1227:LEU:HD23 | 1:C:1227:LEU:C | 2.32 | 0.49 |
| 1:B:1601:GLN:CG | 1:B:1604:LYS:HD2 | 2.39 | 0.49 |
| 2:F:182:UNK:O | 2:F:183:UNK:C | 2.61 | 0.49 |
| 1:C:1154:VAL:HG11 | 1:C:1177:LEU:HA | 1.94 | 0.49 |
| 1:A:1377:THR:O | 1:A:1381:HIS:HB2 | 2.12 | 0.49 |
| 1:B:1167:SER:C | 1:B:1169:VAL:N | 2.62 | 0.49 |
| 1:B:1150:TRP:HA | 1:B:1153:LEU:HB3 | 1.94 | 0.49 |
| 2:D:154:ARG:CB | 2:D:154:ARG:HH11 | 2.26 | 0.49 |
| 1:A:1188:GLU:C | 1:A:1190:ILE:N | 2.66 | 0.49 |
| 1:A:1292:ASP:HA | 2:F:97:GLN:CG | 2.42 | 0.49 |
| 1:C:1496:ALA:HB2 | 1:C:1514:LEU:HD13 | 1.95 | 0.49 |
| 1:A:1277:VAL:CG2 | 1:A:1278:VAL:N | 2.70 | 0.49 |
| 1:C:1231:LEU:O | 1:C:1232:VAL:O | 2.31 | 0.49 |
| 1:A:1580:ASP:OD1 | 1:C:1605:GLU:CB | 2.61 | 0.49 |
| 1:C:1166:GLU:HB2 | 1:C:1168:TYR:CZ | 2.48 | 0.49 |
| 1:C:1405:TYR:CE2 | 1:C:1434:ARG:NH1 | 2.81 | 0.49 |
| 1:A:1428:PRO:O | 1:A:1429:ARG:HB2 | 2.12 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1198:ILE:HG22 | 1:A:1198:ILE:O | 2.12 | 0.49 |
| 2:E:105:TRP:CA | 2:E:108:GLU:HG3 | 2.41 | 0.49 |
| 1:B:1137:TYR:CA | 1:B:1138:MET:HB2 | 2.38 | 0.49 |
| 1:C:1278:VAL:CG1 | 1:C:1278:VAL:O | 2.54 | 0.48 |
| 1:B:1578:ARG:NE | 1:B:1583:LEU:HD23 | 2.24 | 0.48 |
| 1:C:1597:PRO:HB3 | 1:C:1601:GLN:NE2 | 2.23 | 0.48 |
| 1:C:1572:THR:CG2 | 1:C:1599:PHE:CD2 | 2.94 | 0.48 |
| 1:C:1182:ARG:C | 1:C:1183:LEU:HD23 | 2.33 | 0.48 |
| 2:D:125:GLN:CD | 2:D:125:GLN:C | 2.72 | 0.48 |
| 1:B:1193:PRO:HG2 | 1:B:1194:ASN:H | 1.78 | 0.48 |
| 1:B:1130:LYS:O | 1:B:1133:ASP:O | 2.31 | 0.48 |
| 1:B:1234:LEU:C | 1:B:1236:GLU:H | 2.10 | 0.48 |
| 1:C:1273:GLY:O | 1:C:1277:VAL:HG13 | 2.13 | 0.48 |
| 1:B:1273:GLY:O | 1:B:1277:VAL:HG13 | 2.12 | 0.48 |
| 1:A:1587:TRP:C | 1:A:1589:HIS:N | 2.66 | 0.48 |
| 2:E:114:GLN:CG | 2:E:115:GLU:N | 2.26 | 0.48 |
| 1:A:1414:PHE:O | 2:F:130:LYS:HD3 | 2.12 | 0.48 |
| 1:B:1335:HIS:C | 1:B:1335:HIS:ND1 | 2.66 | 0.48 |
| 1:B:1389:GLY:O | 1:B:1392:LYS:HB2 | 2.13 | 0.48 |
| 2:E:154:ARG:CB | 2:E:154:ARG:HH11 | 2.26 | 0.48 |
| 1:B:1513:TYR:HA | 1:B:1516:LYS:HG2 | 1.95 | 0.48 |
| 2:E:180:UNK:O | 2:E:181:UNK:O | 2.30 | 0.48 |
| 1:B:1203:ASP:HB3 | 2:D:60:UNK:CB | 2.43 | 0.48 |
| 2:D:131:ALA:HA | 2:D:134:ASP:OD2 | 2.13 | 0.48 |
| 2:F:155:ILE:O | 2:F:156:ALA:CB | 2.61 | 0.48 |
| 1:B:1272:CYS:O | 1:B:1276:ILE:HG23 | 2.14 | 0.48 |
| 1:B:1111:LEU:O | 1:B:1115:GLN:HB2 | 2.14 | 0.48 |
| 2:E:155:ILE:O | 2:E:156:ALA:CB | 2.61 | 0.48 |
| 1:C:1620:ARG:CB | 1:C:1620:ARG:NH1 | 2.54 | 0.48 |
| 1:B:1624:GLU:C | 1:B:1626:ALA:N | 2.64 | 0.48 |
| 1:C:1335:HIS:C | 1:C:1335:HIS:ND1 | 2.66 | 0.48 |
| 1:C:1577:LEU:N | 1:C:1577:LEU:HD23 | 2.29 | 0.48 |
| 1:C:1578:ARG:NE | 1:C:1583:LEU:HD23 | 2.24 | 0.48 |
| 1:C:1586:ALA:HB1 | 1:C:1590:ASN:ND2 | 2.17 | 0.48 |
| 1:C:1198:ILE:O | 1:C:1201:VAL:CG2 | 2.61 | 0.48 |
| 1:A:1469:ASN:HD21 | 1:A:1498:ARG:HH12 | 1.59 | 0.48 |
| 2:F:125:GLN:CD | 2:F:125:GLN:C | 2.72 | 0.48 |
| 1:B:1167:SER:C | 1:B:1168:TYR:CG | 2.85 | 0.48 |
| 1:B:1193:PRO:O | 1:B:1194:ASN:O | 2.30 | 0.48 |
| 2:D:102:ILE:O | 2:D:106:ARG:CB | 2.61 | 0.48 |
| 1:A:1345:ILE:H | 1:A:1346:PRO:CD | 2.18 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:1317:PHE:CD1 | 1:B:1339:PHE:HB3 | 2.47 | 0.48 |
| 1:C:1461:LYS:HG2 | 1:C:1489:ASN:ND2 | 2.28 | 0.48 |
| 1:B:1461:LYS:HG2 | 1:B:1489:ASN:ND2 | 2.29 | 0.48 |
| 1:A:1295:TYR:O | 1:A:1296:PHE:CG | 2.67 | 0.48 |
| 1:B:1577:LEU:HD23 | 1:B:1577:LEU:N | 2.29 | 0.48 |
| 1:C:1569:CYS:O | 1:C:1572:THR:OG1 | 2.32 | 0.48 |
| 1:C:1595:ALA:C | 1:C:1596:MET:HG3 | 2.32 | 0.48 |
| 1:B:1588:ARG:NE | 2:F:190:UNK:O | 2.47 | 0.48 |
| 1:C:1214:ALA:O | 1:C:1218:TYR:CB | 2.57 | 0.48 |
| 1:B:1358:TRP:CE2 | 1:B:1381:HIS:CG | 3.01 | 0.48 |
| 1:A:1414:PHE:C | 1:A:1416:PRO:HD3 | 2.22 | 0.48 |
| 1:B:1452:LEU:HD13 | 1:B:1467:LEU:CD1 | 2.43 | 0.48 |
| 1:B:1161:ARG:HE | 1:B:1173:LEU:HD23 | 1.76 | 0.48 |
| 1:B:1188:GLU:C | 1:B:1190:ILE:N | 2.66 | 0.48 |
| 1:B:1254:LYS:HD2 | 1:B:1285:GLU:CG | 2.43 | 0.48 |
| 1:A:1572:THR:CG2 | 1:A:1599:PHE:HD2 | 2.26 | 0.48 |
| 1:B:1569:CYS:O | 1:B:1572:THR:OG1 | 2.32 | 0.48 |
| 1:C:1168:TYR:CA | 1:C:1172:GLU:OE2 | 2.61 | 0.48 |
| 1:C:1175:PHE:CD1 | 1:C:1200:GLN:HB3 | 2.48 | 0.48 |
| 2:F:133:LYS:CE | 2:F:133:LYS:HA | 2.41 | 0.48 |
| 1:A:1083:GLN:HE21 | 1:A:1106:ALA:CB | 2.27 | 0.48 |
| 1:A:1121:VAL:CG1 | 1:A:1125:ILE:HB | 2.43 | 0.48 |
| 1:A:1389:GLY:O | 1:A:1392:LYS:HB2 | 2.13 | 0.48 |
| 1:B:1301:THR:O | 1:B:1304:GLU:HB2 | 2.12 | 0.48 |
| 1:A:1234:LEU:C | 1:A:1236:GLU:H | 2.10 | 0.48 |
| 1:A:1150:TRP:HA | 1:A:1153:LEU:HB3 | 1.96 | 0.48 |
| 1:B:1284:GLU:C | 1:B:1284:GLU:OE2 | 2.52 | 0.48 |
| 1:C:1253:TRP:CE3 | 1:C:1276:ILE:HB | 2.48 | 0.48 |
| 1:C:1279:HIS:CD2 | 1:C:1280:ALA:N | 2.81 | 0.48 |
| 1:C:1329:PRO:O | 1:C:1332:MET:HB3 | 2.14 | 0.48 |
| 1:B:1598:TYR:CZ | 2:D:201:UNK:CB | 2.97 | 0.48 |
| 1:C:1452:LEU:HD13 | 1:C:1467:LEU:CD1 | 2.43 | 0.48 |
| 2:E:129:GLU:HB2 | 2:E:132:LYS:NZ | 2.24 | 0.48 |
| 1:B:1129:ILE:HG13 | 1:B:1130:LYS:N | 2.28 | 0.48 |
| 1:C:1513:TYR:HA | 1:C:1516:LYS:HG2 | 1.96 | 0.48 |
| 2:F:112:ARG:HD3 | 2:F:113:LEU:N | 2.28 | 0.48 |
| 1:A:1551:GLU:HG2 | 1:A:1582:VAL:CG2 | 2.35 | 0.48 |
| 1:C:1592:MET:CG | 1:C:1593:ASP:N | 2.73 | 0.48 |
| 1:C:1365:TYR:CB | 1:C:1374:ALA:HB2 | 2.44 | 0.48 |
| 1:C:1416:PRO:O | 1:C:1419:LEU:HB3 | 2.14 | 0.48 |
| 1:A:1167:SER:O | 1:A:1168:TYR:CE1 | 2.66 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:1230:THR:O | 1:B:1231:LEU:CB | 2.61 | 0.48 |
| 1:A:1446:PRO:O | 1:A:1449:LYS:HB2 | 2.14 | 0.48 |
| 1:A:1452:LEU:HD13 | 1:A:1467:LEU:CD1 | 2.43 | 0.48 |
| 1:B:1329:PRO:O | 1:B:1332:MET:HB3 | 2.14 | 0.48 |
| 2:D:124:GLU:OE1 | 2:D:128:ARG:CZ | 2.62 | 0.48 |
| 1:A:1111:LEU:O | 1:A:1115:GLN:HB2 | 2.14 | 0.48 |
| 1:B:1301:THR:CA | 1:B:1304:GLU:HG3 | 2.32 | 0.48 |
| 1:C:1596:MET:H | 1:C:1597:PRO:CD | 2.09 | 0.48 |
| 1:C:1133:ASP:HB2 | 1:C:1134:PRO:CD | 2.44 | 0.48 |
| 1:C:1446:PRO:O | 1:C:1449:LYS:HB2 | 2.14 | 0.48 |
| 1:A:1395:ILE:HG23 | 1:A:1396:THR:N | 2.29 | 0.48 |
| 2:F:124:GLU:OE1 | 2:F:128:ARG:CZ | 2.62 | 0.48 |
| 1:C:1190:ILE:HG12 | 1:C:1216:LEU:HD11 | 1.94 | 0.48 |
| 1:A:1149:ASN:O | 1:A:1153:LEU:HB3 | 2.13 | 0.48 |
| 1:B:1421:ASP:O | 1:B:1424:MET:HB2 | 2.14 | 0.48 |
| 1:C:1284:GLU:OE2 | 1:C:1284:GLU:C | 2.52 | 0.48 |
| 1:B:1254:LYS:HD2 | 1:B:1285:GLU:CD | 2.34 | 0.47 |
| 1:A:1577:LEU:HD23 | 1:A:1577:LEU:N | 2.28 | 0.47 |
| 1:A:1602:VAL:CG1 | 2:F:202:UNK:O | 2.62 | 0.47 |
| 1:B:1600:ILE:HA | 1:B:1603:MET:CE | 2.43 | 0.47 |
| 2:F:193:UNK:C | 2:F:195:UNK:N | 2.76 | 0.47 |
| 1:A:1602:VAL:HG21 | 2:F:202:UNK:CB | 2.44 | 0.47 |
| 1:C:1137:TYR:O | 1:C:1141:VAL:HG23 | 2.14 | 0.47 |
| 1:B:1361:LEU:HD21 | 1:B:1365:TYR:HE2 | 1.40 | 0.47 |
| 1:C:1408:ILE:HG22 | 1:C:1412:LEU:CG | 2.43 | 0.47 |
| 2:E:124:GLU:OE1 | 2:E:128:ARG:CZ | 2.62 | 0.47 |
| 1:B:1420:ASN:HA | 1:B:1423:LEU:CG | 2.44 | 0.47 |
| 1:A:1167:SER:HB3 | 1:A:1168:TYR:HD1 | 1.78 | 0.47 |
| 1:A:1375:ILE:HG23 | 1:A:1391:PHE:CZ | 2.49 | 0.47 |
| 1:A:1387:LYS:HB2 | 1:A:1390:GLN:CG | 2.41 | 0.47 |
| 1:B:1524:SER:C | 1:B:1526:GLU:H | 2.17 | 0.47 |
| 1:A:1524:SER:C | 1:A:1526:GLU:H | 2.17 | 0.47 |
| 1:A:1206:TYR:CE1 | 1:A:1230:THR:CB | 2.97 | 0.47 |
| 1:C:1208:GLU:CA | 1:C:1208:GLU:OE1 | 2.62 | 0.47 |
| 1:A:1272:CYS:O | 1:A:1276:ILE:HG23 | 2.14 | 0.47 |
| 1:C:1253:TRP:HZ3 | 1:C:1276:ILE:CG2 | 2.05 | 0.47 |
| 1:A:1569:CYS:O | 1:A:1572:THR:OG1 | 2.32 | 0.47 |
| 1:C:1175:PHE:HE1 | 1:C:1200:GLN:CB | 2.26 | 0.47 |
| 1:B:1405:TYR:CE2 | 1:B:1434:ARG:NH1 | 2.81 | 0.47 |
| 1:B:1387:LYS:HB2 | 1:B:1390:GLN:CG | 2.41 | 0.47 |
| 1:A:1091:ASN:ND2 | 1:A:1092:LEU:N | 2.61 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:C:1329:PRO:O | 1:C:1332:MET:N | 2.45 | 0.47 |
| 1:B:1578:ARG:CD | 1:B:1582:VAL:HB | 2.43 | 0.47 |
| 2:F:127:TRP:CA | 2:F:130:LYS:HE3 | 2.42 | 0.47 |
| 2:D:127:TRP:CA | 2:D:130:LYS:HE3 | 2.41 | 0.47 |
| 1:C:1092:LEU:O | 1:C:1094:ARG:CA | 2.54 | 0.47 |
| 1:B:1375:ILE:HG23 | 1:B:1391:PHE:CZ | 2.49 | 0.47 |
| 1:B:1234:LEU:CG | 1:B:1235:GLY:N | 2.75 | 0.47 |
| 1:C:1495:LEU:O | 1:C:1499:LEU:HG | 2.15 | 0.47 |
| 1:A:1513:TYR:HD1 | 1:A:1516:LYS:CE | 2.23 | 0.47 |
| 2:F:98:GLU:O | 2:F:102:ILE:HG23 | 2.14 | 0.47 |
| 1:A:1335:HIS:C | 1:A:1335:HIS:ND1 | 2.67 | 0.47 |
| 1:B:1253:TRP:CE3 | 1:B:1276:ILE:HB | 2.48 | 0.47 |
| 2:D:191:UNK:O | 2:D:193:UNK:N | 2.48 | 0.47 |
| 1:C:1504:LEU:CG | 2:E:149:ASN:ND2 | 2.69 | 0.47 |
| 1:A:1416:PRO:O | 1:A:1419:LEU:HB3 | 2.14 | 0.47 |
| 1:A:1475:GLU:CD | 2:F:149:ASN:HD21 | 2.18 | 0.47 |
| 1:A:1469:ASN:ND2 | 1:A:1498:ARG:NH2 | 2.62 | 0.47 |
| 1:A:1362:VAL:CG2 | 1:A:1377:THR:CB | 2.83 | 0.47 |
| 1:B:1408:ILE:HG22 | 1:B:1412:LEU:CG | 2.43 | 0.47 |
| 1:B:1375:ILE:HA | 1:B:1378:MET:HE3 | 1.96 | 0.47 |
| 1:B:1083:GLN:HE21 | 1:B:1106:ALA:HB3 | 1.76 | 0.47 |
| 2:D:102:ILE:HG13 | 2:D:103:ARG:N | 2.30 | 0.47 |
| 1:C:1368:TYR:CE1 | 1:C:1370:GLU:OE2 | 2.68 | 0.47 |
| 1:A:1113:LYS:HG2 | 1:A:1117:GLN:NE2 | 2.30 | 0.47 |
| 1:C:1324:TYR:CD2 | 1:C:1332:MET:HA | 2.44 | 0.47 |
| 1:A:1567:GLY:O | 1:A:1571:PHE:CD1 | 2.67 | 0.47 |
| 1:B:1564:GLU:O | 1:B:1568:ALA:N | 2.46 | 0.47 |
| 1:C:1567:GLY:O | 1:C:1571:PHE:CD1 | 2.67 | 0.47 |
| 1:C:1588:ARG:CG | 1:C:1589:HIS:N | 2.77 | 0.47 |
| 1:C:1111:LEU:O | 1:C:1115:GLN:HB2 | 2.14 | 0.47 |
| 1:A:1408:ILE:O | 1:A:1412:LEU:HB3 | 2.15 | 0.47 |
| 1:A:1129:ILE:HG13 | 1:A:1130:LYS:N | 2.29 | 0.47 |
| 1:A:1461:LYS:HG2 | 1:A:1489:ASN:ND2 | 2.29 | 0.47 |
| 1:C:1078:ASN:CB | 1:C:1098:PHE:CZ | 2.97 | 0.47 |
| 1:C:1085:LEU:C | 1:C:1086:ILE:O | 2.45 | 0.47 |
| 1:C:1553:LEU:O | 1:C:1556:TRP:HB3 | 2.15 | 0.47 |
| 2:F:178:UNK:C | 2:F:180:UNK:N | 2.74 | 0.47 |
| 1:C:1448:VAL:O | 1:C:1451:TYR:HB3 | 2.14 | 0.47 |
| 1:A:1082:VAL:O | 1:A:1085:LEU:HG | 2.14 | 0.47 |
| 2:D:153:ASN:ND2 | 2:D:158:LYS:CB | 2.77 | 0.47 |
| 1:C:1461:LYS:O | 1:C:1465:GLU:HB2 | 2.15 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:1610:VAL:O | 1:B:1614:ASP:CG | 2.53 | 0.47 |
| 1:B:1113:LYS:HG2 | 1:B:1117:GLN:NE2 | 2.30 | 0.47 |
| 1:A:1258:PHE:CA | 1:A:1289:TYR:CD1 | 2.96 | 0.47 |
| 1:A:1279:HIS:HE1 | 1:A:1283:LEU:CD1 | 2.09 | 0.47 |
| 1:A:1295:TYR:O | 1:A:1296:PHE:CB | 2.61 | 0.47 |
| 1:A:1329:PRO:O | 1:A:1332:MET:HB3 | 2.14 | 0.47 |
| 1:C:1272:CYS:O | 1:C:1276:ILE:HG23 | 2.14 | 0.47 |
| 1:A:1599:PHE:CE2 | 1:A:1600:ILE:HG13 | 2.50 | 0.47 |
| 1:B:1598:TYR:HE2 | 2:D:200:UNK:CB | 2.23 | 0.47 |
| 1:C:1561:GLU:HA | 1:C:1561:GLU:OE2 | 2.15 | 0.47 |
| 1:C:1572:THR:HG22 | 1:C:1578:ARG:HB3 | 1.96 | 0.47 |
| 2:F:183:UNK:N | 2:F:188:UNK:CB | 2.77 | 0.47 |
| 1:A:1561:GLU:OE2 | 1:A:1561:GLU:HA | 2.14 | 0.47 |
| 1:C:1171:THR:HG21 | 1:C:1200:GLN:OE1 | 2.14 | 0.47 |
| 1:C:1197:HIS:O | 1:C:1198:ILE:C | 2.53 | 0.47 |
| 1:C:1126:ASP:O | 1:C:1156:TYR:CE1 | 2.68 | 0.47 |
| 1:C:1145:ASN:O | 1:C:1150:TRP:CE2 | 2.68 | 0.47 |
| 2:E:122:VAL:HG23 | 2:E:123:MET:SD | 2.54 | 0.47 |
| 2:E:125:GLN:CD | 2:E:125:GLN:C | 2.72 | 0.47 |
| 1:A:1448:VAL:O | 1:A:1451:TYR:HB3 | 2.14 | 0.47 |
| 2:F:133:LYS:CA | 2:F:133:LYS:CE | 2.93 | 0.47 |
| 1:A:1365:TYR:CB | 1:A:1374:ALA:HB2 | 2.44 | 0.47 |
| 1:B:1335:HIS:ND1 | 1:B:1336:LEU:N | 2.63 | 0.47 |
| 1:B:1401:VAL:O | 1:B:1404:TYR:HD1 | 1.98 | 0.47 |
| 1:B:1448:VAL:O | 1:B:1451:TYR:HB3 | 2.15 | 0.47 |
| 1:A:1168:TYR:CA | 1:A:1172:GLU:OE2 | 2.63 | 0.47 |
| 1:A:1193:PRO:HG2 | 1:A:1194:ASN:H | 1.80 | 0.47 |
| 2:D:173:UNK:C | 2:D:176:UNK:CB | 2.92 | 0.47 |
| 1:B:1509:ARG:CZ | 2:D:166:ALA:CB | 2.93 | 0.47 |
| 1:B:1491:ASP:O | 1:B:1493:ILE:N | 2.48 | 0.47 |
| 1:B:1214:ALA:O | 1:B:1218:TYR:CB | 2.57 | 0.47 |
| 1:A:1368:TYR:CE1 | 1:A:1370:GLU:OE2 | 2.68 | 0.47 |
| 1:A:1301:THR:HG22 | 1:A:1301:THR:O | 2.15 | 0.47 |
| 1:A:1230:THR:O | 1:A:1231:LEU:CB | 2.61 | 0.47 |
| 1:A:1284:GLU:C | 1:A:1284:GLU:OE2 | 2.52 | 0.47 |
| 1:C:1421:ASP:O | 1:C:1424:MET:HB2 | 2.15 | 0.47 |
| 1:A:1258:PHE:HA | 1:A:1289:TYR:CD1 | 2.50 | 0.47 |
| 1:C:1335:HIS:ND1 | 1:C:1336:LEU:N | 2.63 | 0.47 |
| 1:B:1599:PHE:CE2 | 1:B:1600:ILE:HG13 | 2.50 | 0.47 |
| 1:B:1605:GLU:O | 1:B:1609:LYS:N | 2.48 | 0.47 |
| 1:C:1408:ILE:O | 1:C:1412:LEU:HB3 | 2.15 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:1490:PHE:CE2 | 1:B:1492:ASN:OD1 | 2.65 | 0.47 |
| 1:B:1085:LEU:CD2 | 1:B:1125:ILE:HD11 | 2.43 | 0.47 |
| 1:A:1421:ASP:O | 1:A:1424:MET:HB2 | 2.14 | 0.47 |
| 1:A:1290:TYR:CD1 | 1:A:1295:TYR:CE2 | 3.03 | 0.47 |
| 1:C:1274:LEU:CA | 1:C:1277:VAL:CG2 | 2.86 | 0.47 |
| 1:C:1564:GLU:O | 1:C:1568:ALA:N | 2.46 | 0.47 |
| 2:F:187:UNK:O | 2:F:188:UNK:C | 2.62 | 0.47 |
| 1:C:1150:TRP:HA | 1:C:1153:LEU:HB3 | 1.97 | 0.47 |
| 1:C:1475:GLU:OE1 | 2:E:145:GLN:HB2 | 2.15 | 0.47 |
| 1:A:1412:LEU:HD12 | 1:A:1419:LEU:HD21 | 1.66 | 0.47 |
| 1:A:1405:TYR:CE2 | 1:A:1434:ARG:NH1 | 2.81 | 0.47 |
| 2:F:118:ALA:CA | 2:F:121:LYS:HE3 | 2.41 | 0.47 |
| 2:F:122:VAL:HG23 | 2:F:123:MET:SD | 2.55 | 0.47 |
| 1:A:1414:PHE:CD1 | 2:F:127:TRP:CE3 | 3.03 | 0.47 |
| 1:C:1091:ASN:O | 1:C:1092:LEU:CB | 2.62 | 0.47 |
| 1:B:1371:TYR:CB | 1:B:1394:ILE:HG22 | 2.43 | 0.47 |
| 1:C:1375:ILE:HG23 | 1:C:1391:PHE:CZ | 2.49 | 0.47 |
| 1:B:1135:SER:O | 1:B:1136:SER:C | 2.53 | 0.47 |
| 1:C:1524:SER:C | 1:C:1526:GLU:H | 2.16 | 0.47 |
| 1:C:1301:THR:HG22 | 1:C:1301:THR:O | 2.15 | 0.47 |
| 1:B:1495:LEU:O | 1:B:1499:LEU:HG | 2.15 | 0.47 |
| 1:A:1145:ASN:HD22 | 1:A:1153:LEU:CD2 | 2.28 | 0.47 |
| 1:C:1113:LYS:HG2 | 1:C:1117:GLN:NE2 | 2.30 | 0.47 |
| 1:A:1495:LEU:O | 1:A:1499:LEU:HG | 2.15 | 0.47 |
| 1:A:1605:GLU:O | 1:A:1609:LYS:N | 2.48 | 0.47 |
| 1:B:1596:MET:H | 1:B:1597:PRO:CD | 2.13 | 0.47 |
| 1:C:1588:ARG:O | 1:C:1589:HIS:O | 2.32 | 0.47 |
| 1:C:1456:GLN:HG3 | 1:C:1456:GLN:O | 2.07 | 0.47 |
| 1:C:1098:PHE:O | 1:C:1102:CYS:CB | 2.62 | 0.47 |
| 1:A:1610:VAL:O | 1:A:1614:ASP:CG | 2.54 | 0.47 |
| 1:A:1553:LEU:O | 1:A:1556:TRP:HB3 | 2.15 | 0.47 |
| 1:B:1553:LEU:O | 1:B:1556:TRP:HB3 | 2.15 | 0.47 |
| 1:C:1244:ALA:HB1 | 1:C:1275:HIS:C | 2.35 | 0.46 |
| 1:A:1561:GLU:HG3 | 1:A:1562:LYS:N | 2.30 | 0.46 |
| 1:B:1561:GLU:OE2 | 1:B:1561:GLU:HA | 2.14 | 0.46 |
| 1:B:1587:TRP:NE1 | 1:B:1594:PHE:CE2 | 2.75 | 0.46 |
| 1:C:1605:GLU:O | 1:C:1609:LYS:N | 2.48 | 0.46 |
| 1:C:1106:ALA:O | 1:C:1107:VAL:C | 2.53 | 0.46 |
| 1:B:1365:TYR:CB | 1:B:1374:ALA:HB2 | 2.44 | 0.46 |
| 1:C:1395:ILE:HG23 | 1:C:1396:THR:N | 2.29 | 0.46 |
| 2:E:133:LYS:CA | 2:E:133:LYS:CE | 2.93 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:1474:GLU:O | 2:E:141:ARG:HG2 | 2.15 | 0.46 |
| 1:A:1408:ILE:HG22 | 1:A:1412:LEU:CG | 2.42 | 0.46 |
| 1:B:1450:PRO:O | 1:B:1453:ARG:HB2 | 2.15 | 0.46 |
| 1:A:1107:VAL:HG12 | 1:A:1111:LEU:CB | 2.43 | 0.46 |
| 1:C:1297:GLU:CA | 1:C:1300:ILE:HG12 | 2.45 | 0.46 |
| 1:B:1561:GLU:HG3 | 1:B:1562:LYS:N | 2.30 | 0.46 |
| 2:D:179:UNK:C | 2:D:181:UNK:N | 2.78 | 0.46 |
| 1:A:1451:TYR:O | 1:A:1455:VAL:HG23 | 2.16 | 0.46 |
| 1:B:1408:ILE:O | 1:B:1412:LEU:HB3 | 2.16 | 0.46 |
| 1:B:1472:ILE:CG2 | 1:B:1498:ARG:HE | 2.21 | 0.46 |
| 2:D:122:VAL:HG23 | 2:D:123:MET:SD | 2.55 | 0.46 |
| 2:D:133:LYS:CE | 2:D:133:LYS:CA | 2.93 | 0.46 |
| 2:E:144:GLU:O | 2:E:148:LYS:N | 2.45 | 0.46 |
| 1:A:1232:VAL:O | 1:A:1233:HIS:CB | 2.63 | 0.46 |
| 1:B:1461:LYS:O | 1:B:1465:GLU:HB2 | 2.15 | 0.46 |
| 1:A:1563:ARG:O | 1:A:1565:CYS:N | 2.48 | 0.46 |
| 1:B:1567:GLY:O | 1:B:1571:PHE:CD1 | 2.68 | 0.46 |
| 1:C:1167:SER:HA | 1:C:1171:THR:CB | 2.45 | 0.46 |
| 1:C:1469:ASN:ND2 | 1:C:1498:ARG:NH2 | 2.62 | 0.46 |
| 1:C:1530:LYS:HG2 | 1:C:1531:ASP:N | 2.30 | 0.46 |
| 1:A:1167:SER:C | 1:A:1169:VAL:N | 2.66 | 0.46 |
| 2:F:114:GLN:CG | 2:F:115:GLU:N | 2.26 | 0.46 |
| 1:B:1514:LEU:CD2 | 1:B:1514:LEU:C | 2.81 | 0.46 |
| 1:A:1491:ASP:O | 1:A:1493:ILE:N | 2.48 | 0.46 |
| 1:B:1111:LEU:HD22 | 1:B:1111:LEU:C | 2.29 | 0.46 |
| 2:D:95:LEU:HA | 2:D:99:PRO:HD2 | 1.97 | 0.46 |
| 1:B:1368:TYR:CE1 | 1:B:1370:GLU:OE2 | 2.68 | 0.46 |
| 1:A:1461:LYS:O | 1:A:1465:GLU:HB2 | 2.15 | 0.46 |
| 2:F:102:ILE:O | 2:F:104:LYS:N | 2.49 | 0.46 |
| 1:C:1600:ILE:HB | 1:C:1601:GLN:OE1 | 2.16 | 0.46 |
| 1:C:1137:TYR:HB2 | 1:C:1169:VAL:CG2 | 2.46 | 0.46 |
| 1:B:1358:TRP:CZ3 | 1:B:1381:HIS:CE1 | 2.70 | 0.46 |
| 1:C:1425:VAL:CG2 | 1:C:1426:LEU:H | 2.19 | 0.46 |
| 1:C:1450:PRO:O | 1:C:1453:ARG:HB2 | 2.15 | 0.46 |
| 1:B:1395:ILE:HG23 | 1:B:1396:THR:N | 2.29 | 0.46 |
| 1:B:1448:VAL:HA | 1:B:1451:TYR:HB3 | 1.98 | 0.46 |
| 1:A:1161:ARG:HH22 | 1:A:1174:ILE:CG1 | 2.28 | 0.46 |
| 1:A:1108:TRP:CD1 | 1:A:1131:ALA:CB | 2.93 | 0.46 |
| 1:B:1303:LEU:HD12 | 1:B:1320:LEU:CD1 | 2.35 | 0.46 |
| 1:A:1335:HIS:ND1 | 1:A:1336:LEU:N | 2.63 | 0.46 |
| 2:F:183:UNK:HA | 2:F:188:UNK:CB | 2.45 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:F:191:UNK:O | 2:F:194:UNK:N | 2.49 | 0.46 |
| 1:C:1147:SER:OG | 1:C:1148:GLY:N | 2.48 | 0.46 |
| 1:C:1414:PHE:C | 1:C:1416:PRO:HD3 | 2.21 | 0.46 |
| 1:C:1448:VAL:HA | 1:C:1451:TYR:HB3 | 1.97 | 0.46 |
| 2:E:101:SER:O | 2:E:105:TRP:HE3 | 1.99 | 0.46 |
| 1:C:1491:ASP:O | 1:C:1493:ILE:N | 2.48 | 0.46 |
| 2:F:148:LYS:O | 2:F:151:ILE:HG23 | 2.16 | 0.46 |
| 1:B:1301:THR:O | 1:B:1301:THR:HG22 | 2.15 | 0.46 |
| 1:A:1307:LEU:HD11 | 1:A:1316:MET:HB3 | 1.97 | 0.46 |
| 1:C:1610:VAL:O | 1:C:1614:ASP:CG | 2.53 | 0.46 |
| 1:C:1254:LYS:CD | 1:C:1285:GLU:HG2 | 2.45 | 0.46 |
| 1:A:1578:ARG:CD | 1:A:1582:VAL:HB | 2.43 | 0.46 |
| 1:A:1578:ARG:NH2 | 1:A:1583:LEU:HD23 | 2.28 | 0.46 |
| 1:B:1446:PRO:O | 1:B:1449:LYS:HB2 | 2.15 | 0.46 |
| 2:E:94:ARG:NH2 | 2:E:98:GLU:HG2 | 2.30 | 0.46 |
| 1:B:1307:LEU:HD11 | 1:B:1316:MET:HB3 | 1.97 | 0.46 |
| 1:A:1132:ASP:C | 1:A:1133:ASP:O | 2.52 | 0.46 |
| 1:A:1244:ALA:HB2 | 1:A:1275:HIS:ND1 | 2.14 | 0.46 |
| 1:C:1263:GLY:O | 1:C:1264:LYS:CB | 2.61 | 0.46 |
| 1:C:1561:GLU:HG3 | 1:C:1562:LYS:N | 2.30 | 0.46 |
| 1:C:1362:VAL:CG2 | 1:C:1377:THR:CB | 2.83 | 0.46 |
| 2:E:137:GLU:HG3 | 2:E:141:ARG:NH2 | 2.31 | 0.46 |
| 1:A:1401:VAL:O | 1:A:1404:TYR:HD1 | 1.98 | 0.46 |
| 1:A:1420:ASN:HA | 1:A:1423:LEU:CG | 2.44 | 0.46 |
| 1:B:1460:ASN:HB3 | 1:B:1463:VAL:HG23 | 1.98 | 0.46 |
| 1:A:1167:SER:HB3 | 1:A:1168:TYR:CE1 | 2.50 | 0.46 |
| 1:A:1111:LEU:CD2 | 1:A:1115:GLN:CG | 2.94 | 0.46 |
| 2:E:148:LYS:O | 2:E:151:ILE:HG23 | 2.16 | 0.46 |
| 2:D:185:UNK:CA | 2:D:189:UNK:C | 2.86 | 0.46 |
| 1:C:1499:LEU:HB2 | 1:C:1511:ALA:CB | 2.42 | 0.46 |
| 2:D:147:GLU:HA | 2:D:147:GLU:OE1 | 2.05 | 0.46 |
| 2:E:147:GLU:HA | 2:E:147:GLU:OE1 | 2.05 | 0.46 |
| 1:A:1315:GLY:O | 1:A:1319:GLU:HG2 | 2.16 | 0.46 |
| 1:A:1564:GLU:O | 1:A:1568:ALA:N | 2.46 | 0.46 |
| 1:B:1596:MET:SD | 1:B:1599:PHE:CZ | 3.09 | 0.46 |
| 1:C:1565:CYS:O | 1:C:1569:CYS:SG | 2.74 | 0.46 |
| 1:C:1599:PHE:CE2 | 1:C:1600:ILE:HG13 | 2.50 | 0.46 |
| 2:E:192:UNK:O | 2:E:193:UNK:O | 2.33 | 0.46 |
| 1:C:1126:ASP:O | 1:C:1156:TYR:CZ | 2.68 | 0.46 |
| 1:C:1401:VAL:O | 1:C:1404:TYR:HD1 | 1.98 | 0.46 |
| 1:C:1427:SER:HB2 | 1:C:1428:PRO:HD2 | 1.88 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:1474:GLU:O | 2:E:141:ARG:CD | 2.63 | 0.46 |
| 1:C:1475:GLU:OE1 | 2:E:141:ARG:O | 2.34 | 0.46 |
| 1:A:1450:PRO:O | 1:A:1453:ARG:HB2 | 2.15 | 0.46 |
| 2:F:133:LYS:HA | 2:F:133:LYS:HZ2 | 1.75 | 0.46 |
| 1:B:1416:PRO:O | 1:B:1419:LEU:HB3 | 2.14 | 0.46 |
| 1:B:1451:TYR:O | 1:B:1455:VAL:HG23 | 2.16 | 0.46 |
| 1:B:1214:ALA:O | 1:B:1218:TYR:CG | 2.69 | 0.46 |
| 2:D:155:ILE:CD1 | 2:D:155:ILE:N | 2.78 | 0.46 |
| 1:A:1273:GLY:C | 1:A:1275:HIS:H | 2.20 | 0.46 |
| 1:B:1273:GLY:C | 1:B:1275:HIS:H | 2.19 | 0.46 |
| 1:A:1600:ILE:HB | 1:A:1601:GLN:OE1 | 2.16 | 0.46 |
| 1:B:1577:LEU:C | 1:B:1579:PRO:HD3 | 2.37 | 0.46 |
| 2:D:204:UNK:O | 2:D:205:UNK:O | 2.34 | 0.46 |
| 2:F:184:UNK:C | 2:F:186:UNK:N | 2.79 | 0.46 |
| 1:C:1080:SER:C | 1:C:1082:VAL:H | 2.19 | 0.46 |
| 1:C:1444:GLN:HE21 | 2:E:130:LYS:HD2 | 1.79 | 0.46 |
| 2:D:118:ALA:CA | 2:D:121:LYS:HE3 | 2.41 | 0.46 |
| 1:B:1136:SER:HB3 | 1:B:1141:VAL:CG1 | 2.39 | 0.46 |
| 1:B:1161:ARG:NH1 | 1:B:1193:PRO:C | 2.68 | 0.46 |
| 1:B:1111:LEU:CD2 | 1:B:1115:GLN:CG | 2.94 | 0.46 |
| 2:D:148:LYS:O | 2:D:151:ILE:HG23 | 2.16 | 0.46 |
| 1:A:1345:ILE:HB | 1:A:1368:TYR:CE2 | 2.51 | 0.46 |
| 1:C:1078:ASN:CB | 1:C:1098:PHE:CE2 | 2.99 | 0.46 |
| 1:B:1315:GLY:O | 1:B:1319:GLU:HG2 | 2.16 | 0.46 |
| 2:E:107:GLU:OE1 | 2:E:107:GLU:HA | 2.16 | 0.46 |
| 1:A:1290:TYR:CZ | 1:A:1295:TYR:CE2 | 3.04 | 0.46 |
| 1:C:1211:TYR:CB | 1:C:1231:LEU:HD22 | 2.43 | 0.46 |
| 1:B:1572:THR:CB | 1:B:1599:PHE:HD2 | 2.28 | 0.46 |
| 1:B:1588:ARG:CZ | 2:F:195:UNK:CB | 2.94 | 0.46 |
| 1:B:1530:LYS:HG2 | 1:B:1531:ASP:N | 2.31 | 0.46 |
| 1:A:1490:PHE:CZ | 1:A:1492:ASN:CG | 2.87 | 0.46 |
| 1:C:1307:LEU:HD11 | 1:C:1316:MET:HB3 | 1.97 | 0.46 |
| 2:F:137:GLU:HG3 | 2:F:141:ARG:NH2 | 2.31 | 0.46 |
| 1:B:1482:THR:HA | 1:B:1485:ASP:CG | 2.37 | 0.46 |
| 1:A:1326:LYS:HG3 | 1:A:1327:PHE:CE1 | 2.51 | 0.45 |
| 1:C:1277:VAL:O | 1:C:1279:HIS:CB | 2.65 | 0.45 |
| 1:B:1579:PRO:O | 1:B:1583:LEU:HG | 2.16 | 0.45 |
| 1:C:1111:LEU:CD2 | 1:C:1115:GLN:CG | 2.94 | 0.45 |
| 1:C:1111:LEU:CD1 | 1:C:1129:ILE:HG21 | 2.45 | 0.45 |
| 1:C:1358:TRP:CH2 | 1:C:1381:HIS:ND1 | 2.61 | 0.45 |
| 1:A:1161:ARG:HG2 | 1:A:1173:LEU:HD22 | 1.97 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:1206:TYR:CE1 | 1:B:1230:THR:HB | 2.50 | 0.45 |
| 1:C:1079:THR:CG2 | 1:C:1079:THR:O | 2.56 | 0.45 |
| 1:B:1340:TRP:CD1 | 1:B:1340:TRP:N | 2.84 | 0.45 |
| 1:C:1629:THR:O | 1:C:1629:THR:HG22 | 2.16 | 0.45 |
| 1:A:1244:ALA:N | 1:A:1275:HIS:HE1 | 2.13 | 0.45 |
| 1:A:1279:HIS:CE1 | 1:A:1282:GLU:HB3 | 2.51 | 0.45 |
| 1:B:1588:ARG:CG | 1:B:1588:ARG:HH11 | 2.14 | 0.45 |
| 1:B:1600:ILE:HB | 1:B:1601:GLN:OE1 | 2.16 | 0.45 |
| 1:C:1579:PRO:O | 1:C:1583:LEU:HG | 2.16 | 0.45 |
| 1:C:1572:THR:CB | 1:C:1599:PHE:CD2 | 2.99 | 0.45 |
| 1:A:1214:ALA:O | 1:A:1218:TYR:CG | 2.69 | 0.45 |
| 1:C:1181:ASN:CG | 1:C:1185:GLU:HB2 | 2.37 | 0.45 |
| 2:E:127:TRP:CA | 2:E:130:LYS:HE3 | 2.41 | 0.45 |
| 1:A:1469:ASN:ND2 | 1:A:1469:ASN:O | 2.49 | 0.45 |
| 2:D:123:MET:O | 2:D:127:TRP:CD2 | 2.70 | 0.45 |
| 1:B:1167:SER:CB | 1:B:1168:TYR:HD1 | 2.28 | 0.45 |
| 1:C:1490:PHE:CZ | 1:C:1492:ASN:CG | 2.88 | 0.45 |
| 1:B:1232:VAL:O | 1:B:1233:HIS:CB | 2.63 | 0.45 |
| 1:C:1482:THR:HA | 1:C:1485:ASP:CG | 2.37 | 0.45 |
| 1:B:1588:ARG:HD2 | 1:B:1588:ARG:HA | 1.41 | 0.45 |
| 1:C:1561:GLU:HG3 | 1:C:1563:ARG:H | 1.82 | 0.45 |
| 1:C:1601:GLN:HA | 1:C:1604:LYS:CG | 2.47 | 0.45 |
| 1:A:1408:ILE:HD13 | 1:A:1422:LEU:HD11 | 1.98 | 0.45 |
| 1:A:1408:ILE:CG2 | 1:A:1412:LEU:HB2 | 2.23 | 0.45 |
| 1:A:1455:VAL:CG1 | 1:A:1456:GLN:H | 1.95 | 0.45 |
| 1:A:1361:LEU:HD22 | 1:A:1365:TYR:HE2 | 1.72 | 0.45 |
| 1:B:1469:ASN:ND2 | 1:B:1498:ARG:NH2 | 2.63 | 0.45 |
| 1:B:1345:ILE:N | 1:B:1346:PRO:HD2 | 2.20 | 0.45 |
| 1:B:1230:THR:O | 1:B:1231:LEU:CG | 2.64 | 0.45 |
| 2:F:103:ARG:HA | 2:F:106:ARG:HB2 | 1.98 | 0.45 |
| 1:C:1315:GLY:O | 1:C:1319:GLU:HG2 | 2.15 | 0.45 |
| 1:C:1340:TRP:CD1 | 1:C:1340:TRP:N | 2.84 | 0.45 |
| 1:B:1518:ASN:O | 1:B:1518:ASN:CG | 2.55 | 0.45 |
| 1:A:1255:GLU:C | 1:A:1289:TYR:OH | 2.55 | 0.45 |
| 1:C:1406:ARG:O | 1:C:1409:GLN:CB | 2.65 | 0.45 |
| 1:A:1458:HIS:C | 1:A:1460:ASN:H | 2.20 | 0.45 |
| 1:A:1490:PHE:CE2 | 1:A:1492:ASN:OD1 | 2.66 | 0.45 |
| 1:A:1617:GLU:CG | 1:A:1621:LYS:NZ | 2.80 | 0.45 |
| 1:A:1340:TRP:CD1 | 1:A:1340:TRP:N | 2.84 | 0.45 |
| 1:A:1244:ALA:H | 1:A:1275:HIS:CE1 | 2.35 | 0.45 |
| 1:A:1295:TYR:CE2 | 1:A:1299:LEU:CB | 2.94 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1565:CYS:O | 1:A:1569:CYS:SG | 2.75 | 0.45 |
| 1:A:1579:PRO:O | 1:A:1583:LEU:HG | 2.16 | 0.45 |
| 1:B:1601:GLN:HA | 1:B:1604:LYS:CG | 2.46 | 0.45 |
| 1:C:1146:THR:O | 1:C:1147:SER:O | 2.34 | 0.45 |
| 1:C:1214:ALA:O | 1:C:1218:TYR:CG | 2.69 | 0.45 |
| 1:A:1455:VAL:O | 1:A:1456:GLN:CB | 2.65 | 0.45 |
| 1:A:1456:GLN:HG3 | 1:A:1456:GLN:O | 2.08 | 0.45 |
| 1:B:1474:GLU:C | 1:B:1475:GLU:HG3 | 2.37 | 0.45 |
| 1:A:1181:ASN:O | 1:A:1182:ARG:HG2 | 2.16 | 0.45 |
| 1:B:1080:SER:C | 1:B:1082:VAL:H | 2.19 | 0.45 |
| 1:C:1617:GLU:CG | 1:C:1621:LYS:NZ | 2.80 | 0.45 |
| 1:A:1561:GLU:CG | 1:A:1562:LYS:N | 2.80 | 0.45 |
| 1:A:1601:GLN:HA | 1:A:1604:LYS:CG | 2.46 | 0.45 |
| 1:C:1154:VAL:HG21 | 1:C:1180:THR:HG21 | 1.95 | 0.45 |
| 1:C:1408:ILE:O | 1:C:1412:LEU:CA | 2.64 | 0.45 |
| 1:A:1400:ASN:OD1 | 1:A:1402:GLU:HB3 | 2.17 | 0.45 |
| 1:B:1333:ARG:HB2 | 1:B:1360:GLU:HG2 | 1.94 | 0.45 |
| 1:A:1162:LYS:HE3 | 1:A:1162:LYS:HB2 | 1.71 | 0.45 |
| 1:A:1530:LYS:HG2 | 1:A:1531:ASP:N | 2.31 | 0.45 |
| 1:A:1333:ARG:HB2 | 1:A:1360:GLU:HG3 | 1.90 | 0.45 |
| 1:C:1230:THR:O | 1:C:1230:THR:HG22 | 2.17 | 0.45 |
| 1:C:1326:LYS:HG3 | 1:C:1327:PHE:CE1 | 2.52 | 0.45 |
| 1:B:1274:LEU:H | 1:B:1274:LEU:CD1 | 2.20 | 0.45 |
| 1:A:1598:TYR:HE2 | 2:F:199:UNK:N | 2.15 | 0.45 |
| 1:C:1198:ILE:CG2 | 1:C:1221:VAL:HG23 | 2.46 | 0.45 |
| 1:C:1451:TYR:O | 1:C:1455:VAL:HG23 | 2.16 | 0.45 |
| 1:A:1474:GLU:C | 1:A:1475:GLU:HG3 | 2.37 | 0.45 |
| 1:B:1326:LYS:HG3 | 1:B:1327:PHE:CE1 | 2.51 | 0.45 |
| 1:B:1329:PRO:O | 1:B:1332:MET:N | 2.45 | 0.45 |
| 1:B:1324:TYR:CD2 | 1:B:1332:MET:HA | 2.44 | 0.45 |
| 1:B:1408:ILE:HD13 | 1:B:1422:LEU:HD11 | 1.98 | 0.45 |
| 1:B:1095:ALA:HA | 1:B:1098:PHE:CZ | 2.52 | 0.45 |
| 1:A:1122:LYS:CG | 1:A:1123:GLU:N | 2.70 | 0.45 |
| 1:B:1090:GLY:HA2 | 1:B:1094:ARG:CZ | 2.46 | 0.45 |
| 1:B:1113:LYS:HG3 | 1:B:1139:GLU:OE1 | 2.17 | 0.45 |
| 1:C:1232:VAL:O | 1:C:1233:HIS:CB | 2.65 | 0.45 |
| 1:C:1332:MET:SD | 1:C:1360:GLU:CB | 3.05 | 0.45 |
| 1:B:1254:LYS:HD2 | 1:B:1285:GLU:OE2 | 2.17 | 0.45 |
| 1:A:1601:GLN:N | 1:A:1601:GLN:OE1 | 2.50 | 0.45 |
| 1:B:1565:CYS:O | 1:B:1569:CYS:SG | 2.75 | 0.45 |
| 1:B:1591:ILE:HG12 | 1:B:1592:MET:N | 2.31 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:1106:ALA:O | 1:C:1107:VAL:O | 2.35 | 0.45 |
| 1:C:1145:ASN:OD1 | 1:C:1179:LYS:NZ | 2.36 | 0.45 |
| 1:A:1460:ASN:HB3 | 1:A:1463:VAL:HG23 | 1.98 | 0.45 |
| 1:B:1467:LEU:HG | 1:B:1471:PHE:HE2 | 1.82 | 0.45 |
| 1:A:1080:SER:C | 1:A:1082:VAL:N | 2.70 | 0.45 |
| 1:A:1482:THR:HA | 1:A:1485:ASP:CG | 2.36 | 0.45 |
| 1:A:1204:ARG:O | 1:A:1208:GLU:N | 2.49 | 0.45 |
| 1:C:1277:VAL:C | 1:C:1279:HIS:H | 2.17 | 0.45 |
| 1:C:1270:GLN:CD | 1:C:1298:GLU:CB | 2.78 | 0.45 |
| 1:B:1601:GLN:N | 1:B:1601:GLN:OE1 | 2.50 | 0.45 |
| 1:C:1161:ARG:HH21 | 1:C:1170:GLU:CG | 2.30 | 0.45 |
| 1:C:1400:ASN:OD1 | 1:C:1402:GLU:HB3 | 2.17 | 0.45 |
| 1:C:1444:GLN:HE22 | 2:E:130:LYS:HD2 | 1.77 | 0.45 |
| 1:B:1332:MET:SD | 1:B:1360:GLU:CB | 3.05 | 0.45 |
| 1:B:1413:GLU:HA | 1:B:1413:GLU:OE1 | 2.17 | 0.45 |
| 1:B:1466:SER:O | 1:B:1469:ASN:HB3 | 2.17 | 0.45 |
| 1:A:1123:GLU:OE1 | 2:F:7:UNK:CB | 2.65 | 0.45 |
| 1:A:1206:TYR:CE1 | 1:A:1226:ARG:HA | 2.52 | 0.45 |
| 1:A:1230:THR:HG22 | 1:A:1230:THR:O | 2.17 | 0.45 |
| 1:A:1230:THR:O | 1:A:1231:LEU:CG | 2.65 | 0.45 |
| 1:B:1518:ASN:O | 1:B:1518:ASN:ND2 | 2.50 | 0.45 |
| 1:A:1332:MET:SD | 1:A:1360:GLU:CB | 3.05 | 0.45 |
| 1:B:1561:GLU:CG | 1:B:1562:LYS:N | 2.80 | 0.45 |
| 1:B:1598:TYR:CA | 1:C:1584:GLU:OE2 | 2.61 | 0.45 |
| 1:C:1458:HIS:C | 1:C:1460:ASN:H | 2.19 | 0.45 |
| 1:A:1448:VAL:HA | 1:A:1451:TYR:HB3 | 1.98 | 0.45 |
| 2:F:123:MET:O | 2:F:127:TRP:CD2 | 2.70 | 0.45 |
| 1:B:1332:MET:HG3 | 1:B:1357:LEU:HD12 | 1.99 | 0.45 |
| 1:B:1333:ARG:HA | 1:B:1360:GLU:CG | 2.47 | 0.45 |
| 1:B:1456:GLN:O | 1:B:1456:GLN:HG3 | 2.07 | 0.45 |
| 1:B:1161:ARG:HG2 | 1:B:1173:LEU:HD22 | 1.97 | 0.45 |
| 1:A:1503:GLU:HG3 | 1:A:1504:LEU:H | 1.82 | 0.45 |
| 1:B:1083:GLN:C | 1:B:1085:LEU:N | 2.70 | 0.45 |
| 1:A:1087:GLU:H | 1:A:1087:GLU:HG2 | 1.52 | 0.45 |
| 1:A:1089:ILE:HD12 | 1:A:1089:ILE:N | 2.31 | 0.45 |
| 1:A:1145:ASN:HD22 | 1:A:1153:LEU:HD22 | 1.82 | 0.45 |
| 1:B:1204:ARG:O | 1:B:1208:GLU:N | 2.48 | 0.45 |
| 1:A:1261:VAL:HG13 | 1:A:1295:TYR:CE1 | 2.52 | 0.44 |
| 1:B:1277:VAL:C | 1:B:1279:HIS:HD1 | 2.20 | 0.44 |
| 1:B:1282:GLU:C | 1:B:1283:LEU:CD1 | 2.86 | 0.44 |
| 1:C:1561:GLU:CG | 1:C:1562:LYS:N | 2.80 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:E:189:UNK:CA | 2:E:194:UNK:CB | 2.96 | 0.44 |
| 1:C:1166:GLU:HB2 | 1:C:1168:TYR:OH | 2.17 | 0.44 |
| 1:C:1167:SER:CA | 1:C:1171:THR:H | 2.28 | 0.44 |
| 1:A:1362:VAL:HG23 | 1:A:1377:THR:HG21 | 1.99 | 0.44 |
| 2:D:174:UNK:CA | 2:D:175:UNK:CB | 2.95 | 0.44 |
| 1:B:1617:GLU:CG | 1:B:1621:LYS:NZ | 2.80 | 0.44 |
| 1:A:1237:TYR:CG | 1:A:1237:TYR:O | 2.70 | 0.44 |
| 1:A:1333:ARG:HB2 | 1:A:1360:GLU:HG2 | 1.94 | 0.44 |
| 1:A:1592:MET:HG2 | 1:A:1593:ASP:H | 1.81 | 0.44 |
| 1:A:1408:ILE:O | 1:A:1412:LEU:CA | 2.64 | 0.44 |
| 1:A:1452:LEU:HD13 | 1:A:1467:LEU:HD13 | 1.99 | 0.44 |
| 1:B:1455:VAL:O | 1:B:1456:GLN:CB | 2.65 | 0.44 |
| 1:B:1458:HIS:C | 1:B:1460:ASN:H | 2.19 | 0.44 |
| 1:B:1137:TYR:HB3 | 1:B:1172:GLU:HG2 | 1.99 | 0.44 |
| 1:B:1080:SER:C | 1:B:1082:VAL:N | 2.70 | 0.44 |
| 1:A:1085:LEU:HD11 | 1:A:1111:LEU:HG | 1.99 | 0.44 |
| 1:A:1111:LEU:CD1 | 1:A:1125:ILE:HG13 | 2.44 | 0.44 |
| 2:D:91:GLN:NE2 | 2:D:94:ARG:HD2 | 2.32 | 0.44 |
| 1:B:1235:GLY:O | 1:B:1238:GLN:HB2 | 2.17 | 0.44 |
| 1:A:1302:MET:C | 1:A:1304:GLU:N | 2.69 | 0.44 |
| 2:F:112:ARG:C | 2:F:113:LEU:O | 2.54 | 0.44 |
| 1:A:1324:TYR:CD2 | 1:A:1332:MET:HA | 2.43 | 0.44 |
| 1:C:1274:LEU:O | 1:C:1277:VAL:CG2 | 2.65 | 0.44 |
| 1:B:1245:ARG:O | 1:B:1246:LYS:CB | 2.66 | 0.44 |
| 1:B:1274:LEU:O | 1:B:1277:VAL:CG2 | 2.65 | 0.44 |
| 1:A:1611:ASP:CG | 1:B:1607:LEU:HD22 | 2.34 | 0.44 |
| 1:C:1420:ASN:HA | 1:C:1423:LEU:CG | 2.44 | 0.44 |
| 1:A:1395:ILE:CG2 | 1:A:1396:THR:N | 2.81 | 0.44 |
| 1:B:1130:LYS:HZ3 | 1:B:1155:LYS:CG | 2.29 | 0.44 |
| 1:B:1144:ALA:CA | 1:B:1149:ASN:HB2 | 2.46 | 0.44 |
| 1:A:1084:VAL:O | 1:A:1086:ILE:N | 2.49 | 0.44 |
| 2:D:94:ARG:NE | 2:D:98:GLU:OE1 | 2.47 | 0.44 |
| 1:B:1345:ILE:HB | 1:B:1368:TYR:CE2 | 2.51 | 0.44 |
| 2:D:48:UNK:C | 2:D:50:UNK:N | 2.80 | 0.44 |
| 1:A:1274:LEU:O | 1:A:1277:VAL:CG2 | 2.65 | 0.44 |
| 1:C:1258:PHE:CZ | 1:C:1293:ARG:CZ | 3.01 | 0.44 |
| 1:C:1297:GLU:OE1 | 1:C:1297:GLU:HA | 2.18 | 0.44 |
| 1:C:1577:LEU:C | 1:C:1579:PRO:HD3 | 2.36 | 0.44 |
| 1:A:1580:ASP:OD2 | 1:C:1605:GLU:HG3 | 2.17 | 0.44 |
| 1:B:1588:ARG:NH1 | 2:F:195:UNK:CB | 2.81 | 0.44 |
| 1:C:1460:ASN:HB3 | 1:C:1463:VAL:HG23 | 1.98 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:E:123:MET:O | 2:E:127:TRP:CD2 | 2.70 | 0.44 |
| 1:B:1333:ARG:HB2 | 1:B:1360:GLU:HG3 | 1.90 | 0.44 |
| 1:A:1162:LYS:C | 1:A:1162:LYS:CB | 2.80 | 0.44 |
| 1:A:1136:SER:HB2 | 1:A:1172:GLU:HB3 | 1.99 | 0.44 |
| 1:B:1163:LYS:O | 2:D:38:UNK:N | 2.48 | 0.44 |
| 1:B:1181:ASN:CG | 1:B:1182:ARG:N | 2.71 | 0.44 |
| 1:B:1086:ILE:HG22 | 1:B:1087:GLU:HG3 | 1.99 | 0.44 |
| 1:B:1133:ASP:HA | 1:B:1134:PRO:HA | 1.57 | 0.44 |
| 1:A:1095:ALA:HA | 1:A:1098:PHE:CZ | 2.52 | 0.44 |
| 2:F:7:UNK:O | 2:F:8:UNK:C | 2.66 | 0.44 |
| 2:F:94:ARG:HH21 | 2:F:94:ARG:CG | 2.30 | 0.44 |
| 1:C:1566:PHE:CE2 | 2:E:181:UNK:CA | 3.00 | 0.44 |
| 1:C:1518:ASN:CG | 1:C:1518:ASN:O | 2.55 | 0.44 |
| 1:C:1254:LYS:CD | 1:C:1285:GLU:CG | 2.83 | 0.44 |
| 1:B:1254:LYS:HA | 1:B:1289:TYR:CE2 | 2.52 | 0.44 |
| 1:C:1127:SER:HA | 1:C:1156:TYR:HH | 1.79 | 0.44 |
| 1:C:1452:LEU:HD13 | 1:C:1467:LEU:HD13 | 1.99 | 0.44 |
| 1:C:1474:GLU:C | 1:C:1475:GLU:HG3 | 2.37 | 0.44 |
| 1:A:1407:ALA:C | 1:A:1409:GLN:H | 2.21 | 0.44 |
| 1:A:1474:GLU:HG3 | 1:A:1476:ASP:H | 1.82 | 0.44 |
| 1:B:1400:ASN:OD1 | 1:B:1402:GLU:HB3 | 2.17 | 0.44 |
| 1:B:1481:ARG:NH1 | 1:B:1510:ILE:HD12 | 2.31 | 0.44 |
| 1:A:1206:TYR:CD1 | 1:A:1230:THR:HB | 2.52 | 0.44 |
| 1:C:1085:LEU:O | 1:C:1085:LEU:HD12 | 2.18 | 0.44 |
| 1:B:1291:GLN:O | 1:B:1294:GLY:N | 2.43 | 0.44 |
| 1:C:1237:TYR:CG | 1:C:1237:TYR:O | 2.70 | 0.44 |
| 1:A:1297:GLU:HA | 1:A:1297:GLU:OE1 | 2.18 | 0.44 |
| 1:B:1279:HIS:HD2 | 1:B:1280:ALA:N | 1.96 | 0.44 |
| 1:A:1561:GLU:HG3 | 1:A:1563:ARG:H | 1.82 | 0.44 |
| 1:B:1561:GLU:HG3 | 1:B:1563:ARG:H | 1.82 | 0.44 |
| 1:C:1601:GLN:N | 1:C:1601:GLN:OE1 | 2.50 | 0.44 |
| 1:C:1132:ASP:O | 1:C:1133:ASP:CB | 2.65 | 0.44 |
| 1:C:1174:ILE:CD1 | 1:C:1174:ILE:N | 2.81 | 0.44 |
| 1:C:1198:ILE:CG2 | 1:C:1221:VAL:CG2 | 2.95 | 0.44 |
| 1:C:1455:VAL:O | 1:C:1456:GLN:CB | 2.65 | 0.44 |
| 1:B:1330:GLN:HG3 | 1:B:1331:LYS:HG3 | 2.00 | 0.44 |
| 1:B:1474:GLU:HG3 | 1:B:1476:ASP:H | 1.83 | 0.44 |
| 1:A:1371:TYR:CB | 1:A:1394:ILE:HG22 | 2.43 | 0.44 |
| 1:C:1302:MET:C | 1:C:1304:GLU:N | 2.69 | 0.44 |
| 1:A:1206:TYR:CG | 1:A:1226:ARG:HG3 | 2.52 | 0.44 |
| 1:C:1459:ASN:O | 1:C:1489:ASN:HB3 | 2.18 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:E:112:ARG:C | 2:E:113:LEU:O | 2.54 | 0.44 |
| 1:A:1518:ASN:O | 1:A:1518:ASN:ND2 | 2.50 | 0.44 |
| 1:A:1480:LEU:HA | 1:A:1483:SER:HB3 | 2.00 | 0.44 |
| 1:B:1480:LEU:HA | 1:B:1483:SER:HB3 | 2.00 | 0.44 |
| 1:A:1165:ARG:O | 1:A:1165:ARG:HG3 | 2.18 | 0.44 |
| 1:A:1154:VAL:HG13 | 1:A:1181:ASN:HD21 | 1.82 | 0.44 |
| 1:A:1411:TYR:HA | 1:A:1415:LYS:HB2 | 1.90 | 0.44 |
| 2:E:105:TRP:HA | 2:E:108:GLU:CG | 2.48 | 0.44 |
| 1:C:1187:GLU:O | 1:C:1190:ILE:HG22 | 2.18 | 0.44 |
| 2:D:103:ARG:CZ | 2:D:106:ARG:HG3 | 2.48 | 0.44 |
| 1:C:1095:ALA:HA | 1:C:1098:PHE:CZ | 2.52 | 0.44 |
| 1:B:1237:TYR:O | 1:B:1237:TYR:CG | 2.70 | 0.44 |
| 1:A:1333:ARG:CB | 1:A:1360:GLU:HG2 | 2.48 | 0.44 |
| 1:A:1562:LYS:C | 1:A:1564:GLU:N | 2.70 | 0.44 |
| 2:F:196:UNK:O | 2:F:197:UNK:O | 2.36 | 0.44 |
| 1:C:1413:GLU:HA | 1:C:1413:GLU:OE1 | 2.18 | 0.44 |
| 1:A:1469:ASN:ND2 | 1:A:1498:ARG:HH12 | 2.16 | 0.44 |
| 1:B:1297:GLU:OE1 | 1:B:1297:GLU:HA | 2.18 | 0.44 |
| 1:B:1407:ALA:C | 1:B:1409:GLN:H | 2.21 | 0.44 |
| 1:B:1469:ASN:ND2 | 1:B:1498:ARG:HH12 | 2.15 | 0.44 |
| 1:B:1163:LYS:O | 1:B:1164:ALA:CB | 2.64 | 0.44 |
| 1:B:1177:LEU:O | 1:B:1180:THR:N | 2.51 | 0.44 |
| 1:A:1481:ARG:NH1 | 1:A:1510:ILE:HD12 | 2.32 | 0.44 |
| 1:A:1155:LYS:O | 1:A:1158:GLN:HB3 | 2.18 | 0.44 |
| 1:C:1345:ILE:HB | 1:C:1368:TYR:CE2 | 2.52 | 0.44 |
| 1:A:1090:GLY:HA2 | 1:A:1094:ARG:CZ | 2.48 | 0.44 |
| 1:C:1518:ASN:ND2 | 1:C:1518:ASN:O | 2.50 | 0.44 |
| 1:C:1548:GLU:CD | 1:C:1548:GLU:H | 2.21 | 0.44 |
| 1:C:1273:GLY:C | 1:C:1275:HIS:H | 2.20 | 0.44 |
| 1:B:1546:ASP:O | 1:B:1547:THR:C | 2.56 | 0.44 |
| 1:C:1609:LYS:HG2 | 1:C:1612:LYS:CD | 2.44 | 0.44 |
| 1:A:1416:PRO:O | 1:A:1417:LEU:C | 2.56 | 0.44 |
| 1:A:1235:GLY:O | 1:A:1238:GLN:HB2 | 2.18 | 0.44 |
| 1:A:1430:LEU:HD12 | 1:A:1431:ASP:H | 1.83 | 0.44 |
| 1:A:1459:ASN:O | 1:A:1489:ASN:HB3 | 2.18 | 0.44 |
| 1:A:1577:LEU:C | 1:A:1579:PRO:HD3 | 2.36 | 0.43 |
| 2:D:191:UNK:C | 2:D:196:UNK:CB | 2.95 | 0.43 |
| 1:C:1469:ASN:ND2 | 1:C:1498:ARG:HH12 | 2.16 | 0.43 |
| 1:A:1416:PRO:HD3 | 2:F:130:LYS:CD | 2.37 | 0.43 |
| 1:A:1425:VAL:CG2 | 1:A:1426:LEU:H | 2.18 | 0.43 |
| 1:A:1159:MET:SD | 1:A:1162:LYS:CB | 3.04 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:1390:GLN:HB2 | 1:B:1390:GLN:HE21 | 1.64 | 0.43 |
| 1:A:1080:SER:C | 1:A:1082:VAL:H | 2.19 | 0.43 |
| 1:C:1477:TYR:O | 1:C:1481:ARG:HB2 | 2.19 | 0.43 |
| 1:C:1566:PHE:CD2 | 2:E:181:UNK:HA | 2.52 | 0.43 |
| 1:C:1155:LYS:O | 1:C:1158:GLN:HB3 | 2.18 | 0.43 |
| 1:A:1204:ARG:NH1 | 1:A:1207:ASP:OD2 | 2.51 | 0.43 |
| 1:A:1175:PHE:HE1 | 1:A:1200:GLN:HB3 | 1.82 | 0.43 |
| 1:A:1546:ASP:O | 1:A:1547:THR:C | 2.56 | 0.43 |
| 1:C:1562:LYS:C | 1:C:1564:GLU:N | 2.71 | 0.43 |
| 1:C:1395:ILE:CG2 | 1:C:1396:THR:N | 2.81 | 0.43 |
| 1:C:1467:LEU:HG | 1:C:1471:PHE:HE2 | 1.82 | 0.43 |
| 1:C:1474:GLU:HG3 | 1:C:1476:ASP:H | 1.82 | 0.43 |
| 1:C:1434:ARG:HB2 | 2:E:7:UNK:CB | 2.48 | 0.43 |
| 1:A:1413:GLU:HA | 1:A:1413:GLU:OE1 | 2.18 | 0.43 |
| 1:B:1406:ARG:O | 1:B:1409:GLN:CB | 2.64 | 0.43 |
| 1:B:1435:ALA:O | 1:B:1439:PHE:HD2 | 2.01 | 0.43 |
| 1:A:1181:ASN:O | 1:A:1182:ARG:NE | 2.52 | 0.43 |
| 1:B:1082:VAL:CG1 | 1:B:1083:GLN:N | 2.69 | 0.43 |
| 1:B:1085:LEU:H | 1:B:1085:LEU:HG | 1.69 | 0.43 |
| 1:A:1083:GLN:NE2 | 1:A:1106:ALA:HB3 | 2.32 | 0.43 |
| 1:C:1619:LEU:N | 1:C:1619:LEU:HD22 | 2.33 | 0.43 |
| 1:A:1187:GLU:O | 1:A:1190:ILE:HG22 | 2.18 | 0.43 |
| 2:F:147:GLU:HA | 2:F:147:GLU:OE1 | 2.05 | 0.43 |
| 1:A:1092:LEU:C | 1:A:1094:ARG:N | 2.72 | 0.43 |
| 1:B:1154:VAL:HG11 | 1:B:1183:LEU:HB3 | 2.01 | 0.43 |
| 1:A:1282:GLU:C | 1:A:1283:LEU:CD1 | 2.86 | 0.43 |
| 1:C:1563:ARG:NH2 | 2:E:182:UNK:N | 2.66 | 0.43 |
| 1:C:1080:SER:C | 1:C:1082:VAL:N | 2.70 | 0.43 |
| 1:C:1407:ALA:C | 1:C:1409:GLN:H | 2.21 | 0.43 |
| 1:A:1466:SER:O | 1:A:1469:ASN:HB3 | 2.18 | 0.43 |
| 1:A:1177:LEU:CA | 1:A:1180:THR:HG1 | 2.29 | 0.43 |
| 1:A:1477:TYR:O | 1:A:1481:ARG:HB2 | 2.19 | 0.43 |
| 1:A:1477:TYR:CD1 | 1:A:1478:GLN:N | 2.87 | 0.43 |
| 1:B:1230:THR:O | 1:B:1230:THR:HG22 | 2.17 | 0.43 |
| 1:A:1333:ARG:HA | 1:A:1360:GLU:CG | 2.47 | 0.43 |
| 1:C:1329:PRO:O | 1:C:1330:GLN:C | 2.56 | 0.43 |
| 1:C:1578:ARG:NH2 | 1:C:1583:LEU:HD23 | 2.28 | 0.43 |
| 1:C:1572:THR:OG1 | 1:C:1599:PHE:CD2 | 2.61 | 0.43 |
| 1:C:1416:PRO:O | 1:C:1417:LEU:C | 2.57 | 0.43 |
| 1:B:1395:ILE:CG2 | 1:B:1396:THR:N | 2.81 | 0.43 |
| 1:B:1435:ALA:HB1 | 1:B:1439:PHE:HE2 | 1.84 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:1333:ARG:HA | 1:C:1360:GLU:CG | 2.48 | 0.43 |
| 1:A:1563:ARG:C | 1:A:1565:CYS:N | 2.72 | 0.43 |
| 1:A:1580:ASP:OD1 | 1:C:1605:GLU:CG | 2.67 | 0.43 |
| 1:C:1419:LEU:HD23 | 1:C:1447:LEU:HD13 | 2.01 | 0.43 |
| 1:C:1455:VAL:CG1 | 1:C:1456:GLN:N | 2.64 | 0.43 |
| 1:C:1480:LEU:HA | 1:C:1483:SER:HB3 | 2.00 | 0.43 |
| 1:A:1469:ASN:C | 1:A:1469:ASN:HD22 | 2.21 | 0.43 |
| 1:A:1414:PHE:CD1 | 2:F:127:TRP:CB | 3.01 | 0.43 |
| 1:B:1298:GLU:OE1 | 1:B:1298:GLU:HA | 2.19 | 0.43 |
| 1:B:1408:ILE:O | 1:B:1412:LEU:CA | 2.64 | 0.43 |
| 1:A:1193:PRO:O | 1:A:1194:ASN:O | 2.36 | 0.43 |
| 1:B:1477:TYR:CD1 | 1:B:1478:GLN:N | 2.87 | 0.43 |
| 1:B:1111:LEU:HD21 | 1:B:1115:GLN:HG2 | 2.00 | 0.43 |
| 1:A:1345:ILE:HG21 | 1:A:1368:TYR:HD2 | 1.83 | 0.43 |
| 2:D:185:UNK:CA | 2:D:189:UNK:O | 2.54 | 0.43 |
| 2:E:91:GLN:O | 2:E:92:ALA:HB2 | 2.18 | 0.43 |
| 1:B:1190:ILE:CD1 | 1:B:1216:LEU:HG | 2.49 | 0.43 |
| 1:A:1298:GLU:OE1 | 1:A:1298:GLU:HA | 2.19 | 0.43 |
| 1:A:1467:LEU:HG | 1:A:1471:PHE:HE2 | 1.82 | 0.43 |
| 1:B:1181:ASN:CG | 1:B:1182:ARG:H | 2.21 | 0.43 |
| 1:B:1503:GLU:HG3 | 1:B:1504:LEU:H | 1.82 | 0.43 |
| 1:C:1190:ILE:HG12 | 1:C:1216:LEU:CG | 2.49 | 0.43 |
| 1:B:1083:GLN:NE2 | 1:B:1107:VAL:HG23 | 2.34 | 0.43 |
| 1:B:1155:LYS:O | 1:B:1158:GLN:HB3 | 2.18 | 0.43 |
| 1:B:1145:ASN:HA | 1:B:1153:LEU:HD22 | 2.01 | 0.43 |
| 1:B:1459:ASN:O | 1:B:1489:ASN:HB3 | 2.18 | 0.43 |
| 1:C:1430:LEU:HD12 | 1:C:1431:ASP:H | 1.84 | 0.43 |
| 1:C:1477:TYR:CD1 | 1:C:1478:GLN:N | 2.87 | 0.43 |
| 1:A:1436:VAL:HG11 | 1:A:1462:SER:HB2 | 2.00 | 0.43 |
| 1:A:1329:PRO:O | 1:A:1330:GLN:C | 2.57 | 0.43 |
| 1:A:1590:ASN:HB2 | 1:A:1592:MET:O | 2.19 | 0.43 |
| 1:B:1578:ARG:NH2 | 1:B:1583:LEU:HD23 | 2.28 | 0.43 |
| 1:C:1596:MET:SD | 1:C:1597:PRO:CD | 3.01 | 0.43 |
| 1:C:1122:LYS:CG | 1:C:1123:GLU:N | 2.71 | 0.43 |
| 1:C:1157:LEU:HD12 | 1:C:1173:LEU:CD1 | 2.48 | 0.43 |
| 1:C:1193:PRO:O | 1:C:1194:ASN:CB | 2.67 | 0.43 |
| 1:C:1198:ILE:C | 1:C:1201:VAL:HG23 | 2.38 | 0.43 |
| 1:C:1348:VAL:O | 1:C:1352:ALA:N | 2.52 | 0.43 |
| 1:C:1467:LEU:O | 1:C:1470:LEU:HB2 | 2.19 | 0.43 |
| 2:E:145:GLN:O | 2:E:149:ASN:ND2 | 2.52 | 0.43 |
| 1:B:1329:PRO:O | 1:B:1330:GLN:C | 2.56 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:1452:LEU:HD13 | 1:B:1467:LEU:HD13 | 1.99 | 0.43 |
| 1:C:1091:ASN:HA | 1:C:1091:ASN:HD22 | 1.51 | 0.43 |
| 1:B:1411:TYR:HA | 1:B:1415:LYS:HB2 | 1.89 | 0.43 |
| 1:B:1135:SER:O | 1:B:1136:SER:O | 2.36 | 0.43 |
| 1:C:1344:ASN:CG | 1:C:1345:ILE:N | 2.72 | 0.43 |
| 1:B:1189:PHE:O | 1:B:1217:LEU:CD2 | 2.66 | 0.43 |
| 1:B:1619:LEU:N | 1:B:1619:LEU:HD22 | 2.32 | 0.43 |
| 1:C:1159:MET:HA | 1:C:1162:LYS:HD3 | 2.00 | 0.43 |
| 1:A:1183:LEU:CG | 1:A:1184:ALA:N | 2.82 | 0.43 |
| 1:A:1626:ALA:O | 1:A:1629:THR:O | 2.36 | 0.43 |
| 1:C:1332:MET:SD | 1:C:1360:GLU:HB2 | 2.59 | 0.43 |
| 1:B:1244:ALA:N | 1:B:1275:HIS:HE1 | 2.16 | 0.43 |
| 1:B:1583:LEU:O | 1:B:1594:PHE:CZ | 2.70 | 0.43 |
| 2:D:201:UNK:O | 2:D:202:UNK:C | 2.66 | 0.43 |
| 1:C:1376:ILE:HA | 1:C:1379:MET:HG3 | 2.01 | 0.43 |
| 1:C:1469:ASN:O | 1:C:1469:ASN:ND2 | 2.49 | 0.43 |
| 1:A:1376:ILE:HA | 1:A:1379:MET:HG3 | 2.01 | 0.43 |
| 1:A:1435:ALA:O | 1:A:1439:PHE:HD2 | 2.01 | 0.43 |
| 1:A:1348:VAL:O | 1:A:1352:ALA:N | 2.52 | 0.43 |
| 1:B:1416:PRO:O | 1:B:1417:LEU:C | 2.56 | 0.43 |
| 1:B:1168:TYR:CA | 1:B:1172:GLU:OE2 | 2.63 | 0.43 |
| 1:A:1505:ILE:O | 1:A:1506:GLU:C | 2.57 | 0.43 |
| 1:B:1477:TYR:O | 1:B:1481:ARG:HB2 | 2.19 | 0.43 |
| 1:C:1190:ILE:HG22 | 1:C:1191:ASN:ND2 | 2.34 | 0.43 |
| 1:C:1142:GLN:C | 1:C:1142:GLN:CD | 2.78 | 0.43 |
| 1:B:1204:ARG:NH1 | 1:B:1207:ASP:OD2 | 2.51 | 0.43 |
| 1:B:1520:ARG:H | 1:B:1520:ARG:CD | 2.32 | 0.43 |
| 1:A:1332:MET:HG3 | 1:A:1357:LEU:HD12 | 1.99 | 0.43 |
| 1:A:1609:LYS:HA | 1:A:1612:LYS:CG | 2.48 | 0.43 |
| 1:C:1588:ARG:HH21 | 2:D:193:UNK:HA | 1.75 | 0.43 |
| 1:C:1505:ILE:O | 1:C:1506:GLU:C | 2.57 | 0.43 |
| 2:E:108:GLU:O | 2:E:108:GLU:OE1 | 2.37 | 0.43 |
| 1:B:1198:ILE:HG23 | 1:B:1201:VAL:CG2 | 2.49 | 0.43 |
| 2:D:173:UNK:C | 2:D:176:UNK:N | 2.82 | 0.43 |
| 1:B:1484:ILE:C | 1:B:1484:ILE:HD12 | 2.39 | 0.43 |
| 1:C:1190:ILE:HG21 | 1:C:1216:LEU:HD21 | 2.01 | 0.43 |
| 1:B:1132:ASP:C | 1:B:1133:ASP:O | 2.56 | 0.43 |
| 1:A:1085:LEU:H | 1:A:1085:LEU:HG | 1.63 | 0.43 |
| 1:A:1619:LEU:N | 1:A:1619:LEU:HD22 | 2.32 | 0.43 |
| 2:F:91:GLN:HE21 | 2:F:91:GLN:HB3 | 1.67 | 0.43 |
| 1:B:1436:VAL:HG11 | 1:B:1462:SER:HB2 | 2.00 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1279:HIS:NE2 | 1:A:1282:GLU:HB3 | 2.34 | 0.43 |
| 1:C:1230:THR:C | 1:C:1231:LEU:CG | 2.86 | 0.43 |
| 1:B:1253:TRP:HZ3 | 1:B:1276:ILE:CG2 | 2.04 | 0.43 |
| 1:A:1554:LEU:HD23 | 1:A:1582:VAL:CG1 | 2.49 | 0.43 |
| 1:B:1562:LYS:C | 1:B:1564:GLU:N | 2.71 | 0.43 |
| 1:B:1590:ASN:HB2 | 1:B:1592:MET:O | 2.19 | 0.43 |
| 2:F:195:UNK:O | 2:F:197:UNK:N | 2.49 | 0.43 |
| 1:B:1362:VAL:HG23 | 1:B:1377:THR:HG21 | 1.99 | 0.43 |
| 1:C:1466:SER:O | 1:C:1469:ASN:HB3 | 2.18 | 0.43 |
| 1:A:1467:LEU:O | 1:A:1470:LEU:HB2 | 2.18 | 0.43 |
| 1:B:1420:ASN:C | 1:B:1422:LEU:N | 2.73 | 0.43 |
| 2:D:126:GLU:HG3 | 2:D:130:LYS:HZ1 | 1.80 | 0.43 |
| 1:C:1371:TYR:CB | 1:C:1394:ILE:HG22 | 2.43 | 0.43 |
| 1:A:1484:ILE:HD12 | 1:A:1484:ILE:C | 2.39 | 0.43 |
| 1:A:1111:LEU:HD21 | 1:A:1115:GLN:HG2 | 1.99 | 0.43 |
| 1:A:1230:THR:O | 1:A:1231:LEU:HG | 2.19 | 0.43 |
| 1:A:1517:GLY:C | 1:A:1519:ASN:N | 2.72 | 0.43 |
| 1:A:1283:LEU:CD2 | 1:A:1313:HIS:CE1 | 3.00 | 0.42 |
| 1:C:1298:GLU:OE1 | 1:C:1298:GLU:HA | 2.19 | 0.42 |
| 1:C:1329:PRO:HB2 | 1:C:1330:GLN:H | 1.62 | 0.42 |
| 1:C:1330:GLN:HG3 | 1:C:1331:LYS:HG3 | 2.01 | 0.42 |
| 1:B:1535:LYS:HZ1 | 1:B:1563:ARG:HH12 | 1.63 | 0.42 |
| 1:A:1157:LEU:HD13 | 1:A:1177:LEU:HD21 | 2.00 | 0.42 |
| 1:B:1206:TYR:CE1 | 1:B:1226:ARG:CA | 3.02 | 0.42 |
| 1:B:1142:GLN:C | 1:B:1142:GLN:CD | 2.78 | 0.42 |
| 2:F:190:UNK:C | 2:F:192:UNK:N | 2.79 | 0.42 |
| 1:C:1435:ALA:O | 1:C:1439:PHE:HD2 | 2.01 | 0.42 |
| 1:A:1443:LYS:O | 1:A:1444:GLN:HG3 | 2.20 | 0.42 |
| 1:B:1332:MET:SD | 1:B:1360:GLU:HB2 | 2.59 | 0.42 |
| 1:B:1333:ARG:CG | 1:B:1360:GLU:HG3 | 2.49 | 0.42 |
| 1:B:1467:LEU:O | 1:B:1470:LEU:HB2 | 2.19 | 0.42 |
| 1:B:1505:ILE:O | 1:B:1506:GLU:C | 2.57 | 0.42 |
| 1:A:1388:GLU:CG | 1:A:1389:GLY:N | 2.82 | 0.42 |
| 1:B:1302:MET:C | 1:B:1304:GLU:N | 2.69 | 0.42 |
| 1:A:1344:ASN:OD1 | 1:A:1345:ILE:N | 2.52 | 0.42 |
| 1:A:1520:ARG:H | 1:A:1520:ARG:CD | 2.32 | 0.42 |
| 1:A:1258:PHE:HB2 | 1:A:1289:TYR:CZ | 2.27 | 0.42 |
| 1:C:1276:ILE:HG13 | 1:C:1277:VAL:N | 2.34 | 0.42 |
| 1:C:1587:TRP:CD1 | 1:C:1587:TRP:N | 2.86 | 0.42 |
| 1:C:1141:VAL:HG11 | 1:C:1168:TYR:O | 2.19 | 0.42 |
| 2:F:145:GLN:O | 2:F:149:ASN:ND2 | 2.52 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:1401:VAL:HA | 1:B:1404:TYR:HD1 | 1.83 | 0.42 |
| 1:A:1167:SER:CB | 1:A:1168:TYR:CD1 | 3.03 | 0.42 |
| 1:A:1481:ARG:NH1 | 1:A:1510:ILE:HG13 | 2.35 | 0.42 |
| 1:B:1130:LYS:HZ3 | 1:B:1155:LYS:CD | 2.31 | 0.42 |
| 2:D:137:GLU:HG3 | 2:D:141:ARG:HH12 | 1.84 | 0.42 |
| 1:B:1187:GLU:O | 1:B:1190:ILE:HG22 | 2.19 | 0.42 |
| 1:C:1520:ARG:H | 1:C:1520:ARG:CD | 2.32 | 0.42 |
| 1:C:1282:GLU:OE2 | 1:C:1285:GLU:CB | 2.62 | 0.42 |
| 1:A:1594:PHE:O | 1:A:1596:MET:HE2 | 2.20 | 0.42 |
| 1:C:1535:LYS:HZ1 | 1:C:1563:ARG:HH12 | 1.63 | 0.42 |
| 1:C:1401:VAL:HG22 | 1:C:1429:ARG:HH21 | 1.84 | 0.42 |
| 2:E:1:UNK:C | 2:E:3:UNK:N | 2.80 | 0.42 |
| 2:E:106:ARG:C | 2:E:108:GLU:H | 2.23 | 0.42 |
| 2:E:105:TRP:O | 2:E:108:GLU:CD | 2.58 | 0.42 |
| 1:B:1136:SER:HA | 1:B:1137:TYR:C | 2.38 | 0.42 |
| 1:C:1344:ASN:OD1 | 1:C:1345:ILE:N | 2.52 | 0.42 |
| 1:C:1370:GLU:HA | 1:C:1370:GLU:OE1 | 2.19 | 0.42 |
| 1:B:1345:ILE:HG21 | 1:B:1368:TYR:HD2 | 1.83 | 0.42 |
| 1:A:1303:LEU:HD23 | 1:A:1303:LEU:H | 1.85 | 0.42 |
| 1:B:1430:LEU:HD12 | 1:B:1431:ASP:H | 1.84 | 0.42 |
| 1:B:1340:TRP:CZ3 | 1:B:1367:LYS:HD2 | 2.54 | 0.42 |
| 1:A:1175:PHE:O | 1:A:1178:ALA:HB3 | 2.20 | 0.42 |
| 1:C:1436:VAL:HG11 | 1:C:1462:SER:HB2 | 2.00 | 0.42 |
| 1:A:1244:ALA:CA | 1:A:1275:HIS:CE1 | 3.02 | 0.42 |
| 1:A:1330:GLN:HG3 | 1:A:1331:LYS:HG3 | 2.00 | 0.42 |
| 1:C:1254:LYS:HD2 | 1:C:1285:GLU:OE2 | 2.18 | 0.42 |
| 1:A:1590:ASN:O | 1:A:1591:ILE:C | 2.58 | 0.42 |
| 1:C:1599:PHE:H | 1:C:1599:PHE:HD1 | 1.62 | 0.42 |
| 1:C:1136:SER:C | 1:C:1136:SER:N | 2.58 | 0.42 |
| 1:C:1161:ARG:HH22 | 1:C:1195:ASN:HB3 | 1.81 | 0.42 |
| 1:C:1204:ARG:NH1 | 1:C:1207:ASP:OD2 | 2.52 | 0.42 |
| 1:C:1503:GLU:HG3 | 1:C:1504:LEU:H | 1.82 | 0.42 |
| 1:A:1160:ALA:C | 1:A:1162:LYS:N | 2.72 | 0.42 |
| 2:E:104:LYS:C | 2:E:108:GLU:HG2 | 2.36 | 0.42 |
| 2:F:162:GLN:CB | 2:F:166:ALA:CB | 2.96 | 0.42 |
| 1:B:1083:GLN:O | 1:B:1086:ILE:HG13 | 2.19 | 0.42 |
| 1:B:1112:ALA:CB | 1:B:1140:VAL:HG21 | 2.46 | 0.42 |
| 1:A:1370:GLU:HA | 1:A:1370:GLU:OE1 | 2.20 | 0.42 |
| 1:B:1344:ASN:CG | 1:B:1345:ILE:N | 2.72 | 0.42 |
| 2:F:94:ARG:HG2 | 2:F:94:ARG:HH21 | 1.84 | 0.42 |
| 1:A:1340:TRP:CZ3 | 1:A:1367:LYS:HD2 | 2.54 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1256:VAL:CA | 1:A:1289:TYR:OH | 2.68 | 0.42 |
| 1:A:1332:MET:SD | 1:A:1360:GLU:HB2 | 2.59 | 0.42 |
| 1:A:1592:MET:O | 1:A:1593:ASP:OD1 | 2.37 | 0.42 |
| 1:B:1590:ASN:O | 1:B:1591:ILE:C | 2.57 | 0.42 |
| 1:C:1592:MET:HG2 | 1:C:1593:ASP:N | 2.34 | 0.42 |
| 1:C:1596:MET:SD | 1:C:1599:PHE:CZ | 3.12 | 0.42 |
| 1:A:1420:ASN:C | 1:A:1422:LEU:N | 2.72 | 0.42 |
| 1:B:1333:ARG:CA | 1:B:1360:GLU:CG | 2.98 | 0.42 |
| 1:B:1412:LEU:HA | 1:B:1419:LEU:HD13 | 2.00 | 0.42 |
| 1:B:1466:SER:O | 1:B:1470:LEU:N | 2.52 | 0.42 |
| 1:B:1469:ASN:ND2 | 1:B:1498:ARG:NH1 | 2.68 | 0.42 |
| 1:A:1521:TRP:CZ3 | 1:A:1525:VAL:HG11 | 2.55 | 0.42 |
| 1:B:1370:GLU:OE1 | 1:B:1370:GLU:HA | 2.20 | 0.42 |
| 1:B:1431:ASP:C | 1:B:1433:THR:N | 2.73 | 0.42 |
| 1:B:1513:TYR:O | 1:B:1516:LYS:N | 2.53 | 0.42 |
| 2:F:102:ILE:C | 2:F:104:LYS:H | 2.23 | 0.42 |
| 1:A:1517:GLY:C | 1:A:1519:ASN:H | 2.22 | 0.42 |
| 1:C:1517:GLY:C | 1:C:1519:ASN:H | 2.23 | 0.42 |
| 1:C:1517:GLY:C | 1:C:1519:ASN:N | 2.73 | 0.42 |
| 1:C:1332:MET:HG3 | 1:C:1357:LEU:HD12 | 1.99 | 0.42 |
| 1:B:1555:GLN:OE1 | 1:B:1585:THR:CG2 | 2.68 | 0.42 |
| 1:B:1609:LYS:HA | 1:B:1612:LYS:CG | 2.49 | 0.42 |
| 1:C:1609:LYS:HA | 1:C:1612:LYS:CG | 2.48 | 0.42 |
| 1:C:1161:ARG:NH1 | 1:C:1195:ASN:HB3 | 2.34 | 0.42 |
| 1:C:1414:PHE:CD2 | 2:E:123:MET:HG3 | 2.55 | 0.42 |
| 1:C:1469:ASN:ND2 | 1:C:1498:ARG:NH1 | 2.68 | 0.42 |
| 1:A:1165:ARG:NH2 | 1:A:1194:ASN:OD1 | 2.52 | 0.42 |
| 2:D:144:GLU:O | 2:D:148:LYS:N | 2.45 | 0.42 |
| 1:C:1345:ILE:HG21 | 1:C:1368:TYR:HD2 | 1.84 | 0.42 |
| 1:A:1344:ASN:CG | 1:A:1345:ILE:N | 2.72 | 0.42 |
| 1:A:1142:GLN:C | 1:A:1142:GLN:CD | 2.78 | 0.42 |
| 1:B:1340:TRP:H | 1:B:1340:TRP:HD1 | 1.68 | 0.42 |
| 1:A:1518:ASN:O | 1:A:1518:ASN:CG | 2.55 | 0.42 |
| 1:B:1175:PHE:O | 1:B:1178:ALA:HB3 | 2.19 | 0.42 |
| 1:A:1274:LEU:CD1 | 1:A:1274:LEU:H | 2.20 | 0.42 |
| 1:A:1295:TYR:HD2 | 1:A:1299:LEU:HD22 | 1.83 | 0.42 |
| 1:C:1325:SER:OG | 1:C:1326:LYS:HE3 | 2.20 | 0.42 |
| 1:B:1258:PHE:C | 1:B:1260:CYS:H | 2.23 | 0.42 |
| 1:A:1435:ALA:HB1 | 1:A:1439:PHE:HE2 | 1.84 | 0.42 |
| 1:B:1329:PRO:HB2 | 1:B:1330:GLN:H | 1.62 | 0.42 |
| 1:B:1476:ASP:CG | 1:B:1479:ALA:HB3 | 2.39 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1194:ASN:O | 1:A:1195:ASN:C | 2.58 | 0.42 |
| 1:C:1626:ALA:O | 1:C:1630:GLN:HB2 | 2.19 | 0.42 |
| 1:A:1109:SER:HA | 1:A:1134:PRO:HG3 | 2.02 | 0.42 |
| 1:A:1326:LYS:C | 1:A:1327:PHE:CG | 2.93 | 0.42 |
| 1:A:1592:MET:HG2 | 1:A:1593:ASP:N | 2.34 | 0.42 |
| 1:C:1189:PHE:O | 1:C:1193:PRO:HG3 | 2.20 | 0.42 |
| 1:C:1193:PRO:C | 1:C:1194:ASN:CG | 2.76 | 0.42 |
| 1:A:1456:GLN:HE22 | 1:A:1467:LEU:CD2 | 2.33 | 0.42 |
| 1:A:1466:SER:O | 1:A:1470:LEU:N | 2.52 | 0.42 |
| 1:B:1147:SER:OG | 1:B:1148:GLY:N | 2.53 | 0.42 |
| 1:C:1521:TRP:CZ3 | 1:C:1525:VAL:HG11 | 2.55 | 0.42 |
| 1:B:1368:TYR:HD1 | 1:B:1368:TYR:O | 2.03 | 0.42 |
| 1:A:1276:ILE:HG13 | 1:A:1277:VAL:N | 2.34 | 0.42 |
| 1:C:1333:ARG:CB | 1:C:1360:GLU:HG2 | 2.48 | 0.42 |
| 2:D:145:GLN:O | 2:D:149:ASN:ND2 | 2.52 | 0.42 |
| 2:E:105:TRP:CA | 2:E:108:GLU:CG | 2.98 | 0.42 |
| 1:A:1513:TYR:O | 1:A:1516:LYS:N | 2.53 | 0.42 |
| 1:B:1213:ALA:O | 1:B:1217:LEU:HB2 | 2.20 | 0.42 |
| 1:C:1270:GLN:HA | 1:C:1270:GLN:OE1 | 2.19 | 0.41 |
| 1:B:1280:ALA:C | 1:B:1282:GLU:H | 2.22 | 0.41 |
| 1:B:1569:CYS:C | 1:B:1571:PHE:N | 2.74 | 0.41 |
| 1:C:1170:GLU:CG | 1:C:1171:THR:N | 2.83 | 0.41 |
| 1:C:1175:PHE:O | 1:C:1178:ALA:HB3 | 2.19 | 0.41 |
| 1:C:1443:LYS:O | 1:C:1444:GLN:HG3 | 2.20 | 0.41 |
| 1:C:1474:GLU:O | 1:C:1475:GLU:CB | 2.68 | 0.41 |
| 2:F:126:GLU:HG3 | 2:F:130:LYS:HZ3 | 1.76 | 0.41 |
| 1:B:1325:SER:OG | 1:B:1326:LYS:HE3 | 2.20 | 0.41 |
| 1:B:1376:ILE:HA | 1:B:1379:MET:HG3 | 2.01 | 0.41 |
| 1:B:1469:ASN:O | 1:B:1469:ASN:ND2 | 2.49 | 0.41 |
| 1:A:1170:GLU:O | 1:A:1173:LEU:N | 2.53 | 0.41 |
| 1:C:1492:ASN:O | 1:C:1493:ILE:CD1 | 2.68 | 0.41 |
| 1:C:1490:PHE:CE2 | 1:C:1492:ASN:OD1 | 2.66 | 0.41 |
| 1:A:1206:TYR:CZ | 1:A:1230:THR:OG1 | 2.67 | 0.41 |
| 1:A:1431:ASP:C | 1:A:1433:THR:N | 2.73 | 0.41 |
| 1:C:1431:ASP:C | 1:C:1433:THR:N | 2.73 | 0.41 |
| 2:F:107:GLU:O | 2:F:110:ARG:HG2 | 2.20 | 0.41 |
| 1:C:1162:LYS:HD2 | 1:C:1162:LYS:H | 1.85 | 0.41 |
| 1:A:1325:SER:OG | 1:A:1326:LYS:HE3 | 2.20 | 0.41 |
| 1:A:1333:ARG:CA | 1:A:1360:GLU:CG | 2.98 | 0.41 |
| 1:C:1270:GLN:CG | 1:C:1298:GLU:CG | 2.87 | 0.41 |
| 1:C:1254:LYS:CA | 1:C:1289:TYR:CE2 | 3.02 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:1283:LEU:CD2 | 1:B:1313:HIS:NE2 | 2.74 | 0.41 |
| 1:C:1194:ASN:HD22 | 1:C:1194:ASN:C | 2.24 | 0.41 |
| 1:B:1348:VAL:O | 1:B:1352:ALA:N | 2.52 | 0.41 |
| 1:C:1362:VAL:HG23 | 1:C:1377:THR:HG21 | 1.99 | 0.41 |
| 1:A:1412:LEU:HA | 1:A:1419:LEU:HD13 | 1.98 | 0.41 |
| 1:A:1471:PHE:HD1 | 1:A:1476:ASP:HB3 | 1.85 | 0.41 |
| 1:B:1419:LEU:HD23 | 1:B:1447:LEU:HD13 | 2.01 | 0.41 |
| 1:B:1443:LYS:O | 1:B:1444:GLN:HG3 | 2.20 | 0.41 |
| 1:A:1161:ARG:HE | 1:A:1173:LEU:CD2 | 2.29 | 0.41 |
| 1:C:1387:LYS:HD2 | 1:C:1390:GLN:CD | 2.41 | 0.41 |
| 1:A:1387:LYS:O | 1:A:1389:GLY:N | 2.53 | 0.41 |
| 1:B:1345:ILE:HB | 1:B:1368:TYR:HE2 | 1.85 | 0.41 |
| 1:B:1230:THR:O | 1:B:1231:LEU:HG | 2.19 | 0.41 |
| 2:F:102:ILE:C | 2:F:104:LYS:N | 2.73 | 0.41 |
| 1:B:1094:ARG:O | 1:B:1097:GLU:HB2 | 2.20 | 0.41 |
| 1:B:1517:GLY:C | 1:B:1519:ASN:N | 2.73 | 0.41 |
| 1:A:1255:GLU:O | 1:A:1289:TYR:CE2 | 2.72 | 0.41 |
| 1:C:1258:PHE:C | 1:C:1260:CYS:H | 2.24 | 0.41 |
| 1:C:1599:PHE:HA | 1:C:1602:VAL:CG2 | 2.50 | 0.41 |
| 2:E:189:UNK:N | 2:E:194:UNK:CB | 2.83 | 0.41 |
| 1:C:1145:ASN:O | 1:C:1150:TRP:CZ2 | 2.73 | 0.41 |
| 1:C:1170:GLU:O | 1:C:1173:LEU:N | 2.53 | 0.41 |
| 1:C:1422:LEU:C | 1:C:1422:LEU:HD13 | 2.40 | 0.41 |
| 1:C:1434:ARG:HH21 | 2:E:5:UNK:CB | 2.33 | 0.41 |
| 1:C:1476:ASP:CG | 1:C:1479:ALA:HB3 | 2.39 | 0.41 |
| 1:B:1323:LEU:O | 1:B:1327:PHE:CD2 | 2.73 | 0.41 |
| 1:B:1425:VAL:CG2 | 1:B:1426:LEU:H | 2.18 | 0.41 |
| 1:A:1167:SER:OG | 1:A:1168:TYR:N | 2.53 | 0.41 |
| 1:B:1170:GLU:CG | 1:B:1171:THR:N | 2.83 | 0.41 |
| 1:B:1493:ILE:O | 1:B:1494:SER:C | 2.59 | 0.41 |
| 1:B:1387:LYS:O | 1:B:1389:GLY:N | 2.54 | 0.41 |
| 1:B:1521:TRP:CZ3 | 1:B:1525:VAL:HG11 | 2.55 | 0.41 |
| 1:A:1292:ASP:HA | 2:F:97:GLN:HG2 | 2.00 | 0.41 |
| 1:B:1499:LEU:HB2 | 1:B:1511:ALA:CB | 2.43 | 0.41 |
| 1:A:1499:LEU:HB2 | 1:A:1511:ALA:CB | 2.42 | 0.41 |
| 1:A:1323:LEU:O | 1:A:1327:PHE:CD2 | 2.73 | 0.41 |
| 1:A:1580:ASP:OD1 | 1:C:1605:GLU:N | 2.54 | 0.41 |
| 1:C:1561:GLU:CG | 1:C:1562:LYS:H | 2.34 | 0.41 |
| 1:C:1417:LEU:HD22 | 1:C:1417:LEU:HA | 1.90 | 0.41 |
| 1:A:1406:ARG:O | 1:A:1409:GLN:CB | 2.64 | 0.41 |
| 1:A:1469:ASN:ND2 | 1:A:1498:ARG:NH1 | 2.68 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1471:PHE:HA | 1:A:1474:GLU:CG | 2.44 | 0.41 |
| 1:A:1476:ASP:CG | 1:A:1479:ALA:HB3 | 2.40 | 0.41 |
| 1:A:1181:ASN:C | 1:A:1182:ARG:HG2 | 2.40 | 0.41 |
| 1:B:1166:GLU:C | 1:B:1167:SER:O | 2.59 | 0.41 |
| 1:B:1481:ARG:O | 1:B:1484:ILE:HG13 | 2.20 | 0.41 |
| 1:B:1521:TRP:CZ3 | 1:B:1522:LYS:CD | 3.02 | 0.41 |
| 2:F:144:GLU:O | 2:F:148:LYS:N | 2.45 | 0.41 |
| 2:D:148:LYS:C | 2:D:151:ILE:HG23 | 2.41 | 0.41 |
| 1:C:1368:TYR:O | 1:C:1368:TYR:HD1 | 2.03 | 0.41 |
| 1:B:1517:GLY:C | 1:B:1519:ASN:H | 2.22 | 0.41 |
| 1:A:1258:PHE:C | 1:A:1260:CYS:H | 2.23 | 0.41 |
| 1:A:1329:PRO:HB2 | 1:A:1330:GLN:H | 1.63 | 0.41 |
| 1:A:1333:ARG:CG | 1:A:1360:GLU:HG3 | 2.50 | 0.41 |
| 1:C:1333:ARG:CG | 1:C:1360:GLU:HG3 | 2.49 | 0.41 |
| 1:A:1561:GLU:CG | 1:A:1562:LYS:H | 2.34 | 0.41 |
| 1:A:1598:TYR:CE2 | 2:F:199:UNK:N | 2.89 | 0.41 |
| 1:C:1533:LEU:O | 1:C:1535:LYS:N | 2.53 | 0.41 |
| 1:B:1318:THR:HG22 | 1:B:1347:LYS:NZ | 2.36 | 0.41 |
| 1:C:1412:LEU:HA | 1:C:1419:LEU:HD13 | 1.99 | 0.41 |
| 1:C:1435:ALA:HB1 | 1:C:1439:PHE:HE2 | 1.83 | 0.41 |
| 1:C:1472:ILE:CG2 | 1:C:1498:ARG:HE | 2.21 | 0.41 |
| 2:E:134:ASP:HA | 2:E:137:GLU:OE1 | 2.21 | 0.41 |
| 2:E:98:GLU:HA | 2:E:98:GLU:OE1 | 2.21 | 0.41 |
| 1:A:1387:LYS:HD2 | 1:A:1390:GLN:CD | 2.41 | 0.41 |
| 2:D:103:ARG:HD2 | 2:D:103:ARG:HA | 1.59 | 0.41 |
| 1:B:1344:ASN:OD1 | 1:B:1345:ILE:N | 2.53 | 0.41 |
| 2:D:186:UNK:C | 2:D:188:UNK:N | 2.83 | 0.41 |
| 1:A:1209:LYS:CB | 1:A:1231:LEU:HB3 | 2.48 | 0.41 |
| 1:C:1513:TYR:O | 1:C:1516:LYS:N | 2.53 | 0.41 |
| 2:D:107:GLU:O | 2:D:110:ARG:HG2 | 2.20 | 0.41 |
| 1:A:1183:LEU:HD12 | 1:A:1184:ALA:N | 2.35 | 0.41 |
| 1:C:1340:TRP:H | 1:C:1340:TRP:HD1 | 1.68 | 0.41 |
| 1:C:1340:TRP:CZ3 | 1:C:1367:LYS:HD2 | 2.55 | 0.41 |
| 1:A:1340:TRP:HD1 | 1:A:1340:TRP:H | 1.67 | 0.41 |
| 1:A:1253:TRP:HZ3 | 1:A:1276:ILE:CG2 | 2.04 | 0.41 |
| 1:A:1290:TYR:CD2 | 1:A:1299:LEU:CD1 | 2.92 | 0.41 |
| 1:B:1276:ILE:HG13 | 1:B:1277:VAL:N | 2.34 | 0.41 |
| 1:A:1554:LEU:HB2 | 1:A:1571:PHE:CE2 | 2.56 | 0.41 |
| 1:A:1596:MET:SD | 1:A:1599:PHE:CZ | 3.13 | 0.41 |
| 1:B:1602:VAL:HG13 | 2:D:205:UNK:C | 2.51 | 0.41 |
| 1:B:1605:GLU:CB | 1:C:1580:ASP:OD1 | 2.62 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1401:VAL:HG22 | 1:A:1429:ARG:HH21 | 1.84 | 0.41 |
| 1:B:1456:GLN:HE22 | 1:B:1467:LEU:CD2 | 2.33 | 0.41 |
| 1:C:1094:ARG:O | 1:C:1097:GLU:HB2 | 2.20 | 0.41 |
| 2:E:94:ARG:C | 2:E:96:THR:N | 2.73 | 0.41 |
| 1:B:1170:GLU:O | 1:B:1173:LEU:N | 2.53 | 0.41 |
| 1:C:1213:ALA:O | 1:C:1217:LEU:HB2 | 2.20 | 0.41 |
| 1:A:1105:PRO:CG | 1:A:1108:TRP:CZ2 | 3.04 | 0.41 |
| 2:E:148:LYS:C | 2:E:151:ILE:HG23 | 2.41 | 0.41 |
| 1:C:1345:ILE:HB | 1:C:1368:TYR:HE2 | 1.85 | 0.41 |
| 1:B:1342:ARG:O | 1:B:1343:VAL:HB | 2.21 | 0.41 |
| 1:C:1323:LEU:O | 1:C:1327:PHE:CD2 | 2.73 | 0.41 |
| 1:B:1587:TRP:CD1 | 1:B:1587:TRP:N | 2.87 | 0.41 |
| 1:C:1472:ILE:CG2 | 1:C:1498:ARG:HH21 | 2.34 | 0.41 |
| 2:E:133:LYS:HA | 2:E:133:LYS:HZ2 | 1.74 | 0.41 |
| 1:A:1420:ASN:HA | 1:A:1423:LEU:CD1 | 2.51 | 0.41 |
| 1:A:1472:ILE:CG2 | 1:A:1498:ARG:HH21 | 2.34 | 0.41 |
| 1:A:1474:GLU:O | 1:A:1475:GLU:HB2 | 2.21 | 0.41 |
| 1:B:1422:LEU:C | 1:B:1422:LEU:HD13 | 2.40 | 0.41 |
| 1:B:1137:TYR:HB2 | 1:B:1138:MET:CE | 2.51 | 0.41 |
| 1:A:1481:ARG:NH1 | 1:A:1510:ILE:CD1 | 2.84 | 0.41 |
| 1:B:1504:LEU:HA | 1:B:1504:LEU:HD23 | 1.79 | 0.41 |
| 1:B:1496:ALA:CB | 1:B:1515:PHE:CZ | 3.02 | 0.41 |
| 1:B:1083:GLN:NE2 | 1:B:1106:ALA:CB | 2.81 | 0.41 |
| 1:A:1303:LEU:HD12 | 1:A:1320:LEU:CD1 | 2.34 | 0.41 |
| 1:C:1303:LEU:H | 1:C:1303:LEU:HD23 | 1.84 | 0.41 |
| 1:A:1211:TYR:HB2 | 1:A:1231:LEU:HD11 | 2.02 | 0.41 |
| 1:A:1295:TYR:HE2 | 1:A:1299:LEU:HD13 | 1.85 | 0.41 |
| 1:B:1244:ALA:H | 1:B:1275:HIS:CE1 | 2.39 | 0.41 |
| 1:B:1561:GLU:CG | 1:B:1562:LYS:H | 2.34 | 0.41 |
| 2:F:182:UNK:C | 2:F:188:UNK:CB | 2.99 | 0.41 |
| 2:F:196:UNK:O | 2:F:199:UNK:CB | 2.69 | 0.41 |
| 1:C:1167:SER:O | 1:C:1172:GLU:N | 2.54 | 0.41 |
| 2:E:134:ASP:HA | 2:E:137:GLU:HB2 | 2.03 | 0.41 |
| 1:A:1419:LEU:HD23 | 1:A:1447:LEU:HD13 | 2.01 | 0.41 |
| 1:B:1401:VAL:HG22 | 1:B:1429:ARG:HH21 | 1.85 | 0.41 |
| 1:B:1469:ASN:C | 1:B:1469:ASN:HD22 | 2.21 | 0.41 |
| 1:B:1471:PHE:HD1 | 1:B:1476:ASP:HB3 | 1.86 | 0.41 |
| 1:A:1504:LEU:HA | 1:A:1504:LEU:HD23 | 1.79 | 0.41 |
| 1:B:1481:ARG:NH1 | 1:B:1510:ILE:CD1 | 2.83 | 0.41 |
| 1:B:1508:ARG:CZ | 1:B:1530:LYS:HD3 | 2.50 | 0.41 |
| 1:A:1493:ILE:O | 1:A:1494:SER:C | 2.59 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:1130:LYS:NZ | 1:B:1155:LYS:HD3 | 2.35 | 0.41 |
| 1:C:1521:TRP:CH2 | 1:C:1525:VAL:HG11 | 2.56 | 0.41 |
| 1:C:1224:PHE:HA | 1:C:1227:LEU:HB3 | 2.03 | 0.41 |
| 1:B:1211:TYR:HB2 | 1:B:1231:LEU:HD11 | 2.01 | 0.41 |
| 1:A:1094:ARG:O | 1:A:1097:GLU:HB2 | 2.20 | 0.41 |
| 1:C:1151:GLU:HB3 | 1:C:1152:GLU:OE2 | 2.21 | 0.41 |
| 1:A:1261:VAL:HG11 | 1:A:1295:TYR:CE1 | 2.53 | 0.41 |
| 1:B:1258:PHE:CE1 | 1:B:1293:ARG:HD2 | 2.56 | 0.41 |
| 1:A:1584:GLU:C | 1:A:1586:ALA:H | 2.25 | 0.41 |
| 1:A:1599:PHE:HA | 1:A:1602:VAL:CG2 | 2.51 | 0.41 |
| 1:B:1533:LEU:O | 1:B:1535:LYS:N | 2.54 | 0.41 |
| 1:C:1108:TRP:CE3 | 1:C:1108:TRP:CA | 2.98 | 0.41 |
| 1:C:1136:SER:CB | 1:C:1140:VAL:CG2 | 2.97 | 0.41 |
| 1:A:1280:ALA:N | 1:A:1280:ALA:C | 2.59 | 0.41 |
| 1:B:1361:LEU:HD22 | 1:B:1365:TYR:HE2 | 1.72 | 0.41 |
| 1:C:1466:SER:O | 1:C:1470:LEU:N | 2.52 | 0.41 |
| 1:C:1456:GLN:HE22 | 1:C:1467:LEU:CD2 | 2.34 | 0.41 |
| 1:C:1379:MET:SD | 1:C:1403:LEU:HD21 | 2.61 | 0.41 |
| 1:A:1422:LEU:HD13 | 1:A:1422:LEU:C | 2.41 | 0.41 |
| 1:A:1474:GLU:O | 1:A:1475:GLU:CB | 2.69 | 0.41 |
| 1:B:1427:SER:HB2 | 1:B:1428:PRO:HD2 | 1.88 | 0.41 |
| 2:D:126:GLU:OE2 | 2:D:129:GLU:CD | 2.59 | 0.41 |
| 1:A:1154:VAL:HG13 | 1:A:1180:THR:HG21 | 2.02 | 0.41 |
| 1:A:1161:ARG:O | 1:A:1164:ALA:O | 2.38 | 0.41 |
| 2:E:105:TRP:HA | 2:E:108:GLU:OE2 | 2.20 | 0.41 |
| 1:A:1481:ARG:O | 1:A:1484:ILE:HG13 | 2.21 | 0.41 |
| 1:B:1509:ARG:NH2 | 2:D:163:GLN:CA | 2.50 | 0.41 |
| 1:B:1115:GLN:OE1 | 1:B:1121:VAL:HG21 | 2.21 | 0.41 |
| 1:B:1126:ASP:OD1 | 1:B:1156:TYR:OH | 2.38 | 0.41 |
| 1:C:1387:LYS:O | 1:C:1389:GLY:N | 2.53 | 0.41 |
| 1:B:1387:LYS:HD2 | 1:B:1390:GLN:CD | 2.41 | 0.41 |
| 1:B:1388:GLU:CG | 1:B:1389:GLY:N | 2.82 | 0.41 |
| 1:A:1521:TRP:CZ3 | 1:A:1522:LYS:CD | 3.02 | 0.41 |
| 1:A:1621:LYS:HB3 | 1:A:1625:GLN:NE2 | 2.36 | 0.41 |
| 1:C:1617:GLU:HA | 1:C:1620:ARG:CZ | 2.51 | 0.41 |
| 1:C:1621:LYS:HB3 | 1:C:1625:GLN:NE2 | 2.36 | 0.41 |
| 2:D:151:ILE:CG1 | 2:D:152:ASN:N | 2.84 | 0.41 |
| 1:A:1236:GLU:HB3 | 1:A:1237:TYR:H | 1.77 | 0.41 |
| 2:E:91:GLN:OE1 | 2:E:92:ALA:HA | 2.21 | 0.41 |
| 2:E:178:UNK:O | 2:E:180:UNK:N | 2.54 | 0.41 |
| 2:F:134:ASP:HA | 2:F:137:GLU:OE1 | 2.21 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:1092:LEU:C | 1:B:1094:ARG:N | 2.71 | 0.41 |
| 1:A:1277:VAL:C | 1:A:1279:HIS:HD1 | 2.20 | 0.41 |
| 1:A:1329:PRO:O | 1:A:1332:MET:N | 2.45 | 0.41 |
| 1:C:1253:TRP:O | 1:C:1289:TYR:CZ | 2.74 | 0.41 |
| 1:A:1563:ARG:O | 1:A:1564:GLU:C | 2.59 | 0.41 |
| 1:B:1567:GLY:O | 1:B:1569:CYS:N | 2.54 | 0.41 |
| 1:C:1554:LEU:HB2 | 1:C:1571:PHE:CE2 | 2.56 | 0.41 |
| 1:C:1198:ILE:C | 1:C:1201:VAL:CG2 | 2.90 | 0.41 |
| 1:C:1381:HIS:N | 1:C:1382:PRO:CD | 2.82 | 0.41 |
| 1:C:1471:PHE:HD1 | 1:C:1476:ASP:HB3 | 1.85 | 0.41 |
| 1:A:1161:ARG:HA | 1:A:1161:ARG:HD3 | 1.84 | 0.41 |
| 1:B:1481:ARG:NH1 | 1:B:1510:ILE:HG13 | 2.35 | 0.41 |
| 1:A:1082:VAL:HG11 | 1:A:1105:PRO:CB | 2.44 | 0.41 |
| 2:D:103:ARG:HA | 2:D:106:ARG:HB2 | 2.03 | 0.41 |
| 1:A:1342:ARG:O | 1:A:1343:VAL:HB | 2.21 | 0.41 |
| 1:A:1345:ILE:HB | 1:A:1368:TYR:HE2 | 1.85 | 0.41 |
| 1:A:1213:ALA:O | 1:A:1217:LEU:HB2 | 2.20 | 0.41 |
| 2:F:134:ASP:HA | 2:F:137:GLU:HB2 | 2.03 | 0.41 |
| 1:C:1151:GLU:O | 1:C:1151:GLU:CG | 2.69 | 0.41 |
| 2:D:12:UNK:C | 2:D:14:UNK:N | 2.84 | 0.41 |
| 1:A:1251:ARG:C | 1:A:1253:TRP:H | 2.25 | 0.40 |
| 1:A:1257:CYS:SG | 1:A:1290:TYR:HE1 | 2.41 | 0.40 |
| 1:A:1601:GLN:HA | 1:A:1604:LYS:CD | 2.51 | 0.40 |
| 1:B:1533:LEU:CD2 | 1:B:1535:LYS:HB2 | 2.51 | 0.40 |
| 1:C:1599:PHE:HA | 1:C:1602:VAL:HG23 | 2.03 | 0.40 |
| 1:A:1381:HIS:N | 1:A:1382:PRO:CD | 2.83 | 0.40 |
| 2:D:126:GLU:HG3 | 2:D:130:LYS:CE | 2.52 | 0.40 |
| 1:A:1163:LYS:O | 1:A:1164:ALA:CB | 2.68 | 0.40 |
| 1:A:1378:MET:SD | 1:A:1391:PHE:HD2 | 2.45 | 0.40 |
| 1:B:1170:GLU:C | 1:B:1172:GLU:H | 2.25 | 0.40 |
| 1:A:1137:TYR:HB2 | 1:A:1138:MET:CE | 2.51 | 0.40 |
| 1:B:1224:PHE:HA | 1:B:1227:LEU:HB3 | 2.03 | 0.40 |
| 1:B:1146:THR:OG1 | 1:B:1147:SER:N | 2.54 | 0.40 |
| 1:C:1619:LEU:O | 1:C:1620:ARG:C | 2.59 | 0.40 |
| 1:A:1619:LEU:O | 1:A:1620:ARG:C | 2.59 | 0.40 |
| 2:F:151:ILE:CG1 | 2:F:152:ASN:N | 2.84 | 0.40 |
| 1:A:1151:GLU:HB3 | 1:A:1152:GLU:OE2 | 2.21 | 0.40 |
| 1:A:1244:ALA:N | 1:A:1275:HIS:CE1 | 2.89 | 0.40 |
| 1:C:1234:LEU:HD23 | 1:C:1264:LYS:HZ3 | 1.51 | 0.40 |
| 1:C:1280:ALA:C | 1:C:1282:GLU:N | 2.74 | 0.40 |
| 1:A:1551:GLU:CG | 1:A:1582:VAL:CG2 | 2.93 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1551:GLU:OE1 | 1:A:1582:VAL:HG22 | 2.21 | 0.40 |
| 1:A:1587:TRP:CD1 | 1:A:1587:TRP:N | 2.87 | 0.40 |
| 1:C:1567:GLY:O | 1:C:1569:CYS:N | 2.55 | 0.40 |
| 1:C:1134:PRO:O | 1:C:1135:SER:O | 2.39 | 0.40 |
| 1:C:1167:SER:CB | 1:C:1171:THR:HG1 | 2.34 | 0.40 |
| 1:C:1376:ILE:CD1 | 1:C:1403:LEU:HD23 | 2.50 | 0.40 |
| 1:C:1474:GLU:O | 1:C:1475:GLU:HB2 | 2.21 | 0.40 |
| 1:B:1379:MET:SD | 1:B:1403:LEU:HD21 | 2.61 | 0.40 |
| 1:B:1474:GLU:O | 1:B:1475:GLU:CB | 2.69 | 0.40 |
| 1:B:1472:ILE:CG2 | 1:B:1498:ARG:HH21 | 2.34 | 0.40 |
| 1:A:1157:LEU:CD1 | 1:A:1177:LEU:CD2 | 2.95 | 0.40 |
| 1:B:1107:VAL:HG12 | 1:B:1111:LEU:CB | 2.43 | 0.40 |
| 1:C:1388:GLU:CG | 1:C:1389:GLY:N | 2.82 | 0.40 |
| 2:D:95:LEU:O | 2:D:99:PRO:HD2 | 2.21 | 0.40 |
| 1:A:1368:TYR:O | 1:A:1368:TYR:HD1 | 2.03 | 0.40 |
| 1:A:1206:TYR:CE1 | 1:A:1230:THR:OG1 | 2.70 | 0.40 |
| 1:A:1209:LYS:HG3 | 1:A:1209:LYS:H | 1.65 | 0.40 |
| 1:C:1240:ALA:C | 1:C:1242:ASP:N | 2.74 | 0.40 |
| 1:C:1251:ARG:C | 1:C:1253:TRP:H | 2.25 | 0.40 |
| 1:B:1554:LEU:HB2 | 1:B:1571:PHE:CE2 | 2.56 | 0.40 |
| 1:C:1533:LEU:CD2 | 1:C:1535:LYS:HB2 | 2.51 | 0.40 |
| 1:C:1469:ASN:HD22 | 1:C:1469:ASN:C | 2.21 | 0.40 |
| 2:E:126:GLU:OE2 | 2:E:129:GLU:CD | 2.59 | 0.40 |
| 1:C:1475:GLU:OE1 | 2:E:145:GLN:CB | 2.70 | 0.40 |
| 1:A:1401:VAL:HG12 | 1:A:1401:VAL:O | 2.22 | 0.40 |
| 1:A:1414:PHE:CE1 | 2:F:127:TRP:CE3 | 3.09 | 0.40 |
| 1:B:1456:GLN:NE2 | 1:B:1467:LEU:CD2 | 2.85 | 0.40 |
| 1:A:1170:GLU:CG | 1:A:1171:THR:N | 2.83 | 0.40 |
| 1:C:1493:ILE:O | 1:C:1494:SER:C | 2.59 | 0.40 |
| 1:B:1102:CYS:O | 1:B:1103:ASN:CB | 2.69 | 0.40 |
| 1:C:1521:TRP:CZ3 | 1:C:1522:LYS:CD | 3.03 | 0.40 |
| 2:D:186:UNK:C | 2:D:188:UNK:H | 2.34 | 0.40 |
| 1:A:1151:GLU:CG | 1:A:1151:GLU:O | 2.69 | 0.40 |
| 1:B:1517:GLY:O | 1:B:1519:ASN:N | 2.55 | 0.40 |
| 1:C:1333:ARG:CA | 1:C:1360:GLU:CG | 2.98 | 0.40 |
| 1:B:1599:PHE:HA | 1:B:1602:VAL:CG2 | 2.51 | 0.40 |
| 1:C:1584:GLU:C | 1:C:1586:ALA:H | 2.25 | 0.40 |
| 1:C:1108:TRP:NE1 | 1:C:1131:ALA:CB | 2.84 | 0.40 |
| 1:C:1449:LYS:O | 1:C:1453:ARG:NH1 | 2.55 | 0.40 |
| 1:A:1402:GLU:CD | 1:A:1402:GLU:C | 2.80 | 0.40 |
| 1:B:1402:GLU:CD | 1:B:1402:GLU:C | 2.80 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:1474:GLU:O | 1:B:1475:GLU:HB2 | 2.21 | 0.40 |
| 1:B:1170:GLU:OE1 | 1:B:1194:ASN:HB3 | 2.22 | 0.40 |
| 1:A:1130:LYS:HZ3 | 1:A:1155:LYS:CG | 2.34 | 0.40 |
| 1:B:1521:TRP:CH2 | 1:B:1525:VAL:HG11 | 2.56 | 0.40 |
| 2:F:148:LYS:C | 2:F:151:ILE:HG23 | 2.41 | 0.40 |
| 2:E:151:ILE:CG1 | 2:E:152:ASN:N | 2.84 | 0.40 |
| 1:B:1240:ALA:C | 1:B:1242:ASP:N | 2.74 | 0.40 |
| 1:A:1132:ASP:O | 1:A:1133:ASP:O | 2.39 | 0.40 |
| 1:C:1233:HIS:ND1 | 1:C:1236:GLU:CD | 2.75 | 0.40 |
| 1:A:1596:MET:SD | 1:A:1597:PRO:CD | 3.00 | 0.40 |
| 1:B:1561:GLU:CD | 1:B:1562:LYS:H | 2.25 | 0.40 |
| 1:B:1596:MET:SD | 1:B:1599:PHE:HZ | 2.43 | 0.40 |
| 1:C:1578:ARG:HH12 | 1:C:1594:PHE:HZ | 1.69 | 0.40 |
| 1:A:1224:PHE:HA | 1:A:1227:LEU:HB3 | 2.03 | 0.40 |
| 1:C:1420:ASN:C | 1:C:1422:LEU:N | 2.73 | 0.40 |
| 1:B:1333:ARG:CB | 1:B:1360:GLU:HG2 | 2.48 | 0.40 |
| 1:B:1401:VAL:O | 1:B:1401:VAL:HG12 | 2.22 | 0.40 |
| 1:B:1166:GLU:O | 1:B:1169:VAL:HB | 2.21 | 0.40 |
| 1:B:1502:HIS:O | 1:B:1508:ARG:HD2 | 2.22 | 0.40 |
| 1:A:1232:VAL:O | 1:A:1233:HIS:HB3 | 2.22 | 0.40 |
| 1:A:1517:GLY:O | 1:A:1519:ASN:N | 2.54 | 0.40 |

All (5) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|--------------------------|--------------------------|-------------------|
| 1:B:1340:TRP:CZ2 | 1:C:1222:SER:OG[12_655] | 1.80 | 0.40 |
| 1:C:1304:GLU:OE2 | 1:C:1334:GLU:OE2[15_645] | 1.98 | 0.22 |
| 1:A:1199:GLN:NE2 | 1:A:1431:ASP:OD2[10_555] | 2.13 | 0.07 |
| 1:B:1340:TRP:CZ2 | 1:C:1222:SER:CB[12_655] | 2.15 | 0.05 |
| 1:B:1341:SER:OG | 1:C:1203:ASP:OD2[12_655] | 2.18 | 0.02 |

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 X-ray entries followed by that with respect to entries of similar resolution.

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 | 551/624 (88%) | 322 (58%) | 152 (28%) | 77 (14%) | 0 | 6 |
| 1 | B | 551/624 (88%) | 319 (58%) | 161 (29%) | 71 (13%) | 0 | 7 |
| 1 | C | 551/624 (88%) | 309 (56%) | 164 (30%) | 78 (14%) | 0 | 6 |
| 2 | D | 77/190 (40%) | 50 (65%) | 16 (21%) | 11 (14%) | 0 | 6 |
| 2 | E | 66/190 (35%) | 35 (53%) | 21 (32%) | 10 (15%) | 0 | 5 |
| 2 | F | 76/190 (40%) | 42 (55%) | 20 (26%) | 14 (18%) | 0 | 4 |
| All | All | 1872/2442 (77%) | 1077 (58%) | 534 (28%) | 261 (14%) | 0 | 6 |

All (261) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | A | 1087 | GLU |
| 1 | A | 1091 | ASN |
| 1 | A | 1105 | PRO |
| 1 | A | 1122 | LYS |
| 1 | A | 1130 | LYS |
| 1 | A | 1165 | ARG |
| 1 | A | 1168 | TYR |
| 1 | A | 1181 | ASN |
| 1 | A | 1193 | PRO |
| 1 | A | 1194 | ASN |
| 1 | A | 1198 | ILE |
| 1 | A | 1231 | LEU |
| 1 | A | 1251 | ARG |
| 1 | A | 1278 | VAL |
| 1 | A | 1283 | LEU |
| 1 | A | 1297 | GLU |
| 1 | A | 1327 | PHE |
| 1 | A | 1329 | PRO |
| 1 | A | 1330 | GLN |
| 1 | A | 1427 | SER |
| 1 | A | 1493 | ILE |
| 1 | A | 1547 | THR |
| 1 | A | 1590 | ASN |
| 1 | A | 1594 | PHE |
| 1 | A | 1596 | MET |
| 1 | A | 1597 | PRO |
| 1 | B | 1105 | PRO |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | B | 1121 | VAL |
| 1 | B | 1130 | LYS |
| 1 | B | 1164 | ALA |
| 1 | B | 1167 | SER |
| 1 | B | 1168 | TYR |
| 1 | B | 1181 | ASN |
| 1 | B | 1184 | ALA |
| 1 | B | 1193 | PRO |
| 1 | B | 1194 | ASN |
| 1 | B | 1231 | LEU |
| 1 | B | 1246 | LYS |
| 1 | B | 1247 | ALA |
| 1 | B | 1251 | ARG |
| 1 | B | 1278 | VAL |
| 1 | B | 1280 | ALA |
| 1 | B | 1283 | LEU |
| 1 | B | 1297 | GLU |
| 1 | B | 1327 | PHE |
| 1 | B | 1329 | PRO |
| 1 | B | 1330 | GLN |
| 1 | B | 1427 | SER |
| 1 | B | 1493 | ILE |
| 1 | B | 1547 | THR |
| 1 | B | 1588 | ARG |
| 1 | B | 1594 | PHE |
| 1 | B | 1596 | MET |
| 1 | B | 1597 | PRO |
| 1 | B | 1625 | GLN |
| 1 | C | 1088 | HIS |
| 1 | C | 1093 | ASP |
| 1 | C | 1105 | PRO |
| 1 | C | 1106 | ALA |
| 1 | C | 1107 | VAL |
| 1 | C | 1122 | LYS |
| 1 | C | 1133 | ASP |
| 1 | C | 1137 | TYR |
| 1 | C | 1147 | SER |
| 1 | C | 1149 | ASN |
| 1 | C | 1167 | SER |
| 1 | C | 1194 | ASN |
| 1 | C | 1198 | ILE |
| 1 | C | 1199 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | C | 1200 | GLN |
| 1 | C | 1223 | ASN |
| 1 | C | 1231 | LEU |
| 1 | C | 1232 | VAL |
| 1 | C | 1234 | LEU |
| 1 | C | 1235 | GLY |
| 1 | C | 1251 | ARG |
| 1 | C | 1278 | VAL |
| 1 | C | 1280 | ALA |
| 1 | C | 1283 | LEU |
| 1 | C | 1297 | GLU |
| 1 | C | 1327 | PHE |
| 1 | C | 1329 | PRO |
| 1 | C | 1330 | GLN |
| 1 | C | 1427 | SER |
| 1 | C | 1493 | ILE |
| 1 | C | 1547 | THR |
| 1 | C | 1589 | HIS |
| 1 | C | 1591 | ILE |
| 1 | C | 1594 | PHE |
| 1 | C | 1596 | MET |
| 1 | C | 1597 | PRO |
| 2 | D | 113 | LEU |
| 2 | D | 156 | ALA |
| 2 | D | 157 | ASP |
| 2 | E | 95 | LEU |
| 2 | F | 156 | ALA |
| 2 | F | 157 | ASP |
| 2 | F | 163 | GLN |
| 2 | F | 167 | ASP |
| 1 | A | 1093 | ASP |
| 1 | A | 1145 | ASN |
| 1 | A | 1151 | GLU |
| 1 | A | 1160 | ALA |
| 1 | A | 1164 | ALA |
| 1 | A | 1195 | ASN |
| 1 | A | 1294 | GLY |
| 1 | A | 1296 | PHE |
| 1 | A | 1358 | TRP |
| 1 | A | 1382 | PRO |
| 1 | A | 1416 | PRO |
| 1 | A | 1517 | GLY |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | A | 1588 | ARG |
| 1 | B | 1086 | ILE |
| 1 | B | 1093 | ASP |
| 1 | B | 1103 | ASN |
| 1 | B | 1136 | SER |
| 1 | B | 1145 | ASN |
| 1 | B | 1358 | TRP |
| 1 | B | 1382 | PRO |
| 1 | B | 1416 | PRO |
| 1 | B | 1517 | GLY |
| 1 | B | 1585 | THR |
| 1 | C | 1089 | ILE |
| 1 | C | 1092 | LEU |
| 1 | C | 1103 | ASN |
| 1 | C | 1121 | VAL |
| 1 | C | 1145 | ASN |
| 1 | C | 1151 | GLU |
| 1 | C | 1358 | TRP |
| 1 | C | 1382 | PRO |
| 1 | C | 1416 | PRO |
| 1 | C | 1517 | GLY |
| 1 | C | 1585 | THR |
| 1 | C | 1590 | ASN |
| 2 | D | 94 | ARG |
| 2 | D | 115 | GLU |
| 2 | D | 160 | PHE |
| 2 | E | 113 | LEU |
| 2 | E | 115 | GLU |
| 2 | F | 113 | LEU |
| 2 | F | 115 | GLU |
| 1 | A | 1088 | HIS |
| 1 | A | 1138 | MET |
| 1 | A | 1148 | GLY |
| 1 | A | 1182 | ARG |
| 1 | A | 1216 | LEU |
| 1 | A | 1236 | GLU |
| 1 | A | 1254 | LYS |
| 1 | A | 1281 | ASP |
| 1 | A | 1345 | ILE |
| 1 | A | 1383 | THR |
| 1 | A | 1388 | GLU |
| 1 | A | 1432 | HIS |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | A | 1505 | ILE |
| 1 | A | 1568 | ALA |
| 1 | A | 1585 | THR |
| 1 | A | 1591 | ILE |
| 1 | B | 1091 | ASN |
| 1 | B | 1138 | MET |
| 1 | B | 1151 | GLU |
| 1 | B | 1195 | ASN |
| 1 | B | 1216 | LEU |
| 1 | B | 1221 | VAL |
| 1 | B | 1236 | GLU |
| 1 | B | 1254 | LYS |
| 1 | B | 1345 | ILE |
| 1 | B | 1383 | THR |
| 1 | B | 1388 | GLU |
| 1 | B | 1432 | HIS |
| 1 | B | 1505 | ILE |
| 1 | B | 1528 | CYS |
| 1 | B | 1568 | ALA |
| 1 | C | 1134 | PRO |
| 1 | C | 1135 | SER |
| 1 | C | 1216 | LEU |
| 1 | C | 1221 | VAL |
| 1 | C | 1254 | LYS |
| 1 | C | 1345 | ILE |
| 1 | C | 1383 | THR |
| 1 | C | 1388 | GLU |
| 1 | C | 1432 | HIS |
| 1 | C | 1505 | ILE |
| 1 | C | 1568 | ALA |
| 2 | D | 95 | LEU |
| 2 | D | 98 | GLU |
| 2 | E | 107 | GLU |
| 2 | F | 101 | SER |
| 2 | F | 162 | GLN |
| 1 | A | 1221 | VAL |
| 1 | A | 1264 | LYS |
| 1 | A | 1429 | ARG |
| 1 | A | 1548 | GLU |
| 1 | A | 1589 | HIS |
| 1 | B | 1084 | VAL |
| 1 | B | 1264 | LYS |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | B | 1429 | ARG |
| 1 | B | 1548 | GLU |
| 1 | B | 1590 | ASN |
| 1 | C | 1165 | ARG |
| 1 | C | 1247 | ALA |
| 1 | C | 1264 | LYS |
| 1 | C | 1295 | TYR |
| 1 | C | 1429 | ARG |
| 2 | E | 94 | ARG |
| 2 | F | 103 | ARG |
| 1 | A | 1132 | ASP |
| 1 | A | 1247 | ALA |
| 1 | A | 1316 | MET |
| 1 | A | 1408 | ILE |
| 1 | A | 1424 | MET |
| 1 | A | 1575 | ASP |
| 1 | B | 1080 | SER |
| 1 | B | 1259 | ALA |
| 1 | B | 1316 | MET |
| 1 | B | 1408 | ILE |
| 1 | B | 1424 | MET |
| 1 | C | 1080 | SER |
| 1 | C | 1166 | GLU |
| 1 | C | 1259 | ALA |
| 1 | C | 1316 | MET |
| 1 | C | 1408 | ILE |
| 1 | C | 1424 | MET |
| 1 | C | 1625 | GLN |
| 2 | D | 116 | LEU |
| 2 | E | 92 | ALA |
| 2 | E | 98 | GLU |
| 2 | E | 112 | ARG |
| 2 | E | 116 | LEU |
| 2 | F | 112 | ARG |
| 2 | F | 116 | LEU |
| 2 | F | 149 | ASN |
| 1 | A | 1080 | SER |
| 1 | A | 1121 | VAL |
| 1 | A | 1131 | ALA |
| 1 | A | 1259 | ALA |
| 1 | A | 1544 | SER |
| 1 | B | 1088 | HIS |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | B | 1147 | SER |
| 1 | C | 1192 | GLY |
| 1 | C | 1544 | SER |
| 2 | D | 149 | ASN |
| 2 | E | 149 | ASN |
| 2 | F | 164 | PRO |
| 1 | A | 1134 | PRO |
| 1 | A | 1141 | VAL |
| 1 | A | 1525 | VAL |
| 1 | B | 1141 | VAL |
| 1 | B | 1525 | VAL |
| 1 | C | 1525 | VAL |
| 1 | A | 1133 | ASP |
| 2 | F | 99 | PRO |
| 1 | A | 1343 | VAL |
| 1 | A | 1579 | PRO |
| 1 | B | 1343 | VAL |
| 1 | B | 1579 | PRO |
| 1 | C | 1343 | VAL |
| 1 | C | 1579 | PRO |
| 1 | B | 1148 | GLY |
| 2 | D | 99 | PRO |
| 1 | C | 1193 | PRO |
| 1 | C | 1256 | VAL |

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 X-ray entries followed by that with respect to entries of similar resolution.

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 | 485/541 (90%) | 409 (84%) | 76 (16%) | 3 | 21 |
| 1 | B | 485/541 (90%) | 404 (83%) | 81 (17%) | 3 | 19 |
| 1 | C | 485/541 (90%) | 395 (81%) | 90 (19%) | 2 | 14 |
| 2 | D | 62/73 (85%) | 45 (73%) | 17 (27%) | 0 | 4 |
| 2 | E | 61/73 (84%) | 42 (69%) | 19 (31%) | 0 | 2 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles |
|-----|-------|-----------------|------------|-----------|-------------|
| 2 | F | 62/73 (85%) | 42 (68%) | 20 (32%) | 0 2 |
| All | All | 1640/1842 (89%) | 1337 (82%) | 303 (18%) | 2 14 |

All (303) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | A | 1085 | LEU |
| 1 | A | 1086 | ILE |
| 1 | A | 1087 | GLU |
| 1 | A | 1096 | TYR |
| 1 | A | 1098 | PHE |
| 1 | A | 1102 | CYS |
| 1 | A | 1108 | TRP |
| 1 | A | 1111 | LEU |
| 1 | A | 1126 | ASP |
| 1 | A | 1133 | ASP |
| 1 | A | 1136 | SER |
| 1 | A | 1137 | TYR |
| 1 | A | 1154 | VAL |
| 1 | A | 1156 | TYR |
| 1 | A | 1168 | TYR |
| 1 | A | 1172 | GLU |
| 1 | A | 1175 | PHE |
| 1 | A | 1181 | ASN |
| 1 | A | 1209 | LYS |
| 1 | A | 1212 | ASP |
| 1 | A | 1217 | LEU |
| 1 | A | 1221 | VAL |
| 1 | A | 1226 | ARG |
| 1 | A | 1227 | LEU |
| 1 | A | 1245 | ARG |
| 1 | A | 1258 | PHE |
| 1 | A | 1261 | VAL |
| 1 | A | 1262 | ASP |
| 1 | A | 1274 | LEU |
| 1 | A | 1290 | TYR |
| 1 | A | 1295 | TYR |
| 1 | A | 1303 | LEU |
| 1 | A | 1311 | ARG |
| 1 | A | 1317 | PHE |
| 1 | A | 1326 | LYS |
| 1 | A | 1340 | TRP |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | A | 1344 | ASN |
| 1 | A | 1345 | ILE |
| 1 | A | 1350 | ARG |
| 1 | A | 1354 | GLN |
| 1 | A | 1377 | THR |
| 1 | A | 1383 | THR |
| 1 | A | 1384 | ASP |
| 1 | A | 1390 | GLN |
| 1 | A | 1417 | LEU |
| 1 | A | 1419 | LEU |
| 1 | A | 1422 | LEU |
| 1 | A | 1424 | MET |
| 1 | A | 1447 | LEU |
| 1 | A | 1458 | HIS |
| 1 | A | 1460 | ASN |
| 1 | A | 1469 | ASN |
| 1 | A | 1489 | ASN |
| 1 | A | 1490 | PHE |
| 1 | A | 1504 | LEU |
| 1 | A | 1510 | ILE |
| 1 | A | 1526 | GLU |
| 1 | A | 1527 | LEU |
| 1 | A | 1529 | LYS |
| 1 | A | 1536 | ASP |
| 1 | A | 1540 | TYR |
| 1 | A | 1549 | LEU |
| 1 | A | 1574 | TYR |
| 1 | A | 1577 | LEU |
| 1 | A | 1578 | ARG |
| 1 | A | 1588 | ARG |
| 1 | A | 1591 | ILE |
| 1 | A | 1592 | MET |
| 1 | A | 1593 | ASP |
| 1 | A | 1594 | PHE |
| 1 | A | 1596 | MET |
| 1 | A | 1597 | PRO |
| 1 | A | 1598 | TYR |
| 1 | A | 1601 | GLN |
| 1 | A | 1611 | ASP |
| 1 | A | 1620 | ARG |
| 1 | B | 1085 | LEU |
| 1 | B | 1091 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | B | 1096 | TYR |
| 1 | B | 1098 | PHE |
| 1 | B | 1104 | GLU |
| 1 | B | 1108 | TRP |
| 1 | B | 1111 | LEU |
| 1 | B | 1120 | MET |
| 1 | B | 1121 | VAL |
| 1 | B | 1126 | ASP |
| 1 | B | 1136 | SER |
| 1 | B | 1137 | TYR |
| 1 | B | 1154 | VAL |
| 1 | B | 1156 | TYR |
| 1 | B | 1168 | TYR |
| 1 | B | 1172 | GLU |
| 1 | B | 1175 | PHE |
| 1 | B | 1183 | LEU |
| 1 | B | 1197 | HIS |
| 1 | B | 1209 | LYS |
| 1 | B | 1212 | ASP |
| 1 | B | 1217 | LEU |
| 1 | B | 1221 | VAL |
| 1 | B | 1222 | SER |
| 1 | B | 1226 | ARG |
| 1 | B | 1227 | LEU |
| 1 | B | 1245 | ARG |
| 1 | B | 1258 | PHE |
| 1 | B | 1261 | VAL |
| 1 | B | 1262 | ASP |
| 1 | B | 1274 | LEU |
| 1 | B | 1281 | ASP |
| 1 | B | 1290 | TYR |
| 1 | B | 1295 | TYR |
| 1 | B | 1303 | LEU |
| 1 | B | 1311 | ARG |
| 1 | B | 1317 | PHE |
| 1 | B | 1326 | LYS |
| 1 | B | 1339 | PHE |
| 1 | B | 1340 | TRP |
| 1 | B | 1344 | ASN |
| 1 | B | 1345 | ILE |
| 1 | B | 1350 | ARG |
| 1 | B | 1354 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | B | 1377 | THR |
| 1 | B | 1383 | THR |
| 1 | B | 1384 | ASP |
| 1 | B | 1390 | GLN |
| 1 | B | 1417 | LEU |
| 1 | B | 1419 | LEU |
| 1 | B | 1422 | LEU |
| 1 | B | 1424 | MET |
| 1 | B | 1447 | LEU |
| 1 | B | 1458 | HIS |
| 1 | B | 1460 | ASN |
| 1 | B | 1469 | ASN |
| 1 | B | 1489 | ASN |
| 1 | B | 1490 | PHE |
| 1 | B | 1504 | LEU |
| 1 | B | 1510 | ILE |
| 1 | B | 1526 | GLU |
| 1 | B | 1527 | LEU |
| 1 | B | 1529 | LYS |
| 1 | B | 1536 | ASP |
| 1 | B | 1540 | TYR |
| 1 | B | 1549 | LEU |
| 1 | B | 1574 | TYR |
| 1 | B | 1577 | LEU |
| 1 | B | 1578 | ARG |
| 1 | B | 1588 | ARG |
| 1 | B | 1591 | ILE |
| 1 | B | 1592 | MET |
| 1 | B | 1593 | ASP |
| 1 | B | 1594 | PHE |
| 1 | B | 1596 | MET |
| 1 | B | 1597 | PRO |
| 1 | B | 1598 | TYR |
| 1 | B | 1601 | GLN |
| 1 | B | 1611 | ASP |
| 1 | B | 1620 | ARG |
| 1 | B | 1629 | THR |
| 1 | C | 1085 | LEU |
| 1 | C | 1086 | ILE |
| 1 | C | 1087 | GLU |
| 1 | C | 1089 | ILE |
| 1 | C | 1091 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | C | 1092 | LEU |
| 1 | C | 1096 | TYR |
| 1 | C | 1098 | PHE |
| 1 | C | 1101 | ARG |
| 1 | C | 1102 | CYS |
| 1 | C | 1103 | ASN |
| 1 | C | 1104 | GLU |
| 1 | C | 1108 | TRP |
| 1 | C | 1111 | LEU |
| 1 | C | 1121 | VAL |
| 1 | C | 1126 | ASP |
| 1 | C | 1133 | ASP |
| 1 | C | 1137 | TYR |
| 1 | C | 1149 | ASN |
| 1 | C | 1154 | VAL |
| 1 | C | 1156 | TYR |
| 1 | C | 1159 | MET |
| 1 | C | 1168 | TYR |
| 1 | C | 1172 | GLU |
| 1 | C | 1174 | ILE |
| 1 | C | 1175 | PHE |
| 1 | C | 1191 | ASN |
| 1 | C | 1194 | ASN |
| 1 | C | 1198 | ILE |
| 1 | C | 1208 | GLU |
| 1 | C | 1212 | ASP |
| 1 | C | 1217 | LEU |
| 1 | C | 1221 | VAL |
| 1 | C | 1226 | ARG |
| 1 | C | 1227 | LEU |
| 1 | C | 1231 | LEU |
| 1 | C | 1232 | VAL |
| 1 | C | 1245 | ARG |
| 1 | C | 1258 | PHE |
| 1 | C | 1261 | VAL |
| 1 | C | 1262 | ASP |
| 1 | C | 1274 | LEU |
| 1 | C | 1281 | ASP |
| 1 | C | 1290 | TYR |
| 1 | C | 1295 | TYR |
| 1 | C | 1303 | LEU |
| 1 | C | 1311 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | C | 1317 | PHE |
| 1 | C | 1326 | LYS |
| 1 | C | 1340 | TRP |
| 1 | C | 1344 | ASN |
| 1 | C | 1345 | ILE |
| 1 | C | 1350 | ARG |
| 1 | C | 1354 | GLN |
| 1 | C | 1377 | THR |
| 1 | C | 1383 | THR |
| 1 | C | 1384 | ASP |
| 1 | C | 1390 | GLN |
| 1 | C | 1417 | LEU |
| 1 | C | 1419 | LEU |
| 1 | C | 1422 | LEU |
| 1 | C | 1424 | MET |
| 1 | C | 1447 | LEU |
| 1 | C | 1458 | HIS |
| 1 | C | 1460 | ASN |
| 1 | C | 1469 | ASN |
| 1 | C | 1489 | ASN |
| 1 | C | 1490 | PHE |
| 1 | C | 1504 | LEU |
| 1 | C | 1526 | GLU |
| 1 | C | 1527 | LEU |
| 1 | C | 1529 | LYS |
| 1 | C | 1536 | ASP |
| 1 | C | 1540 | TYR |
| 1 | C | 1549 | LEU |
| 1 | C | 1574 | TYR |
| 1 | C | 1577 | LEU |
| 1 | C | 1578 | ARG |
| 1 | C | 1588 | ARG |
| 1 | C | 1589 | HIS |
| 1 | C | 1590 | ASN |
| 1 | C | 1591 | ILE |
| 1 | C | 1592 | MET |
| 1 | C | 1593 | ASP |
| 1 | C | 1594 | PHE |
| 1 | C | 1596 | MET |
| 1 | C | 1597 | PRO |
| 1 | C | 1601 | GLN |
| 1 | C | 1611 | ASP |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | C | 1620 | ARG |
| 2 | D | 103 | ARG |
| 2 | D | 105 | TRP |
| 2 | D | 106 | ARG |
| 2 | D | 108 | GLU |
| 2 | D | 110 | ARG |
| 2 | D | 112 | ARG |
| 2 | D | 114 | GLN |
| 2 | D | 116 | LEU |
| 2 | D | 120 | SER |
| 2 | D | 123 | MET |
| 2 | D | 125 | GLN |
| 2 | D | 127 | TRP |
| 2 | D | 130 | LYS |
| 2 | D | 133 | LYS |
| 2 | D | 137 | GLU |
| 2 | D | 153 | ASN |
| 2 | D | 155 | ILE |
| 2 | E | 91 | GLN |
| 2 | E | 93 | ASP |
| 2 | E | 94 | ARG |
| 2 | E | 98 | GLU |
| 2 | E | 100 | GLU |
| 2 | E | 110 | ARG |
| 2 | E | 112 | ARG |
| 2 | E | 114 | GLN |
| 2 | E | 116 | LEU |
| 2 | E | 120 | SER |
| 2 | E | 123 | MET |
| 2 | E | 125 | GLN |
| 2 | E | 127 | TRP |
| 2 | E | 130 | LYS |
| 2 | E | 133 | LYS |
| 2 | E | 137 | GLU |
| 2 | E | 140 | GLN |
| 2 | E | 153 | ASN |
| 2 | E | 155 | ILE |
| 2 | F | 91 | GLN |
| 2 | F | 93 | ASP |
| 2 | F | 94 | ARG |
| 2 | F | 97 | GLN |
| 2 | F | 105 | TRP |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | F | 106 | ARG |
| 2 | F | 108 | GLU |
| 2 | F | 110 | ARG |
| 2 | F | 112 | ARG |
| 2 | F | 114 | GLN |
| 2 | F | 116 | LEU |
| 2 | F | 120 | SER |
| 2 | F | 123 | MET |
| 2 | F | 125 | GLN |
| 2 | F | 127 | TRP |
| 2 | F | 130 | LYS |
| 2 | F | 133 | LYS |
| 2 | F | 137 | GLU |
| 2 | F | 140 | GLN |
| 2 | F | 153 | ASN |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (63) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | A | 1083 | GLN |
| 1 | A | 1091 | ASN |
| 1 | A | 1103 | ASN |
| 1 | A | 1117 | GLN |
| 1 | A | 1145 | ASN |
| 1 | A | 1191 | ASN |
| 1 | A | 1354 | GLN |
| 1 | A | 1380 | ASN |
| 1 | A | 1381 | HIS |
| 1 | A | 1390 | GLN |
| 1 | A | 1456 | GLN |
| 1 | A | 1457 | ASN |
| 1 | A | 1468 | ASN |
| 1 | A | 1469 | ASN |
| 1 | A | 1489 | ASN |
| 1 | A | 1518 | ASN |
| 1 | A | 1523 | GLN |
| 1 | A | 1539 | GLN |
| 1 | A | 1630 | GLN |
| 1 | B | 1083 | GLN |
| 1 | B | 1091 | ASN |
| 1 | B | 1117 | GLN |
| 1 | B | 1145 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | B | 1191 | ASN |
| 1 | B | 1194 | ASN |
| 1 | B | 1354 | GLN |
| 1 | B | 1380 | ASN |
| 1 | B | 1381 | HIS |
| 1 | B | 1390 | GLN |
| 1 | B | 1456 | GLN |
| 1 | B | 1457 | ASN |
| 1 | B | 1468 | ASN |
| 1 | B | 1469 | ASN |
| 1 | B | 1489 | ASN |
| 1 | B | 1518 | ASN |
| 1 | B | 1523 | GLN |
| 1 | B | 1539 | GLN |
| 1 | B | 1630 | GLN |
| 1 | C | 1091 | ASN |
| 1 | C | 1149 | ASN |
| 1 | C | 1191 | ASN |
| 1 | C | 1194 | ASN |
| 1 | C | 1354 | GLN |
| 1 | C | 1380 | ASN |
| 1 | C | 1381 | HIS |
| 1 | C | 1390 | GLN |
| 1 | C | 1444 | GLN |
| 1 | C | 1456 | GLN |
| 1 | C | 1457 | ASN |
| 1 | C | 1468 | ASN |
| 1 | C | 1469 | ASN |
| 1 | C | 1489 | ASN |
| 1 | C | 1518 | ASN |
| 1 | C | 1523 | GLN |
| 1 | C | 1539 | GLN |
| 1 | C | 1590 | ASN |
| 2 | D | 91 | GLN |
| 2 | D | 149 | ASN |
| 2 | D | 153 | ASN |
| 2 | E | 149 | ASN |
| 2 | E | 153 | ASN |
| 2 | F | 149 | ASN |
| 2 | F | 153 | ASN |

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates 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 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|-----------------|--------|----------------|-----------------------|-------|
| 1 | A | 553/624 (88%) | 4.12 | 342 (61%) 0 3 | 306, 348, 348, 348 | 0 |
| 1 | B | 553/624 (88%) | 4.91 | 368 (66%) 0 3 | 257, 257, 318, 319 | 0 |
| 1 | C | 553/624 (88%) | 2.81 | 238 (43%) 0 4 | 232, 232, 308, 309 | 0 |
| 2 | D | 79/190 (41%) | 4.22 | 62 (78%) 0 2 | 298, 298, 298, 298 | 0 |
| 2 | E | 68/190 (35%) | 1.97 | 26 (38%) 0 4 | 314, 314, 314, 314 | 0 |
| 2 | F | 78/190 (41%) | 3.16 | 33 (42%) 0 4 | 339, 339, 339, 339 | 0 |
| All | All | 1884/2442 (77%) | 3.85 | 1069 (56%) 0 3 | 232, 307, 348, 348 | 0 |

All (1069) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 1 | C | 1091 | ASN | 38.3 |
| 1 | C | 1078 | ASN | 36.0 |
| 1 | C | 1090 | GLY | 34.7 |
| 1 | C | 1079 | THR | 33.3 |
| 1 | B | 1106 | ALA | 29.6 |
| 1 | B | 1105 | PRO | 28.3 |
| 1 | C | 1088 | HIS | 28.1 |
| 1 | C | 1089 | ILE | 27.0 |
| 1 | C | 1087 | GLU | 26.4 |
| 1 | C | 1080 | SER | 26.2 |
| 1 | B | 1123 | GLU | 24.8 |
| 1 | A | 1079 | THR | 23.5 |
| 1 | C | 1081 | ALA | 22.1 |
| 1 | A | 1629 | THR | 22.0 |
| 1 | B | 1083 | GLN | 21.9 |
| 1 | A | 1080 | SER | 21.6 |
| 1 | B | 1104 | GLU | 21.3 |
| 1 | B | 1223 | ASN | 21.1 |
| 1 | A | 1094 | ARG | 20.0 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 1 | A | 1083 | GLN | 19.2 |
| 1 | C | 1109 | SER | 19.2 |
| 1 | B | 1078 | ASN | 19.1 |
| 1 | A | 1109 | SER | 18.9 |
| 1 | B | 1129 | ILE | 18.2 |
| 1 | B | 1134 | PRO | 18.2 |
| 1 | B | 1132 | ASP | 18.1 |
| 1 | B | 1122 | LYS | 18.0 |
| 1 | B | 1133 | ASP | 17.9 |
| 1 | B | 1115 | GLN | 17.7 |
| 1 | B | 1128 | TYR | 17.7 |
| 1 | B | 1096 | TYR | 17.6 |
| 1 | B | 1103 | ASN | 17.6 |
| 1 | B | 1182 | ARG | 17.3 |
| 1 | B | 1126 | ASP | 17.2 |
| 1 | B | 1125 | ILE | 17.2 |
| 1 | B | 1088 | HIS | 17.1 |
| 1 | B | 1130 | LYS | 16.9 |
| 1 | B | 1086 | ILE | 16.7 |
| 1 | B | 1131 | ALA | 16.7 |
| 1 | B | 1121 | VAL | 16.7 |
| 1 | B | 1087 | GLU | 16.5 |
| 1 | B | 1120 | MET | 16.4 |
| 1 | A | 1088 | HIS | 16.3 |
| 1 | B | 1212 | ASP | 16.2 |
| 1 | A | 1134 | PRO | 16.1 |
| 1 | B | 1214 | ALA | 15.9 |
| 1 | B | 1085 | LEU | 15.8 |
| 1 | B | 1089 | ILE | 15.8 |
| 1 | B | 1230 | THR | 15.8 |
| 1 | B | 1079 | THR | 15.6 |
| 1 | B | 1082 | VAL | 15.6 |
| 1 | B | 1108 | TRP | 15.4 |
| 1 | B | 1151 | GLU | 15.4 |
| 1 | A | 1628 | GLU | 15.4 |
| 1 | A | 1093 | ASP | 15.1 |
| 1 | C | 1086 | ILE | 15.1 |
| 1 | A | 1136 | SER | 15.0 |
| 1 | B | 1213 | ALA | 14.9 |
| 1 | A | 1082 | VAL | 14.8 |
| 1 | B | 1107 | VAL | 14.7 |
| 1 | B | 1093 | ASP | 14.6 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 1 | B | 1156 | TYR | 14.3 |
| 1 | B | 1124 | ALA | 14.2 |
| 1 | C | 1110 | GLN | 14.2 |
| 1 | B | 1109 | SER | 14.2 |
| 1 | A | 1081 | ALA | 14.1 |
| 1 | A | 1096 | TYR | 14.1 |
| 1 | B | 1080 | SER | 14.0 |
| 1 | A | 1135 | SER | 14.0 |
| 2 | F | 101 | SER | 13.9 |
| 1 | B | 1222 | SER | 13.8 |
| 1 | A | 1262 | ASP | 13.7 |
| 1 | B | 1099 | ALA | 13.7 |
| 1 | A | 1330 | GLN | 13.3 |
| 1 | B | 1211 | TYR | 13.3 |
| 1 | B | 1210 | MET | 13.3 |
| 2 | D | 163 | GLN | 13.1 |
| 1 | A | 1087 | GLU | 13.0 |
| 1 | A | 1078 | ASN | 13.0 |
| 1 | A | 1261 | VAL | 12.9 |
| 1 | B | 1111 | LEU | 12.9 |
| 1 | B | 1226 | ARG | 12.9 |
| 1 | B | 1137 | TYR | 12.8 |
| 1 | A | 1097 | GLU | 12.7 |
| 1 | A | 1270 | GLN | 12.6 |
| 1 | B | 1189 | PHE | 12.6 |
| 1 | B | 1181 | ASN | 12.5 |
| 1 | A | 1095 | ALA | 12.5 |
| 2 | D | 162 | GLN | 12.4 |
| 1 | B | 1139 | GLU | 12.3 |
| 1 | C | 1098 | PHE | 12.3 |
| 1 | A | 1152 | GLU | 12.2 |
| 1 | A | 1112 | ALA | 12.1 |
| 1 | B | 1095 | ALA | 12.1 |
| 1 | A | 1298 | GLU | 12.0 |
| 1 | C | 1105 | PRO | 12.0 |
| 1 | C | 1114 | ALA | 11.9 |
| 1 | C | 1083 | GLN | 11.9 |
| 1 | B | 1091 | ASN | 11.9 |
| 2 | F | 102 | ILE | 11.8 |
| 1 | B | 1148 | GLY | 11.8 |
| 1 | A | 1085 | LEU | 11.7 |
| 1 | A | 1091 | ASN | 11.7 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 1 | C | 1082 | VAL | 11.6 |
| 1 | A | 1110 | GLN | 11.6 |
| 1 | B | 1140 | VAL | 11.6 |
| 1 | B | 1161 | ARG | 11.6 |
| 1 | B | 1165 | ARG | 11.5 |
| 1 | C | 1094 | ARG | 11.5 |
| 1 | A | 1329 | PRO | 11.5 |
| 2 | F | 104 | LYS | 11.5 |
| 1 | A | 1265 | GLU | 11.4 |
| 1 | B | 1262 | ASP | 11.3 |
| 2 | F | 107 | GLU | 11.3 |
| 1 | B | 1127 | SER | 11.3 |
| 1 | C | 1134 | PRO | 11.3 |
| 1 | A | 1084 | VAL | 11.2 |
| 1 | B | 1147 | SER | 11.2 |
| 1 | A | 1151 | GLU | 11.1 |
| 1 | B | 1264 | LYS | 11.1 |
| 1 | A | 1098 | PHE | 11.1 |
| 1 | B | 1118 | LYS | 11.1 |
| 1 | C | 1120 | MET | 11.0 |
| 1 | A | 1223 | ASN | 11.0 |
| 1 | B | 1100 | GLU | 11.0 |
| 1 | B | 1102 | CYS | 11.0 |
| 1 | A | 1148 | GLY | 11.0 |
| 1 | C | 1107 | VAL | 10.8 |
| 1 | C | 1085 | LEU | 10.8 |
| 1 | B | 1216 | LEU | 10.8 |
| 1 | A | 1120 | MET | 10.8 |
| 1 | B | 1157 | LEU | 10.7 |
| 1 | B | 1081 | ALA | 10.6 |
| 1 | C | 1101 | ARG | 10.5 |
| 1 | A | 1212 | ASP | 10.5 |
| 1 | B | 1110 | GLN | 10.5 |
| 1 | B | 1092 | LEU | 10.5 |
| 1 | A | 1211 | TYR | 10.5 |
| 1 | A | 1092 | LEU | 10.4 |
| 1 | A | 1196 | ALA | 10.4 |
| 1 | B | 1183 | LEU | 10.3 |
| 2 | D | 91 | GLN | 10.3 |
| 2 | F | 103 | ARG | 10.3 |
| 2 | E | 112 | ARG | 10.2 |
| 1 | C | 1113 | LYS | 10.2 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 1 | C | 1097 | GLU | 10.1 |
| 1 | C | 1128 | TYR | 10.1 |
| 1 | C | 1093 | ASP | 10.1 |
| 2 | D | 164 | PRO | 10.1 |
| 1 | A | 1149 | ASN | 10.1 |
| 1 | A | 1627 | THR | 10.1 |
| 1 | A | 1386 | TRP | 10.0 |
| 1 | B | 1152 | GLU | 10.0 |
| 1 | C | 1118 | LYS | 10.0 |
| 1 | B | 1149 | ASN | 9.9 |
| 2 | D | 165 | ASP | 9.9 |
| 2 | F | 108 | GLU | 9.9 |
| 1 | B | 1206 | TYR | 9.9 |
| 1 | A | 1165 | ARG | 9.9 |
| 1 | C | 1115 | GLN | 9.8 |
| 1 | B | 1218 | TYR | 9.7 |
| 1 | B | 1112 | ALA | 9.7 |
| 1 | B | 1184 | ALA | 9.7 |
| 1 | A | 1113 | LYS | 9.6 |
| 1 | B | 1188 | GLU | 9.6 |
| 1 | A | 1626 | ALA | 9.6 |
| 1 | B | 1191 | ASN | 9.6 |
| 1 | B | 1192 | GLY | 9.6 |
| 1 | A | 1086 | ILE | 9.5 |
| 1 | B | 1506 | GLU | 9.5 |
| 1 | C | 1462 | SER | 9.5 |
| 1 | A | 1331 | LYS | 9.5 |
| 1 | B | 1160 | ALA | 9.5 |
| 2 | F | 93 | ASP | 9.4 |
| 1 | B | 1164 | ALA | 9.4 |
| 1 | A | 1396 | THR | 9.4 |
| 1 | C | 1092 | LEU | 9.4 |
| 1 | C | 1129 | ILE | 9.4 |
| 1 | A | 1327 | PHE | 9.4 |
| 1 | B | 1158 | GLN | 9.4 |
| 1 | B | 1116 | LEU | 9.3 |
| 1 | A | 1431 | ASP | 9.3 |
| 1 | B | 1136 | SER | 9.3 |
| 1 | C | 1108 | TRP | 9.3 |
| 1 | B | 1190 | ILE | 9.2 |
| 1 | B | 1280 | ALA | 9.2 |
| 1 | C | 1112 | ALA | 9.2 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 1 | B | 1197 | HIS | 9.2 |
| 1 | A | 1267 | ARG | 9.2 |
| 1 | A | 1395 | ILE | 9.1 |
| 1 | A | 1106 | ALA | 9.1 |
| 1 | C | 1095 | ALA | 9.1 |
| 1 | B | 1114 | ALA | 9.1 |
| 2 | F | 109 | GLN | 9.1 |
| 1 | A | 1192 | GLY | 9.1 |
| 1 | B | 1162 | LYS | 9.0 |
| 2 | F | 112 | ARG | 9.0 |
| 1 | B | 1185 | GLU | 9.0 |
| 1 | B | 1084 | VAL | 8.9 |
| 1 | A | 1266 | PHE | 8.9 |
| 2 | F | 110 | ARG | 8.9 |
| 2 | D | 166 | ALA | 8.8 |
| 1 | A | 1239 | ALA | 8.8 |
| 1 | B | 1278 | VAL | 8.8 |
| 2 | E | 113 | LEU | 8.8 |
| 1 | B | 1198 | ILE | 8.8 |
| 1 | A | 1156 | TYR | 8.8 |
| 1 | A | 1630 | GLN | 8.7 |
| 1 | B | 1254 | LYS | 8.7 |
| 1 | B | 1625 | GLN | 8.7 |
| 1 | A | 1306 | ALA | 8.7 |
| 1 | A | 1247 | ALA | 8.7 |
| 2 | F | 106 | ARG | 8.6 |
| 1 | A | 1123 | GLU | 8.6 |
| 1 | B | 1215 | LYS | 8.6 |
| 1 | B | 1458 | HIS | 8.6 |
| 1 | A | 1099 | ALA | 8.6 |
| 1 | B | 1279 | HIS | 8.5 |
| 1 | C | 1520 | ARG | 8.5 |
| 1 | B | 1094 | ARG | 8.5 |
| 1 | A | 1197 | HIS | 8.5 |
| 1 | B | 1135 | SER | 8.5 |
| 1 | A | 1248 | ASN | 8.5 |
| 1 | A | 1222 | SER | 8.4 |
| 1 | C | 1130 | LYS | 8.4 |
| 1 | B | 1542 | SER | 8.4 |
| 1 | B | 1443 | LYS | 8.4 |
| 1 | A | 1242 | ASP | 8.4 |
| 1 | B | 1187 | GLU | 8.4 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 1 | B | 1252 | THR | 8.3 |
| 1 | A | 1240 | ALA | 8.3 |
| 1 | A | 1280 | ALA | 8.3 |
| 1 | A | 1111 | LEU | 8.3 |
| 1 | A | 1189 | PHE | 8.3 |
| 1 | A | 1326 | LYS | 8.3 |
| 1 | B | 1263 | GLY | 8.3 |
| 1 | B | 1163 | LYS | 8.3 |
| 2 | F | 111 | LYS | 8.3 |
| 1 | B | 1520 | ARG | 8.3 |
| 1 | C | 1096 | TYR | 8.3 |
| 1 | B | 1119 | GLY | 8.3 |
| 1 | C | 1126 | ASP | 8.3 |
| 2 | D | 93 | ASP | 8.3 |
| 1 | A | 1178 | ALA | 8.2 |
| 1 | C | 1111 | LEU | 8.2 |
| 1 | A | 1105 | PRO | 8.2 |
| 1 | B | 1225 | GLY | 8.2 |
| 1 | B | 1444 | GLN | 8.1 |
| 1 | A | 1328 | LYS | 8.1 |
| 1 | B | 1504 | LEU | 8.1 |
| 1 | A | 1107 | VAL | 8.1 |
| 1 | A | 1147 | SER | 8.0 |
| 1 | A | 1121 | VAL | 8.0 |
| 1 | B | 1251 | ARG | 8.0 |
| 1 | C | 1135 | SER | 8.0 |
| 1 | B | 1523 | GLN | 8.0 |
| 2 | E | 110 | ARG | 8.0 |
| 1 | B | 1203 | ASP | 8.0 |
| 1 | B | 1380 | ASN | 8.0 |
| 1 | A | 1179 | LYS | 8.0 |
| 1 | A | 1622 | GLU | 7.9 |
| 1 | B | 1169 | VAL | 7.9 |
| 1 | A | 1153 | LEU | 7.9 |
| 1 | B | 1159 | MET | 7.8 |
| 2 | F | 96 | THR | 7.8 |
| 1 | C | 1104 | GLU | 7.8 |
| 1 | A | 1140 | VAL | 7.8 |
| 1 | C | 1119 | GLY | 7.8 |
| 1 | B | 1090 | GLY | 7.8 |
| 2 | F | 105 | TRP | 7.8 |
| 1 | B | 1414 | PHE | 7.8 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 1 | B | 1154 | VAL | 7.8 |
| 1 | A | 1300 | ILE | 7.8 |
| 1 | A | 1313 | HIS | 7.8 |
| 1 | C | 1434 | ARG | 7.8 |
| 1 | A | 1118 | LYS | 7.7 |
| 1 | C | 1489 | ASN | 7.7 |
| 1 | B | 1573 | CYS | 7.7 |
| 1 | A | 1264 | LYS | 7.7 |
| 1 | A | 1108 | TRP | 7.7 |
| 1 | B | 1204 | ARG | 7.7 |
| 1 | A | 1089 | ILE | 7.6 |
| 1 | A | 1254 | LYS | 7.6 |
| 2 | E | 115 | GLU | 7.6 |
| 1 | A | 1573 | CYS | 7.6 |
| 1 | B | 1200 | GLN | 7.6 |
| 1 | A | 1133 | ASP | 7.6 |
| 1 | A | 1225 | GLY | 7.6 |
| 1 | A | 1224 | PHE | 7.6 |
| 1 | A | 1297 | GLU | 7.6 |
| 2 | D | 134 | ASP | 7.6 |
| 1 | A | 1229 | SER | 7.5 |
| 1 | B | 1217 | LEU | 7.5 |
| 1 | C | 1106 | ALA | 7.5 |
| 1 | C | 1099 | ALA | 7.5 |
| 1 | B | 1277 | VAL | 7.5 |
| 2 | E | 114 | GLN | 7.5 |
| 1 | A | 1230 | THR | 7.5 |
| 1 | A | 1290 | TYR | 7.5 |
| 1 | B | 1097 | GLU | 7.5 |
| 1 | A | 1180 | THR | 7.4 |
| 1 | B | 1208 | GLU | 7.4 |
| 1 | A | 1141 | VAL | 7.4 |
| 1 | B | 1231 | LEU | 7.4 |
| 1 | B | 1138 | MET | 7.4 |
| 1 | B | 1261 | VAL | 7.4 |
| 1 | B | 1168 | TYR | 7.4 |
| 1 | A | 1311 | ARG | 7.4 |
| 1 | A | 1193 | PRO | 7.4 |
| 1 | C | 1144 | ALA | 7.3 |
| 1 | B | 1113 | LYS | 7.3 |
| 1 | A | 1128 | TYR | 7.3 |
| 2 | D | 159 | ALA | 7.3 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 1 | A | 1241 | VAL | 7.2 |
| 1 | B | 1224 | PHE | 7.2 |
| 2 | E | 155 | ILE | 7.2 |
| 1 | B | 1155 | LYS | 7.2 |
| 1 | A | 1115 | GLN | 7.2 |
| 1 | B | 1326 | LYS | 7.2 |
| 1 | B | 1628 | GLU | 7.2 |
| 2 | D | 136 | GLU | 7.1 |
| 1 | B | 1201 | VAL | 7.1 |
| 1 | B | 1209 | LYS | 7.1 |
| 1 | A | 1150 | TRP | 7.1 |
| 1 | A | 1214 | ALA | 7.0 |
| 1 | B | 1186 | LEU | 7.0 |
| 1 | A | 1271 | MET | 7.0 |
| 1 | A | 1398 | VAL | 7.0 |
| 1 | B | 1265 | GLU | 7.0 |
| 1 | A | 1623 | GLU | 6.9 |
| 1 | B | 1153 | LEU | 6.9 |
| 1 | C | 1156 | TYR | 6.9 |
| 2 | D | 94 | ARG | 6.8 |
| 1 | B | 1150 | TRP | 6.8 |
| 1 | A | 1090 | GLY | 6.8 |
| 1 | A | 1275 | HIS | 6.8 |
| 1 | A | 1119 | GLY | 6.8 |
| 1 | A | 1400 | ASN | 6.8 |
| 1 | B | 1117 | GLN | 6.8 |
| 1 | C | 1149 | ASN | 6.8 |
| 1 | B | 1293 | ARG | 6.8 |
| 1 | A | 1154 | VAL | 6.8 |
| 1 | A | 1137 | TYR | 6.7 |
| 2 | E | 109 | GLN | 6.7 |
| 1 | A | 1397 | LYS | 6.7 |
| 1 | A | 1385 | ALA | 6.7 |
| 1 | A | 1356 | HIS | 6.7 |
| 1 | C | 1084 | VAL | 6.7 |
| 1 | B | 1306 | ALA | 6.7 |
| 1 | B | 1141 | VAL | 6.7 |
| 1 | B | 1193 | PRO | 6.7 |
| 1 | A | 1228 | ALA | 6.7 |
| 1 | A | 1243 | GLY | 6.7 |
| 1 | A | 1268 | LEU | 6.6 |
| 1 | C | 1116 | LEU | 6.6 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 1 | A | 1160 | ALA | 6.6 |
| 1 | B | 1220 | ASN | 6.6 |
| 1 | B | 1475 | GLU | 6.6 |
| 1 | A | 1625 | GLN | 6.6 |
| 2 | D | 167 | ASP | 6.6 |
| 1 | B | 1379 | MET | 6.6 |
| 2 | E | 111 | LYS | 6.6 |
| 1 | A | 1263 | GLY | 6.5 |
| 1 | A | 1139 | GLU | 6.5 |
| 1 | A | 1213 | ALA | 6.5 |
| 1 | A | 1226 | ARG | 6.5 |
| 2 | D | 115 | GLU | 6.5 |
| 1 | A | 1432 | HIS | 6.5 |
| 1 | A | 1101 | ARG | 6.5 |
| 1 | C | 1133 | ASP | 6.5 |
| 1 | A | 1394 | ILE | 6.4 |
| 1 | B | 1227 | LEU | 6.4 |
| 1 | B | 1202 | GLY | 6.4 |
| 1 | C | 1136 | SER | 6.4 |
| 1 | A | 1117 | GLN | 6.4 |
| 1 | A | 1357 | LEU | 6.4 |
| 1 | A | 1274 | LEU | 6.4 |
| 1 | A | 1293 | ARG | 6.4 |
| 1 | A | 1227 | LEU | 6.4 |
| 1 | A | 1231 | LEU | 6.3 |
| 1 | A | 1237 | TYR | 6.3 |
| 1 | B | 1250 | THR | 6.3 |
| 1 | A | 1199 | GLN | 6.3 |
| 2 | D | 132 | LYS | 6.3 |
| 1 | B | 1228 | ALA | 6.3 |
| 1 | B | 1166 | GLU | 6.2 |
| 1 | A | 1399 | ALA | 6.2 |
| 1 | A | 1575 | ASP | 6.2 |
| 1 | A | 1302 | MET | 6.2 |
| 1 | A | 1246 | LYS | 6.2 |
| 1 | A | 1200 | GLN | 6.2 |
| 2 | D | 131 | ALA | 6.2 |
| 1 | A | 1175 | PHE | 6.2 |
| 1 | B | 1629 | THR | 6.2 |
| 1 | C | 1395 | ILE | 6.1 |
| 1 | C | 1523 | GLN | 6.1 |
| 2 | E | 107 | GLU | 6.1 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 1 | A | 1273 | GLY | 6.1 |
| 1 | B | 1199 | GLN | 6.1 |
| 1 | A | 1218 | TYR | 6.1 |
| 1 | A | 1277 | VAL | 6.0 |
| 1 | A | 1430 | LEU | 6.0 |
| 1 | A | 1198 | ILE | 6.0 |
| 1 | A | 1157 | LEU | 6.0 |
| 1 | A | 1335 | HIS | 6.0 |
| 1 | C | 1100 | GLU | 6.0 |
| 1 | C | 1121 | VAL | 6.0 |
| 1 | A | 1354 | GLN | 6.0 |
| 1 | A | 1351 | ALA | 6.0 |
| 1 | C | 1141 | VAL | 5.9 |
| 1 | C | 1125 | ILE | 5.9 |
| 1 | B | 1575 | ASP | 5.8 |
| 2 | D | 138 | TRP | 5.8 |
| 1 | A | 1238 | GLN | 5.8 |
| 1 | A | 1100 | GLU | 5.8 |
| 1 | B | 1442 | VAL | 5.8 |
| 1 | A | 1433 | THR | 5.8 |
| 1 | B | 1456 | GLN | 5.8 |
| 2 | E | 106 | ARG | 5.8 |
| 1 | C | 1438 | TYR | 5.8 |
| 2 | D | 92 | ALA | 5.7 |
| 1 | A | 1339 | PHE | 5.7 |
| 1 | B | 1266 | PHE | 5.7 |
| 1 | B | 1219 | ASN | 5.7 |
| 1 | C | 1169 | VAL | 5.7 |
| 1 | A | 1315 | GLY | 5.7 |
| 1 | B | 1207 | ASP | 5.7 |
| 1 | C | 1179 | LYS | 5.7 |
| 1 | B | 1416 | PRO | 5.7 |
| 2 | D | 107 | GLU | 5.7 |
| 1 | A | 1429 | ARG | 5.6 |
| 1 | B | 1101 | ARG | 5.6 |
| 2 | D | 168 | ILE | 5.6 |
| 1 | A | 1210 | MET | 5.6 |
| 1 | B | 1229 | SER | 5.6 |
| 1 | A | 1289 | TYR | 5.6 |
| 1 | C | 1140 | VAL | 5.6 |
| 1 | C | 1175 | PHE | 5.6 |
| 1 | C | 1122 | LYS | 5.6 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 1 | C | 1515 | PHE | 5.6 |
| 1 | A | 1171 | THR | 5.6 |
| 1 | B | 1438 | TYR | 5.5 |
| 2 | D | 169 | ILE | 5.5 |
| 1 | B | 1255 | GLU | 5.5 |
| 1 | C | 1514 | LEU | 5.5 |
| 1 | B | 1295 | TYR | 5.5 |
| 1 | B | 1462 | SER | 5.5 |
| 2 | F | 113 | LEU | 5.5 |
| 1 | A | 1292 | ASP | 5.5 |
| 1 | A | 1324 | TYR | 5.5 |
| 1 | B | 1410 | PHE | 5.5 |
| 1 | A | 1332 | MET | 5.5 |
| 1 | B | 1289 | TYR | 5.5 |
| 1 | B | 1524 | SER | 5.5 |
| 1 | B | 1178 | ALA | 5.4 |
| 1 | C | 1102 | CYS | 5.4 |
| 2 | D | 117 | ASP | 5.4 |
| 1 | B | 1205 | CYS | 5.4 |
| 1 | A | 1278 | VAL | 5.4 |
| 1 | A | 1355 | ALA | 5.4 |
| 1 | C | 1197 | HIS | 5.4 |
| 1 | A | 1288 | ASN | 5.4 |
| 1 | A | 1388 | GLU | 5.4 |
| 1 | C | 1521 | TRP | 5.4 |
| 1 | A | 1125 | ILE | 5.4 |
| 1 | C | 1544 | SER | 5.4 |
| 1 | A | 1403 | LEU | 5.3 |
| 1 | B | 1375 | ILE | 5.3 |
| 1 | C | 1153 | LEU | 5.3 |
| 1 | C | 1458 | HIS | 5.3 |
| 1 | B | 1395 | ILE | 5.3 |
| 1 | A | 1572 | THR | 5.3 |
| 1 | B | 1543 | GLU | 5.3 |
| 1 | A | 1323 | LEU | 5.3 |
| 1 | B | 1539 | GLN | 5.3 |
| 1 | B | 1521 | TRP | 5.3 |
| 1 | B | 1384 | ASP | 5.2 |
| 1 | A | 1130 | LYS | 5.2 |
| 1 | B | 1412 | LEU | 5.2 |
| 2 | E | 156 | ALA | 5.2 |
| 2 | D | 98 | GLU | 5.2 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 1 | B | 1180 | THR | 5.2 |
| 1 | C | 1137 | TYR | 5.2 |
| 1 | C | 1534 | TYR | 5.2 |
| 1 | A | 1116 | LEU | 5.2 |
| 1 | A | 1316 | MET | 5.2 |
| 2 | D | 137 | GLU | 5.2 |
| 1 | B | 1451 | TYR | 5.2 |
| 1 | B | 1221 | VAL | 5.2 |
| 2 | D | 133 | LYS | 5.2 |
| 1 | B | 1179 | LYS | 5.2 |
| 1 | C | 1145 | ASN | 5.1 |
| 1 | A | 1325 | SER | 5.1 |
| 1 | C | 1164 | ALA | 5.1 |
| 1 | A | 1142 | GLN | 5.1 |
| 1 | B | 1474 | GLU | 5.1 |
| 2 | D | 145 | GLN | 5.1 |
| 1 | B | 1434 | ARG | 5.1 |
| 1 | B | 1256 | VAL | 5.1 |
| 1 | B | 1413 | GLU | 5.1 |
| 1 | B | 1403 | LEU | 5.1 |
| 1 | A | 1114 | ALA | 5.0 |
| 1 | C | 1498 | ARG | 5.0 |
| 1 | B | 1248 | ASN | 5.0 |
| 1 | C | 1385 | ALA | 5.0 |
| 2 | F | 92 | ALA | 5.0 |
| 2 | D | 141 | ARG | 5.0 |
| 1 | B | 1242 | ASP | 5.0 |
| 1 | B | 1275 | HIS | 5.0 |
| 1 | B | 1311 | ARG | 5.0 |
| 1 | A | 1216 | LEU | 5.0 |
| 1 | A | 1342 | ARG | 5.0 |
| 1 | B | 1098 | PHE | 5.0 |
| 1 | B | 1307 | LEU | 5.0 |
| 2 | D | 116 | LEU | 5.0 |
| 1 | C | 1461 | LYS | 5.0 |
| 1 | A | 1272 | CYS | 5.0 |
| 1 | A | 1542 | SER | 5.0 |
| 1 | B | 1382 | PRO | 5.0 |
| 2 | D | 152 | ASN | 5.0 |
| 1 | A | 1122 | LYS | 5.0 |
| 1 | A | 1202 | GLY | 4.9 |
| 1 | A | 1319 | GLU | 4.9 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 1 | A | 1164 | ALA | 4.9 |
| 1 | B | 1515 | PHE | 4.9 |
| 1 | A | 1195 | ASN | 4.9 |
| 1 | A | 1220 | ASN | 4.9 |
| 1 | A | 1382 | PRO | 4.9 |
| 2 | F | 99 | PRO | 4.9 |
| 2 | D | 135 | LEU | 4.9 |
| 1 | C | 1382 | PRO | 4.9 |
| 2 | D | 160 | PHE | 4.9 |
| 1 | C | 1150 | TRP | 4.9 |
| 2 | F | 98 | GLU | 4.9 |
| 1 | A | 1358 | TRP | 4.9 |
| 2 | D | 127 | TRP | 4.9 |
| 1 | C | 1403 | LEU | 4.8 |
| 1 | A | 1340 | TRP | 4.8 |
| 1 | A | 1169 | VAL | 4.8 |
| 1 | B | 1624 | GLU | 4.8 |
| 2 | F | 100 | GLU | 4.8 |
| 1 | A | 1279 | HIS | 4.8 |
| 1 | B | 1505 | ILE | 4.8 |
| 1 | B | 1244 | ALA | 4.8 |
| 1 | B | 1473 | THR | 4.8 |
| 1 | A | 1245 | ARG | 4.8 |
| 1 | A | 1244 | ALA | 4.7 |
| 1 | B | 1313 | HIS | 4.7 |
| 2 | D | 149 | ASN | 4.7 |
| 1 | B | 1630 | GLN | 4.7 |
| 1 | C | 1139 | GLU | 4.7 |
| 1 | A | 1181 | ASN | 4.7 |
| 1 | C | 1103 | ASN | 4.7 |
| 1 | A | 1188 | GLU | 4.7 |
| 1 | B | 1472 | ILE | 4.7 |
| 1 | B | 1623 | GLU | 4.7 |
| 1 | C | 1124 | ALA | 4.7 |
| 1 | A | 1299 | LEU | 4.6 |
| 1 | A | 1317 | PHE | 4.6 |
| 1 | C | 1154 | VAL | 4.6 |
| 2 | F | 91 | GLN | 4.6 |
| 1 | A | 1337 | GLU | 4.6 |
| 1 | C | 1165 | ARG | 4.6 |
| 1 | A | 1269 | ALA | 4.6 |
| 1 | C | 1538 | MET | 4.6 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 1 | A | 1334 | GLU | 4.6 |
| 1 | A | 1296 | PHE | 4.6 |
| 2 | D | 97 | GLN | 4.6 |
| 1 | C | 1375 | ILE | 4.6 |
| 1 | C | 1540 | TYR | 4.5 |
| 1 | A | 1161 | ARG | 4.5 |
| 1 | C | 1117 | GLN | 4.5 |
| 1 | C | 1441 | LYS | 4.5 |
| 2 | D | 114 | GLN | 4.5 |
| 1 | A | 1201 | VAL | 4.5 |
| 1 | A | 1203 | ASP | 4.5 |
| 1 | A | 1384 | ASP | 4.5 |
| 1 | C | 1628 | GLU | 4.5 |
| 1 | B | 1194 | ASN | 4.5 |
| 1 | C | 1406 | ARG | 4.5 |
| 1 | A | 1285 | GLU | 4.5 |
| 1 | A | 1387 | LYS | 4.5 |
| 1 | A | 1320 | LEU | 4.4 |
| 1 | B | 1394 | ILE | 4.4 |
| 1 | B | 1145 | ASN | 4.4 |
| 1 | B | 1417 | LEU | 4.4 |
| 2 | D | 139 | ASN | 4.4 |
| 1 | A | 1333 | ARG | 4.4 |
| 2 | D | 130 | LYS | 4.4 |
| 1 | B | 1627 | THR | 4.4 |
| 1 | B | 1268 | LEU | 4.4 |
| 2 | D | 99 | PRO | 4.4 |
| 2 | F | 95 | LEU | 4.4 |
| 1 | A | 1206 | TYR | 4.4 |
| 1 | B | 1507 | PHE | 4.4 |
| 1 | C | 1490 | PHE | 4.4 |
| 1 | B | 1290 | TYR | 4.4 |
| 1 | B | 1391 | PHE | 4.4 |
| 1 | A | 1295 | TYR | 4.4 |
| 1 | C | 1512 | ALA | 4.4 |
| 1 | A | 1276 | ILE | 4.3 |
| 1 | A | 1301 | THR | 4.3 |
| 1 | A | 1585 | THR | 4.3 |
| 1 | B | 1285 | GLU | 4.3 |
| 1 | C | 1506 | GLU | 4.3 |
| 2 | D | 140 | GLN | 4.3 |
| 1 | B | 1514 | LEU | 4.3 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 1 | A | 1191 | ASN | 4.3 |
| 1 | A | 1383 | THR | 4.3 |
| 1 | C | 1132 | ASP | 4.3 |
| 1 | A | 1322 | ILE | 4.3 |
| 1 | C | 1384 | ASP | 4.3 |
| 1 | B | 1381 | HIS | 4.3 |
| 1 | B | 1445 | LEU | 4.3 |
| 1 | A | 1166 | GLU | 4.3 |
| 1 | A | 1401 | VAL | 4.3 |
| 1 | B | 1238 | GLN | 4.2 |
| 1 | A | 1462 | SER | 4.2 |
| 1 | A | 1124 | ALA | 4.2 |
| 1 | A | 1194 | ASN | 4.2 |
| 1 | B | 1411 | TYR | 4.2 |
| 1 | A | 1250 | THR | 4.2 |
| 1 | A | 1312 | ALA | 4.2 |
| 1 | B | 1541 | ALA | 4.2 |
| 1 | B | 1358 | TRP | 4.2 |
| 1 | A | 1155 | LYS | 4.2 |
| 1 | A | 1215 | LYS | 4.2 |
| 1 | B | 1535 | LYS | 4.2 |
| 2 | D | 112 | ARG | 4.2 |
| 1 | A | 1309 | LEU | 4.2 |
| 1 | C | 1460 | ASN | 4.2 |
| 1 | A | 1434 | ARG | 4.2 |
| 1 | A | 1183 | LEU | 4.2 |
| 1 | A | 1177 | LEU | 4.2 |
| 1 | A | 1167 | SER | 4.2 |
| 1 | B | 1173 | LEU | 4.2 |
| 1 | A | 1174 | ILE | 4.1 |
| 1 | C | 1310 | GLU | 4.1 |
| 1 | C | 1451 | TYR | 4.1 |
| 1 | B | 1247 | ALA | 4.1 |
| 1 | C | 1378 | MET | 4.1 |
| 1 | B | 1509 | ARG | 4.1 |
| 1 | C | 1541 | ALA | 4.1 |
| 1 | C | 1172 | GLU | 4.1 |
| 1 | A | 1132 | ASP | 4.1 |
| 1 | A | 1176 | ALA | 4.1 |
| 1 | C | 1204 | ARG | 4.1 |
| 1 | B | 1259 | ALA | 4.1 |
| 1 | B | 1578 | ARG | 4.1 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 1 | B | 1253 | TRP | 4.1 |
| 1 | B | 1439 | PHE | 4.0 |
| 1 | A | 1168 | TYR | 4.0 |
| 1 | A | 1221 | VAL | 4.0 |
| 1 | A | 1126 | ASP | 4.0 |
| 1 | C | 1383 | THR | 4.0 |
| 1 | C | 1507 | PHE | 4.0 |
| 1 | A | 1102 | CYS | 4.0 |
| 1 | A | 1138 | MET | 4.0 |
| 1 | B | 1432 | HIS | 4.0 |
| 1 | A | 1534 | TYR | 4.0 |
| 1 | B | 1146 | THR | 4.0 |
| 1 | B | 1574 | TYR | 4.0 |
| 1 | C | 1511 | ALA | 4.0 |
| 1 | B | 1292 | ASP | 3.9 |
| 1 | C | 1359 | ALA | 3.9 |
| 1 | B | 1143 | ALA | 3.9 |
| 1 | B | 1196 | ALA | 3.9 |
| 1 | B | 1503 | GLU | 3.9 |
| 2 | F | 159 | ALA | 3.9 |
| 1 | A | 1380 | ASN | 3.9 |
| 1 | B | 1577 | LEU | 3.9 |
| 1 | A | 1144 | ALA | 3.9 |
| 2 | D | 108 | GLU | 3.9 |
| 1 | B | 1144 | ALA | 3.9 |
| 1 | C | 1524 | SER | 3.9 |
| 1 | A | 1233 | HIS | 3.9 |
| 1 | C | 1444 | GLN | 3.9 |
| 1 | C | 1410 | PHE | 3.9 |
| 2 | D | 161 | TYR | 3.9 |
| 1 | A | 1392 | LYS | 3.9 |
| 1 | C | 1452 | LEU | 3.9 |
| 1 | B | 1142 | GLN | 3.9 |
| 1 | C | 1573 | CYS | 3.9 |
| 1 | B | 1170 | GLU | 3.9 |
| 2 | F | 161 | TYR | 3.9 |
| 1 | B | 1351 | ALA | 3.8 |
| 1 | C | 1416 | PRO | 3.8 |
| 1 | C | 1148 | GLY | 3.8 |
| 1 | B | 1463 | VAL | 3.8 |
| 1 | B | 1167 | SER | 3.8 |
| 1 | A | 1352 | ALA | 3.8 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 1 | B | 1249 | SER | 3.8 |
| 1 | A | 1391 | PHE | 3.8 |
| 1 | B | 1460 | ASN | 3.8 |
| 1 | C | 1560 | GLU | 3.8 |
| 1 | B | 1425 | VAL | 3.8 |
| 1 | C | 1131 | ALA | 3.7 |
| 1 | B | 1240 | ALA | 3.7 |
| 1 | A | 1185 | GLU | 3.7 |
| 1 | C | 1196 | ALA | 3.7 |
| 2 | D | 105 | TRP | 3.7 |
| 1 | C | 1157 | LEU | 3.7 |
| 1 | B | 1436 | VAL | 3.7 |
| 1 | B | 1368 | TYR | 3.7 |
| 1 | B | 1576 | LEU | 3.7 |
| 1 | B | 1441 | LYS | 3.7 |
| 2 | F | 114 | GLN | 3.7 |
| 1 | B | 1288 | ASN | 3.7 |
| 1 | A | 1578 | ARG | 3.7 |
| 1 | B | 1518 | ASN | 3.7 |
| 1 | B | 1386 | TRP | 3.7 |
| 1 | C | 1379 | MET | 3.7 |
| 2 | D | 113 | LEU | 3.7 |
| 1 | A | 1483 | SER | 3.7 |
| 1 | C | 1430 | LEU | 3.7 |
| 2 | D | 120 | SER | 3.7 |
| 1 | A | 1257 | CYS | 3.6 |
| 1 | A | 1318 | THR | 3.6 |
| 1 | C | 1226 | ARG | 3.6 |
| 1 | C | 1396 | THR | 3.6 |
| 2 | D | 128 | ARG | 3.6 |
| 1 | B | 1354 | GLN | 3.6 |
| 1 | A | 1460 | ASN | 3.6 |
| 1 | B | 1378 | MET | 3.6 |
| 1 | C | 1420 | ASN | 3.6 |
| 1 | B | 1534 | TYR | 3.6 |
| 1 | C | 1357 | LEU | 3.6 |
| 2 | D | 148 | LYS | 3.6 |
| 1 | A | 1336 | LEU | 3.6 |
| 1 | B | 1453 | ARG | 3.6 |
| 1 | B | 1174 | ILE | 3.5 |
| 1 | A | 1520 | ARG | 3.5 |
| 1 | B | 1415 | LYS | 3.5 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 1 | C | 1178 | ALA | 3.5 |
| 1 | B | 1316 | MET | 3.5 |
| 1 | A | 1305 | ALA | 3.5 |
| 1 | A | 1381 | HIS | 3.5 |
| 1 | C | 1432 | HIS | 3.5 |
| 1 | B | 1446 | PRO | 3.5 |
| 1 | B | 1626 | ALA | 3.5 |
| 1 | A | 1145 | ASN | 3.5 |
| 1 | A | 1353 | GLU | 3.5 |
| 1 | C | 1417 | LEU | 3.5 |
| 1 | C | 1356 | HIS | 3.5 |
| 1 | B | 1502 | HIS | 3.5 |
| 1 | B | 1406 | ARG | 3.5 |
| 1 | A | 1368 | TYR | 3.5 |
| 1 | C | 1495 | LEU | 3.4 |
| 2 | F | 162 | GLN | 3.4 |
| 1 | C | 1222 | SER | 3.4 |
| 2 | F | 124 | GLU | 3.4 |
| 1 | C | 1386 | TRP | 3.4 |
| 2 | D | 142 | GLN | 3.4 |
| 1 | C | 1563 | ARG | 3.4 |
| 1 | B | 1294 | GLY | 3.4 |
| 1 | B | 1435 | ALA | 3.4 |
| 1 | A | 1286 | LEU | 3.4 |
| 1 | B | 1175 | PHE | 3.4 |
| 1 | B | 1195 | ASN | 3.4 |
| 1 | A | 1624 | GLU | 3.4 |
| 1 | C | 1143 | ALA | 3.4 |
| 1 | A | 1281 | ASP | 3.4 |
| 1 | B | 1276 | ILE | 3.4 |
| 1 | B | 1303 | LEU | 3.4 |
| 1 | C | 1163 | LYS | 3.4 |
| 1 | B | 1452 | LEU | 3.4 |
| 2 | E | 154 | ARG | 3.4 |
| 1 | A | 1205 | CYS | 3.3 |
| 1 | B | 1544 | SER | 3.3 |
| 1 | C | 1151 | GLU | 3.3 |
| 1 | C | 1423 | LEU | 3.3 |
| 1 | C | 1545 | LYS | 3.3 |
| 1 | A | 1405 | TYR | 3.3 |
| 1 | A | 1234 | LEU | 3.3 |
| 1 | C | 1412 | LEU | 3.3 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 1 | A | 1425 | VAL | 3.3 |
| 1 | C | 1261 | VAL | 3.3 |
| 1 | C | 1402 | GLU | 3.3 |
| 1 | A | 1303 | LEU | 3.3 |
| 1 | A | 1255 | GLU | 3.3 |
| 1 | A | 1426 | LEU | 3.3 |
| 1 | C | 1418 | LEU | 3.3 |
| 1 | A | 1506 | GLU | 3.3 |
| 2 | D | 100 | GLU | 3.3 |
| 1 | A | 1314 | MET | 3.3 |
| 1 | B | 1495 | LEU | 3.3 |
| 1 | B | 1340 | TRP | 3.3 |
| 1 | A | 1217 | LEU | 3.2 |
| 2 | E | 137 | GLU | 3.2 |
| 1 | B | 1467 | LEU | 3.2 |
| 1 | B | 1383 | THR | 3.2 |
| 1 | B | 1312 | ALA | 3.2 |
| 1 | A | 1576 | LEU | 3.2 |
| 1 | A | 1568 | ALA | 3.2 |
| 2 | F | 97 | GLN | 3.2 |
| 1 | C | 1127 | SER | 3.2 |
| 1 | A | 1219 | ASN | 3.2 |
| 1 | B | 1568 | ALA | 3.2 |
| 1 | C | 1629 | THR | 3.2 |
| 1 | B | 1440 | SER | 3.2 |
| 1 | C | 1526 | GLU | 3.2 |
| 1 | B | 1582 | VAL | 3.2 |
| 1 | C | 1525 | VAL | 3.2 |
| 1 | C | 1186 | LEU | 3.2 |
| 1 | C | 1377 | THR | 3.2 |
| 1 | C | 1216 | LEU | 3.2 |
| 1 | C | 1380 | ASN | 3.2 |
| 2 | D | 109 | GLN | 3.2 |
| 1 | A | 1589 | HIS | 3.2 |
| 1 | B | 1177 | LEU | 3.2 |
| 2 | D | 129 | GLU | 3.2 |
| 1 | C | 1422 | LEU | 3.2 |
| 1 | A | 1249 | SER | 3.2 |
| 1 | C | 1522 | LYS | 3.2 |
| 1 | C | 1561 | GLU | 3.2 |
| 1 | C | 1456 | GLN | 3.1 |
| 1 | B | 1258 | PHE | 3.1 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 1 | A | 1294 | GLY | 3.1 |
| 1 | B | 1357 | LEU | 3.1 |
| 1 | C | 1610 | VAL | 3.1 |
| 1 | B | 1447 | LEU | 3.1 |
| 1 | A | 1451 | TYR | 3.1 |
| 1 | B | 1404 | TYR | 3.1 |
| 1 | A | 1393 | ASP | 3.1 |
| 1 | C | 1392 | LYS | 3.1 |
| 1 | A | 1436 | VAL | 3.1 |
| 2 | F | 139 | ASN | 3.1 |
| 1 | B | 1325 | SER | 3.1 |
| 1 | C | 1488 | ASP | 3.1 |
| 1 | C | 1358 | TRP | 3.1 |
| 1 | A | 1291 | GLN | 3.1 |
| 1 | B | 1273 | GLY | 3.1 |
| 1 | C | 1248 | ASN | 3.1 |
| 2 | F | 152 | ASN | 3.1 |
| 1 | A | 1283 | LEU | 3.0 |
| 1 | A | 1423 | LEU | 3.0 |
| 2 | D | 144 | GLU | 3.0 |
| 1 | C | 1405 | TYR | 3.0 |
| 1 | A | 1256 | VAL | 3.0 |
| 1 | B | 1621 | LYS | 3.0 |
| 1 | C | 1473 | THR | 3.0 |
| 2 | E | 117 | ASP | 3.0 |
| 1 | A | 1172 | GLU | 3.0 |
| 1 | C | 1391 | PHE | 3.0 |
| 1 | C | 1528 | CYS | 3.0 |
| 1 | B | 1396 | THR | 3.0 |
| 1 | C | 1578 | ARG | 3.0 |
| 1 | A | 1260 | CYS | 3.0 |
| 1 | A | 1582 | VAL | 3.0 |
| 2 | E | 121 | LYS | 3.0 |
| 1 | C | 1433 | THR | 3.0 |
| 1 | B | 1471 | PHE | 3.0 |
| 1 | A | 1390 | GLN | 2.9 |
| 1 | C | 1200 | GLN | 2.9 |
| 1 | A | 1143 | ALA | 2.9 |
| 1 | A | 1375 | ILE | 2.9 |
| 2 | F | 94 | ARG | 2.9 |
| 1 | A | 1258 | PHE | 2.9 |
| 1 | C | 1497 | GLN | 2.9 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 1 | C | 1160 | ALA | 2.9 |
| 1 | A | 1173 | LEU | 2.9 |
| 1 | A | 1444 | GLN | 2.9 |
| 1 | B | 1392 | LYS | 2.9 |
| 1 | B | 1560 | GLU | 2.9 |
| 1 | A | 1146 | THR | 2.9 |
| 2 | F | 117 | ASP | 2.9 |
| 1 | B | 1423 | LEU | 2.9 |
| 1 | C | 1381 | HIS | 2.9 |
| 1 | B | 1510 | ILE | 2.9 |
| 1 | B | 1561 | GLU | 2.9 |
| 1 | C | 1152 | GLU | 2.9 |
| 1 | B | 1310 | GLU | 2.9 |
| 1 | B | 1233 | HIS | 2.8 |
| 1 | A | 1307 | LEU | 2.8 |
| 1 | B | 1243 | GLY | 2.8 |
| 2 | D | 95 | LEU | 2.8 |
| 1 | C | 1465 | GLU | 2.8 |
| 1 | C | 1142 | GLN | 2.8 |
| 1 | C | 1435 | ALA | 2.8 |
| 1 | B | 1508 | ARG | 2.8 |
| 1 | B | 1356 | HIS | 2.8 |
| 1 | A | 1236 | GLU | 2.8 |
| 1 | C | 1176 | ALA | 2.8 |
| 1 | C | 1290 | TYR | 2.8 |
| 1 | B | 1371 | TYR | 2.8 |
| 2 | E | 104 | LYS | 2.8 |
| 1 | A | 1378 | MET | 2.8 |
| 1 | A | 1404 | TYR | 2.8 |
| 1 | C | 1472 | ILE | 2.8 |
| 1 | C | 1404 | TYR | 2.8 |
| 1 | A | 1184 | ALA | 2.8 |
| 1 | C | 1123 | GLU | 2.8 |
| 1 | C | 1447 | LEU | 2.8 |
| 1 | A | 1259 | ALA | 2.8 |
| 1 | C | 1171 | THR | 2.8 |
| 2 | E | 108 | GLU | 2.8 |
| 1 | C | 1529 | LYS | 2.8 |
| 1 | C | 1324 | TYR | 2.8 |
| 1 | C | 1394 | ILE | 2.7 |
| 1 | C | 1426 | LEU | 2.7 |
| 1 | C | 1504 | LEU | 2.7 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 1 | B | 1540 | TYR | 2.7 |
| 1 | B | 1449 | LYS | 2.7 |
| 1 | C | 1627 | THR | 2.7 |
| 1 | C | 1212 | ASP | 2.7 |
| 1 | C | 1442 | VAL | 2.7 |
| 1 | B | 1270 | GLN | 2.7 |
| 1 | B | 1236 | GLU | 2.7 |
| 1 | B | 1405 | TYR | 2.7 |
| 2 | E | 95 | LEU | 2.7 |
| 1 | A | 1131 | ALA | 2.7 |
| 1 | B | 1309 | LEU | 2.7 |
| 1 | A | 1535 | LYS | 2.7 |
| 1 | C | 1562 | LYS | 2.7 |
| 1 | B | 1433 | THR | 2.7 |
| 1 | C | 1598 | TYR | 2.7 |
| 1 | B | 1234 | LEU | 2.7 |
| 1 | A | 1190 | ILE | 2.7 |
| 1 | A | 1252 | THR | 2.7 |
| 1 | C | 1302 | MET | 2.7 |
| 1 | B | 1448 | VAL | 2.6 |
| 1 | C | 1468 | ASN | 2.6 |
| 1 | B | 1339 | PHE | 2.6 |
| 1 | B | 1529 | LYS | 2.6 |
| 1 | A | 1574 | TYR | 2.6 |
| 1 | B | 1622 | GLU | 2.6 |
| 1 | B | 1468 | ASN | 2.6 |
| 2 | D | 106 | ARG | 2.6 |
| 1 | B | 1476 | ASP | 2.6 |
| 1 | C | 1572 | THR | 2.6 |
| 1 | C | 1620 | ARG | 2.6 |
| 1 | B | 1516 | LYS | 2.6 |
| 1 | C | 1459 | ASN | 2.6 |
| 1 | C | 1429 | ARG | 2.6 |
| 1 | B | 1426 | LEU | 2.6 |
| 1 | B | 1171 | THR | 2.6 |
| 1 | B | 1455 | VAL | 2.6 |
| 1 | C | 1161 | ARG | 2.6 |
| 1 | B | 1172 | GLU | 2.6 |
| 1 | A | 1524 | SER | 2.5 |
| 1 | C | 1311 | ARG | 2.5 |
| 1 | A | 1402 | GLU | 2.5 |
| 1 | B | 1377 | THR | 2.5 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 1 | A | 1424 | MET | 2.5 |
| 1 | C | 1293 | ARG | 2.5 |
| 1 | C | 1535 | LYS | 2.5 |
| 1 | B | 1372 | ASP | 2.5 |
| 1 | C | 1230 | THR | 2.5 |
| 1 | C | 1360 | GLU | 2.5 |
| 1 | B | 1402 | GLU | 2.5 |
| 1 | A | 1349 | LEU | 2.5 |
| 2 | D | 101 | SER | 2.5 |
| 2 | F | 160 | PHE | 2.5 |
| 1 | C | 1499 | LEU | 2.5 |
| 2 | D | 158 | LYS | 2.5 |
| 1 | C | 1325 | SER | 2.5 |
| 1 | B | 1374 | ALA | 2.5 |
| 1 | C | 1494 | SER | 2.5 |
| 1 | B | 1589 | HIS | 2.5 |
| 1 | B | 1488 | ASP | 2.5 |
| 1 | C | 1166 | GLU | 2.5 |
| 1 | C | 1614 | ASP | 2.5 |
| 1 | B | 1522 | LYS | 2.5 |
| 1 | A | 1186 | LEU | 2.5 |
| 1 | B | 1281 | ASP | 2.5 |
| 1 | B | 1477 | TYR | 2.4 |
| 1 | C | 1606 | TYR | 2.4 |
| 1 | A | 1371 | TYR | 2.4 |
| 1 | C | 1411 | TYR | 2.4 |
| 1 | A | 1348 | VAL | 2.4 |
| 1 | A | 1361 | LEU | 2.4 |
| 1 | B | 1272 | CYS | 2.4 |
| 1 | B | 1595 | ALA | 2.4 |
| 1 | B | 1237 | TYR | 2.4 |
| 1 | C | 1424 | MET | 2.4 |
| 1 | A | 1458 | HIS | 2.4 |
| 2 | D | 111 | LYS | 2.4 |
| 1 | A | 1561 | GLU | 2.4 |
| 1 | C | 1388 | GLU | 2.4 |
| 1 | B | 1614 | ASP | 2.4 |
| 2 | D | 124 | GLU | 2.4 |
| 1 | B | 1585 | THR | 2.4 |
| 1 | B | 1459 | ASN | 2.4 |
| 1 | B | 1513 | TYR | 2.4 |
| 1 | C | 1439 | PHE | 2.4 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 2 | D | 143 | SER | 2.4 |
| 1 | B | 1302 | MET | 2.3 |
| 1 | C | 1254 | LYS | 2.3 |
| 1 | C | 1146 | THR | 2.3 |
| 1 | A | 1595 | ALA | 2.3 |
| 1 | C | 1491 | ASP | 2.3 |
| 2 | D | 123 | MET | 2.3 |
| 1 | A | 1539 | GLN | 2.3 |
| 1 | B | 1454 | SER | 2.3 |
| 1 | A | 1129 | ILE | 2.3 |
| 1 | B | 1430 | LEU | 2.3 |
| 1 | C | 1617 | GLU | 2.3 |
| 1 | A | 1461 | LYS | 2.3 |
| 1 | A | 1521 | TRP | 2.3 |
| 1 | B | 1241 | VAL | 2.3 |
| 1 | C | 1421 | ASP | 2.3 |
| 1 | C | 1427 | SER | 2.3 |
| 1 | C | 1443 | LYS | 2.3 |
| 2 | D | 96 | THR | 2.3 |
| 2 | E | 120 | SER | 2.3 |
| 1 | C | 1509 | ARG | 2.3 |
| 1 | A | 1551 | GLU | 2.3 |
| 1 | B | 1422 | LEU | 2.3 |
| 2 | F | 141 | ARG | 2.3 |
| 1 | A | 1581 | VAL | 2.3 |
| 1 | A | 1204 | ARG | 2.3 |
| 1 | B | 1239 | ALA | 2.3 |
| 1 | B | 1429 | ARG | 2.3 |
| 1 | C | 1252 | THR | 2.3 |
| 1 | A | 1343 | VAL | 2.3 |
| 1 | C | 1211 | TYR | 2.2 |
| 1 | C | 1400 | ASN | 2.2 |
| 2 | E | 151 | ILE | 2.2 |
| 1 | B | 1362 | VAL | 2.2 |
| 1 | B | 1235 | GLY | 2.2 |
| 1 | C | 1407 | ALA | 2.2 |
| 1 | A | 1447 | LEU | 2.2 |
| 1 | C | 1510 | ILE | 2.2 |
| 1 | B | 1511 | ALA | 2.2 |
| 1 | A | 1310 | GLU | 2.2 |
| 1 | B | 1483 | SER | 2.2 |
| 2 | E | 116 | LEU | 2.2 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 1 | B | 1620 | ARG | 2.2 |
| 1 | A | 1158 | GLN | 2.2 |
| 1 | B | 1365 | TYR | 2.2 |
| 1 | A | 1584 | GLU | 2.2 |
| 1 | A | 1377 | THR | 2.2 |
| 1 | A | 1364 | LEU | 2.2 |
| 1 | C | 1502 | HIS | 2.2 |
| 1 | A | 1187 | GLU | 2.2 |
| 1 | C | 1374 | ALA | 2.2 |
| 2 | E | 125 | GLN | 2.2 |
| 2 | E | 134 | ASP | 2.2 |
| 1 | B | 1296 | PHE | 2.2 |
| 1 | C | 1337 | GLU | 2.1 |
| 1 | B | 1350 | ARG | 2.1 |
| 2 | E | 94 | ARG | 2.1 |
| 2 | E | 139 | ASN | 2.1 |
| 2 | D | 125 | GLN | 2.1 |
| 1 | B | 1528 | CYS | 2.1 |
| 1 | C | 1437 | ASN | 2.1 |
| 1 | A | 1251 | ARG | 2.1 |
| 1 | B | 1419 | LEU | 2.1 |
| 1 | B | 1531 | ASP | 2.1 |
| 1 | B | 1398 | VAL | 2.1 |
| 1 | C | 1503 | GLU | 2.1 |
| 1 | B | 1347 | LYS | 2.1 |
| 1 | C | 1295 | TYR | 2.1 |
| 1 | B | 1519 | ASN | 2.1 |
| 1 | B | 1431 | ASP | 2.1 |
| 1 | C | 1147 | SER | 2.1 |
| 1 | A | 1514 | LEU | 2.0 |
| 1 | C | 1408 | ILE | 2.0 |
| 1 | B | 1581 | VAL | 2.0 |
| 1 | A | 1182 | ARG | 2.0 |
| 2 | D | 119 | ALA | 2.0 |
| 1 | A | 1543 | GLU | 2.0 |
| 1 | B | 1536 | ASP | 2.0 |
| 1 | C | 1289 | TYR | 2.0 |
| 2 | E | 96 | THR | 2.0 |
| 1 | A | 1347 | LYS | 2.0 |
| 1 | B | 1257 | CYS | 2.0 |
| 1 | B | 1617 | GLU | 2.0 |
| 1 | A | 1507 | PHE | 2.0 |

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.