



Full wwPDB EM Validation Report ⓘ

Nov 19, 2022 – 10:19 AM EST

PDB ID : 1O1A
EMDB ID : EMD-1001
Title : MOLECULAR MODELS OF AVERAGED RIGOR CROSSBRIDGES FROM
TOMOGRAMS OF INSECT FLIGHT MUSCLE
Authors : Chen, L.F.; Winkler, H.; Reedy, M.K.; Reedy, M.C.; Taylor, K.A.
Deposited on : 2002-11-18
Resolution : 70.00 Å (reported)
Based on initial models : 2MYS, 1ATN

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

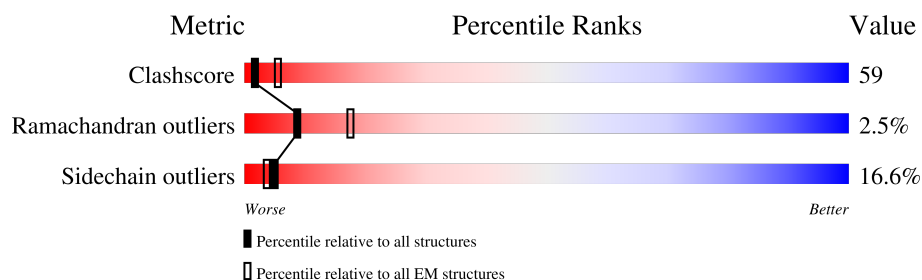
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 70.00 Å.

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



| Metric | Whole archive (#Entries) | EM structures (#Entries) |
|-----------------------|--------------------------|--------------------------|
| Clashscore | 158937 | 4297 |
| Ramachandran outliers | 154571 | 4023 |
| Sidechain outliers | 154315 | 3826 |

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

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|---|
| 1 | A | 840 | <div> <div>100%</div> <div>25% 50% 20% .</div> </div> |
| 1 | D | 840 | <div> <div>100%</div> <div>26% 50% 19% .</div> </div> |
| 1 | G | 840 | <div> <div>100%</div> <div>25% 51% 20% .</div> </div> |
| 1 | J | 840 | <div> <div>100%</div> <div>25% 51% 20% .</div> </div> |
| 1 | M | 840 | <div> <div>100%</div> <div>26% 50% 20% .</div> </div> |
| 1 | P | 840 | <div> <div>100%</div> <div>26% 49% 21% .</div> </div> |
| 2 | B | 145 | <div> <div>100%</div> <div>68% 23% 6% .</div> </div> |
| 2 | E | 145 | <div> <div>100%</div> <div>64% 27% 6% .</div> </div> |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 2 | H | 145 | |
| 2 | K | 145 | |
| 2 | N | 145 | |
| 2 | Q | 145 | |
| 3 | C | 147 | |
| 3 | F | 147 | |
| 3 | I | 147 | |
| 3 | L | 147 | |
| 3 | O | 147 | |
| 3 | R | 147 | |
| 4 | 1 | 375 | |
| 4 | 2 | 375 | |
| 4 | 3 | 375 | |
| 4 | 4 | 375 | |
| 4 | 5 | 375 | |
| 4 | 6 | 375 | |
| 4 | 7 | 375 | |
| 4 | 8 | 375 | |
| 4 | 9 | 375 | |
| 4 | V | 375 | |
| 4 | W | 375 | |
| 4 | X | 375 | |
| 4 | Y | 375 | |
| 4 | Z | 375 | |

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

ria:

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 1 | MLY | A | 505 | - | - | X | - |
| 1 | MLY | A | 553 | - | - | X | - |
| 1 | MLY | A | 764 | - | - | X | - |
| 1 | MLY | A | 837 | - | - | X | - |
| 1 | MLY | A | 839 | - | - | X | - |
| 1 | MLY | D | 553 | - | - | X | - |
| 1 | MLY | D | 764 | - | - | X | - |
| 1 | MLY | D | 782 | - | - | X | - |
| 1 | MLY | G | 505 | - | - | X | - |
| 1 | MLY | G | 553 | - | - | X | - |
| 1 | MLY | G | 764 | - | - | X | - |
| 1 | MLY | G | 84 | - | - | X | - |
| 1 | MLY | J | 505 | - | - | X | - |
| 1 | MLY | J | 553 | - | - | X | - |
| 1 | MLY | J | 839 | - | - | X | - |
| 1 | MLY | J | 84 | - | - | X | - |
| 1 | MLY | M | 839 | - | - | X | - |
| 1 | MLY | P | 839 | - | - | X | - |

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 94966 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called SKELETAL MUSCLE MYOSIN II.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
| 1 | A | 840 | Total | C | N | O | S | 0 | 0 |
| | | | 6797 | 4382 | 1135 | 1243 | 37 | | |
| 1 | D | 840 | Total | C | N | O | S | 0 | 0 |
| | | | 6797 | 4382 | 1135 | 1243 | 37 | | |
| 1 | G | 840 | Total | C | N | O | S | 0 | 0 |
| | | | 6797 | 4382 | 1135 | 1243 | 37 | | |
| 1 | J | 840 | Total | C | N | O | S | 0 | 0 |
| | | | 6797 | 4382 | 1135 | 1243 | 37 | | |
| 1 | M | 840 | Total | C | N | O | S | 0 | 0 |
| | | | 6797 | 4382 | 1135 | 1243 | 37 | | |
| 1 | P | 840 | Total | C | N | O | S | 0 | 0 |
| | | | 6797 | 4382 | 1135 | 1243 | 37 | | |

- Molecule 2 is a protein called SKELETAL MUSCLE MYOSIN II REGULATORY LIGHT CHAIN.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 2 | B | 145 | Total | C | N | O | S | 0 | 0 |
| | | | 1127 | 717 | 177 | 227 | 6 | | |
| 2 | E | 145 | Total | C | N | O | S | 0 | 0 |
| | | | 1127 | 717 | 177 | 227 | 6 | | |
| 2 | H | 145 | Total | C | N | O | S | 0 | 0 |
| | | | 1127 | 717 | 177 | 227 | 6 | | |
| 2 | K | 145 | Total | C | N | O | S | 0 | 0 |
| | | | 1127 | 717 | 177 | 227 | 6 | | |
| 2 | N | 145 | Total | C | N | O | S | 0 | 0 |
| | | | 1127 | 717 | 177 | 227 | 6 | | |
| 2 | Q | 145 | Total | C | N | O | S | 0 | 0 |
| | | | 1127 | 717 | 177 | 227 | 6 | | |

- Molecule 3 is a protein called SKELETAL MUSCLE MYOSIN II ESSENTIAL LIGHT CHAIN.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 3 | C | 147 | Total | C | N | O | S | 0 | 0 |
| | | | 1123 | 698 | 188 | 230 | 7 | | |
| 3 | F | 147 | Total | C | N | O | S | 0 | 0 |
| | | | 1123 | 698 | 188 | 230 | 7 | | |
| 3 | I | 147 | Total | C | N | O | S | 0 | 0 |
| | | | 1123 | 698 | 188 | 230 | 7 | | |
| 3 | L | 147 | Total | C | N | O | S | 0 | 0 |
| | | | 1123 | 698 | 188 | 230 | 7 | | |
| 3 | O | 147 | Total | C | N | O | S | 0 | 0 |
| | | | 1123 | 698 | 188 | 230 | 7 | | |
| 3 | R | 147 | Total | C | N | O | S | 0 | 0 |
| | | | 1123 | 698 | 188 | 230 | 7 | | |

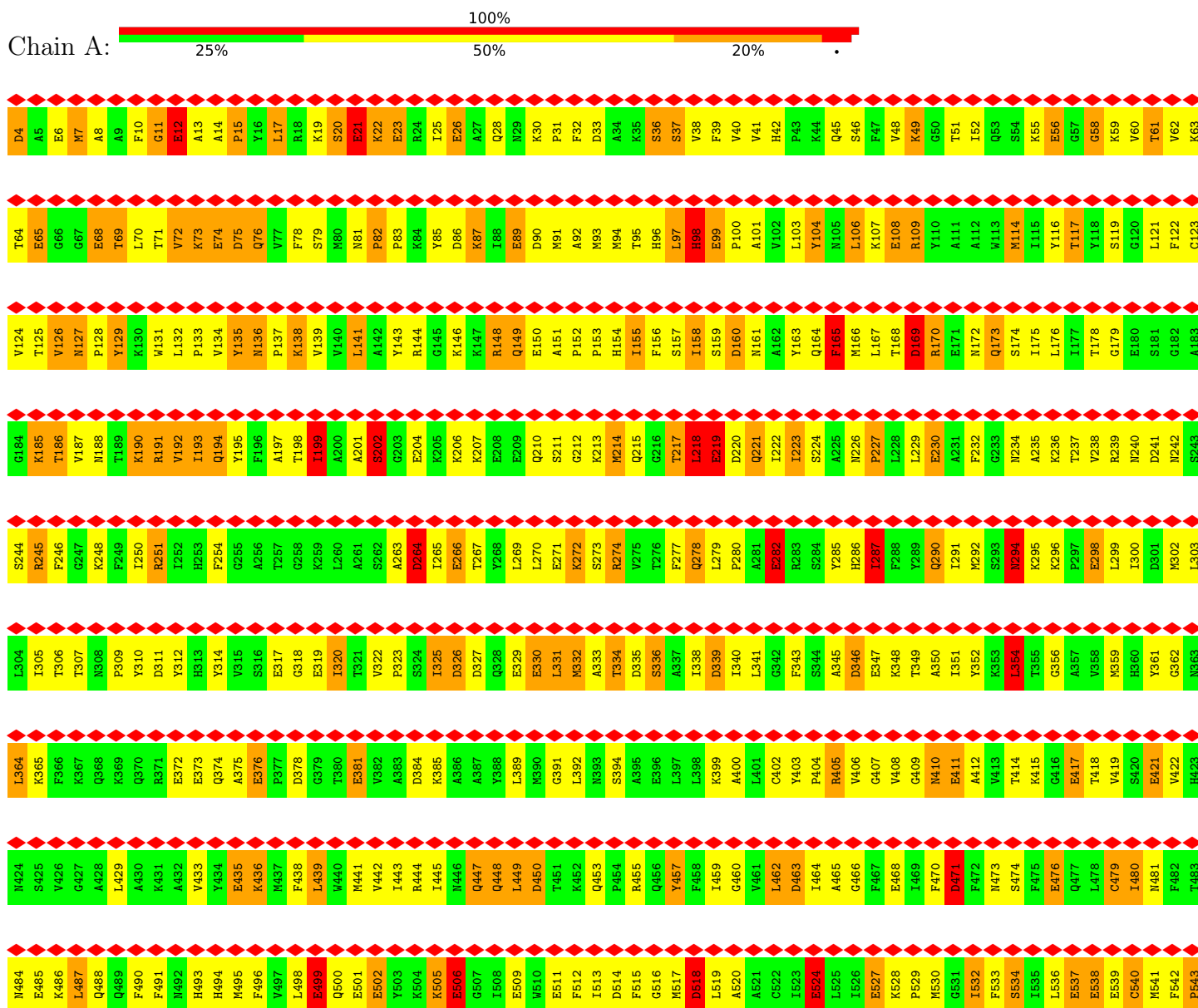
- Molecule 4 is a protein called SKELETAL MUSCLE ACTIN.

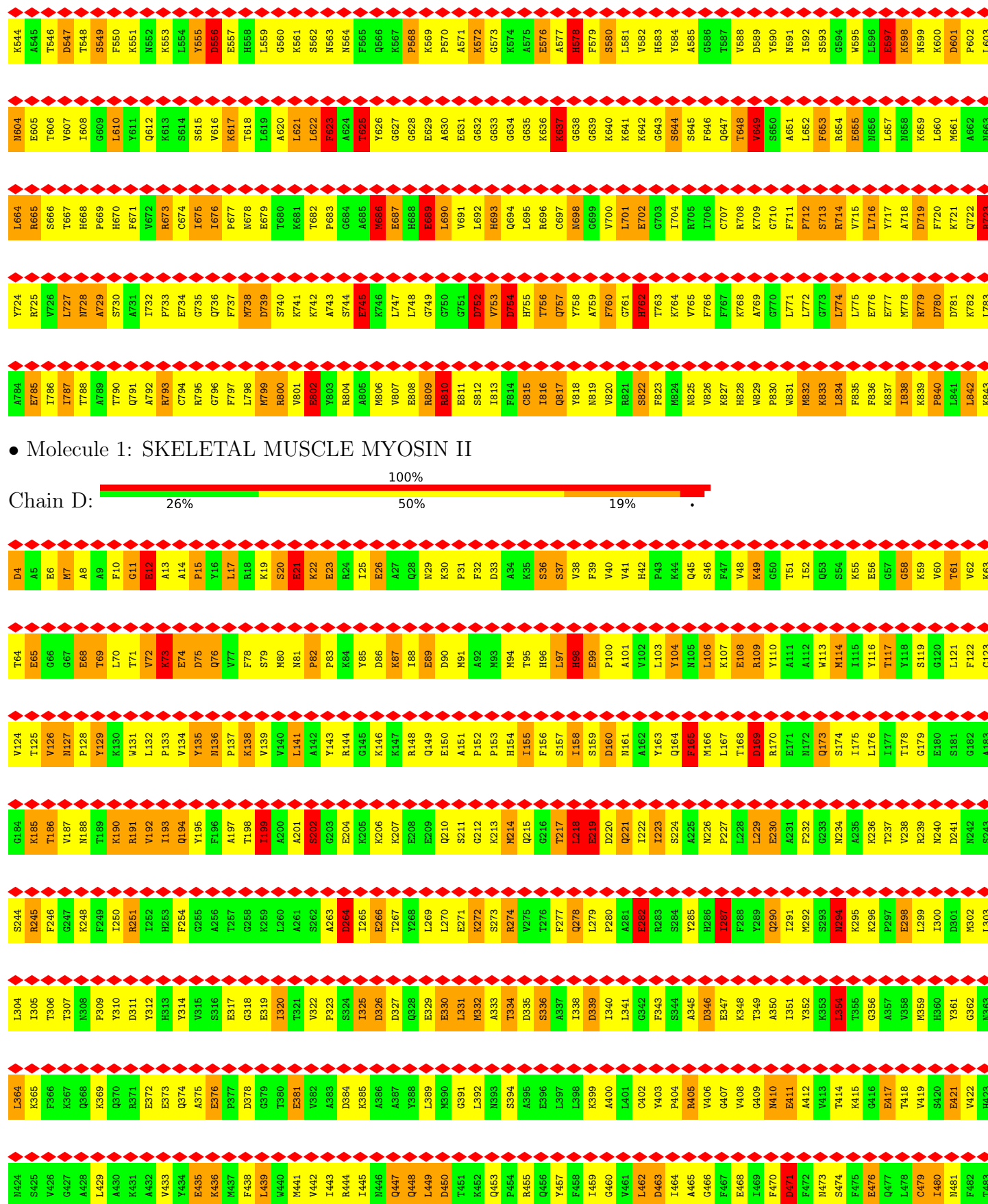
| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 4 | 1 | 372 | Total | C | N | O | S | 0 | 0 |
| | | | 2906 | 1836 | 489 | 561 | 20 | | |
| 4 | 2 | 372 | Total | C | N | O | S | 0 | 0 |
| | | | 2906 | 1836 | 489 | 561 | 20 | | |
| 4 | 3 | 372 | Total | C | N | O | S | 0 | 0 |
| | | | 2906 | 1836 | 489 | 561 | 20 | | |
| 4 | 4 | 372 | Total | C | N | O | S | 0 | 0 |
| | | | 2906 | 1836 | 489 | 561 | 20 | | |
| 4 | 5 | 372 | Total | C | N | O | S | 0 | 0 |
| | | | 2906 | 1836 | 489 | 561 | 20 | | |
| 4 | 6 | 372 | Total | C | N | O | S | 0 | 0 |
| | | | 2906 | 1836 | 489 | 561 | 20 | | |
| 4 | 7 | 372 | Total | C | N | O | S | 0 | 0 |
| | | | 2906 | 1836 | 489 | 561 | 20 | | |
| 4 | 8 | 372 | Total | C | N | O | S | 0 | 0 |
| | | | 2906 | 1836 | 489 | 561 | 20 | | |
| 4 | 9 | 372 | Total | C | N | O | S | 0 | 0 |
| | | | 2906 | 1836 | 489 | 561 | 20 | | |
| 4 | V | 372 | Total | C | N | O | S | 0 | 0 |
| | | | 2906 | 1836 | 489 | 561 | 20 | | |
| 4 | W | 372 | Total | C | N | O | S | 0 | 0 |
| | | | 2906 | 1836 | 489 | 561 | 20 | | |
| 4 | X | 372 | Total | C | N | O | S | 0 | 0 |
| | | | 2906 | 1836 | 489 | 561 | 20 | | |
| 4 | Y | 372 | Total | C | N | O | S | 0 | 0 |
| | | | 2906 | 1836 | 489 | 561 | 20 | | |
| 4 | Z | 372 | Total | C | N | O | S | 0 | 0 |
| | | | 2906 | 1836 | 489 | 561 | 20 | | |

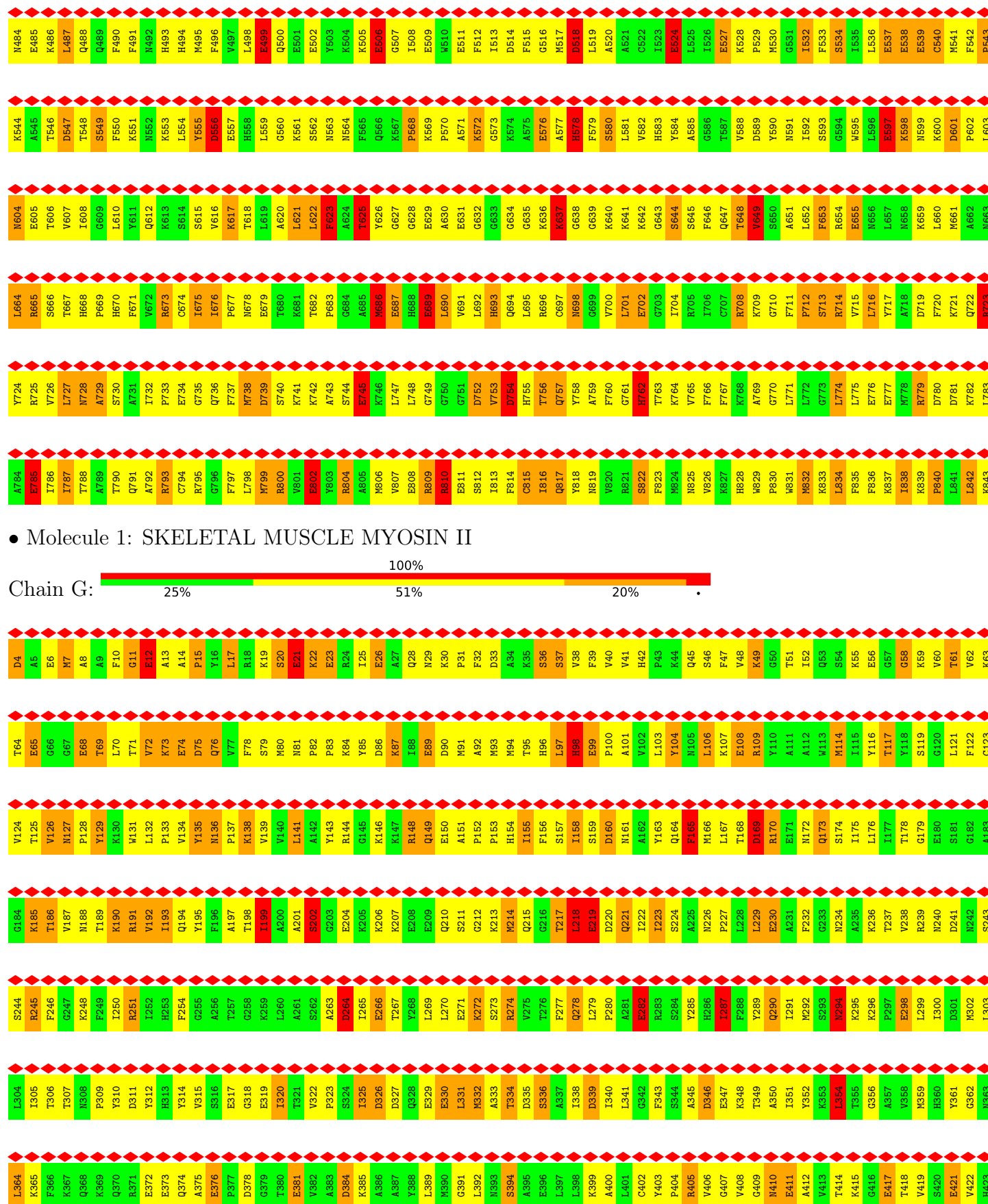
3 Residue-property plots

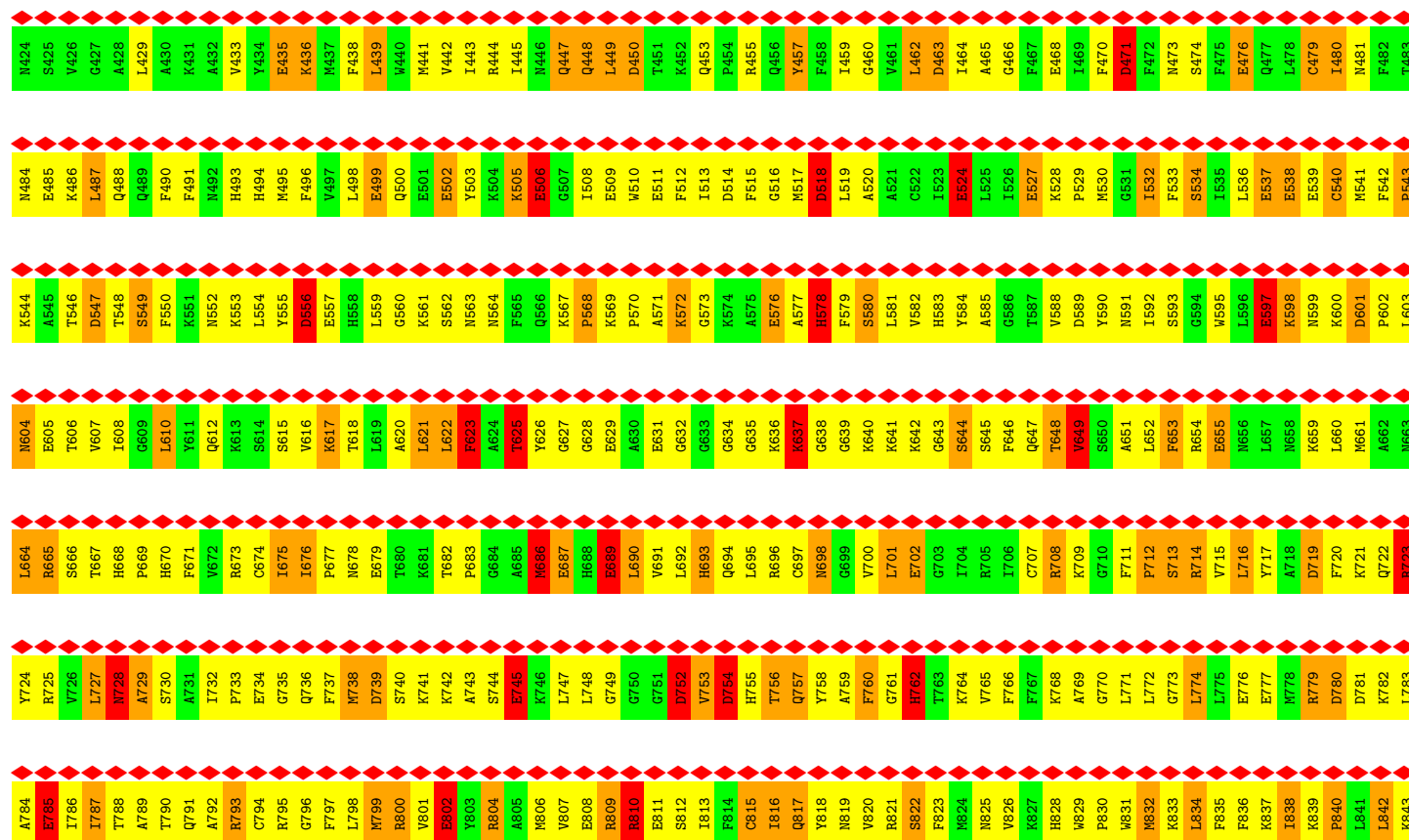
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: SKELETAL MUSCLE MYOSIN II

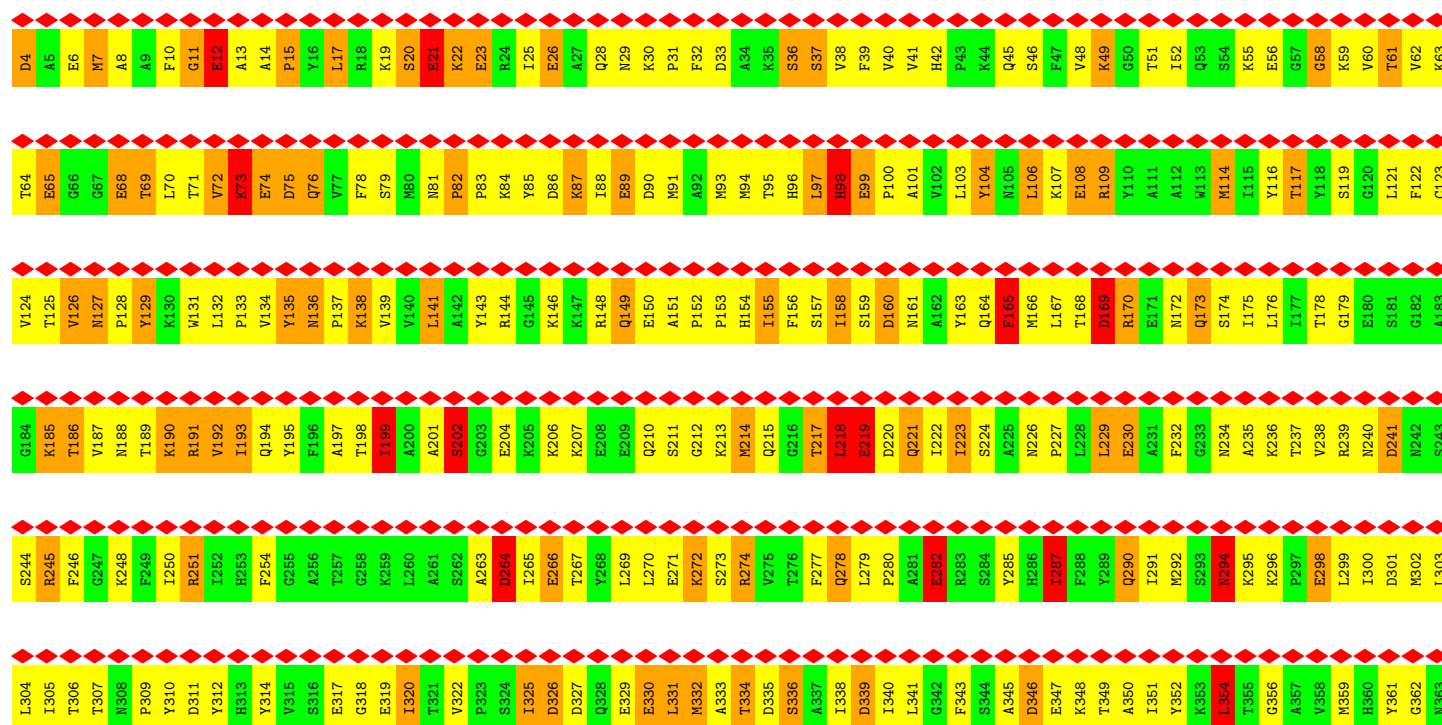








• Molecule 1: SKELETAL MUSCLE MYOSIN II



| | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|
| A784 | R785 | I786 | T787 | A788 | A789 | T790 | Q791 | A792 | R793 | C794 | R795 | G796 | F797 | M798 | M799 | R800 | V801 | E802 | Y803 | R804 | A805 | M806 | V807 | E808 | R809 | R810 | E811 | S812 | L813 | F814 | C815 | L816 | Q817 | Y818 | N819 | V820 | R821 | S822 | F823 | M824 | N825 | V826 | K827 | H828 | V829 | P830 | M831 | N832 | K833 | L834 | F835 | P836 | K837 | T838 | K839 | P840 | L841 | L842 | K843 |
| Y724 | R725 | V726 | L727 | T728 | A729 | S730 | A731 | I732 | P733 | E734 | G735 | Q736 | F737 | M738 | D739 | S740 | K741 | K742 | A743 | S744 | E745 | K746 | L747 | L748 | G749 | G750 | G751 | D752 | V753 | D754 | H755 | T756 | Q757 | Y758 | A759 | F760 | G761 | R762 | T763 | K764 | V765 | F766 | F767 | K768 | A769 | G770 | L771 | L772 | G773 | L774 | L775 | E776 | E777 | M778 | R779 | D780 | D781 | K782 | L783 |
| L664 | R665 | S666 | T667 | H668 | P669 | H670 | F671 | V672 | K673 | C674 | I675 | I676 | P677 | N678 | E679 | T680 | K681 | T682 | P683 | G684 | A685 | M686 | E687 | H688 | E689 | L690 | V691 | L692 | H693 | Q694 | L695 | R696 | C697 | N698 | G699 | V700 | L701 | E702 | G703 | T704 | R705 | I706 | G707 | R708 | K709 | G710 | F711 | P712 | S713 | R714 | V715 | L716 | Y717 | A718 | D719 | F720 | D721 | Q722 | R723 |
| N604 | E605 | T606 | V607 | I608 | G609 | L610 | Y611 | Q612 | K613 | S614 | S615 | V616 | K617 | T618 | L619 | A620 | L621 | L622 | F623 | A624 | Y625 | Y626 | G627 | G628 | E629 | A630 | E631 | G632 | G633 | G634 | G635 | K636 | K637 | G638 | G639 | K640 | K641 | K642 | G643 | S644 | S645 | F646 | Q647 | T648 | V649 | S650 | A651 | L652 | F653 | R654 | E655 | M656 | L657 | M658 | K659 | L660 | M661 | A662 | N663 |
| K544 | A545 | T546 | D547 | T548 | S549 | F550 | K551 | N552 | K553 | L554 | D555 | D556 | E557 | H558 | L559 | G560 | K561 | S562 | N563 | N564 | F565 | Q566 | K567 | P568 | K569 | P570 | A571 | K572 | G573 | K574 | A575 | E576 | A577 | H578 | F579 | S580 | L581 | V582 | H583 | Y584 | A585 | G586 | T587 | V588 | D589 | Y590 | N591 | I592 | F593 | G594 | L595 | E596 | E597 | K598 | N599 | K600 | D601 | P602 | L603 |
| N484 | E485 | K486 | L487 | Q488 | Q489 | F490 | F491 | N492 | H493 | H494 | M495 | F496 | D497 | L498 | E499 | Q500 | E501 | E502 | Y503 | K504 | K505 | E506 | I507 | I508 | E509 | W510 | E511 | F512 | I513 | D514 | F515 | G516 | M517 | D518 | L519 | A520 | A521 | C522 | I523 | E524 | L525 | I526 | E527 | K528 | P529 | M530 | G531 | I532 | F533 | S534 | I535 | L536 | E537 | E538 | E539 | C540 | M541 | F542 | P543 |
| N424 | S425 | V426 | G427 | A428 | L429 | A430 | K431 | A432 | V433 | Y434 | E435 | A436 | M437 | F438 | L439 | M440 | V442 | I443 | R444 | I445 | M446 | Q447 | Q448 | L449 | D450 | T451 | K452 | Q453 | P454 | R455 | Q456 | G457 | F458 | I459 | G460 | V461 | L462 | D463 | I464 | A465 | G466 | F467 | E468 | I469 | F470 | D471 | F472 | N473 | S474 | F475 | E476 | Q477 | L478 | C479 | I480 | M481 | F482 | T483 | |
| L364 | K365 | F366 | K367 | Q368 | K369 | Q370 | R371 | E372 | E373 | Q374 | A375 | E376 | P377 | D378 | G379 | T380 | E381 | V382 | A383 | D384 | K385 | A386 | A387 | L388 | L389 | M390 | G391 | L392 | N393 | S394 | A395 | E396 | L397 | L398 | K399 | A400 | L401 | C402 | Y403 | P404 | R405 | V406 | G407 | V408 | G409 | N410 | E411 | A412 | V413 | T414 | K415 | G416 | E417 | T418 | V419 | S420 | E421 | F422 | H423 |

• Molecule 1: SKELETAL MUSCLE MYOSIN II



| | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|
| D4 | A5 | E6 | M7 | A8 | A9 | F10 | G11 | E12 | A13 | A14 | P15 | Y16 | L17 | R18 | K19 | S20 | E21 | K22 | R23 | I24 | T25 | E26 | Q27 | N28 | K30 | P31 | F32 | D33 | A34 | K35 | S36 | S37 | V38 | F39 | V40 | V41 | H42 | P43 | K44 | Q45 | S46 | F47 | V48 | K49 | G50 | T51 | I52 | Q53 | S54 | K55 | E56 | G58 | K59 | V60 | T61 | V62 | K63 | | |
| T64 | E65 | G66 | G67 | E68 | T69 | L70 | T71 | V72 | K73 | E74 | D75 | Q76 | V77 | F78 | S79 | M80 | N81 | P82 | P83 | K84 | Y85 | D86 | K87 | T88 | E89 | D90 | N91 | A92 | H93 | H94 | T95 | H96 | L97 | H98 | E99 | P100 | A101 | V102 | L103 | Y104 | N105 | L106 | K107 | E108 | R109 | Y110 | A111 | A112 | Q113 | M114 | I115 | Y116 | T117 | Y118 | S119 | G120 | L121 | F122 | C123 |
| V124 | T125 | V126 | N127 | P128 | Y129 | K130 | V131 | L132 | P133 | V134 | Y135 | N136 | P137 | K138 | V139 | Y140 | L141 | A142 | Y143 | G145 | L146 | K147 | L148 | Q149 | E150 | A151 | P152 | P153 | H154 | I155 | F156 | S157 | I158 | S159 | D160 | N161 | A162 | L163 | Q164 | F165 | M166 | L167 | T168 | D169 | R170 | E171 | N172 | Q173 | S174 | I175 | L176 | T177 | T178 | G179 | E180 | S181 | G182 | A183 | |
| G184 | K185 | T186 | V187 | N188 | T189 | K190 | R191 | V192 | I193 | Q194 | Y195 | F196 | A197 | T198 | N199 | A200 | A201 | S202 | G203 | E204 | K206 | K207 | E208 | E209 | Q210 | S211 | G212 | K213 | M214 | Q215 | G216 | T217 | L218 | E219 | D220 | D221 | I222 | L223 | S224 | A225 | N226 | P227 | L228 | L229 | E230 | A231 | F232 | Q233 | N234 | A235 | K236 | T237 | V238 | R239 | N240 | D241 | N242 | S243 | |
| S244 | R245 | F246 | G247 | K248 | F249 | L250 | R251 | L252 | H253 | F254 | G255 | A256 | T257 | G258 | K259 | L260 | A261 | S262 | A263 | D264 | E266 | T267 | Y268 | L269 | L270 | E271 | K272 | S273 | R274 | V275 | T276 | F277 | Q278 | L279 | P280 | A281 | E282 | R283 | S284 | Y285 | H286 | F287 | F288 | Y289 | Q290 | T291 | M292 | S293 | N294 | K295 | K296 | T297 | E298 | L299 | I300 | D301 | K302 | L303 | |

| | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|
| L784 | L785 | L786 | L787 | L788 | L789 | L790 | L791 | L792 | L793 | L794 | L795 | L796 | L797 | L798 | L799 | L800 | L801 | L802 | L803 | L804 | L805 | L806 | L807 | L808 | L809 | L810 | L811 | L812 | L813 | L814 | L815 | L816 | L817 | L818 | L819 | L820 | L821 | L822 | L823 | L824 | L825 | L826 | L827 | L828 | L829 | L830 | L831 | L832 | L833 | L834 | L835 | L836 | L837 | L838 | L839 | L840 | L841 | L842 | L843 |
| Y724 | R725 | V726 | L727 | N728 | A729 | S730 | T731 | I732 | P733 | E734 | G735 | Q736 | F737 | N738 | D739 | K740 | K741 | K742 | A743 | S744 | E745 | K746 | L747 | L748 | G749 | G750 | G751 | D752 | V753 | Q754 | H755 | T756 | Q757 | Y758 | A759 | F760 | G761 | H762 | T763 | K764 | N765 | F766 | F767 | R768 | A769 | G770 | L771 | L772 | G773 | L774 | L775 | E776 | E777 | H778 | R779 | D780 | D781 | K782 | L783 |
| L664 | R665 | S666 | T667 | H668 | P669 | H670 | F671 | V672 | R673 | C674 | L675 | L676 | N677 | N678 | E679 | T680 | K681 | T682 | P683 | G684 | A685 | N686 | E687 | H688 | E689 | L690 | V691 | L692 | H693 | Q694 | L695 | R696 | C697 | N698 | G699 | V700 | L701 | E702 | G703 | I704 | R705 | I706 | C707 | R708 | K709 | G710 | F711 | P712 | S713 | R714 | V715 | L716 | Y717 | A718 | D719 | F720 | K721 | Q722 | R723 |
| M604 | E605 | T606 | V607 | T608 | G609 | L610 | Y611 | Q612 | K613 | S614 | S615 | V616 | K617 | T618 | L619 | A620 | L621 | L622 | F623 | A624 | T625 | Y626 | G627 | G628 | E629 | A630 | E631 | G632 | G633 | G634 | G635 | K636 | K637 | G638 | G639 | K640 | K641 | K642 | G643 | S644 | S645 | F646 | Q647 | T648 | V649 | S650 | A651 | L652 | F653 | R654 | E655 | N656 | L657 | N658 | K659 | L660 | M661 | A662 | N663 |
| K544 | A545 | T546 | D547 | T548 | S549 | F550 | K551 | N552 | K553 | L554 | Y555 | D556 | E557 | H558 | L559 | G560 | K561 | S562 | N563 | N564 | F565 | Q566 | K567 | P568 | K569 | P570 | A571 | K572 | G573 | K574 | A575 | E576 | A577 | H578 | F579 | S580 | L581 | V582 | H583 | Y584 | A585 | G586 | T587 | V588 | D589 | Y590 | N591 | I592 | S593 | G594 | N595 | L596 | E597 | K598 | N599 | K600 | D601 | P602 | L603 |
| N484 | E485 | K486 | L487 | Q488 | Q489 | F490 | K491 | M492 | H493 | H494 | M495 | F496 | V497 | L498 | E499 | Q500 | E501 | E502 | Y503 | K504 | K505 | E506 | G507 | I508 | E509 | W510 | E511 | F512 | I513 | D514 | F515 | G516 | N517 | D518 | L519 | A520 | A521 | C522 | I523 | E524 | L525 | I526 | E527 | K528 | P529 | M530 | G531 | I532 | F533 | S534 | I535 | L536 | E537 | E538 | E539 | C540 | M541 | F542 | P543 |
| N424 | A425 | V426 | G427 | A428 | L429 | A430 | K431 | A432 | V433 | Y434 | E435 | K436 | M437 | F438 | L439 | W440 | M441 | V442 | I443 | R444 | I445 | M446 | Q447 | Q448 | L449 | D450 | T451 | K452 | Q453 | P454 | R455 | Q456 | G457 | F458 | I459 | G460 | V461 | L462 | D463 | I464 | A465 | G466 | F467 | E468 | I469 | F470 | D471 | F472 | N473 | S474 | F475 | E476 | Q477 | L478 | C479 | I480 | N481 | F482 | T483 |
| L364 | K365 | F366 | K367 | Q368 | K369 | Q370 | R371 | E372 | E373 | Q374 | A375 | E376 | P377 | D378 | G379 | T380 | E381 | V382 | A383 | D384 | K385 | A386 | A387 | Y388 | L389 | M390 | E391 | L392 | N393 | S394 | A395 | E396 | G397 | L398 | K399 | A400 | L401 | C402 | Y403 | P404 | A405 | V406 | G407 | V408 | G409 | N410 | E411 | A412 | T414 | K415 | G416 | A417 | T418 | V419 | S420 | N421 | V422 | H423 | |
| L304 | L305 | T306 | T307 | N308 | P309 | Y310 | D311 | Y312 | H313 | Y314 | V315 | S316 | E317 | G318 | E319 | I320 | T321 | V322 | P323 | S324 | I325 | D326 | D327 | Q328 | E329 | E330 | L331 | M332 | A333 | T334 | S335 | S336 | A337 | I338 | D339 | I340 | L341 | G342 | F343 | S344 | A345 | D346 | E347 | K348 | T349 | A350 | I351 | Y352 | K353 | L354 | T355 | G356 | A357 | V358 | M359 | H360 | Y361 | G362 | N363 |

● Molecule 1: SKELETAL MUSCLE MYOSIN II



| | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|
| G184 | K185 | T186 | V187 | N188 | T189 | K190 | R191 | V192 | I193 | Q194 | Y195 | F196 | A197 | T198 | I199 | A200 | A201 | S202 | G203 | E204 | K205 | K206 | K207 | E208 | E209 | Q210 | S211 | G212 | K213 | M214 | Q215 | G216 | T217 | L218 | E219 | D220 | Q221 | I222 | I223 | S224 | A225 | N226 | P227 | L228 | L229 | E230 | A231 | F232 | K233 | N234 | A235 | K236 | T237 | V238 | R239 | N240 | D241 | N242 | S243 |
| V124 | T125 | V126 | N127 | P128 | Y129 | K130 | W131 | L132 | P133 | V134 | Y135 | N136 | P137 | K138 | V139 | V140 | L141 | A142 | Y143 | R144 | G145 | K146 | L147 | R148 | Q149 | Q210 | A151 | P152 | P153 | H154 | I155 | F156 | S157 | I158 | S159 | D160 | N161 | A162 | Y163 | Q164 | F165 | M166 | L167 | T168 | D169 | R170 | E171 | N172 | Q173 | S174 | I175 | L176 | I177 | T178 | G179 | E180 | S181 | G182 | A183 |
| T64 | E65 | G66 | G67 | E68 | T69 | L70 | T71 | V72 | K73 | E74 | D75 | Q76 | V77 | F78 | S79 | M80 | N81 | P82 | P83 | R84 | D86 | K87 | I88 | E89 | D90 | M91 | A92 | M93 | N94 | T95 | H96 | L97 | H98 | E99 | P100 | A101 | V102 | L103 | Y104 | N105 | L106 | I107 | K108 | R109 | Y110 | A111 | A112 | M113 | M114 | I115 | Y116 | T117 | Y118 | S119 | G120 | L121 | F122 | C123 | |
| D4 | A5 | E6 | M7 | A8 | A9 | F10 | G11 | E12 | A13 | A14 | P15 | Y16 | L17 | R18 | K19 | S20 | E21 | K22 | E23 | R24 | I25 | E26 | Q27 | N29 | K30 | P31 | F32 | D33 | A34 | K35 | S36 | S37 | V38 | F39 | V40 | V41 | H42 | P43 | K44 | Q45 | S46 | F47 | V48 | K49 | G50 | T51 | I52 | Q53 | S54 | K55 | E56 | G57 | G58 | K59 | V60 | T61 | V62 | K63 | |



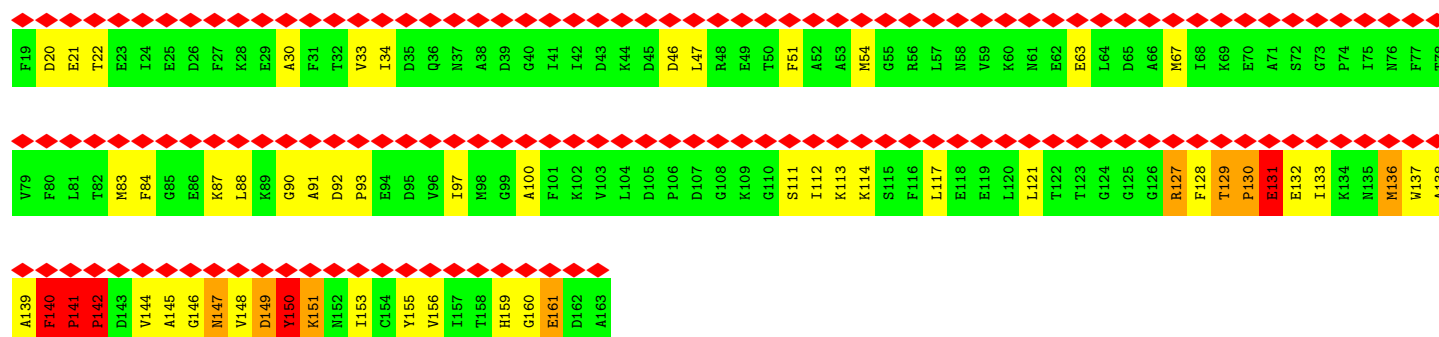
| Device Type | Percentage |
|---------------|------------|
| Smartphones | 100% |
| Tablets | 68% |
| Smart TVs | 23% |
| Other devices | 6% |



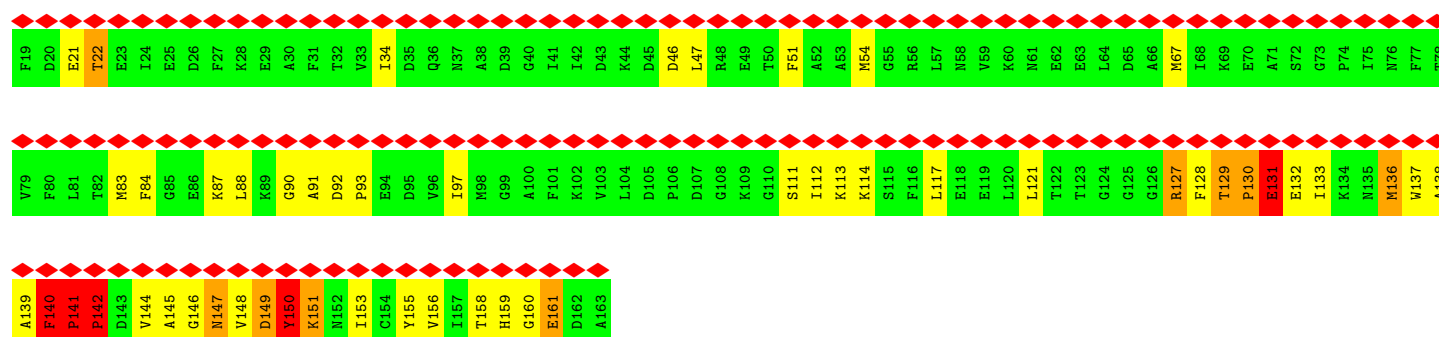
• Molecule 2: SKELETAL MUSCLE MYOSIN II REGULATORY LIGHT CHAIN



• Molecule 2: SKELETAL MUSCLE MYOSIN II REGULATORY LIGHT CHAIN

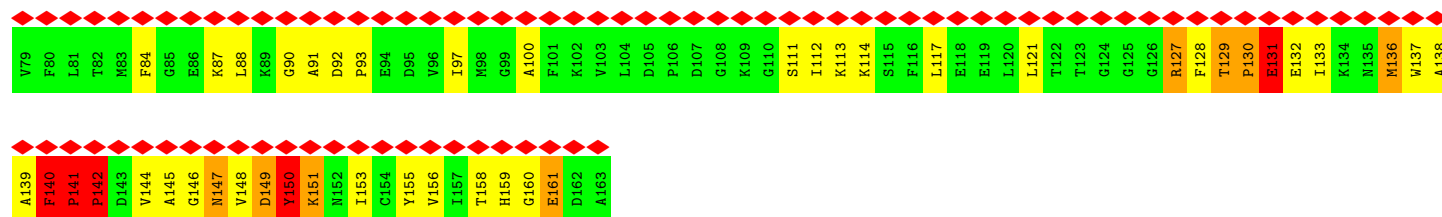


• Molecule 2: SKELETAL MUSCLE MYOSIN II REGULATORY LIGHT CHAIN

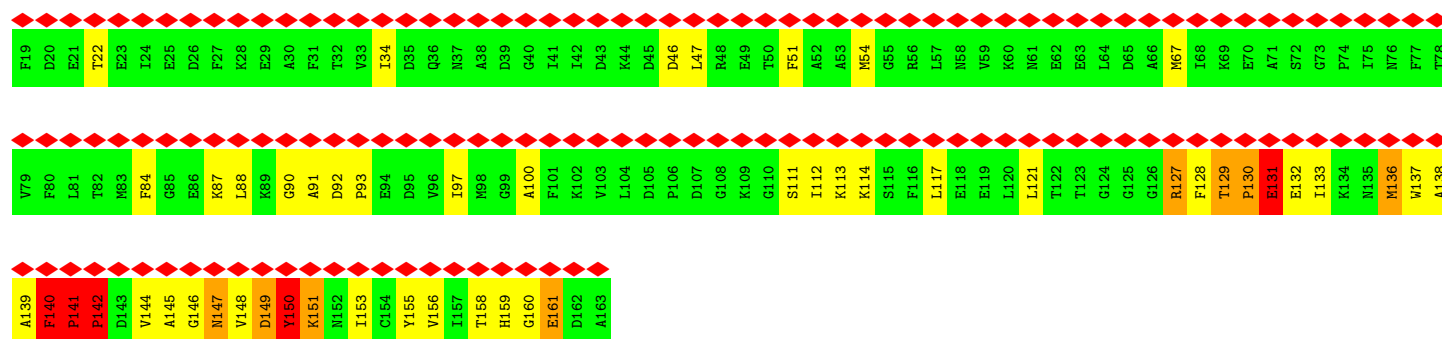


• Molecule 2: SKELETAL MUSCLE MYOSIN II REGULATORY LIGHT CHAIN

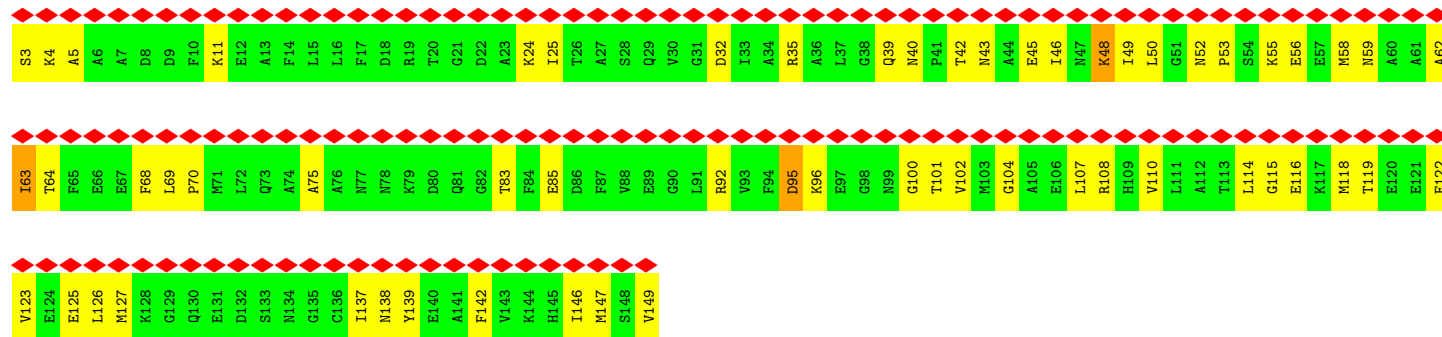




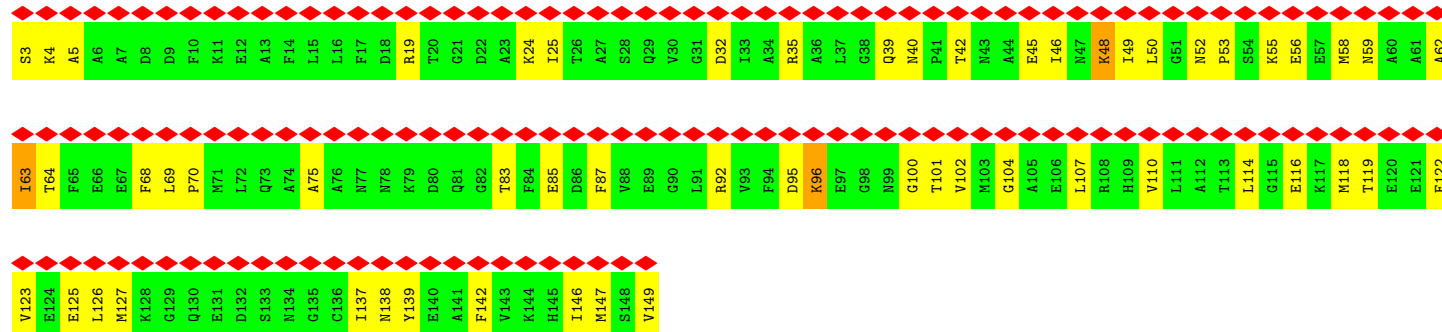
• Molecule 2: SKELETAL MUSCLE MYOSIN II REGULATORY LIGHT CHAIN



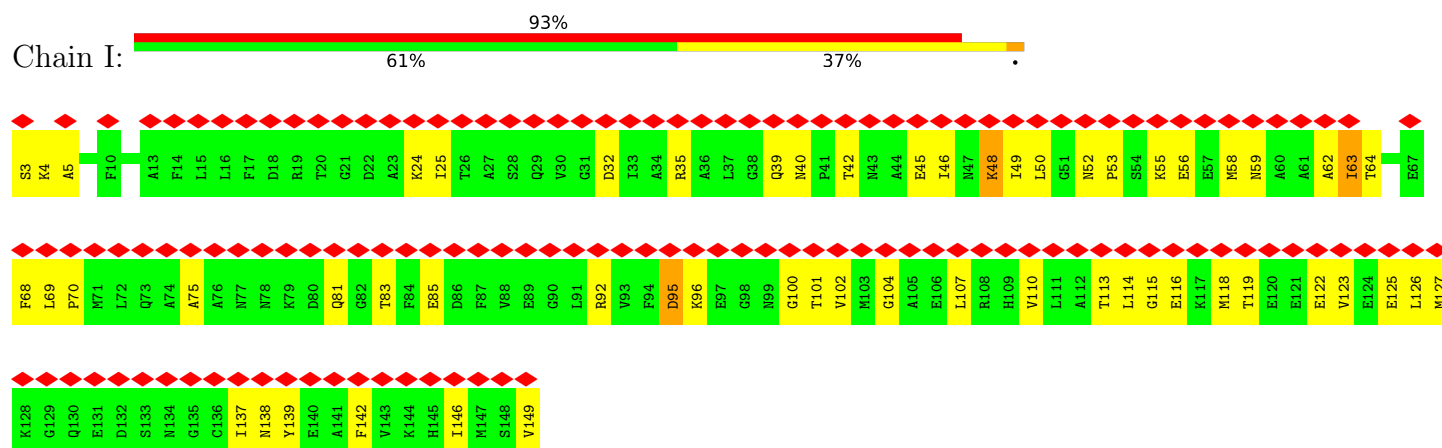
• Molecule 3: SKELETAL MUSCLE MYOSIN II ESSENTIAL LIGHT CHAIN



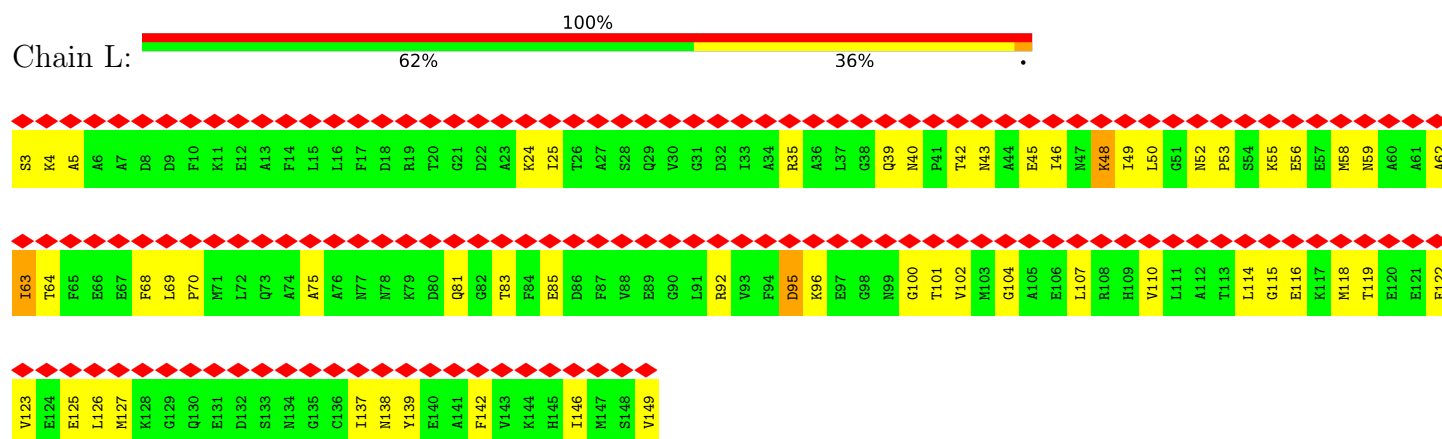
• Molecule 3: SKELETAL MUSCLE MYOSIN II ESSENTIAL LIGHT CHAIN



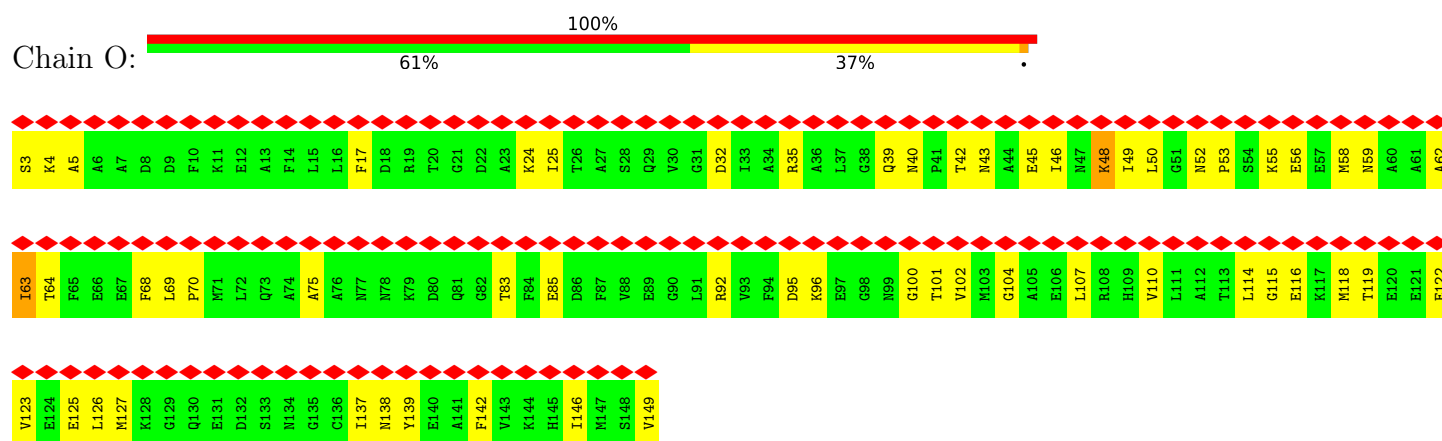
- Molecule 3: SKELETAL MUSCLE MYOSIN II ESSENTIAL LIGHT CHAIN



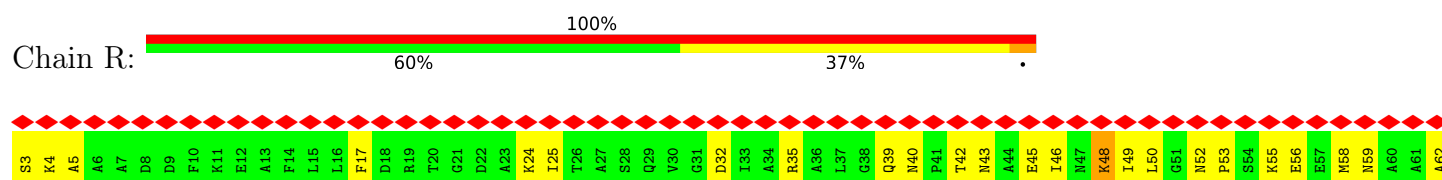
- Molecule 3: SKELETAL MUSCLE MYOSIN II ESSENTIAL LIGHT CHAIN

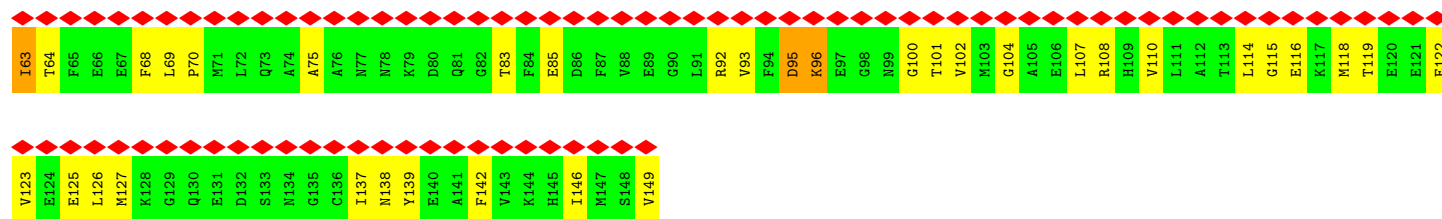


- Molecule 3: SKELETAL MUSCLE MYOSIN II ESSENTIAL LIGHT CHAIN

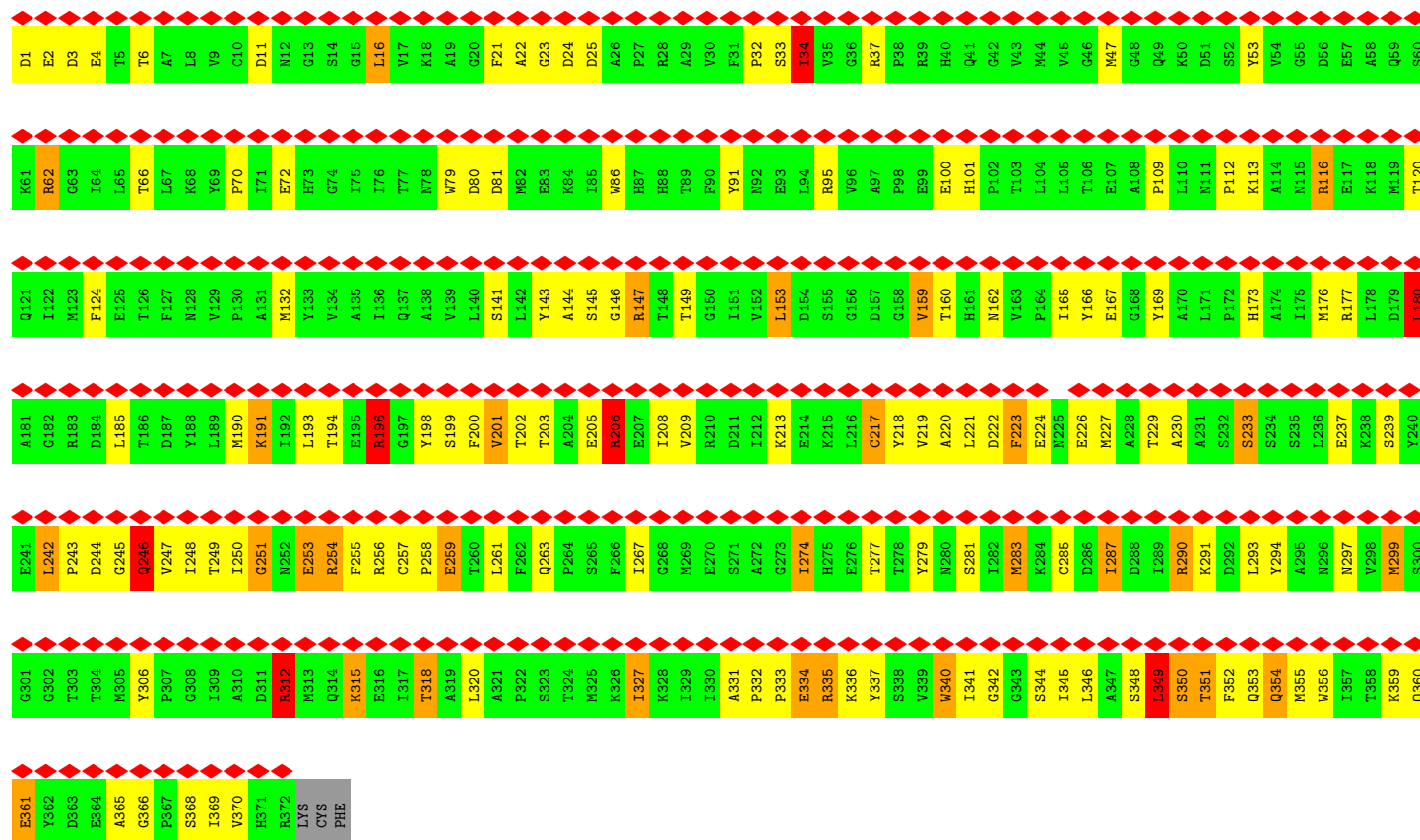


- Molecule 3: SKELETAL MUSCLE MYOSIN II ESSENTIAL LIGHT CHAIN

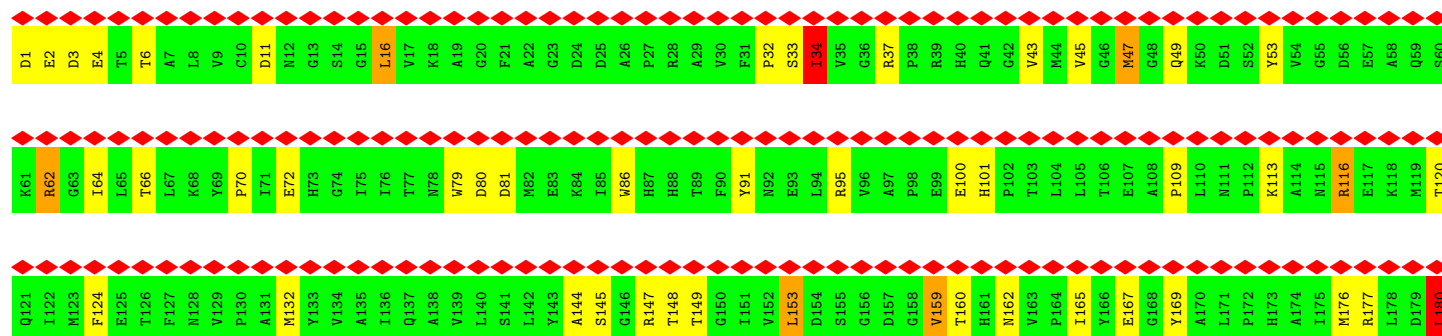




• Molecule 4: SKELETAL MUSCLE ACTIN

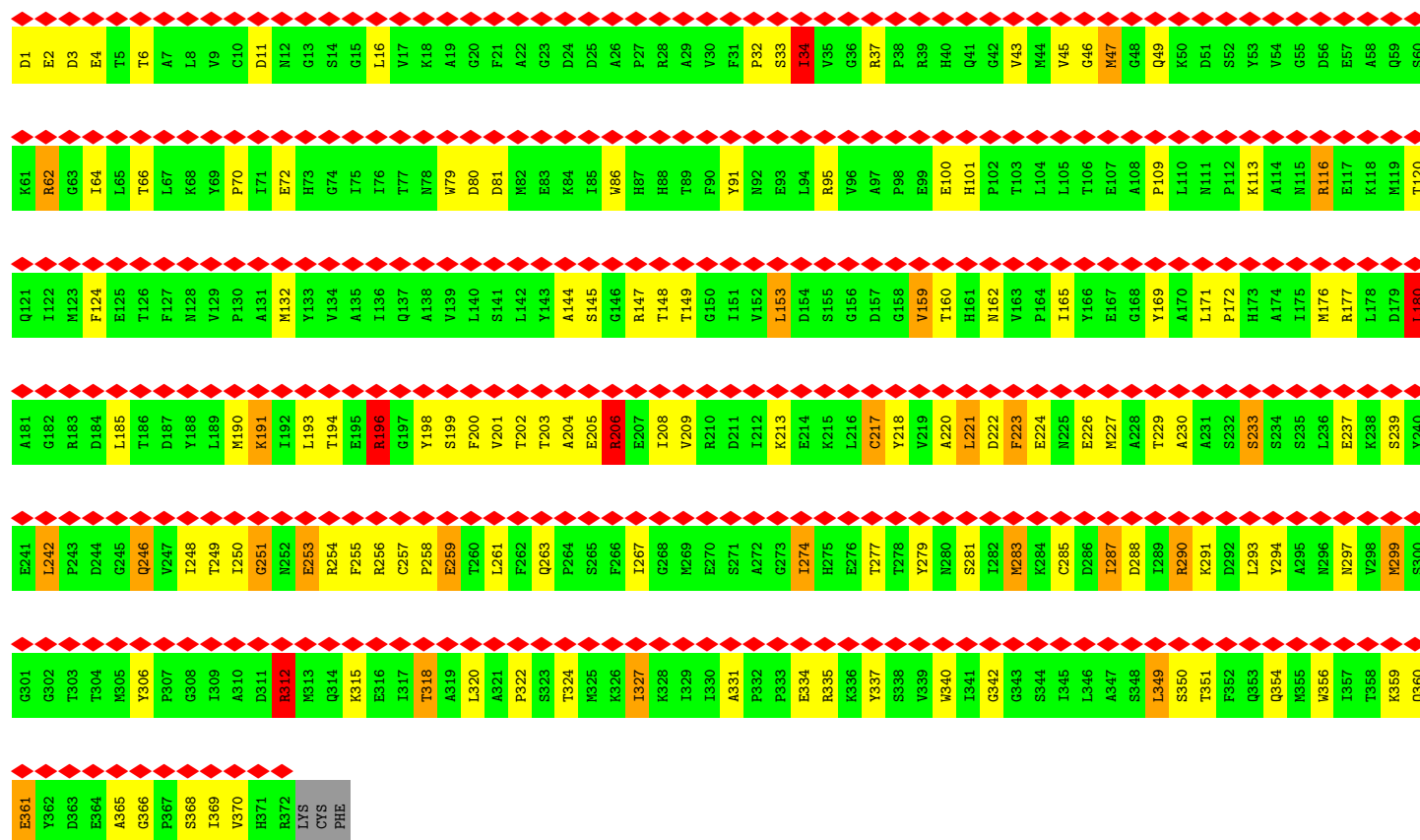


• Molecule 4: SKELETAL MUSCLE ACTIN

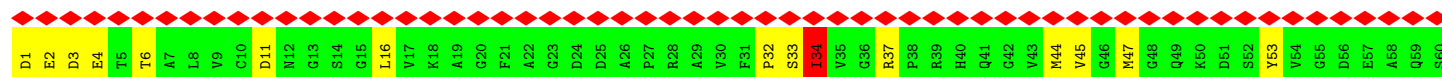


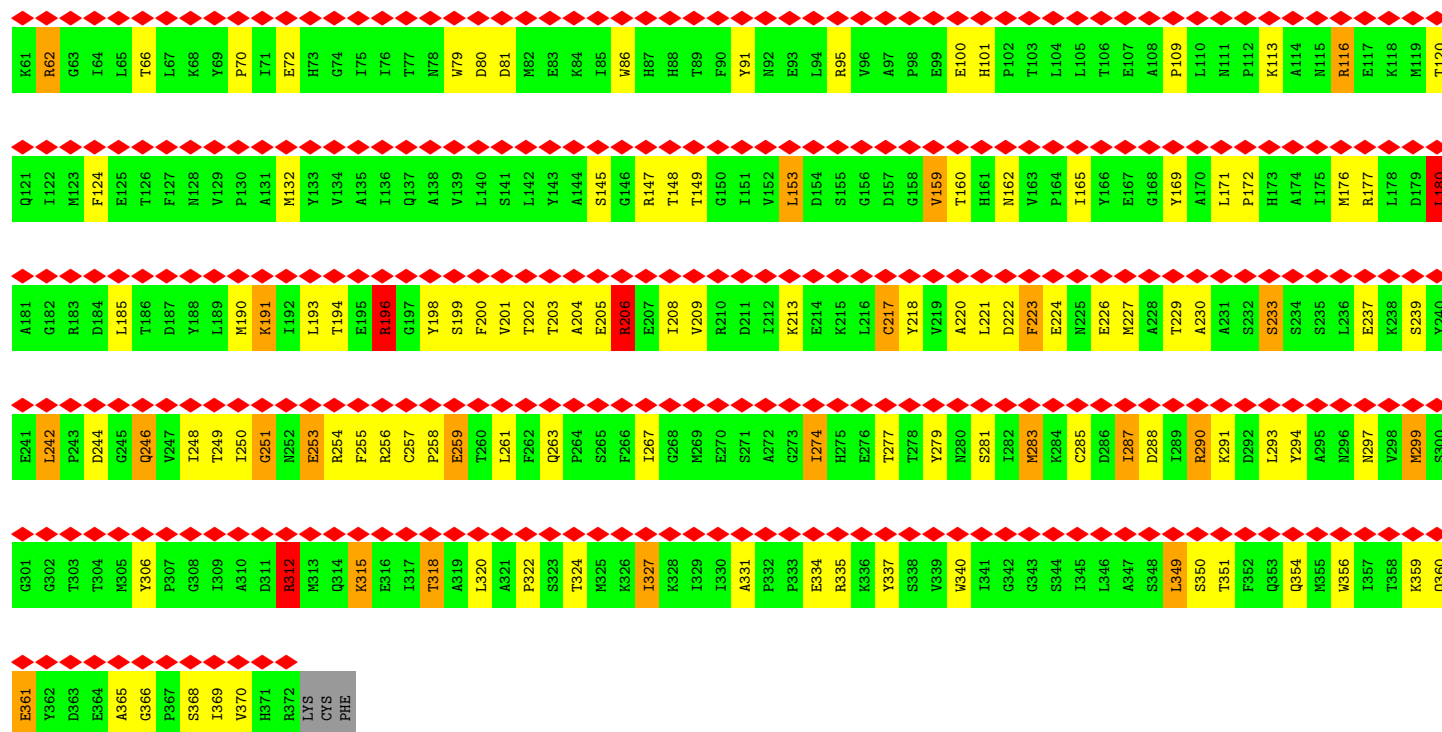


• Molecule 4: SKELETAL MUSCLE ACTIN

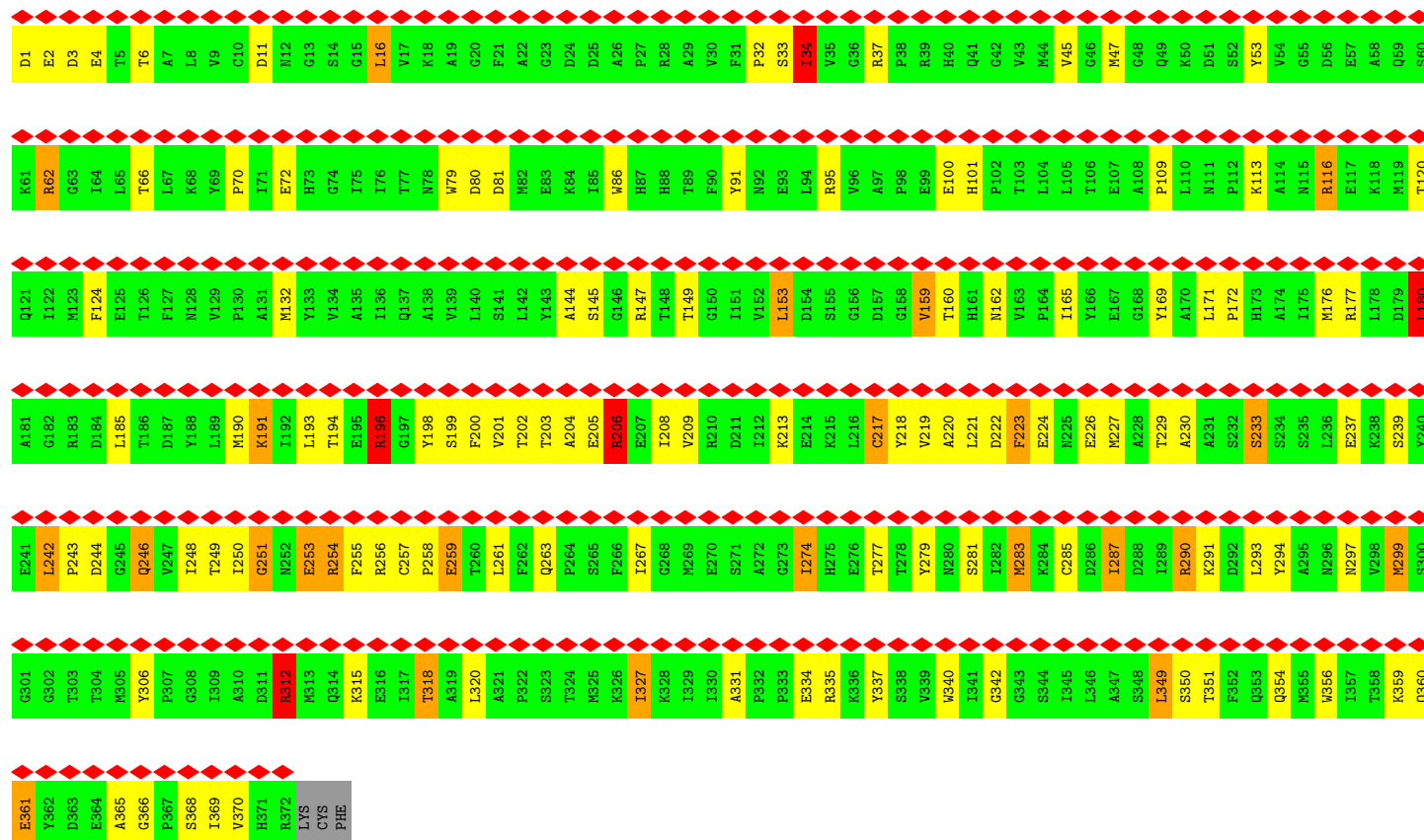


• Molecule 4: SKELETAL MUSCLE ACTIN



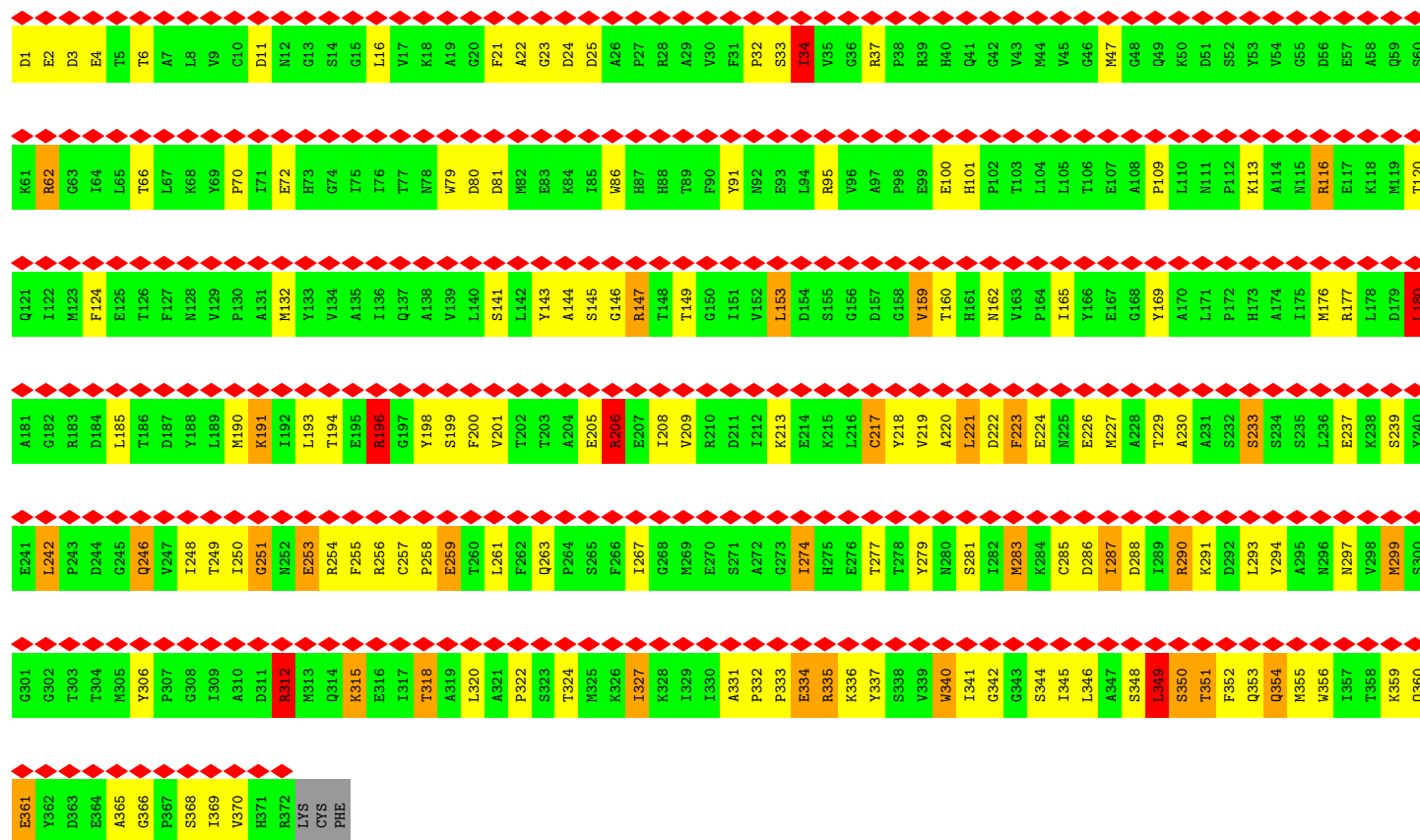


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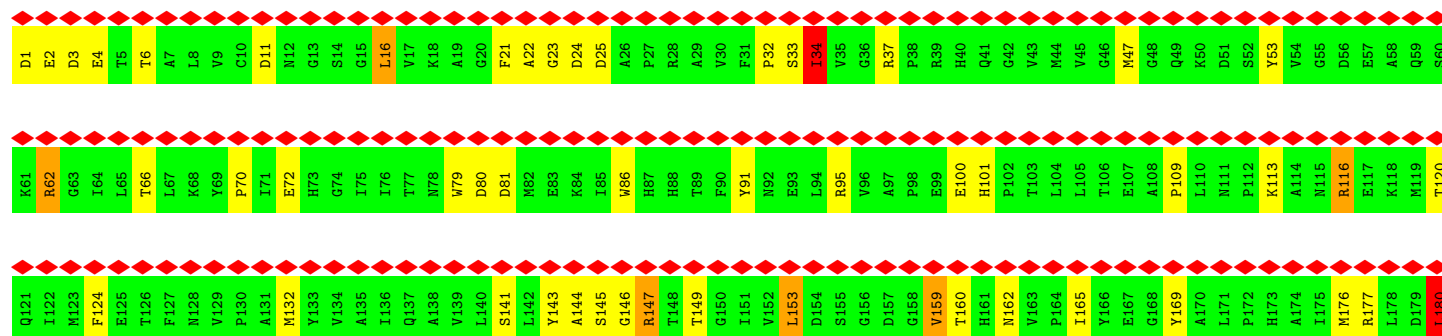


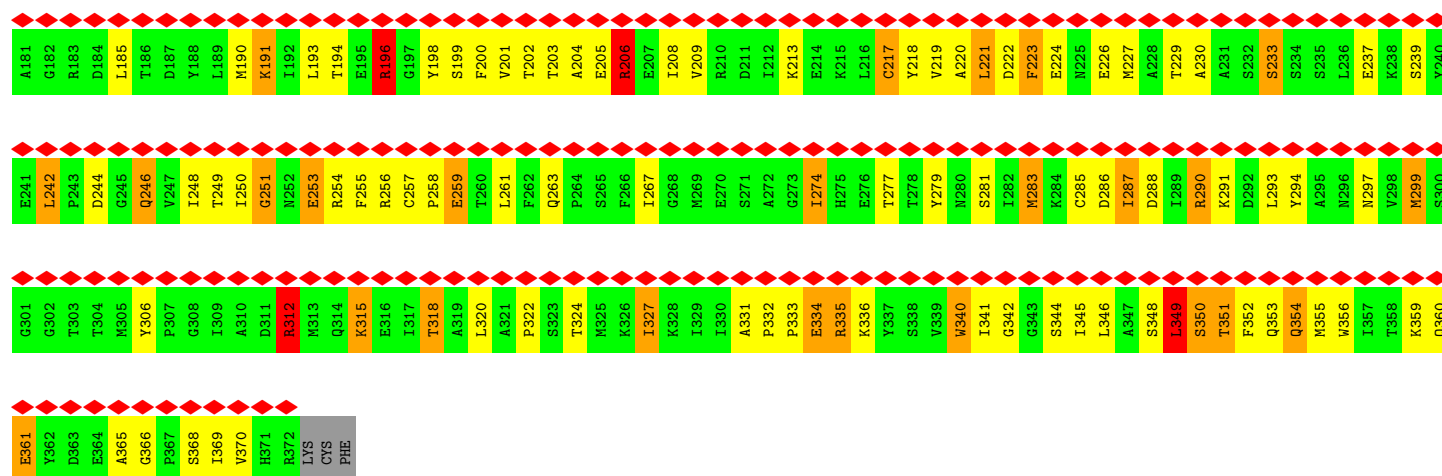


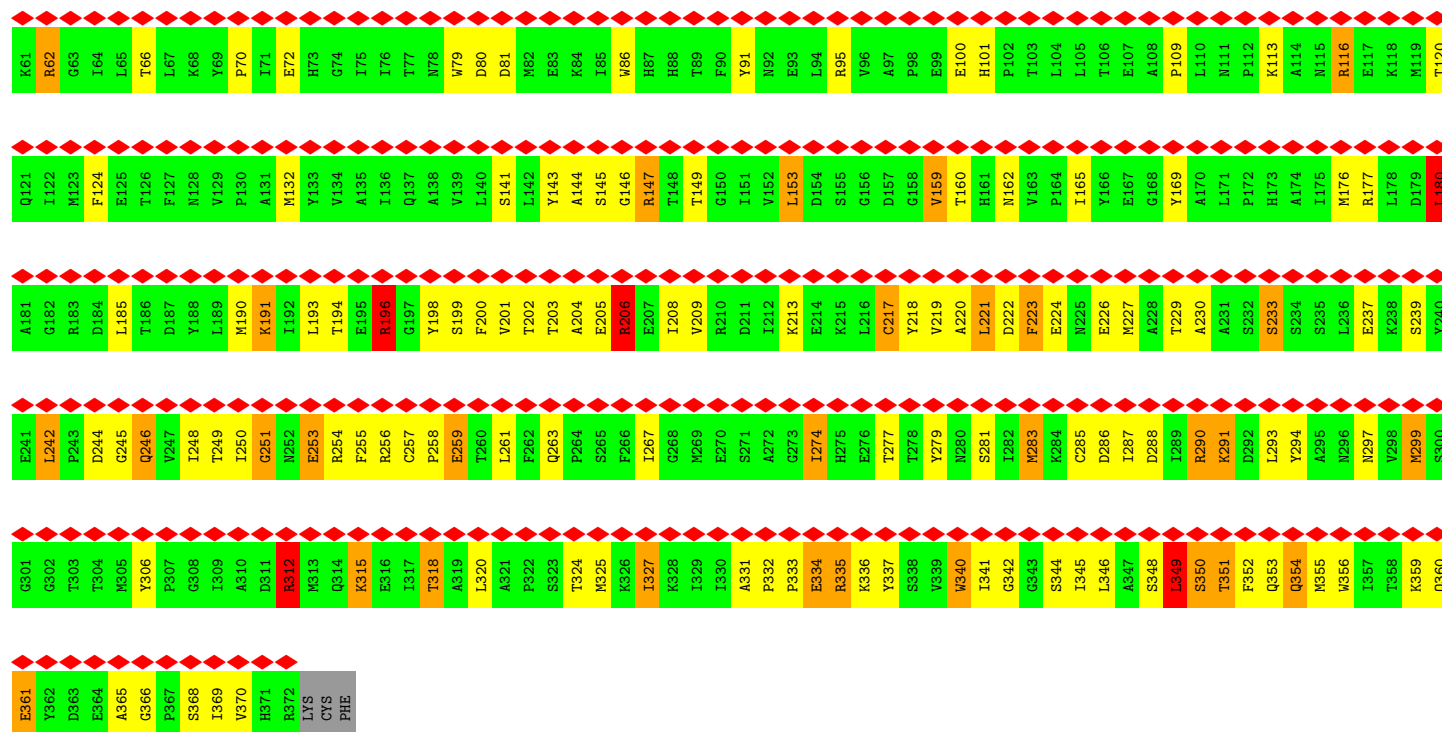
• Molecule 4: SKELETAL MUSCLE ACTIN



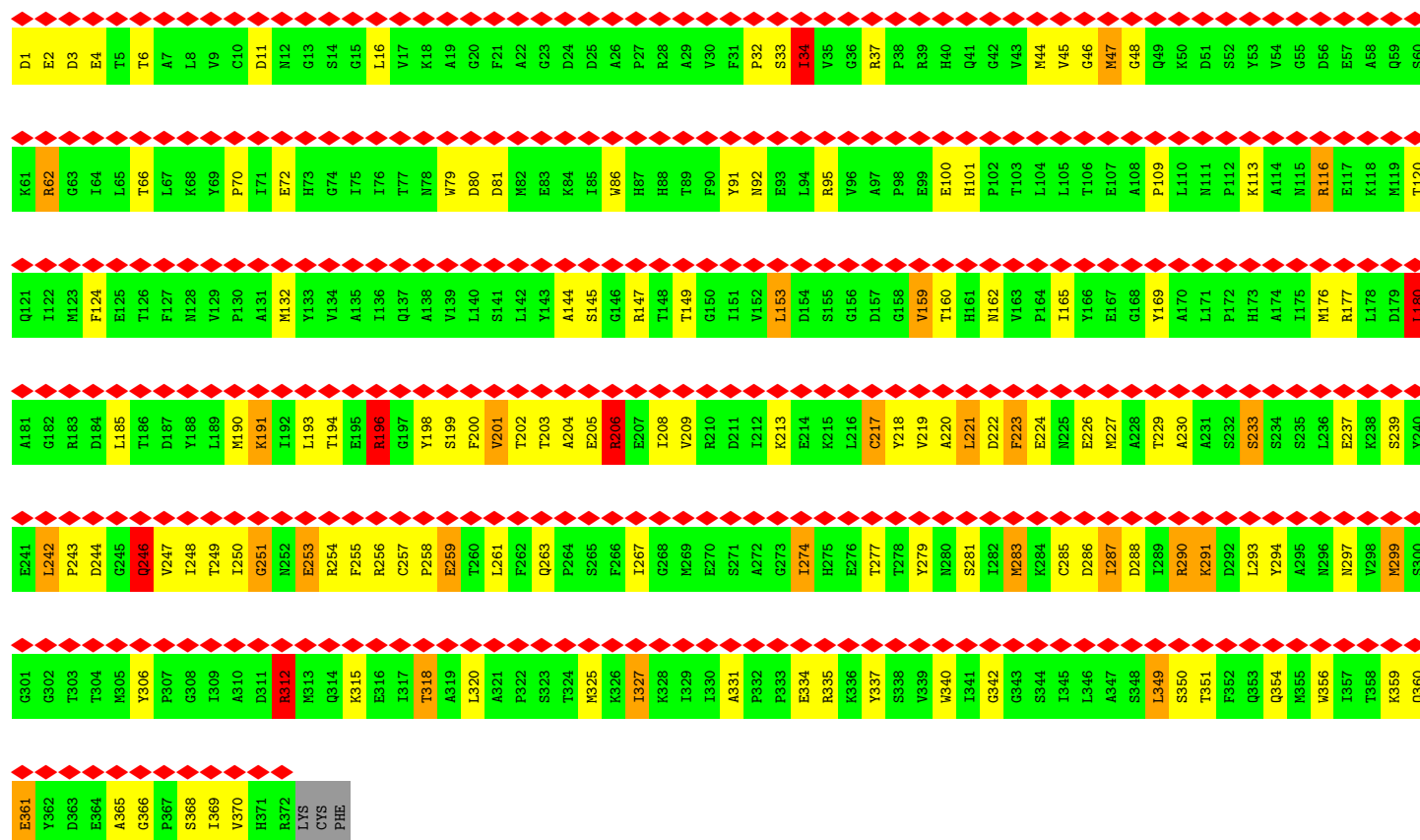
• Molecule 4: SKELETAL MUSCLE ACTIN





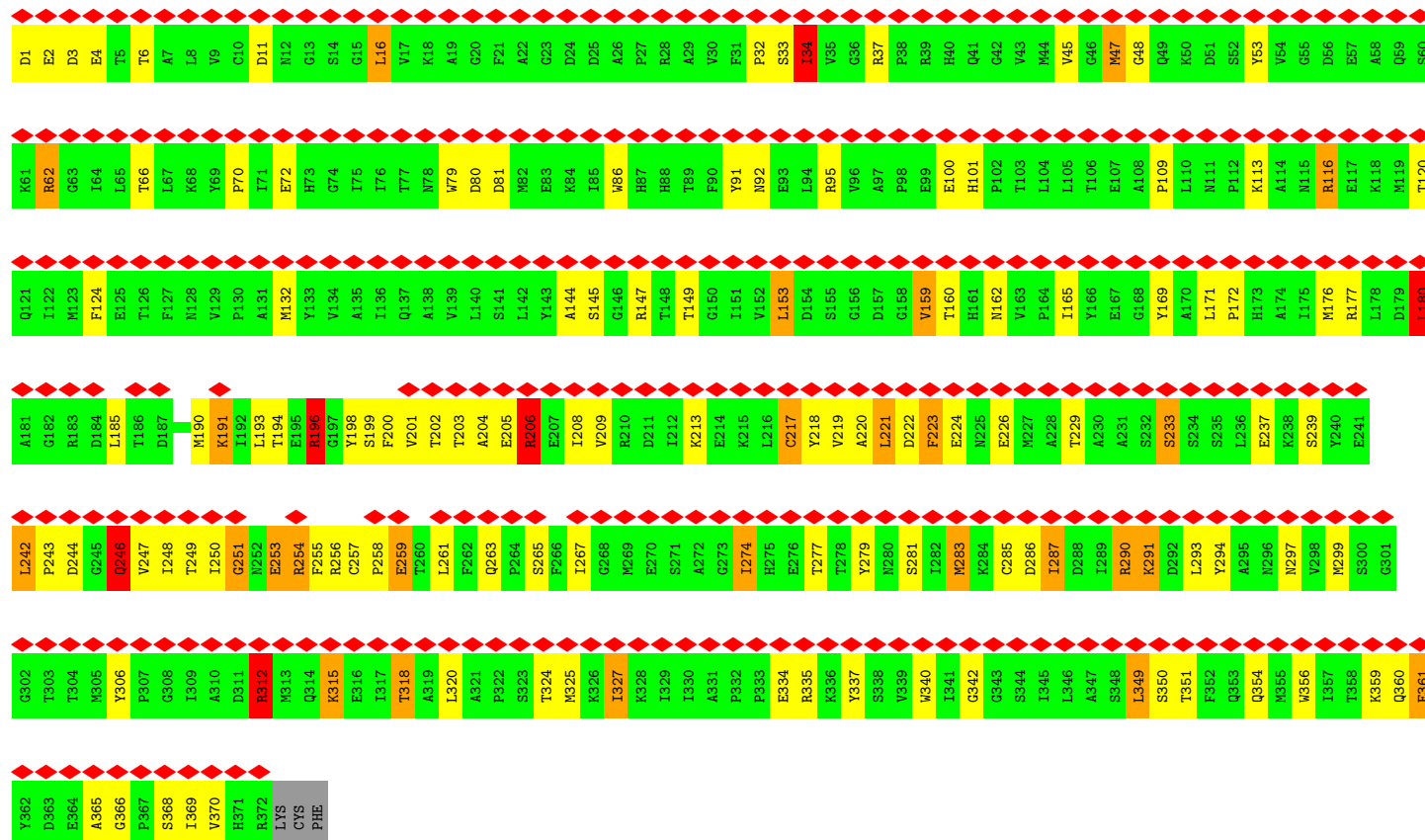


• Molecule 4: SKELETAL MUSCLE ACTIN



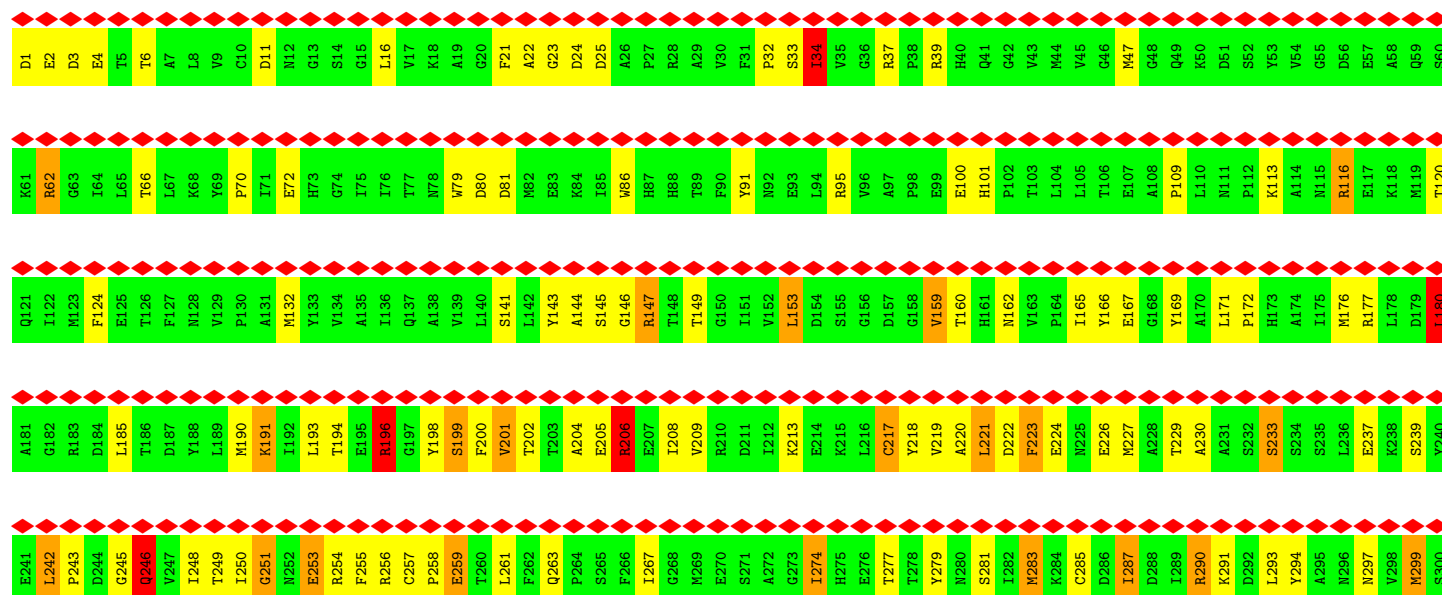
● Molecule 4: SKELETAL MUSCLE ACTIN

Chain Y: 



● Molecule 4: SKELETAL MUSCLE ACTIN

Chain Z: 



| | |
|------|------|
| E361 | G301 |
| Y362 | G302 |
| D363 | T303 |
| E364 | T304 |
| A365 | M305 |
| G366 | Y306 |
| P367 | P307 |
| S368 | G308 |
| T369 | T309 |
| V370 | A310 |
| H371 | D311 |
| R372 | R312 |
| LYS | M313 |
| CYS | Q314 |
| PHE | K315 |
| | E316 |
| | I317 |
| | T318 |
| | A319 |
| | L320 |
| | A321 |
| | P322 |
| | S323 |
| | T324 |
| | M325 |
| | K326 |
| | I327 |
| | K328 |
| | T329 |
| | T330 |
| | A331 |
| | P332 |
| | P333 |
| | E334 |
| | R335 |
| | K336 |
| | Y337 |
| | S338 |
| | V339 |
| | W340 |
| | I341 |
| | G342 |
| | G343 |
| | S344 |
| | T345 |
| | L346 |
| | A347 |
| | S348 |
| | L349 |
| | S350 |
| | T351 |
| | F352 |
| | Q353 |
| | Q354 |
| | M355 |
| | W356 |
| | I357 |
| | T358 |
| | K359 |
| | Q360 |

4 Experimental information

| Property | Value | Source |
|--------------------------------------|---------------------------|-----------|
| EM reconstruction method | TOMOGRAPHY | Depositor |
| Imposed symmetry | POINT, C1 | Depositor |
| Number of tilted images used | Not provided | |
| Resolution determination method | Not provided | |
| CTF correction method | Not provided | |
| Microscope | FEI/PHILIPS EM400 | Depositor |
| Voltage (kV) | 100 | Depositor |
| Electron dose ($e^-/\text{\AA}^2$) | Not provided | |
| Minimum defocus (nm) | Not provided | |
| Maximum defocus (nm) | Not provided | |
| Magnification | 17000 | Depositor |
| Image detector | KODAK SO-163 FILM | Depositor |
| Maximum voxel value | 366.680 | Depositor |
| Minimum voxel value | -417.992 | Depositor |
| Average voxel value | 1.860 | Depositor |
| Voxel value standard deviation | 47.792 | Depositor |
| Recommended contour level | 81.2 | Depositor |
| Tomogram size (\AA) | 9280, 9280, 464 | wwPDB |
| Tomogram dimensions | 600, 600, 30 | wwPDB |
| Tomogram angles ($^\circ$) | 90, 90, 90 | wwPDB |
| Grid spacing (\AA) | 15.4667, 15.4667, 15.4667 | Depositor |

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MLY

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 | 1.77 | 68/6448 (1.1%) | 1.82 | 116/8729 (1.3%) |
| 1 | D | 1.77 | 67/6448 (1.0%) | 1.82 | 115/8729 (1.3%) |
| 1 | G | 1.77 | 69/6449 (1.1%) | 1.83 | 118/8732 (1.4%) |
| 1 | J | 1.77 | 69/6449 (1.1%) | 1.86 | 119/8732 (1.4%) |
| 1 | M | 1.86 | 70/6447 (1.1%) | 1.85 | 120/8726 (1.4%) |
| 1 | P | 1.78 | 68/6447 (1.1%) | 1.87 | 123/8726 (1.4%) |
| 2 | B | 1.22 | 10/1148 (0.9%) | 1.61 | 16/1548 (1.0%) |
| 2 | E | 1.21 | 10/1148 (0.9%) | 1.62 | 16/1548 (1.0%) |
| 2 | H | 1.22 | 10/1148 (0.9%) | 1.62 | 17/1548 (1.1%) |
| 2 | K | 1.22 | 10/1148 (0.9%) | 1.61 | 16/1548 (1.0%) |
| 2 | N | 1.22 | 10/1148 (0.9%) | 1.61 | 16/1548 (1.0%) |
| 2 | Q | 1.22 | 10/1148 (0.9%) | 1.62 | 16/1548 (1.0%) |
| 3 | C | 0.80 | 0/1136 | 0.95 | 4/1525 (0.3%) |
| 3 | F | 0.80 | 0/1136 | 0.95 | 4/1525 (0.3%) |
| 3 | I | 0.80 | 0/1136 | 0.94 | 4/1525 (0.3%) |
| 3 | L | 0.80 | 0/1136 | 0.95 | 4/1525 (0.3%) |
| 3 | O | 0.79 | 0/1136 | 0.95 | 4/1525 (0.3%) |
| 3 | R | 0.80 | 0/1136 | 0.95 | 4/1525 (0.3%) |
| 4 | 1 | 0.89 | 2/2968 (0.1%) | 1.64 | 52/4023 (1.3%) |
| 4 | 2 | 0.89 | 2/2968 (0.1%) | 1.64 | 51/4023 (1.3%) |
| 4 | 3 | 0.89 | 2/2968 (0.1%) | 1.64 | 51/4023 (1.3%) |
| 4 | 4 | 0.89 | 2/2968 (0.1%) | 1.64 | 50/4023 (1.2%) |
| 4 | 5 | 0.89 | 2/2968 (0.1%) | 1.64 | 52/4023 (1.3%) |
| 4 | 6 | 0.89 | 2/2968 (0.1%) | 1.64 | 51/4023 (1.3%) |
| 4 | 7 | 0.89 | 2/2968 (0.1%) | 1.64 | 50/4023 (1.2%) |
| 4 | 8 | 0.89 | 1/2968 (0.0%) | 1.64 | 50/4023 (1.2%) |
| 4 | 9 | 0.89 | 2/2968 (0.1%) | 1.64 | 51/4023 (1.3%) |
| 4 | V | 0.89 | 2/2968 (0.1%) | 1.64 | 51/4023 (1.3%) |
| 4 | W | 0.89 | 2/2968 (0.1%) | 1.64 | 52/4023 (1.3%) |
| 4 | X | 0.89 | 2/2968 (0.1%) | 1.64 | 50/4023 (1.2%) |
| 4 | Y | 0.89 | 2/2968 (0.1%) | 1.64 | 51/4023 (1.3%) |
| 4 | Z | 0.89 | 2/2968 (0.1%) | 1.64 | 51/4023 (1.3%) |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|------------------|-------------|--------------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| All | All | 1.35 | 498/93944 (0.5%) | 1.69 | 1545/127134 (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 | 4 |
| 1 | D | 1 | 4 |
| 1 | G | 1 | 4 |
| 1 | J | 1 | 6 |
| 1 | M | 1 | 4 |
| 1 | P | 1 | 6 |
| 2 | B | 0 | 3 |
| 2 | E | 0 | 3 |
| 2 | H | 0 | 3 |
| 2 | K | 0 | 3 |
| 2 | N | 0 | 3 |
| 2 | Q | 0 | 3 |
| 3 | C | 0 | 2 |
| 3 | F | 0 | 2 |
| 3 | I | 0 | 2 |
| 3 | L | 0 | 2 |
| 3 | O | 0 | 2 |
| 3 | R | 0 | 2 |
| 4 | 1 | 0 | 1 |
| 4 | 2 | 0 | 1 |
| 4 | 3 | 0 | 1 |
| 4 | 4 | 0 | 1 |
| 4 | 5 | 0 | 1 |
| 4 | 6 | 0 | 1 |
| 4 | 7 | 0 | 1 |
| 4 | 8 | 0 | 1 |
| 4 | 9 | 0 | 1 |
| 4 | V | 0 | 1 |
| 4 | W | 0 | 1 |
| 4 | X | 0 | 1 |
| 4 | Y | 0 | 1 |
| 4 | Z | 0 | 1 |
| All | All | 6 | 72 |

All (498) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|--------|-------------|----------|
| 1 | G | 649 | VAL | CB-CG1 | 53.37 | 2.65 | 1.52 |
| 1 | M | 649 | VAL | CB-CG1 | 53.35 | 2.64 | 1.52 |
| 1 | J | 649 | VAL | CB-CG1 | 53.27 | 2.64 | 1.52 |
| 1 | P | 649 | VAL | CB-CG1 | 53.24 | 2.64 | 1.52 |
| 1 | A | 649 | VAL | CB-CG1 | 53.21 | 2.64 | 1.52 |
| 1 | D | 649 | VAL | CB-CG1 | 53.21 | 2.64 | 1.52 |
| 1 | J | 623 | PHE | CB-CG | 48.21 | 2.33 | 1.51 |
| 1 | D | 623 | PHE | CB-CG | 48.20 | 2.33 | 1.51 |
| 1 | P | 623 | PHE | CB-CG | 48.11 | 2.33 | 1.51 |
| 1 | G | 623 | PHE | CB-CG | 48.05 | 2.33 | 1.51 |
| 1 | A | 623 | PHE | CB-CG | 48.04 | 2.33 | 1.51 |
| 1 | M | 623 | PHE | CB-CG | 48.03 | 2.33 | 1.51 |
| 1 | A | 649 | VAL | CB-CG2 | 46.29 | 2.50 | 1.52 |
| 1 | G | 649 | VAL | CB-CG2 | 46.28 | 2.50 | 1.52 |
| 1 | M | 649 | VAL | CB-CG2 | 46.23 | 2.50 | 1.52 |
| 1 | J | 649 | VAL | CB-CG2 | 46.12 | 2.49 | 1.52 |
| 1 | P | 649 | VAL | CB-CG2 | 46.11 | 2.49 | 1.52 |
| 1 | D | 649 | VAL | CB-CG2 | 46.05 | 2.49 | 1.52 |
| 1 | M | 709 | LYS | C-N | 37.12 | 1.99 | 1.33 |
| 1 | D | 648 | THR | CB-OG1 | 34.43 | 2.12 | 1.43 |
| 1 | J | 648 | THR | CB-OG1 | 34.43 | 2.12 | 1.43 |
| 1 | P | 648 | THR | CB-OG1 | 34.41 | 2.12 | 1.43 |
| 1 | A | 648 | THR | CB-OG1 | 34.38 | 2.12 | 1.43 |
| 1 | G | 648 | THR | CB-OG1 | 34.34 | 2.12 | 1.43 |
| 1 | M | 648 | THR | CB-OG1 | 34.32 | 2.11 | 1.43 |
| 1 | D | 648 | THR | CB-CG2 | -30.70 | 0.51 | 1.52 |
| 1 | P | 648 | THR | CB-CG2 | -30.70 | 0.51 | 1.52 |
| 1 | M | 648 | THR | CB-CG2 | -30.69 | 0.51 | 1.52 |
| 1 | A | 648 | THR | CB-CG2 | -30.68 | 0.51 | 1.52 |
| 1 | J | 648 | THR | CB-CG2 | -30.68 | 0.51 | 1.52 |
| 1 | G | 648 | THR | CB-CG2 | -30.64 | 0.51 | 1.52 |
| 1 | M | 806 | MET | C-N | 28.60 | 1.99 | 1.34 |
| 1 | P | 806 | MET | C-N | 19.20 | 1.78 | 1.34 |
| 1 | M | 637 | LYS | C-N | -15.05 | 1.05 | 1.33 |
| 1 | J | 637 | LYS | C-N | -15.04 | 1.05 | 1.33 |
| 1 | P | 637 | LYS | C-N | -15.03 | 1.05 | 1.33 |
| 1 | D | 637 | LYS | C-N | -15.02 | 1.06 | 1.33 |
| 1 | G | 637 | LYS | C-N | -14.76 | 1.06 | 1.33 |
| 1 | A | 637 | LYS | C-N | -14.75 | 1.06 | 1.33 |
| 1 | A | 649 | VAL | C-N | -13.51 | 1.02 | 1.34 |
| 1 | G | 649 | VAL | C-N | -13.50 | 1.02 | 1.34 |
| 1 | D | 649 | VAL | C-N | -13.41 | 1.03 | 1.34 |
| 1 | J | 649 | VAL | C-N | -13.39 | 1.03 | 1.34 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|--------|-------------|----------|
| 1 | P | 649 | VAL | C-N | -13.38 | 1.03 | 1.34 |
| 1 | M | 649 | VAL | C-N | -13.38 | 1.03 | 1.34 |
| 2 | Q | 150 | TYR | CB-CG | -13.36 | 1.31 | 1.51 |
| 2 | N | 150 | TYR | CB-CG | -13.34 | 1.31 | 1.51 |
| 2 | H | 150 | TYR | CB-CG | -13.32 | 1.31 | 1.51 |
| 2 | K | 150 | TYR | CB-CG | -13.32 | 1.31 | 1.51 |
| 2 | B | 150 | TYR | CB-CG | -13.25 | 1.31 | 1.51 |
| 2 | E | 150 | TYR | CB-CG | -13.24 | 1.31 | 1.51 |
| 2 | K | 140 | PHE | C-N | -12.98 | 1.09 | 1.34 |
| 2 | B | 140 | PHE | C-N | -12.97 | 1.09 | 1.34 |
| 2 | E | 140 | PHE | C-N | -12.93 | 1.09 | 1.34 |
| 2 | Q | 140 | PHE | C-N | -12.88 | 1.09 | 1.34 |
| 2 | N | 140 | PHE | C-N | -12.84 | 1.09 | 1.34 |
| 2 | H | 140 | PHE | C-N | -12.79 | 1.09 | 1.34 |
| 2 | B | 150 | TYR | CG-CD2 | -11.33 | 1.24 | 1.39 |
| 2 | N | 150 | TYR | CG-CD2 | -11.27 | 1.24 | 1.39 |
| 2 | Q | 150 | TYR | CG-CD2 | -11.26 | 1.24 | 1.39 |
| 2 | H | 150 | TYR | CG-CD2 | -11.25 | 1.24 | 1.39 |
| 2 | K | 150 | TYR | CG-CD2 | -11.25 | 1.24 | 1.39 |
| 2 | E | 150 | TYR | CG-CD2 | -11.16 | 1.24 | 1.39 |
| 2 | K | 141 | PRO | N-CD | -10.57 | 1.33 | 1.47 |
| 2 | Q | 141 | PRO | N-CD | -10.55 | 1.33 | 1.47 |
| 2 | N | 141 | PRO | N-CD | -10.49 | 1.33 | 1.47 |
| 2 | E | 141 | PRO | N-CD | -10.45 | 1.33 | 1.47 |
| 2 | B | 141 | PRO | N-CD | -10.33 | 1.33 | 1.47 |
| 2 | H | 141 | PRO | N-CD | -10.27 | 1.33 | 1.47 |
| 1 | P | 476 | GLU | CD-OE1 | 8.96 | 1.35 | 1.25 |
| 1 | J | 476 | GLU | CD-OE1 | 8.94 | 1.35 | 1.25 |
| 1 | M | 476 | GLU | CD-OE1 | 8.89 | 1.35 | 1.25 |
| 1 | D | 476 | GLU | CD-OE1 | 8.84 | 1.35 | 1.25 |
| 1 | J | 785 | GLU | C-N | 8.83 | 1.54 | 1.34 |
| 1 | A | 622 | LEU | C-N | 8.76 | 1.54 | 1.34 |
| 1 | J | 622 | LEU | C-N | 8.72 | 1.54 | 1.34 |
| 1 | P | 622 | LEU | C-N | 8.72 | 1.54 | 1.34 |
| 1 | D | 622 | LEU | C-N | 8.67 | 1.53 | 1.34 |
| 1 | A | 476 | GLU | CD-OE1 | 8.66 | 1.35 | 1.25 |
| 1 | G | 476 | GLU | CD-OE1 | 8.65 | 1.35 | 1.25 |
| 1 | M | 622 | LEU | C-N | 8.65 | 1.53 | 1.34 |
| 1 | G | 622 | LEU | C-N | 8.62 | 1.53 | 1.34 |
| 1 | D | 411 | GLU | CD-OE1 | 8.41 | 1.34 | 1.25 |
| 1 | P | 745 | GLU | CD-OE2 | 8.41 | 1.34 | 1.25 |
| 1 | D | 745 | GLU | CD-OE2 | 8.39 | 1.34 | 1.25 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1 | G | 411 | GLU | CD-OE1 | 8.38 | 1.34 | 1.25 |
| 1 | J | 745 | GLU | CD-OE2 | 8.35 | 1.34 | 1.25 |
| 1 | J | 411 | GLU | CD-OE1 | 8.32 | 1.34 | 1.25 |
| 1 | M | 411 | GLU | CD-OE1 | 8.32 | 1.34 | 1.25 |
| 1 | P | 411 | GLU | CD-OE1 | 8.27 | 1.34 | 1.25 |
| 2 | N | 150 | TYR | CA-CB | -8.27 | 1.35 | 1.53 |
| 1 | A | 411 | GLU | CD-OE1 | 8.25 | 1.34 | 1.25 |
| 1 | M | 745 | GLU | CD-OE2 | 8.24 | 1.34 | 1.25 |
| 2 | B | 150 | TYR | CA-CB | -8.22 | 1.35 | 1.53 |
| 2 | K | 150 | TYR | CA-CB | -8.21 | 1.35 | 1.53 |
| 2 | Q | 150 | TYR | CA-CB | -8.19 | 1.35 | 1.53 |
| 2 | H | 150 | TYR | CA-CB | -8.18 | 1.35 | 1.53 |
| 1 | G | 745 | GLU | CD-OE2 | 8.14 | 1.34 | 1.25 |
| 1 | A | 381 | GLU | CD-OE1 | 8.09 | 1.34 | 1.25 |
| 1 | G | 108 | GLU | CD-OE1 | 8.08 | 1.34 | 1.25 |
| 2 | E | 150 | TYR | CA-CB | -8.07 | 1.36 | 1.53 |
| 1 | M | 108 | GLU | CD-OE1 | 7.98 | 1.34 | 1.25 |
| 1 | A | 745 | GLU | CD-OE2 | 7.98 | 1.34 | 1.25 |
| 1 | J | 108 | GLU | CD-OE1 | 7.98 | 1.34 | 1.25 |
| 1 | G | 381 | GLU | CD-OE1 | 7.97 | 1.34 | 1.25 |
| 1 | P | 108 | GLU | CD-OE1 | 7.96 | 1.34 | 1.25 |
| 1 | M | 381 | GLU | CD-OE1 | 7.95 | 1.34 | 1.25 |
| 1 | P | 202 | SER | CB-OG | 7.89 | 1.52 | 1.42 |
| 1 | A | 108 | GLU | CD-OE1 | 7.88 | 1.34 | 1.25 |
| 1 | G | 202 | SER | CB-OG | 7.84 | 1.52 | 1.42 |
| 1 | D | 202 | SER | CB-OG | 7.82 | 1.52 | 1.42 |
| 1 | D | 381 | GLU | CD-OE1 | 7.82 | 1.34 | 1.25 |
| 1 | J | 202 | SER | CB-OG | 7.78 | 1.52 | 1.42 |
| 1 | J | 381 | GLU | CD-OE1 | 7.78 | 1.34 | 1.25 |
| 1 | D | 108 | GLU | CD-OE1 | 7.71 | 1.34 | 1.25 |
| 1 | M | 202 | SER | CB-OG | 7.70 | 1.52 | 1.42 |
| 1 | P | 381 | GLU | CD-OE1 | 7.68 | 1.34 | 1.25 |
| 1 | A | 202 | SER | CB-OG | 7.66 | 1.52 | 1.42 |
| 1 | M | 689 | GLU | CD-OE2 | 7.62 | 1.34 | 1.25 |
| 1 | G | 689 | GLU | CD-OE2 | 7.58 | 1.33 | 1.25 |
| 1 | D | 689 | GLU | CD-OE2 | 7.46 | 1.33 | 1.25 |
| 1 | A | 689 | GLU | CD-OE2 | 7.42 | 1.33 | 1.25 |
| 1 | J | 347 | GLU | CD-OE1 | 7.41 | 1.33 | 1.25 |
| 1 | P | 347 | GLU | CD-OE1 | 7.38 | 1.33 | 1.25 |
| 1 | D | 23 | GLU | CD-OE1 | 7.38 | 1.33 | 1.25 |
| 1 | J | 689 | GLU | CD-OE2 | 7.33 | 1.33 | 1.25 |
| 1 | P | 689 | GLU | CD-OE2 | 7.33 | 1.33 | 1.25 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 1 | M | 347 | GLU | CD-OE1 | 7.32 | 1.33 | 1.25 |
| 1 | A | 347 | GLU | CD-OE1 | 7.31 | 1.33 | 1.25 |
| 1 | J | 23 | GLU | CD-OE1 | 7.31 | 1.33 | 1.25 |
| 1 | M | 23 | GLU | CD-OE1 | 7.30 | 1.33 | 1.25 |
| 1 | D | 68 | GLU | CD-OE2 | 7.27 | 1.33 | 1.25 |
| 1 | P | 23 | GLU | CD-OE1 | 7.26 | 1.33 | 1.25 |
| 1 | G | 23 | GLU | CD-OE1 | 7.26 | 1.33 | 1.25 |
| 1 | D | 347 | GLU | CD-OE1 | 7.25 | 1.33 | 1.25 |
| 1 | G | 347 | GLU | CD-OE1 | 7.23 | 1.33 | 1.25 |
| 1 | M | 524 | GLU | CD-OE1 | 7.21 | 1.33 | 1.25 |
| 1 | M | 511 | GLU | CD-OE1 | 7.19 | 1.33 | 1.25 |
| 1 | A | 23 | GLU | CD-OE1 | 7.17 | 1.33 | 1.25 |
| 1 | P | 511 | GLU | CD-OE1 | 7.16 | 1.33 | 1.25 |
| 1 | A | 511 | GLU | CD-OE1 | 7.13 | 1.33 | 1.25 |
| 1 | J | 511 | GLU | CD-OE1 | 7.13 | 1.33 | 1.25 |
| 1 | P | 811 | GLU | CD-OE1 | 7.12 | 1.33 | 1.25 |
| 1 | G | 26 | GLU | CD-OE1 | 7.07 | 1.33 | 1.25 |
| 1 | G | 68 | GLU | CD-OE2 | 7.06 | 1.33 | 1.25 |
| 1 | M | 811 | GLU | CD-OE1 | 7.05 | 1.33 | 1.25 |
| 1 | J | 330 | GLU | CD-OE1 | 7.03 | 1.33 | 1.25 |
| 1 | D | 376 | GLU | CD-OE1 | 7.03 | 1.33 | 1.25 |
| 1 | D | 524 | GLU | CD-OE1 | 7.02 | 1.33 | 1.25 |
| 1 | D | 811 | GLU | CD-OE1 | 7.02 | 1.33 | 1.25 |
| 1 | M | 330 | GLU | CD-OE1 | 7.01 | 1.33 | 1.25 |
| 1 | A | 524 | GLU | CD-OE1 | 7.01 | 1.33 | 1.25 |
| 1 | P | 524 | GLU | CD-OE1 | 7.00 | 1.33 | 1.25 |
| 1 | D | 511 | GLU | CD-OE1 | 6.97 | 1.33 | 1.25 |
| 1 | J | 26 | GLU | CD-OE1 | 6.96 | 1.33 | 1.25 |
| 1 | J | 811 | GLU | CD-OE1 | 6.96 | 1.33 | 1.25 |
| 1 | P | 330 | GLU | CD-OE1 | 6.94 | 1.33 | 1.25 |
| 1 | M | 68 | GLU | CD-OE2 | 6.93 | 1.33 | 1.25 |
| 1 | G | 524 | GLU | CD-OE1 | 6.92 | 1.33 | 1.25 |
| 1 | J | 376 | GLU | CD-OE1 | 6.91 | 1.33 | 1.25 |
| 1 | A | 26 | GLU | CD-OE1 | 6.90 | 1.33 | 1.25 |
| 1 | D | 26 | GLU | CD-OE1 | 6.90 | 1.33 | 1.25 |
| 1 | P | 655 | GLU | CD-OE1 | 6.89 | 1.33 | 1.25 |
| 1 | M | 376 | GLU | CD-OE1 | 6.89 | 1.33 | 1.25 |
| 1 | P | 68 | GLU | CD-OE2 | 6.88 | 1.33 | 1.25 |
| 1 | A | 376 | GLU | CD-OE1 | 6.88 | 1.33 | 1.25 |
| 1 | A | 330 | GLU | CD-OE1 | 6.88 | 1.33 | 1.25 |
| 1 | P | 26 | GLU | CD-OE1 | 6.88 | 1.33 | 1.25 |
| 1 | A | 68 | GLU | CD-OE2 | 6.87 | 1.33 | 1.25 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1 | J | 68 | GLU | CD-OE2 | 6.87 | 1.33 | 1.25 |
| 1 | J | 524 | GLU | CD-OE1 | 6.87 | 1.33 | 1.25 |
| 1 | G | 376 | GLU | CD-OE1 | 6.86 | 1.33 | 1.25 |
| 1 | A | 655 | GLU | CD-OE1 | 6.84 | 1.33 | 1.25 |
| 1 | G | 330 | GLU | CD-OE1 | 6.84 | 1.33 | 1.25 |
| 1 | M | 26 | GLU | CD-OE1 | 6.83 | 1.33 | 1.25 |
| 1 | P | 376 | GLU | CD-OE1 | 6.81 | 1.33 | 1.25 |
| 1 | D | 330 | GLU | CD-OE1 | 6.80 | 1.33 | 1.25 |
| 1 | M | 319 | GLU | CD-OE1 | 6.80 | 1.33 | 1.25 |
| 1 | G | 511 | GLU | CD-OE1 | 6.80 | 1.33 | 1.25 |
| 1 | M | 655 | GLU | CD-OE1 | 6.79 | 1.33 | 1.25 |
| 1 | P | 538 | GLU | CD-OE1 | 6.76 | 1.33 | 1.25 |
| 1 | J | 655 | GLU | CD-OE1 | 6.76 | 1.33 | 1.25 |
| 1 | A | 811 | GLU | CD-OE1 | 6.75 | 1.33 | 1.25 |
| 1 | G | 811 | GLU | CD-OE1 | 6.71 | 1.33 | 1.25 |
| 1 | A | 266 | GLU | CD-OE2 | 6.69 | 1.33 | 1.25 |
| 1 | J | 538 | GLU | CD-OE1 | 6.69 | 1.33 | 1.25 |
| 1 | G | 655 | GLU | CD-OE1 | 6.67 | 1.32 | 1.25 |
| 1 | G | 319 | GLU | CD-OE1 | 6.67 | 1.32 | 1.25 |
| 1 | J | 319 | GLU | CD-OE1 | 6.62 | 1.32 | 1.25 |
| 1 | M | 538 | GLU | CD-OE1 | 6.62 | 1.32 | 1.25 |
| 1 | G | 785 | GLU | C-N | 6.60 | 1.49 | 1.34 |
| 1 | P | 319 | GLU | CD-OE1 | 6.60 | 1.32 | 1.25 |
| 1 | G | 538 | GLU | CD-OE1 | 6.58 | 1.32 | 1.25 |
| 1 | A | 538 | GLU | CD-OE1 | 6.58 | 1.32 | 1.25 |
| 1 | D | 655 | GLU | CD-OE1 | 6.56 | 1.32 | 1.25 |
| 2 | B | 150 | TYR | CD2-CE2 | -6.55 | 1.29 | 1.39 |
| 1 | M | 266 | GLU | CD-OE2 | 6.55 | 1.32 | 1.25 |
| 1 | J | 266 | GLU | CD-OE2 | 6.54 | 1.32 | 1.25 |
| 1 | A | 319 | GLU | CD-OE1 | 6.53 | 1.32 | 1.25 |
| 1 | D | 538 | GLU | CD-OE1 | 6.51 | 1.32 | 1.25 |
| 1 | D | 89 | GLU | CD-OE1 | 6.51 | 1.32 | 1.25 |
| 1 | D | 99 | GLU | CD-OE2 | 6.50 | 1.32 | 1.25 |
| 2 | E | 150 | TYR | CD2-CE2 | -6.50 | 1.29 | 1.39 |
| 1 | G | 89 | GLU | CD-OE1 | 6.49 | 1.32 | 1.25 |
| 1 | P | 266 | GLU | CD-OE2 | 6.48 | 1.32 | 1.25 |
| 1 | P | 89 | GLU | CD-OE1 | 6.46 | 1.32 | 1.25 |
| 1 | G | 99 | GLU | CD-OE2 | 6.46 | 1.32 | 1.25 |
| 1 | M | 538 | GLU | CD-OE2 | -6.45 | 1.18 | 1.25 |
| 1 | M | 99 | GLU | CD-OE2 | 6.45 | 1.32 | 1.25 |
| 1 | P | 808 | GLU | CD-OE1 | 6.44 | 1.32 | 1.25 |
| 1 | J | 89 | GLU | CD-OE1 | 6.44 | 1.32 | 1.25 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2 | Q | 150 | TYR | CD2-CE2 | -6.44 | 1.29 | 1.39 |
| 1 | J | 808 | GLU | CD-OE1 | 6.44 | 1.32 | 1.25 |
| 1 | G | 808 | GLU | CD-OE1 | 6.42 | 1.32 | 1.25 |
| 1 | A | 605 | GLU | CD-OE1 | 6.42 | 1.32 | 1.25 |
| 1 | G | 502 | GLU | CD-OE2 | 6.42 | 1.32 | 1.25 |
| 1 | D | 502 | GLU | CD-OE2 | 6.41 | 1.32 | 1.25 |
| 1 | D | 266 | GLU | CD-OE2 | 6.41 | 1.32 | 1.25 |
| 1 | P | 502 | GLU | CD-OE2 | 6.41 | 1.32 | 1.25 |
| 1 | D | 808 | GLU | CD-OE1 | 6.41 | 1.32 | 1.25 |
| 1 | J | 99 | GLU | CD-OE2 | 6.41 | 1.32 | 1.25 |
| 2 | K | 150 | TYR | CD2-CE2 | -6.40 | 1.29 | 1.39 |
| 1 | A | 538 | GLU | CD-OE2 | -6.40 | 1.18 | 1.25 |
| 1 | G | 266 | GLU | CD-OE2 | 6.39 | 1.32 | 1.25 |
| 4 | 3 | 259 | GLU | CG-CD | 6.39 | 1.61 | 1.51 |
| 1 | A | 89 | GLU | CD-OE1 | 6.39 | 1.32 | 1.25 |
| 1 | D | 6 | GLU | CD-OE1 | 6.38 | 1.32 | 1.25 |
| 1 | G | 605 | GLU | CD-OE1 | 6.38 | 1.32 | 1.25 |
| 1 | P | 802 | GLU | CD-OE1 | 6.38 | 1.32 | 1.25 |
| 1 | M | 502 | GLU | CD-OE2 | 6.38 | 1.32 | 1.25 |
| 1 | D | 538 | GLU | CD-OE2 | -6.37 | 1.18 | 1.25 |
| 2 | N | 150 | TYR | CD2-CE2 | -6.37 | 1.29 | 1.39 |
| 1 | D | 319 | GLU | CD-OE1 | 6.36 | 1.32 | 1.25 |
| 1 | P | 6 | GLU | CD-OE1 | 6.36 | 1.32 | 1.25 |
| 1 | A | 502 | GLU | CD-OE2 | 6.35 | 1.32 | 1.25 |
| 1 | J | 6 | GLU | CD-OE1 | 6.35 | 1.32 | 1.25 |
| 1 | M | 89 | GLU | CD-OE1 | 6.35 | 1.32 | 1.25 |
| 2 | B | 150 | TYR | N-CA | -6.34 | 1.33 | 1.46 |
| 1 | G | 6 | GLU | CD-OE1 | 6.34 | 1.32 | 1.25 |
| 4 | 5 | 259 | GLU | CG-CD | 6.34 | 1.61 | 1.51 |
| 1 | P | 538 | GLU | CD-OE2 | -6.34 | 1.18 | 1.25 |
| 1 | A | 6 | GLU | CD-OE1 | 6.33 | 1.32 | 1.25 |
| 1 | J | 502 | GLU | CD-OE2 | 6.32 | 1.32 | 1.25 |
| 1 | D | 802 | GLU | CD-OE1 | 6.30 | 1.32 | 1.25 |
| 1 | J | 802 | GLU | CD-OE1 | 6.30 | 1.32 | 1.25 |
| 1 | M | 808 | GLU | CD-OE1 | 6.30 | 1.32 | 1.25 |
| 4 | Y | 259 | GLU | CG-CD | 6.30 | 1.61 | 1.51 |
| 1 | A | 808 | GLU | CD-OE1 | 6.28 | 1.32 | 1.25 |
| 4 | 2 | 259 | GLU | CG-CD | 6.28 | 1.61 | 1.51 |
| 1 | J | 538 | GLU | CD-OE2 | -6.28 | 1.18 | 1.25 |
| 1 | P | 99 | GLU | CD-OE2 | 6.28 | 1.32 | 1.25 |
| 4 | 9 | 259 | GLU | CG-CD | 6.26 | 1.61 | 1.51 |
| 2 | H | 150 | TYR | CD2-CE2 | -6.26 | 1.29 | 1.39 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 4 | 8 | 259 | GLU | CG-CD | 6.26 | 1.61 | 1.51 |
| 4 | X | 259 | GLU | CG-CD | 6.25 | 1.61 | 1.51 |
| 1 | G | 538 | GLU | CD-OE2 | -6.25 | 1.18 | 1.25 |
| 4 | W | 259 | GLU | CG-CD | 6.25 | 1.61 | 1.51 |
| 1 | D | 605 | GLU | CD-OE1 | 6.25 | 1.32 | 1.25 |
| 4 | 6 | 259 | GLU | CG-CD | 6.24 | 1.61 | 1.51 |
| 4 | V | 259 | GLU | CG-CD | 6.24 | 1.61 | 1.51 |
| 1 | D | 509 | GLU | CD-OE1 | 6.23 | 1.32 | 1.25 |
| 4 | Z | 259 | GLU | CG-CD | 6.23 | 1.61 | 1.51 |
| 2 | K | 150 | TYR | N-CA | -6.23 | 1.33 | 1.46 |
| 2 | N | 150 | TYR | N-CA | -6.22 | 1.33 | 1.46 |
| 4 | 4 | 259 | GLU | CG-CD | 6.22 | 1.61 | 1.51 |
| 1 | M | 802 | GLU | CD-OE1 | 6.21 | 1.32 | 1.25 |
| 1 | A | 99 | GLU | CD-OE2 | 6.21 | 1.32 | 1.25 |
| 1 | G | 802 | GLU | CD-OE1 | 6.20 | 1.32 | 1.25 |
| 4 | 1 | 259 | GLU | CG-CD | 6.20 | 1.61 | 1.51 |
| 1 | M | 329 | GLU | CD-OE1 | 6.20 | 1.32 | 1.25 |
| 1 | J | 329 | GLU | CD-OE1 | 6.19 | 1.32 | 1.25 |
| 1 | P | 509 | GLU | CD-OE1 | 6.18 | 1.32 | 1.25 |
| 1 | J | 605 | GLU | CD-OE1 | 6.17 | 1.32 | 1.25 |
| 4 | 7 | 259 | GLU | CG-CD | 6.16 | 1.61 | 1.51 |
| 2 | Q | 150 | TYR | N-CA | -6.16 | 1.34 | 1.46 |
| 1 | M | 6 | GLU | CD-OE1 | 6.14 | 1.32 | 1.25 |
| 2 | H | 150 | TYR | N-CA | -6.14 | 1.34 | 1.46 |
| 1 | P | 605 | GLU | CD-OE1 | 6.14 | 1.32 | 1.25 |
| 1 | M | 605 | GLU | CD-OE1 | 6.13 | 1.32 | 1.25 |
| 1 | G | 509 | GLU | CD-OE1 | 6.13 | 1.32 | 1.25 |
| 1 | G | 329 | GLU | CD-OE1 | 6.12 | 1.32 | 1.25 |
| 1 | A | 329 | GLU | CD-OE1 | 6.12 | 1.32 | 1.25 |
| 2 | E | 150 | TYR | N-CA | -6.12 | 1.34 | 1.46 |
| 1 | A | 509 | GLU | CD-OE1 | 6.11 | 1.32 | 1.25 |
| 1 | G | 476 | GLU | CD-OE2 | -6.10 | 1.19 | 1.25 |
| 1 | J | 509 | GLU | CD-OE1 | 6.10 | 1.32 | 1.25 |
| 1 | M | 509 | GLU | CD-OE1 | 6.09 | 1.32 | 1.25 |
| 1 | J | 230 | GLU | CD-OE2 | 6.07 | 1.32 | 1.25 |
| 1 | A | 417 | GLU | CD-OE1 | 6.07 | 1.32 | 1.25 |
| 1 | P | 329 | GLU | CD-OE1 | 6.04 | 1.32 | 1.25 |
| 1 | D | 417 | GLU | CD-OE1 | 6.03 | 1.32 | 1.25 |
| 1 | M | 417 | GLU | CD-OE1 | 6.00 | 1.32 | 1.25 |
| 1 | P | 230 | GLU | CD-OE2 | 6.00 | 1.32 | 1.25 |
| 1 | A | 802 | GLU | CD-OE1 | 5.98 | 1.32 | 1.25 |
| 1 | G | 230 | GLU | CD-OE2 | 5.97 | 1.32 | 1.25 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1 | G | 540 | CYS | CB-SG | -5.97 | 1.72 | 1.81 |
| 1 | G | 417 | GLU | CD-OE1 | 5.95 | 1.32 | 1.25 |
| 1 | M | 230 | GLU | CD-OE2 | 5.94 | 1.32 | 1.25 |
| 1 | D | 329 | GLU | CD-OE1 | 5.92 | 1.32 | 1.25 |
| 1 | A | 597 | GLU | CD-OE1 | 5.89 | 1.32 | 1.25 |
| 1 | D | 230 | GLU | CD-OE2 | 5.88 | 1.32 | 1.25 |
| 1 | M | 540 | CYS | CB-SG | -5.87 | 1.72 | 1.81 |
| 1 | G | 218 | LEU | CB-CG | 5.86 | 1.69 | 1.52 |
| 1 | P | 417 | GLU | CD-OE1 | 5.85 | 1.32 | 1.25 |
| 1 | M | 527 | GLU | CD-OE1 | 5.84 | 1.32 | 1.25 |
| 1 | A | 540 | CYS | CB-SG | -5.84 | 1.72 | 1.81 |
| 1 | P | 74 | GLU | CD-OE2 | 5.83 | 1.32 | 1.25 |
| 1 | A | 230 | GLU | CD-OE2 | 5.83 | 1.32 | 1.25 |
| 1 | J | 527 | GLU | CD-OE1 | 5.81 | 1.32 | 1.25 |
| 1 | D | 468 | GLU | CD-OE1 | 5.80 | 1.32 | 1.25 |
| 1 | J | 421 | GLU | CD-OE2 | 5.80 | 1.32 | 1.25 |
| 1 | M | 74 | GLU | CD-OE2 | 5.80 | 1.32 | 1.25 |
| 1 | M | 499 | GLU | CD-OE2 | 5.80 | 1.32 | 1.25 |
| 1 | P | 527 | GLU | CD-OE1 | 5.80 | 1.32 | 1.25 |
| 1 | P | 476 | GLU | CD-OE2 | -5.79 | 1.19 | 1.25 |
| 1 | P | 499 | GLU | CD-OE2 | 5.79 | 1.32 | 1.25 |
| 1 | G | 527 | GLU | CD-OE1 | 5.79 | 1.32 | 1.25 |
| 1 | M | 476 | GLU | CD-OE2 | -5.79 | 1.19 | 1.25 |
| 1 | J | 417 | GLU | CD-OE1 | 5.79 | 1.32 | 1.25 |
| 1 | J | 499 | GLU | CD-OE2 | 5.79 | 1.32 | 1.25 |
| 1 | M | 468 | GLU | CD-OE1 | 5.79 | 1.32 | 1.25 |
| 1 | P | 540 | CYS | CB-SG | -5.79 | 1.72 | 1.81 |
| 1 | M | 421 | GLU | CD-OE2 | 5.77 | 1.31 | 1.25 |
| 1 | J | 540 | CYS | CB-SG | -5.77 | 1.72 | 1.81 |
| 1 | D | 597 | GLU | CD-OE1 | 5.76 | 1.31 | 1.25 |
| 1 | P | 785 | GLU | CD-OE2 | 5.76 | 1.31 | 1.25 |
| 1 | A | 468 | GLU | CD-OE1 | 5.75 | 1.31 | 1.25 |
| 1 | J | 74 | GLU | CD-OE2 | 5.74 | 1.31 | 1.25 |
| 1 | D | 785 | GLU | CD-OE2 | 5.74 | 1.31 | 1.25 |
| 1 | A | 625 | THR | CB-CG2 | 5.73 | 1.71 | 1.52 |
| 1 | J | 468 | GLU | CD-OE1 | 5.73 | 1.31 | 1.25 |
| 1 | G | 597 | GLU | CD-OE1 | 5.72 | 1.31 | 1.25 |
| 1 | P | 468 | GLU | CD-OE1 | 5.72 | 1.31 | 1.25 |
| 1 | A | 527 | GLU | CD-OE1 | 5.72 | 1.31 | 1.25 |
| 1 | G | 74 | GLU | CD-OE2 | 5.72 | 1.31 | 1.25 |
| 1 | M | 218 | LEU | CB-CG | 5.72 | 1.69 | 1.52 |
| 1 | D | 625 | THR | CB-CG2 | 5.72 | 1.71 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1 | A | 421 | GLU | CD-OE2 | 5.72 | 1.31 | 1.25 |
| 1 | J | 476 | GLU | CD-OE2 | -5.72 | 1.19 | 1.25 |
| 1 | A | 74 | GLU | CD-OE2 | 5.71 | 1.31 | 1.25 |
| 1 | G | 785 | GLU | CD-OE2 | 5.71 | 1.31 | 1.25 |
| 1 | J | 625 | THR | CB-CG2 | 5.71 | 1.71 | 1.52 |
| 1 | A | 476 | GLU | CD-OE2 | -5.71 | 1.19 | 1.25 |
| 1 | D | 218 | LEU | CB-CG | 5.71 | 1.69 | 1.52 |
| 1 | P | 421 | GLU | CD-OE2 | 5.70 | 1.31 | 1.25 |
| 1 | P | 597 | GLU | CD-OE1 | 5.70 | 1.31 | 1.25 |
| 1 | P | 218 | LEU | CB-CG | 5.69 | 1.69 | 1.52 |
| 1 | A | 785 | GLU | CD-OE2 | 5.69 | 1.31 | 1.25 |
| 1 | D | 540 | CYS | CB-SG | -5.68 | 1.72 | 1.81 |
| 1 | P | 625 | THR | CB-CG2 | 5.68 | 1.71 | 1.52 |
| 1 | D | 476 | GLU | CD-OE2 | -5.68 | 1.19 | 1.25 |
| 1 | M | 625 | THR | CB-CG2 | 5.68 | 1.71 | 1.52 |
| 1 | A | 218 | LEU | CB-CG | 5.67 | 1.69 | 1.52 |
| 1 | G | 625 | THR | CB-CG2 | 5.67 | 1.71 | 1.52 |
| 1 | M | 687 | GLU | CD-OE1 | 5.67 | 1.31 | 1.25 |
| 1 | J | 218 | LEU | CB-CG | 5.67 | 1.69 | 1.52 |
| 1 | J | 597 | GLU | CD-OE1 | 5.67 | 1.31 | 1.25 |
| 1 | D | 687 | GLU | CD-OE1 | 5.64 | 1.31 | 1.25 |
| 1 | G | 687 | GLU | CD-OE1 | 5.64 | 1.31 | 1.25 |
| 1 | D | 499 | GLU | CD-OE2 | 5.60 | 1.31 | 1.25 |
| 1 | J | 785 | GLU | CD-OE2 | 5.59 | 1.31 | 1.25 |
| 1 | P | 373 | GLU | CD-OE1 | 5.59 | 1.31 | 1.25 |
| 1 | M | 785 | GLU | CD-OE2 | 5.58 | 1.31 | 1.25 |
| 1 | J | 687 | GLU | CD-OE1 | 5.58 | 1.31 | 1.25 |
| 1 | D | 373 | GLU | CD-OE1 | 5.58 | 1.31 | 1.25 |
| 1 | M | 597 | GLU | CD-OE1 | 5.58 | 1.31 | 1.25 |
| 1 | A | 499 | GLU | CD-OE2 | 5.57 | 1.31 | 1.25 |
| 1 | A | 687 | GLU | CD-OE1 | 5.57 | 1.31 | 1.25 |
| 1 | D | 74 | GLU | CD-OE2 | 5.57 | 1.31 | 1.25 |
| 1 | M | 373 | GLU | CD-OE1 | 5.56 | 1.31 | 1.25 |
| 1 | J | 777 | GLU | CD-OE2 | 5.55 | 1.31 | 1.25 |
| 1 | J | 373 | GLU | CD-OE1 | 5.55 | 1.31 | 1.25 |
| 1 | G | 421 | GLU | CD-OE2 | 5.53 | 1.31 | 1.25 |
| 1 | D | 777 | GLU | CD-OE2 | 5.53 | 1.31 | 1.25 |
| 1 | A | 777 | GLU | CD-OE2 | 5.52 | 1.31 | 1.25 |
| 1 | D | 421 | GLU | CD-OE2 | 5.51 | 1.31 | 1.25 |
| 1 | G | 499 | GLU | CD-OE2 | 5.51 | 1.31 | 1.25 |
| 2 | K | 150 | TYR | CE1-CZ | 5.50 | 1.45 | 1.38 |
| 2 | H | 150 | TYR | CE1-CZ | 5.50 | 1.45 | 1.38 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 2 | N | 131 | GLU | N-CA | 5.49 | 1.57 | 1.46 |
| 1 | P | 777 | GLU | CD-OE2 | 5.49 | 1.31 | 1.25 |
| 2 | B | 150 | TYR | CE1-CZ | 5.49 | 1.45 | 1.38 |
| 1 | D | 527 | GLU | CD-OE1 | 5.49 | 1.31 | 1.25 |
| 2 | N | 150 | TYR | CE1-CZ | 5.49 | 1.45 | 1.38 |
| 2 | E | 150 | TYR | CE1-CZ | 5.49 | 1.45 | 1.38 |
| 1 | G | 468 | GLU | CD-OE1 | 5.48 | 1.31 | 1.25 |
| 2 | K | 131 | GLU | N-CA | 5.47 | 1.57 | 1.46 |
| 1 | A | 373 | GLU | CD-OE1 | 5.47 | 1.31 | 1.25 |
| 1 | A | 506 | GLU | CD-OE2 | 5.46 | 1.31 | 1.25 |
| 1 | G | 373 | GLU | CD-OE1 | 5.46 | 1.31 | 1.25 |
| 1 | P | 298 | GLU | CD-OE2 | 5.46 | 1.31 | 1.25 |
| 1 | P | 687 | GLU | CD-OE1 | 5.46 | 1.31 | 1.25 |
| 1 | G | 298 | GLU | CD-OE2 | 5.45 | 1.31 | 1.25 |
| 2 | Q | 131 | GLU | N-CA | 5.45 | 1.57 | 1.46 |
| 1 | J | 298 | GLU | CD-OE2 | 5.43 | 1.31 | 1.25 |
| 2 | Q | 150 | TYR | CE1-CZ | 5.43 | 1.45 | 1.38 |
| 1 | A | 65 | GLU | CD-OE1 | 5.42 | 1.31 | 1.25 |
| 1 | A | 479 | CYS | CB-SG | -5.40 | 1.73 | 1.81 |
| 1 | G | 479 | CYS | CB-SG | -5.40 | 1.73 | 1.81 |
| 1 | J | 479 | CYS | CB-SG | -5.40 | 1.73 | 1.81 |
| 1 | D | 298 | GLU | CD-OE2 | 5.39 | 1.31 | 1.25 |
| 2 | E | 131 | GLU | N-CA | 5.39 | 1.57 | 1.46 |
| 2 | H | 131 | GLU | N-CA | 5.38 | 1.57 | 1.46 |
| 1 | M | 218 | LEU | C-N | -5.38 | 1.21 | 1.34 |
| 1 | M | 777 | GLU | CD-OE2 | 5.38 | 1.31 | 1.25 |
| 1 | P | 218 | LEU | C-N | -5.37 | 1.21 | 1.34 |
| 2 | B | 131 | GLU | N-CA | 5.36 | 1.57 | 1.46 |
| 1 | G | 506 | GLU | CD-OE2 | 5.36 | 1.31 | 1.25 |
| 1 | M | 298 | GLU | CD-OE2 | 5.34 | 1.31 | 1.25 |
| 1 | G | 777 | GLU | CD-OE2 | 5.34 | 1.31 | 1.25 |
| 1 | D | 218 | LEU | C-N | -5.34 | 1.21 | 1.34 |
| 1 | J | 679 | GLU | CD-OE2 | 5.33 | 1.31 | 1.25 |
| 1 | M | 679 | GLU | CD-OE2 | 5.32 | 1.31 | 1.25 |
| 1 | M | 479 | CYS | CB-SG | -5.31 | 1.73 | 1.81 |
| 1 | D | 679 | GLU | CD-OE2 | 5.31 | 1.31 | 1.25 |
| 1 | P | 479 | CYS | CB-SG | -5.31 | 1.73 | 1.81 |
| 1 | A | 218 | LEU | C-N | -5.30 | 1.21 | 1.34 |
| 2 | K | 149 | ASP | CB-CG | 5.29 | 1.62 | 1.51 |
| 1 | G | 218 | LEU | C-N | -5.29 | 1.21 | 1.34 |
| 1 | J | 218 | LEU | C-N | -5.28 | 1.22 | 1.34 |
| 1 | D | 65 | GLU | CD-OE1 | 5.27 | 1.31 | 1.25 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1 | D | 282 | GLU | CD-OE1 | 5.27 | 1.31 | 1.25 |
| 1 | A | 298 | GLU | CD-OE2 | 5.27 | 1.31 | 1.25 |
| 1 | J | 65 | GLU | CD-OE1 | 5.27 | 1.31 | 1.25 |
| 1 | G | 679 | GLU | CD-OE2 | 5.27 | 1.31 | 1.25 |
| 1 | P | 65 | GLU | CD-OE1 | 5.26 | 1.31 | 1.25 |
| 1 | P | 12 | GLU | CD-OE2 | 5.24 | 1.31 | 1.25 |
| 1 | A | 21 | GLU | CD-OE2 | 5.24 | 1.31 | 1.25 |
| 1 | P | 527 | GLU | CD-OE2 | -5.24 | 1.19 | 1.25 |
| 1 | G | 21 | GLU | CD-OE2 | 5.24 | 1.31 | 1.25 |
| 1 | D | 506 | GLU | CD-OE2 | 5.22 | 1.31 | 1.25 |
| 1 | M | 21 | GLU | CD-OE2 | 5.21 | 1.31 | 1.25 |
| 2 | B | 149 | ASP | CB-CG | 5.21 | 1.62 | 1.51 |
| 2 | Q | 149 | ASP | CB-CG | 5.21 | 1.62 | 1.51 |
| 1 | P | 282 | GLU | CD-OE1 | 5.21 | 1.31 | 1.25 |
| 1 | J | 282 | GLU | CD-OE1 | 5.20 | 1.31 | 1.25 |
| 1 | D | 479 | CYS | CB-SG | -5.19 | 1.73 | 1.81 |
| 1 | J | 702 | GLU | CD-OE2 | 5.19 | 1.31 | 1.25 |
| 1 | P | 679 | GLU | CD-OE2 | 5.19 | 1.31 | 1.25 |
| 1 | J | 527 | GLU | CD-OE2 | -5.19 | 1.20 | 1.25 |
| 1 | M | 65 | GLU | CD-OE1 | 5.19 | 1.31 | 1.25 |
| 1 | G | 65 | GLU | CD-OE1 | 5.18 | 1.31 | 1.25 |
| 1 | A | 150 | GLU | CD-OE1 | 5.18 | 1.31 | 1.25 |
| 1 | G | 697 | CYS | CB-SG | 5.17 | 1.91 | 1.82 |
| 1 | M | 12 | GLU | CD-OE2 | 5.17 | 1.31 | 1.25 |
| 2 | E | 149 | ASP | CB-CG | 5.16 | 1.62 | 1.51 |
| 1 | M | 702 | GLU | CD-OE2 | 5.16 | 1.31 | 1.25 |
| 1 | A | 702 | GLU | CD-OE2 | 5.16 | 1.31 | 1.25 |
| 1 | G | 702 | GLU | CD-OE2 | 5.16 | 1.31 | 1.25 |
| 1 | J | 21 | GLU | CD-OE2 | 5.16 | 1.31 | 1.25 |
| 1 | P | 506 | GLU | CD-OE2 | 5.16 | 1.31 | 1.25 |
| 2 | N | 149 | ASP | CB-CG | 5.15 | 1.62 | 1.51 |
| 1 | M | 150 | GLU | CD-OE1 | 5.14 | 1.31 | 1.25 |
| 1 | P | 702 | GLU | CD-OE2 | 5.14 | 1.31 | 1.25 |
| 1 | D | 702 | GLU | CD-OE2 | 5.14 | 1.31 | 1.25 |
| 1 | G | 12 | GLU | CD-OE2 | 5.13 | 1.31 | 1.25 |
| 1 | P | 21 | GLU | CD-OE2 | 5.13 | 1.31 | 1.25 |
| 1 | J | 12 | GLU | CD-OE2 | 5.13 | 1.31 | 1.25 |
| 1 | M | 506 | GLU | CD-OE2 | 5.13 | 1.31 | 1.25 |
| 1 | A | 697 | CYS | CB-SG | 5.12 | 1.91 | 1.82 |
| 1 | M | 527 | GLU | CD-OE2 | -5.11 | 1.20 | 1.25 |
| 4 | Z | 259 | GLU | CB-CG | 5.10 | 1.61 | 1.52 |
| 1 | G | 150 | GLU | CD-OE1 | 5.09 | 1.31 | 1.25 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1 | D | 12 | GLU | CD-OE2 | 5.09 | 1.31 | 1.25 |
| 2 | H | 149 | ASP | CB-CG | 5.09 | 1.62 | 1.51 |
| 1 | A | 527 | GLU | CD-OE2 | -5.09 | 1.20 | 1.25 |
| 4 | 4 | 259 | GLU | CB-CG | 5.08 | 1.61 | 1.52 |
| 1 | G | 539 | GLU | CD-OE1 | 5.08 | 1.31 | 1.25 |
| 1 | A | 56 | GLU | CD-OE1 | 5.07 | 1.31 | 1.25 |
| 4 | 6 | 259 | GLU | CB-CG | 5.07 | 1.61 | 1.52 |
| 1 | A | 679 | GLU | CD-OE2 | 5.07 | 1.31 | 1.25 |
| 1 | J | 506 | GLU | CD-OE2 | 5.07 | 1.31 | 1.25 |
| 4 | 1 | 259 | GLU | CB-CG | 5.06 | 1.61 | 1.52 |
| 4 | 7 | 259 | GLU | CB-CG | 5.06 | 1.61 | 1.52 |
| 4 | X | 259 | GLU | CB-CG | 5.06 | 1.61 | 1.52 |
| 4 | V | 259 | GLU | CB-CG | 5.06 | 1.61 | 1.52 |
| 4 | 5 | 259 | GLU | CB-CG | 5.06 | 1.61 | 1.52 |
| 1 | D | 21 | GLU | CD-OE2 | 5.05 | 1.31 | 1.25 |
| 1 | M | 282 | GLU | CD-OE1 | 5.05 | 1.31 | 1.25 |
| 1 | A | 12 | GLU | CD-OE2 | 5.04 | 1.31 | 1.25 |
| 1 | M | 697 | CYS | CB-SG | 5.04 | 1.90 | 1.82 |
| 4 | W | 259 | GLU | CB-CG | 5.04 | 1.61 | 1.52 |
| 4 | 2 | 259 | GLU | CB-CG | 5.04 | 1.61 | 1.52 |
| 1 | P | 150 | GLU | CD-OE1 | 5.03 | 1.31 | 1.25 |
| 4 | 9 | 259 | GLU | CB-CG | 5.03 | 1.61 | 1.52 |
| 1 | J | 150 | GLU | CD-OE1 | 5.03 | 1.31 | 1.25 |
| 4 | Y | 259 | GLU | CB-CG | 5.02 | 1.61 | 1.52 |
| 1 | A | 282 | GLU | CD-OE1 | 5.02 | 1.31 | 1.25 |
| 1 | G | 282 | GLU | CD-OE1 | 5.02 | 1.31 | 1.25 |
| 1 | G | 527 | GLU | CD-OE2 | -5.02 | 1.20 | 1.25 |
| 4 | 3 | 259 | GLU | CB-CG | 5.02 | 1.61 | 1.52 |
| 1 | D | 539 | GLU | CD-OE1 | 5.02 | 1.31 | 1.25 |
| 1 | M | 56 | GLU | CD-OE1 | 5.02 | 1.31 | 1.25 |
| 1 | J | 697 | CYS | CB-SG | 5.01 | 1.90 | 1.82 |
| 1 | J | 539 | GLU | CD-OE1 | 5.01 | 1.31 | 1.25 |
| 1 | D | 697 | CYS | CB-SG | 5.00 | 1.90 | 1.82 |
| 1 | D | 150 | GLU | CD-OE1 | 5.00 | 1.31 | 1.25 |
| 1 | P | 56 | GLU | CD-OE1 | 5.00 | 1.31 | 1.25 |

All (1545) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------|--------|-------------|----------|
| 1 | G | 637 | LYS | O-C-N | -58.52 | 23.72 | 123.20 |
| 1 | M | 637 | LYS | O-C-N | -58.47 | 23.80 | 123.20 |
| 1 | D | 637 | LYS | O-C-N | -58.47 | 23.81 | 123.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|--------|-------------|----------|
| 1 | P | 637 | LYS | O-C-N | -58.47 | 23.81 | 123.20 |
| 1 | A | 637 | LYS | O-C-N | -58.46 | 23.81 | 123.20 |
| 1 | J | 637 | LYS | O-C-N | -58.45 | 23.84 | 123.20 |
| 1 | J | 709 | LYS | O-C-N | -37.56 | 59.35 | 123.20 |
| 1 | G | 649 | VAL | CG1-CB-CG2 | -34.02 | 56.47 | 110.90 |
| 1 | M | 649 | VAL | CG1-CB-CG2 | -34.00 | 56.50 | 110.90 |
| 1 | A | 649 | VAL | CG1-CB-CG2 | -33.99 | 56.52 | 110.90 |
| 1 | J | 649 | VAL | CG1-CB-CG2 | -33.98 | 56.53 | 110.90 |
| 1 | D | 649 | VAL | CG1-CB-CG2 | -33.98 | 56.53 | 110.90 |
| 1 | P | 649 | VAL | CG1-CB-CG2 | -33.97 | 56.56 | 110.90 |
| 1 | A | 648 | THR | CA-CB-OG1 | -31.72 | 42.39 | 109.00 |
| 1 | M | 648 | THR | CA-CB-OG1 | -31.72 | 42.39 | 109.00 |
| 1 | P | 648 | THR | CA-CB-OG1 | -31.72 | 42.39 | 109.00 |
| 1 | J | 648 | THR | CA-CB-OG1 | -31.71 | 42.40 | 109.00 |
| 1 | D | 648 | THR | CA-CB-OG1 | -31.71 | 42.41 | 109.00 |
| 1 | G | 648 | THR | CA-CB-OG1 | -31.67 | 42.48 | 109.00 |
| 1 | P | 785 | GLU | O-C-N | -30.54 | 73.83 | 122.70 |
| 2 | E | 150 | TYR | CB-CG-CD2 | -28.68 | 103.79 | 121.00 |
| 2 | H | 150 | TYR | CB-CG-CD2 | -28.67 | 103.80 | 121.00 |
| 2 | B | 150 | TYR | CB-CG-CD2 | -28.67 | 103.80 | 121.00 |
| 2 | K | 150 | TYR | CB-CG-CD2 | -28.61 | 103.83 | 121.00 |
| 2 | Q | 150 | TYR | CB-CG-CD2 | -28.59 | 103.84 | 121.00 |
| 1 | G | 649 | VAL | CA-CB-CG1 | -28.55 | 68.08 | 110.90 |
| 1 | M | 649 | VAL | CA-CB-CG1 | -28.48 | 68.17 | 110.90 |
| 1 | J | 649 | VAL | CA-CB-CG1 | -28.46 | 68.21 | 110.90 |
| 1 | P | 649 | VAL | CA-CB-CG1 | -28.45 | 68.23 | 110.90 |
| 1 | D | 649 | VAL | CA-CB-CG1 | -28.45 | 68.23 | 110.90 |
| 1 | A | 649 | VAL | CA-CB-CG1 | -28.43 | 68.25 | 110.90 |
| 2 | N | 150 | TYR | CB-CG-CD2 | -28.43 | 103.94 | 121.00 |
| 1 | G | 649 | VAL | CA-CB-CG2 | -28.16 | 68.65 | 110.90 |
| 1 | J | 649 | VAL | CA-CB-CG2 | -28.16 | 68.66 | 110.90 |
| 1 | M | 649 | VAL | CA-CB-CG2 | -28.16 | 68.67 | 110.90 |
| 1 | P | 649 | VAL | CA-CB-CG2 | -28.15 | 68.68 | 110.90 |
| 1 | D | 649 | VAL | CA-CB-CG2 | -28.14 | 68.69 | 110.90 |
| 1 | A | 649 | VAL | CA-CB-CG2 | -28.13 | 68.70 | 110.90 |
| 1 | J | 648 | THR | CA-CB-CG2 | -25.61 | 76.55 | 112.40 |
| 1 | P | 648 | THR | CA-CB-CG2 | -25.51 | 76.69 | 112.40 |
| 1 | D | 648 | THR | CA-CB-CG2 | -25.50 | 76.71 | 112.40 |
| 1 | G | 648 | THR | CA-CB-CG2 | -25.49 | 76.72 | 112.40 |
| 1 | A | 648 | THR | CA-CB-CG2 | -25.48 | 76.73 | 112.40 |
| 1 | M | 648 | THR | CA-CB-CG2 | -25.45 | 76.76 | 112.40 |
| 2 | H | 150 | TYR | CG-CD2-CE2 | -20.93 | 104.56 | 121.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|--------|-------------|----------|
| 2 | E | 150 | TYR | CG-CD2-CE2 | -20.62 | 104.80 | 121.30 |
| 2 | Q | 150 | TYR | CG-CD2-CE2 | -20.54 | 104.87 | 121.30 |
| 2 | B | 150 | TYR | CG-CD2-CE2 | -20.52 | 104.89 | 121.30 |
| 2 | K | 150 | TYR | CG-CD2-CE2 | -20.48 | 104.92 | 121.30 |
| 2 | N | 150 | TYR | CG-CD2-CE2 | -20.47 | 104.92 | 121.30 |
| 2 | Q | 150 | TYR | CD1-CG-CD2 | 19.58 | 139.44 | 117.90 |
| 2 | K | 150 | TYR | CD1-CG-CD2 | 19.56 | 139.41 | 117.90 |
| 2 | E | 150 | TYR | CD1-CG-CD2 | 19.50 | 139.35 | 117.90 |
| 2 | H | 150 | TYR | CD1-CG-CD2 | 19.49 | 139.34 | 117.90 |
| 2 | N | 150 | TYR | CD1-CG-CD2 | 19.42 | 139.27 | 117.90 |
| 2 | B | 150 | TYR | CD1-CG-CD2 | 19.42 | 139.26 | 117.90 |
| 2 | K | 150 | TYR | CG-CD1-CE1 | -18.55 | 106.46 | 121.30 |
| 2 | Q | 150 | TYR | CG-CD1-CE1 | -18.50 | 106.50 | 121.30 |
| 2 | E | 150 | TYR | CG-CD1-CE1 | -18.45 | 106.54 | 121.30 |
| 2 | N | 150 | TYR | CG-CD1-CE1 | -18.44 | 106.55 | 121.30 |
| 2 | H | 150 | TYR | CG-CD1-CE1 | -18.43 | 106.56 | 121.30 |
| 2 | B | 150 | TYR | CG-CD1-CE1 | -18.36 | 106.61 | 121.30 |
| 1 | P | 806 | MET | O-C-N | 17.64 | 150.93 | 122.70 |
| 1 | M | 800 | ARG | NE-CZ-NH2 | -16.63 | 111.98 | 120.30 |
| 1 | J | 800 | ARG | NE-CZ-NH2 | -16.62 | 111.99 | 120.30 |
| 1 | P | 800 | ARG | NE-CZ-NH2 | -16.49 | 112.06 | 120.30 |
| 1 | D | 800 | ARG | NE-CZ-NH2 | -16.40 | 112.10 | 120.30 |
| 1 | A | 800 | ARG | NE-CZ-NH2 | -16.35 | 112.12 | 120.30 |
| 1 | G | 800 | ARG | NE-CZ-NH2 | -16.27 | 112.17 | 120.30 |
| 1 | M | 709 | LYS | C-N-CA | -14.39 | 92.08 | 122.30 |
| 1 | P | 806 | MET | CA-C-N | -14.36 | 85.61 | 117.20 |
| 1 | G | 623 | PHE | CB-CG-CD2 | -13.83 | 111.12 | 120.80 |
| 1 | A | 623 | PHE | CB-CG-CD2 | -13.80 | 111.14 | 120.80 |
| 1 | M | 709 | LYS | O-C-N | 13.79 | 146.65 | 123.20 |
| 1 | M | 623 | PHE | CB-CG-CD2 | -13.76 | 111.17 | 120.80 |
| 1 | P | 785 | GLU | CA-C-N | 13.68 | 147.29 | 117.20 |
| 1 | P | 623 | PHE | CB-CG-CD2 | -13.64 | 111.25 | 120.80 |
| 1 | J | 623 | PHE | CB-CG-CD2 | -13.59 | 111.28 | 120.80 |
| 1 | D | 623 | PHE | CB-CG-CD2 | -13.51 | 111.34 | 120.80 |
| 1 | M | 806 | MET | CA-C-N | -13.18 | 88.19 | 117.20 |
| 1 | M | 709 | LYS | CA-C-N | -13.16 | 89.88 | 116.20 |
| 1 | A | 623 | PHE | CB-CG-CD1 | 12.42 | 129.49 | 120.80 |
| 1 | M | 623 | PHE | CB-CG-CD1 | 12.38 | 129.47 | 120.80 |
| 1 | P | 623 | PHE | CB-CG-CD1 | 12.37 | 129.46 | 120.80 |
| 1 | G | 623 | PHE | CB-CG-CD1 | 12.36 | 129.45 | 120.80 |
| 1 | M | 806 | MET | O-C-N | 12.29 | 142.36 | 122.70 |
| 1 | J | 623 | PHE | CB-CG-CD1 | 12.28 | 129.40 | 120.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|--------|-------------|----------|
| 1 | A | 623 | PHE | CA-CB-CG | -12.28 | 84.43 | 113.90 |
| 1 | P | 623 | PHE | CA-CB-CG | -12.28 | 84.44 | 113.90 |
| 1 | J | 623 | PHE | CA-CB-CG | -12.25 | 84.49 | 113.90 |
| 1 | M | 623 | PHE | CA-CB-CG | -12.23 | 84.54 | 113.90 |
| 1 | G | 623 | PHE | CA-CB-CG | -12.21 | 84.60 | 113.90 |
| 1 | D | 623 | PHE | CA-CB-CG | -12.20 | 84.61 | 113.90 |
| 1 | D | 623 | PHE | CB-CG-CD1 | 12.01 | 129.20 | 120.80 |
| 1 | M | 98 | HIS | CB-CA-C | -11.61 | 87.19 | 110.40 |
| 1 | J | 98 | HIS | CB-CA-C | -11.58 | 87.23 | 110.40 |
| 1 | P | 98 | HIS | CB-CA-C | -11.56 | 87.27 | 110.40 |
| 1 | G | 98 | HIS | CB-CA-C | -11.56 | 87.27 | 110.40 |
| 1 | A | 98 | HIS | CB-CA-C | -11.54 | 87.32 | 110.40 |
| 1 | D | 98 | HIS | CB-CA-C | -11.53 | 87.35 | 110.40 |
| 1 | A | 568 | PRO | O-C-N | 10.70 | 139.82 | 122.70 |
| 1 | G | 568 | PRO | O-C-N | 10.69 | 139.80 | 122.70 |
| 1 | D | 568 | PRO | O-C-N | 10.67 | 139.77 | 122.70 |
| 1 | P | 568 | PRO | O-C-N | 10.63 | 139.71 | 122.70 |
| 1 | J | 568 | PRO | O-C-N | 10.63 | 139.70 | 122.70 |
| 1 | M | 568 | PRO | O-C-N | 10.62 | 139.70 | 122.70 |
| 2 | E | 141 | PRO | CA-N-CD | 10.30 | 126.12 | 111.70 |
| 2 | Q | 141 | PRO | CA-N-CD | 10.26 | 126.06 | 111.70 |
| 2 | K | 141 | PRO | CA-N-CD | 10.25 | 126.06 | 111.70 |
| 2 | H | 141 | PRO | CA-N-CD | 10.25 | 126.05 | 111.70 |
| 2 | N | 141 | PRO | CA-N-CD | 10.20 | 125.98 | 111.70 |
| 2 | B | 141 | PRO | CA-N-CD | 10.17 | 125.94 | 111.70 |
| 1 | G | 625 | THR | CA-CB-CG2 | -10.10 | 98.26 | 112.40 |
| 1 | G | 709 | LYS | O-C-N | 10.10 | 140.38 | 123.20 |
| 1 | J | 327 | ASP | CB-CG-OD1 | -10.07 | 109.24 | 118.30 |
| 1 | A | 625 | THR | CA-CB-CG2 | -10.06 | 98.31 | 112.40 |
| 1 | D | 327 | ASP | CB-CG-OD1 | -10.06 | 109.25 | 118.30 |
| 1 | P | 625 | THR | CA-CB-CG2 | -10.05 | 98.33 | 112.40 |
| 1 | J | 625 | THR | CA-CB-CG2 | -10.04 | 98.34 | 112.40 |
| 1 | M | 625 | THR | CA-CB-CG2 | -10.01 | 98.38 | 112.40 |
| 1 | D | 625 | THR | CA-CB-CG2 | -9.98 | 98.42 | 112.40 |
| 1 | G | 327 | ASP | CB-CG-OD1 | -9.97 | 109.32 | 118.30 |
| 1 | A | 327 | ASP | CB-CG-OD1 | -9.95 | 109.34 | 118.30 |
| 1 | M | 327 | ASP | CB-CG-OD1 | -9.95 | 109.35 | 118.30 |
| 1 | P | 327 | ASP | CB-CG-OD1 | -9.94 | 109.35 | 118.30 |
| 1 | J | 241 | ASP | CB-CG-OD1 | -9.88 | 109.41 | 118.30 |
| 1 | G | 241 | ASP | CB-CG-OD1 | -9.83 | 109.45 | 118.30 |
| 1 | D | 241 | ASP | CB-CG-OD1 | -9.83 | 109.45 | 118.30 |
| 1 | P | 241 | ASP | CB-CG-OD1 | -9.83 | 109.45 | 118.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1 | A | 241 | ASP | CB-CG-OD1 | -9.81 | 109.47 | 118.30 |
| 3 | C | 63 | ILE | O-C-N | 9.74 | 138.28 | 122.70 |
| 3 | R | 63 | ILE | O-C-N | 9.74 | 138.28 | 122.70 |
| 1 | J | 728 | ASN | O-C-N | 9.73 | 138.26 | 122.70 |
| 1 | M | 241 | ASP | CB-CG-OD1 | -9.72 | 109.55 | 118.30 |
| 1 | D | 728 | ASN | O-C-N | 9.72 | 138.26 | 122.70 |
| 1 | M | 728 | ASN | O-C-N | 9.71 | 138.24 | 122.70 |
| 1 | P | 728 | ASN | O-C-N | 9.70 | 138.22 | 122.70 |
| 3 | O | 63 | ILE | O-C-N | 9.70 | 138.22 | 122.70 |
| 3 | F | 63 | ILE | O-C-N | 9.69 | 138.21 | 122.70 |
| 3 | I | 63 | ILE | O-C-N | 9.69 | 138.21 | 122.70 |
| 3 | L | 63 | ILE | O-C-N | 9.68 | 138.19 | 122.70 |
| 1 | A | 728 | ASN | O-C-N | 9.65 | 138.14 | 122.70 |
| 1 | G | 264 | ASP | CB-CG-OD2 | -9.62 | 109.64 | 118.30 |
| 1 | G | 728 | ASN | O-C-N | 9.60 | 138.05 | 122.70 |
| 1 | M | 264 | ASP | CB-CG-OD2 | -9.56 | 109.69 | 118.30 |
| 1 | D | 264 | ASP | CB-CG-OD2 | -9.45 | 109.79 | 118.30 |
| 1 | G | 709 | LYS | CA-C-N | -9.44 | 97.32 | 116.20 |
| 1 | A | 264 | ASP | CB-CG-OD2 | -9.42 | 109.83 | 118.30 |
| 1 | P | 264 | ASP | CB-CG-OD2 | -9.40 | 109.84 | 118.30 |
| 2 | E | 150 | TYR | N-CA-CB | -9.35 | 93.76 | 110.60 |
| 1 | J | 264 | ASP | CB-CG-OD2 | -9.34 | 109.89 | 118.30 |
| 2 | H | 150 | TYR | N-CA-CB | -9.34 | 93.79 | 110.60 |
| 2 | Q | 150 | TYR | N-CA-CB | -9.34 | 93.80 | 110.60 |
| 2 | B | 150 | TYR | N-CA-CB | -9.33 | 93.80 | 110.60 |
| 2 | K | 150 | TYR | N-CA-CB | -9.33 | 93.80 | 110.60 |
| 2 | N | 150 | TYR | N-CA-CB | -9.33 | 93.81 | 110.60 |
| 4 | 9 | 356 | TRP | CD1-CG-CD2 | 9.25 | 113.70 | 106.30 |
| 4 | W | 356 | TRP | CD1-CG-CD2 | 9.22 | 113.68 | 106.30 |
| 4 | Y | 356 | TRP | CD1-CG-CD2 | 9.15 | 113.62 | 106.30 |
| 1 | P | 806 | MET | C-N-CA | -9.13 | 98.86 | 121.70 |
| 4 | 6 | 356 | TRP | CD1-CG-CD2 | 9.13 | 113.61 | 106.30 |
| 4 | 1 | 356 | TRP | CD1-CG-CD2 | 9.12 | 113.59 | 106.30 |
| 4 | Z | 356 | TRP | CD1-CG-CD2 | 9.12 | 113.59 | 106.30 |
| 4 | 3 | 356 | TRP | CD1-CG-CD2 | 9.11 | 113.59 | 106.30 |
| 4 | 7 | 356 | TRP | CD1-CG-CD2 | 9.11 | 113.58 | 106.30 |
| 4 | 8 | 356 | TRP | CD1-CG-CD2 | 9.10 | 113.58 | 106.30 |
| 4 | 2 | 356 | TRP | CD1-CG-CD2 | 9.08 | 113.56 | 106.30 |
| 4 | 5 | 356 | TRP | CD1-CG-CD2 | 9.05 | 113.54 | 106.30 |
| 1 | P | 352 | TYR | CB-CG-CD1 | 9.05 | 126.43 | 121.00 |
| 4 | 4 | 356 | TRP | CD1-CG-CD2 | 9.03 | 113.52 | 106.30 |
| 1 | J | 378 | ASP | CB-CG-OD2 | 9.01 | 126.41 | 118.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 4 | X | 356 | TRP | CD1-CG-CD2 | 9.01 | 113.51 | 106.30 |
| 1 | J | 352 | TYR | CB-CG-CD1 | 9.00 | 126.40 | 121.00 |
| 1 | P | 378 | ASP | CB-CG-OD2 | 8.97 | 126.38 | 118.30 |
| 1 | D | 378 | ASP | CB-CG-OD2 | 8.96 | 126.36 | 118.30 |
| 1 | M | 378 | ASP | CB-CG-OD2 | 8.94 | 126.34 | 118.30 |
| 4 | V | 356 | TRP | CD1-CG-CD2 | 8.93 | 113.44 | 106.30 |
| 1 | G | 378 | ASP | CB-CG-OD2 | 8.85 | 126.27 | 118.30 |
| 1 | D | 352 | TYR | CB-CG-CD1 | 8.81 | 126.29 | 121.00 |
| 1 | A | 378 | ASP | CB-CG-OD2 | 8.80 | 126.22 | 118.30 |
| 2 | N | 138 | ALA | O-C-N | -8.78 | 108.65 | 122.70 |
| 1 | M | 352 | TYR | CB-CG-CD1 | 8.77 | 126.26 | 121.00 |
| 4 | 1 | 177 | ARG | NE-CZ-NH2 | -8.77 | 115.92 | 120.30 |
| 2 | Q | 138 | ALA | O-C-N | -8.76 | 108.69 | 122.70 |
| 2 | K | 138 | ALA | O-C-N | -8.76 | 108.69 | 122.70 |
| 1 | G | 352 | TYR | CB-CG-CD1 | 8.75 | 126.25 | 121.00 |
| 1 | A | 352 | TYR | CB-CG-CD1 | 8.73 | 126.24 | 121.00 |
| 2 | E | 138 | ALA | O-C-N | -8.72 | 108.75 | 122.70 |
| 2 | B | 138 | ALA | O-C-N | -8.69 | 108.79 | 122.70 |
| 4 | 3 | 86 | TRP | CD1-CG-CD2 | 8.69 | 113.25 | 106.30 |
| 2 | H | 138 | ALA | O-C-N | -8.66 | 108.85 | 122.70 |
| 4 | W | 177 | ARG | NE-CZ-NH2 | -8.63 | 115.98 | 120.30 |
| 4 | 3 | 177 | ARG | NE-CZ-NH2 | -8.63 | 115.98 | 120.30 |
| 4 | 2 | 177 | ARG | NE-CZ-NH2 | -8.61 | 116.00 | 120.30 |
| 4 | 8 | 177 | ARG | NE-CZ-NH2 | -8.60 | 116.00 | 120.30 |
| 4 | 5 | 177 | ARG | NE-CZ-NH2 | -8.59 | 116.00 | 120.30 |
| 4 | 4 | 177 | ARG | NE-CZ-NH2 | -8.59 | 116.01 | 120.30 |
| 4 | Z | 177 | ARG | NE-CZ-NH2 | -8.59 | 116.01 | 120.30 |
| 4 | V | 177 | ARG | NE-CZ-NH2 | -8.57 | 116.01 | 120.30 |
| 4 | 5 | 86 | TRP | CD1-CG-CD2 | 8.56 | 113.15 | 106.30 |
| 4 | 1 | 86 | TRP | CD1-CG-CD2 | 8.56 | 113.15 | 106.30 |
| 4 | X | 177 | ARG | NE-CZ-NH2 | -8.55 | 116.02 | 120.30 |
| 4 | Y | 177 | ARG | NE-CZ-NH2 | -8.54 | 116.03 | 120.30 |
| 4 | 8 | 86 | TRP | CD1-CG-CD2 | 8.53 | 113.13 | 106.30 |
| 4 | V | 86 | TRP | CD1-CG-CD2 | 8.53 | 113.13 | 106.30 |
| 1 | M | 601 | ASP | CB-CG-OD1 | -8.53 | 110.62 | 118.30 |
| 4 | Y | 86 | TRP | CD1-CG-CD2 | 8.52 | 113.12 | 106.30 |
| 4 | W | 86 | TRP | CD1-CG-CD2 | 8.51 | 113.11 | 106.30 |
| 1 | A | 601 | ASP | CB-CG-OD1 | -8.50 | 110.65 | 118.30 |
| 1 | G | 601 | ASP | CB-CG-OD1 | -8.50 | 110.65 | 118.30 |
| 1 | J | 33 | ASP | CB-CG-OD1 | -8.49 | 110.66 | 118.30 |
| 4 | 9 | 86 | TRP | CD1-CG-CD2 | 8.49 | 113.10 | 106.30 |
| 1 | P | 33 | ASP | CB-CG-OD1 | -8.48 | 110.66 | 118.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 4 | 9 | 177 | ARG | NE-CZ-NH2 | -8.48 | 116.06 | 120.30 |
| 4 | X | 86 | TRP | CD1-CG-CD2 | 8.48 | 113.08 | 106.30 |
| 1 | J | 601 | ASP | CB-CG-OD1 | -8.46 | 110.68 | 118.30 |
| 4 | Z | 86 | TRP | CD1-CG-CD2 | 8.45 | 113.06 | 106.30 |
| 4 | 2 | 86 | TRP | CD1-CG-CD2 | 8.44 | 113.06 | 106.30 |
| 1 | P | 352 | TYR | CB-CG-CD2 | -8.43 | 115.94 | 121.00 |
| 4 | 6 | 177 | ARG | NE-CZ-NH2 | -8.42 | 116.09 | 120.30 |
| 1 | D | 601 | ASP | CB-CG-OD1 | -8.41 | 110.73 | 118.30 |
| 4 | 7 | 177 | ARG | NE-CZ-NH2 | -8.40 | 116.10 | 120.30 |
| 4 | 7 | 86 | TRP | CD1-CG-CD2 | 8.39 | 113.02 | 106.30 |
| 4 | 4 | 86 | TRP | CD1-CG-CD2 | 8.39 | 113.01 | 106.30 |
| 1 | J | 352 | TYR | CB-CG-CD2 | -8.38 | 115.97 | 121.00 |
| 4 | 6 | 86 | TRP | CD1-CG-CD2 | 8.35 | 112.98 | 106.30 |
| 1 | M | 33 | ASP | CB-CG-OD1 | -8.35 | 110.79 | 118.30 |
| 1 | P | 601 | ASP | CB-CG-OD1 | -8.34 | 110.79 | 118.30 |
| 1 | D | 33 | ASP | CB-CG-OD1 | -8.34 | 110.79 | 118.30 |
| 1 | A | 352 | TYR | CB-CG-CD2 | -8.29 | 116.03 | 121.00 |
| 1 | M | 352 | TYR | CB-CG-CD2 | -8.29 | 116.03 | 121.00 |
| 1 | G | 33 | ASP | CB-CG-OD1 | -8.23 | 110.89 | 118.30 |
| 1 | A | 33 | ASP | CB-CG-OD1 | -8.21 | 110.91 | 118.30 |
| 1 | G | 352 | TYR | CB-CG-CD2 | -8.19 | 116.09 | 121.00 |
| 4 | W | 356 | TRP | CE2-CD2-CG | -8.11 | 100.81 | 107.30 |
| 1 | D | 352 | TYR | CB-CG-CD2 | -8.11 | 116.13 | 121.00 |
| 4 | 9 | 356 | TRP | CE2-CD2-CG | -8.05 | 100.86 | 107.30 |
| 4 | 6 | 356 | TRP | CE2-CD2-CG | -8.02 | 100.88 | 107.30 |
| 4 | 7 | 356 | TRP | CE2-CD2-CG | -8.00 | 100.90 | 107.30 |
| 4 | Y | 356 | TRP | CE2-CD2-CG | -7.97 | 100.92 | 107.30 |
| 4 | 1 | 356 | TRP | CE2-CD2-CG | -7.96 | 100.93 | 107.30 |
| 4 | 2 | 356 | TRP | CE2-CD2-CG | -7.95 | 100.94 | 107.30 |
| 4 | 3 | 356 | TRP | CE2-CD2-CG | -7.94 | 100.95 | 107.30 |
| 4 | 4 | 356 | TRP | CE2-CD2-CG | -7.94 | 100.95 | 107.30 |
| 4 | Z | 356 | TRP | CE2-CD2-CG | -7.94 | 100.95 | 107.30 |
| 1 | A | 637 | LYS | CA-C-N | 7.93 | 132.07 | 116.20 |
| 1 | A | 339 | ASP | CB-CG-OD1 | -7.93 | 111.16 | 118.30 |
| 1 | J | 637 | LYS | CA-C-N | 7.93 | 132.06 | 116.20 |
| 1 | M | 806 | MET | C-N-CA | -7.92 | 101.90 | 121.70 |
| 4 | 5 | 356 | TRP | CE2-CD2-CG | -7.91 | 100.97 | 107.30 |
| 1 | J | 339 | ASP | CB-CG-OD1 | -7.91 | 111.18 | 118.30 |
| 1 | G | 339 | ASP | CB-CG-OD1 | -7.90 | 111.19 | 118.30 |
| 1 | P | 637 | LYS | CA-C-N | 7.90 | 132.00 | 116.20 |
| 1 | D | 637 | LYS | CA-C-N | 7.89 | 131.97 | 116.20 |
| 1 | P | 339 | ASP | CB-CG-OD1 | -7.89 | 111.20 | 118.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 2 | E | 150 | TYR | CD1-CE1-CZ | -7.88 | 112.71 | 119.80 |
| 1 | M | 637 | LYS | CA-C-N | 7.88 | 131.96 | 116.20 |
| 4 | 8 | 356 | TRP | CE2-CD2-CG | -7.87 | 101.00 | 107.30 |
| 1 | G | 637 | LYS | CA-C-N | 7.87 | 131.94 | 116.20 |
| 4 | X | 356 | TRP | CE2-CD2-CG | -7.85 | 101.02 | 107.30 |
| 1 | D | 339 | ASP | CB-CG-OD1 | -7.85 | 111.24 | 118.30 |
| 1 | M | 339 | ASP | CB-CG-OD1 | -7.84 | 111.25 | 118.30 |
| 2 | H | 150 | TYR | CD1-CE1-CZ | -7.83 | 112.76 | 119.80 |
| 4 | 1 | 312 | ARG | NE-CZ-NH2 | 7.82 | 124.21 | 120.30 |
| 2 | B | 150 | TYR | CD1-CE1-CZ | -7.81 | 112.77 | 119.80 |
| 4 | V | 356 | TRP | CE2-CD2-CG | -7.80 | 101.06 | 107.30 |
| 2 | Q | 150 | TYR | CD1-CE1-CZ | -7.79 | 112.79 | 119.80 |
| 2 | N | 150 | TYR | CD1-CE1-CZ | -7.78 | 112.80 | 119.80 |
| 4 | 6 | 312 | ARG | NE-CZ-NH2 | 7.78 | 124.19 | 120.30 |
| 1 | D | 202 | SER | CB-CA-C | -7.78 | 95.32 | 110.10 |
| 4 | 5 | 312 | ARG | NE-CZ-NH2 | 7.76 | 124.18 | 120.30 |
| 1 | A | 202 | SER | CB-CA-C | -7.75 | 95.38 | 110.10 |
| 1 | J | 202 | SER | CB-CA-C | -7.75 | 95.38 | 110.10 |
| 4 | 9 | 312 | ARG | NE-CZ-NH2 | 7.74 | 124.17 | 120.30 |
| 4 | 4 | 312 | ARG | NE-CZ-NH2 | 7.73 | 124.17 | 120.30 |
| 1 | P | 202 | SER | CB-CA-C | -7.73 | 95.42 | 110.10 |
| 1 | M | 202 | SER | CB-CA-C | -7.72 | 95.42 | 110.10 |
| 4 | 3 | 86 | TRP | CE2-CD2-CG | -7.72 | 101.12 | 107.30 |
| 4 | 3 | 312 | ARG | NE-CZ-NH2 | 7.72 | 124.16 | 120.30 |
| 4 | Y | 312 | ARG | NE-CZ-NH2 | 7.70 | 124.15 | 120.30 |
| 1 | M | 653 | PHE | CB-CG-CD1 | -7.70 | 115.41 | 120.80 |
| 4 | W | 312 | ARG | NE-CZ-NH2 | 7.69 | 124.15 | 120.30 |
| 1 | G | 202 | SER | CB-CA-C | -7.69 | 95.50 | 110.10 |
| 4 | Z | 312 | ARG | NE-CZ-NH2 | 7.67 | 124.14 | 120.30 |
| 2 | K | 150 | TYR | CD1-CE1-CZ | -7.67 | 112.89 | 119.80 |
| 4 | 2 | 312 | ARG | NE-CZ-NH2 | 7.66 | 124.13 | 120.30 |
| 4 | 1 | 86 | TRP | CE2-CD2-CG | -7.65 | 101.18 | 107.30 |
| 1 | P | 653 | PHE | CB-CG-CD1 | -7.65 | 115.45 | 120.80 |
| 4 | 5 | 86 | TRP | CE2-CD2-CG | -7.65 | 101.18 | 107.30 |
| 1 | G | 653 | PHE | CB-CG-CD1 | -7.63 | 115.46 | 120.80 |
| 4 | 7 | 312 | ARG | NE-CZ-NH2 | 7.63 | 124.11 | 120.30 |
| 4 | 8 | 86 | TRP | CE2-CD2-CG | -7.61 | 101.21 | 107.30 |
| 1 | J | 653 | PHE | CB-CG-CD1 | -7.60 | 115.48 | 120.80 |
| 4 | 9 | 86 | TRP | CE2-CD2-CG | -7.60 | 101.22 | 107.30 |
| 1 | G | 654 | ARG | NE-CZ-NH1 | 7.59 | 124.09 | 120.30 |
| 4 | W | 86 | TRP | CE2-CD2-CG | -7.58 | 101.23 | 107.30 |
| 4 | Y | 86 | TRP | CE2-CD2-CG | -7.57 | 101.24 | 107.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1 | D | 653 | PHE | CB-CG-CD1 | -7.55 | 115.51 | 120.80 |
| 4 | 8 | 312 | ARG | NE-CZ-NH2 | 7.54 | 124.07 | 120.30 |
| 4 | V | 312 | ARG | NE-CZ-NH2 | 7.54 | 124.07 | 120.30 |
| 1 | A | 654 | ARG | NE-CZ-NH1 | 7.54 | 124.07 | 120.30 |
| 4 | 4 | 86 | TRP | CE2-CD2-CG | -7.54 | 101.27 | 107.30 |
| 4 | V | 86 | TRP | CE2-CD2-CG | -7.53 | 101.27 | 107.30 |
| 4 | X | 312 | ARG | NE-CZ-NH2 | 7.53 | 124.07 | 120.30 |
| 4 | 2 | 86 | TRP | CE2-CD2-CG | -7.53 | 101.28 | 107.30 |
| 4 | X | 86 | TRP | CE2-CD2-CG | -7.52 | 101.28 | 107.30 |
| 3 | L | 63 | ILE | CG1-CB-CG2 | -7.51 | 94.87 | 111.40 |
| 4 | 7 | 86 | TRP | CE2-CD2-CG | -7.51 | 101.29 | 107.30 |
| 4 | Z | 86 | TRP | CE2-CD2-CG | -7.51 | 101.30 | 107.30 |
| 3 | R | 63 | ILE | CG1-CB-CG2 | -7.50 | 94.90 | 111.40 |
| 4 | 6 | 86 | TRP | CE2-CD2-CG | -7.50 | 101.30 | 107.30 |
| 3 | C | 63 | ILE | CG1-CB-CG2 | -7.50 | 94.91 | 111.40 |
| 3 | I | 63 | ILE | CG1-CB-CG2 | -7.49 | 94.92 | 111.40 |
| 3 | F | 63 | ILE | CG1-CB-CG2 | -7.48 | 94.94 | 111.40 |
| 2 | B | 127 | ARG | NE-CZ-NH2 | 7.48 | 124.04 | 120.30 |
| 1 | P | 654 | ARG | NE-CZ-NH1 | 7.48 | 124.04 | 120.30 |
| 1 | P | 518 | ASP | CB-CG-OD1 | -7.47 | 111.58 | 118.30 |
| 1 | A | 653 | PHE | CB-CG-CD1 | -7.46 | 115.58 | 120.80 |
| 1 | M | 518 | ASP | CB-CG-OD1 | -7.46 | 111.58 | 118.30 |
| 3 | O | 63 | ILE | CG1-CB-CG2 | -7.45 | 95.02 | 111.40 |
| 1 | J | 518 | ASP | CB-CG-OD1 | -7.42 | 111.62 | 118.30 |
| 1 | D | 346 | ASP | CB-CG-OD2 | -7.41 | 111.63 | 118.30 |
| 2 | E | 127 | ARG | NE-CZ-NH2 | 7.41 | 124.01 | 120.30 |
| 1 | G | 346 | ASP | CB-CG-OD2 | -7.41 | 111.63 | 118.30 |
| 1 | D | 518 | ASP | CB-CG-OD1 | -7.40 | 111.64 | 118.30 |
| 4 | 5 | 233 | SER | CA-C-N | -7.38 | 100.95 | 117.20 |
| 4 | V | 233 | SER | CA-C-N | -7.38 | 100.97 | 117.20 |
| 4 | X | 233 | SER | CA-C-N | -7.38 | 100.97 | 117.20 |
| 1 | A | 346 | ASP | CB-CG-OD2 | -7.37 | 111.66 | 118.30 |
| 4 | Z | 233 | SER | CA-C-N | -7.37 | 100.98 | 117.20 |
| 4 | 2 | 180 | LEU | CA-CB-CG | 7.37 | 132.25 | 115.30 |
| 4 | 7 | 233 | SER | CA-C-N | -7.37 | 100.98 | 117.20 |
| 3 | R | 63 | ILE | CA-C-N | -7.37 | 100.99 | 117.20 |
| 4 | 8 | 233 | SER | CA-C-N | -7.37 | 100.99 | 117.20 |
| 1 | D | 654 | ARG | NE-CZ-NH1 | 7.37 | 123.98 | 120.30 |
| 4 | W | 233 | SER | CA-C-N | -7.36 | 101.00 | 117.20 |
| 3 | I | 63 | ILE | CA-C-N | -7.36 | 101.00 | 117.20 |
| 4 | 6 | 180 | LEU | CA-CB-CG | 7.36 | 132.23 | 115.30 |
| 3 | O | 63 | ILE | CA-C-N | -7.36 | 101.01 | 117.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 4 | 7 | 180 | LEU | CA-CB-CG | 7.36 | 132.22 | 115.30 |
| 4 | 6 | 233 | SER | CA-C-N | -7.36 | 101.02 | 117.20 |
| 4 | 4 | 180 | LEU | CA-CB-CG | 7.35 | 132.21 | 115.30 |
| 4 | 8 | 180 | LEU | CA-CB-CG | 7.35 | 132.22 | 115.30 |
| 4 | 1 | 233 | SER | CA-C-N | -7.35 | 101.02 | 117.20 |
| 4 | 4 | 233 | SER | CA-C-N | -7.35 | 101.03 | 117.20 |
| 1 | G | 104 | TYR | CB-CG-CD2 | 7.35 | 125.41 | 121.00 |
| 4 | Z | 180 | LEU | CA-CB-CG | 7.35 | 132.19 | 115.30 |
| 4 | 3 | 233 | SER | CA-C-N | -7.34 | 101.04 | 117.20 |
| 4 | X | 180 | LEU | CA-CB-CG | 7.34 | 132.19 | 115.30 |
| 3 | L | 63 | ILE | CA-C-N | -7.34 | 101.05 | 117.20 |
| 4 | 2 | 233 | SER | CA-C-N | -7.34 | 101.06 | 117.20 |
| 4 | W | 180 | LEU | CA-CB-CG | 7.34 | 132.18 | 115.30 |
| 4 | X | 254 | ARG | NE-CZ-NH2 | -7.34 | 116.63 | 120.30 |
| 1 | G | 518 | ASP | CB-CG-OD1 | -7.34 | 111.70 | 118.30 |
| 4 | Y | 233 | SER | CA-C-N | -7.33 | 101.06 | 117.20 |
| 4 | 5 | 180 | LEU | CA-CB-CG | 7.33 | 132.16 | 115.30 |
| 4 | 1 | 180 | LEU | CA-CB-CG | 7.33 | 132.16 | 115.30 |
| 4 | V | 180 | LEU | CA-CB-CG | 7.33 | 132.15 | 115.30 |
| 4 | 9 | 233 | SER | CA-C-N | -7.32 | 101.10 | 117.20 |
| 4 | Y | 180 | LEU | CA-CB-CG | 7.31 | 132.12 | 115.30 |
| 4 | 3 | 180 | LEU | CA-CB-CG | 7.31 | 132.11 | 115.30 |
| 1 | A | 518 | ASP | CB-CG-OD1 | -7.31 | 111.72 | 118.30 |
| 1 | J | 654 | ARG | NE-CZ-NH1 | 7.31 | 123.95 | 120.30 |
| 1 | M | 654 | ARG | NE-CZ-NH1 | 7.30 | 123.95 | 120.30 |
| 2 | Q | 150 | TYR | CB-CG-CD1 | -7.30 | 116.62 | 121.00 |
| 3 | F | 63 | ILE | CA-C-N | -7.29 | 101.15 | 117.20 |
| 3 | C | 63 | ILE | CA-C-N | -7.29 | 101.16 | 117.20 |
| 4 | 9 | 180 | LEU | CA-CB-CG | 7.29 | 132.07 | 115.30 |
| 4 | 4 | 254 | ARG | NE-CZ-NH2 | -7.29 | 116.66 | 120.30 |
| 1 | J | 346 | ASP | CB-CG-OD2 | -7.29 | 111.74 | 118.30 |
| 4 | 5 | 254 | ARG | NE-CZ-NH2 | -7.29 | 116.66 | 120.30 |
| 1 | M | 104 | TYR | CB-CG-CD2 | 7.28 | 125.37 | 121.00 |
| 4 | X | 206 | ARG | NE-CZ-NH1 | 7.28 | 123.94 | 120.30 |
| 4 | Z | 254 | ARG | NE-CZ-NH2 | -7.27 | 116.67 | 120.30 |
| 4 | Z | 79 | TRP | CD1-CG-CD2 | 7.25 | 112.10 | 106.30 |
| 2 | H | 127 | ARG | NE-CZ-NH2 | 7.25 | 123.92 | 120.30 |
| 4 | 1 | 79 | TRP | CD1-CG-CD2 | 7.25 | 112.10 | 106.30 |
| 1 | M | 346 | ASP | CB-CG-OD2 | -7.24 | 111.78 | 118.30 |
| 4 | 1 | 254 | ARG | NE-CZ-NH2 | -7.24 | 116.68 | 120.30 |
| 4 | 3 | 79 | TRP | CD1-CG-CD2 | 7.24 | 112.09 | 106.30 |
| 2 | K | 150 | TYR | CB-CG-CD1 | -7.24 | 116.66 | 121.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1 | P | 346 | ASP | CB-CG-OD2 | -7.24 | 111.79 | 118.30 |
| 4 | 4 | 79 | TRP | CD1-CG-CD2 | 7.23 | 112.08 | 106.30 |
| 4 | 8 | 254 | ARG | NE-CZ-NH2 | -7.22 | 116.69 | 120.30 |
| 1 | A | 104 | TYR | CB-CG-CD2 | 7.22 | 125.33 | 121.00 |
| 4 | 5 | 79 | TRP | CD1-CG-CD2 | 7.21 | 112.07 | 106.30 |
| 4 | 3 | 254 | ARG | NE-CZ-NH2 | -7.21 | 116.70 | 120.30 |
| 4 | 9 | 79 | TRP | CD1-CG-CD2 | 7.21 | 112.06 | 106.30 |
| 4 | V | 254 | ARG | NE-CZ-NH2 | -7.20 | 116.70 | 120.30 |
| 4 | 2 | 254 | ARG | NE-CZ-NH2 | -7.20 | 116.70 | 120.30 |
| 4 | 6 | 79 | TRP | CD1-CG-CD2 | 7.20 | 112.06 | 106.30 |
| 4 | Z | 206 | ARG | NE-CZ-NH1 | 7.19 | 123.89 | 120.30 |
| 4 | 7 | 340 | TRP | CE2-CD2-CG | -7.18 | 101.55 | 107.30 |
| 4 | 7 | 254 | ARG | NE-CZ-NH2 | -7.18 | 116.71 | 120.30 |
| 4 | 8 | 79 | TRP | CD1-CG-CD2 | 7.18 | 112.04 | 106.30 |
| 1 | A | 148 | ARG | NE-CZ-NH2 | -7.18 | 116.71 | 120.30 |
| 2 | N | 150 | TYR | CB-CG-CD1 | -7.18 | 116.69 | 121.00 |
| 4 | V | 206 | ARG | NE-CZ-NH1 | 7.18 | 123.89 | 120.30 |
| 4 | 2 | 79 | TRP | CD1-CG-CD2 | 7.17 | 112.03 | 106.30 |
| 4 | 5 | 206 | ARG | NE-CZ-NH1 | 7.17 | 123.88 | 120.30 |
| 4 | 2 | 206 | ARG | NE-CZ-NH1 | 7.16 | 123.88 | 120.30 |
| 4 | 7 | 79 | TRP | CD1-CG-CD2 | 7.16 | 112.03 | 106.30 |
| 1 | P | 104 | TYR | CB-CG-CD2 | 7.16 | 125.29 | 121.00 |
| 4 | 9 | 340 | TRP | CE2-CD2-CG | -7.15 | 101.58 | 107.30 |
| 4 | Y | 79 | TRP | CD1-CG-CD2 | 7.15 | 112.02 | 106.30 |
| 4 | 6 | 340 | TRP | CE2-CD2-CG | -7.15 | 101.58 | 107.30 |
| 4 | 7 | 206 | ARG | NE-CZ-NH1 | 7.14 | 123.87 | 120.30 |
| 4 | X | 79 | TRP | CD1-CG-CD2 | 7.14 | 112.02 | 106.30 |
| 4 | Y | 340 | TRP | CE2-CD2-CG | -7.14 | 101.58 | 107.30 |
| 1 | A | 568 | PRO | CA-C-N | -7.14 | 101.49 | 117.20 |
| 4 | W | 79 | TRP | CD1-CG-CD2 | 7.14 | 112.02 | 106.30 |
| 4 | V | 79 | TRP | CD1-CG-CD2 | 7.14 | 112.01 | 106.30 |
| 4 | W | 254 | ARG | NE-CZ-NH2 | -7.14 | 116.73 | 120.30 |
| 4 | 3 | 340 | TRP | CE2-CD2-CG | -7.13 | 101.59 | 107.30 |
| 4 | 6 | 254 | ARG | NE-CZ-NH2 | -7.13 | 116.73 | 120.30 |
| 4 | V | 340 | TRP | CE2-CD2-CG | -7.13 | 101.60 | 107.30 |
| 1 | G | 568 | PRO | CA-C-N | -7.13 | 101.52 | 117.20 |
| 1 | M | 568 | PRO | CA-C-N | -7.13 | 101.52 | 117.20 |
| 4 | X | 340 | TRP | CE2-CD2-CG | -7.12 | 101.60 | 107.30 |
| 4 | W | 340 | TRP | CE2-CD2-CG | -7.12 | 101.60 | 107.30 |
| 4 | 6 | 206 | ARG | NE-CZ-NH1 | 7.12 | 123.86 | 120.30 |
| 4 | 8 | 206 | ARG | NE-CZ-NH1 | 7.12 | 123.86 | 120.30 |
| 4 | 5 | 340 | TRP | CE2-CD2-CG | -7.11 | 101.61 | 107.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 4 | 2 | 340 | TRP | CE2-CD2-CG | -7.11 | 101.61 | 107.30 |
| 1 | P | 148 | ARG | NE-CZ-NH2 | -7.10 | 116.75 | 120.30 |
| 4 | 4 | 340 | TRP | CE2-CD2-CG | -7.10 | 101.62 | 107.30 |
| 4 | 3 | 206 | ARG | NE-CZ-NH1 | 7.09 | 123.85 | 120.30 |
| 4 | 8 | 340 | TRP | CE2-CD2-CG | -7.09 | 101.63 | 107.30 |
| 2 | H | 150 | TYR | CB-CG-CD1 | -7.08 | 116.75 | 121.00 |
| 4 | Y | 254 | ARG | NE-CZ-NH2 | -7.07 | 116.76 | 120.30 |
| 4 | 1 | 340 | TRP | CE2-CD2-CG | -7.07 | 101.64 | 107.30 |
| 4 | 4 | 47 | MET | CA-CB-CG | -7.07 | 101.29 | 113.30 |
| 1 | D | 218 | LEU | CB-CG-CD1 | 7.06 | 123.00 | 111.00 |
| 2 | E | 150 | TYR | CB-CG-CD1 | -7.06 | 116.77 | 121.00 |
| 1 | D | 568 | PRO | CA-C-N | -7.05 | 101.68 | 117.20 |
| 1 | J | 568 | PRO | CA-C-N | -7.05 | 101.69 | 117.20 |
| 4 | 1 | 47 | MET | CA-CB-CG | -7.05 | 101.31 | 113.30 |
| 4 | V | 47 | MET | CA-CB-CG | -7.05 | 101.31 | 113.30 |
| 4 | 8 | 47 | MET | CA-CB-CG | -7.05 | 101.32 | 113.30 |
| 4 | Z | 79 | TRP | CE2-CD2-CG | -7.05 | 101.66 | 107.30 |
| 4 | Z | 340 | TRP | CE2-CD2-CG | -7.05 | 101.66 | 107.30 |
| 1 | P | 568 | PRO | CA-C-N | -7.04 | 101.70 | 117.20 |
| 1 | M | 264 | ASP | N-CA-CB | -7.04 | 97.93 | 110.60 |
| 1 | J | 264 | ASP | N-CA-CB | -7.04 | 97.93 | 110.60 |
| 4 | W | 47 | MET | CA-CB-CG | -7.04 | 101.34 | 113.30 |
| 2 | Q | 127 | ARG | NE-CZ-NH2 | 7.03 | 123.82 | 120.30 |
| 1 | P | 264 | ASP | N-CA-CB | -7.03 | 97.94 | 110.60 |
| 4 | 7 | 47 | MET | CA-CB-CG | -7.03 | 101.35 | 113.30 |
| 4 | 9 | 254 | ARG | NE-CZ-NH2 | -7.03 | 116.78 | 120.30 |
| 4 | 3 | 47 | MET | CA-CB-CG | -7.03 | 101.35 | 113.30 |
| 4 | X | 47 | MET | CA-CB-CG | -7.03 | 101.35 | 113.30 |
| 4 | Z | 47 | MET | CA-CB-CG | -7.03 | 101.35 | 113.30 |
| 4 | 2 | 47 | MET | CA-CB-CG | -7.02 | 101.36 | 113.30 |
| 1 | A | 218 | LEU | CB-CG-CD1 | 7.02 | 122.93 | 111.00 |
| 4 | Y | 47 | MET | CA-CB-CG | -7.02 | 101.37 | 113.30 |
| 4 | 5 | 47 | MET | CA-CB-CG | -7.02 | 101.37 | 113.30 |
| 4 | 1 | 79 | TRP | CE2-CD2-CG | -7.01 | 101.69 | 107.30 |
| 4 | Y | 79 | TRP | CE2-CD2-CG | -7.01 | 101.69 | 107.30 |
| 4 | 6 | 47 | MET | CA-CB-CG | -7.01 | 101.38 | 113.30 |
| 4 | X | 79 | TRP | CE2-CD2-CG | -7.01 | 101.69 | 107.30 |
| 4 | 4 | 206 | ARG | NE-CZ-NH1 | 7.00 | 123.80 | 120.30 |
| 1 | J | 104 | TYR | CB-CG-CD2 | 7.00 | 125.20 | 121.00 |
| 4 | 4 | 79 | TRP | CE2-CD2-CG | -7.00 | 101.70 | 107.30 |
| 4 | 2 | 79 | TRP | CE2-CD2-CG | -7.00 | 101.70 | 107.30 |
| 1 | D | 264 | ASP | N-CA-CB | -7.00 | 98.00 | 110.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1 | J | 218 | LEU | CB-CG-CD1 | 7.00 | 122.89 | 111.00 |
| 1 | P | 217 | THR | N-CA-CB | 6.99 | 123.59 | 110.30 |
| 4 | 9 | 47 | MET | CA-CB-CG | -6.99 | 101.41 | 113.30 |
| 4 | 7 | 340 | TRP | CD1-CG-CD2 | 6.99 | 111.89 | 106.30 |
| 4 | 8 | 79 | TRP | CE2-CD2-CG | -6.99 | 101.71 | 107.30 |
| 1 | D | 217 | THR | N-CA-CB | 6.99 | 123.57 | 110.30 |
| 1 | A | 264 | ASP | N-CA-CB | -6.98 | 98.03 | 110.60 |
| 4 | 9 | 206 | ARG | NE-CZ-NH1 | 6.98 | 123.79 | 120.30 |
| 4 | 3 | 79 | TRP | CE2-CD2-CG | -6.98 | 101.71 | 107.30 |
| 1 | J | 148 | ARG | NE-CZ-NH2 | -6.98 | 116.81 | 120.30 |
| 1 | G | 217 | THR | N-CA-CB | 6.98 | 123.56 | 110.30 |
| 1 | M | 217 | THR | N-CA-CB | 6.98 | 123.56 | 110.30 |
| 1 | M | 218 | LEU | CB-CG-CD1 | 6.98 | 122.86 | 111.00 |
| 1 | J | 217 | THR | N-CA-CB | 6.97 | 123.55 | 110.30 |
| 2 | K | 127 | ARG | NE-CZ-NH2 | 6.97 | 123.79 | 120.30 |
| 4 | X | 340 | TRP | CD1-CG-CD2 | 6.97 | 111.88 | 106.30 |
| 2 | N | 127 | ARG | NE-CZ-NH2 | 6.97 | 123.78 | 120.30 |
| 4 | W | 79 | TRP | CE2-CD2-CG | -6.97 | 101.72 | 107.30 |
| 1 | A | 217 | THR | N-CA-CB | 6.97 | 123.53 | 110.30 |
| 1 | P | 218 | LEU | CB-CG-CD1 | 6.96 | 122.84 | 111.00 |
| 1 | G | 264 | ASP | N-CA-CB | -6.96 | 98.07 | 110.60 |
| 1 | D | 104 | TYR | CB-CG-CD2 | 6.96 | 125.17 | 121.00 |
| 4 | 6 | 79 | TRP | CE2-CD2-CG | -6.96 | 101.74 | 107.30 |
| 4 | V | 79 | TRP | CE2-CD2-CG | -6.95 | 101.74 | 107.30 |
| 4 | 9 | 340 | TRP | CD1-CG-CD2 | 6.95 | 111.86 | 106.30 |
| 4 | 6 | 340 | TRP | CD1-CG-CD2 | 6.95 | 111.86 | 106.30 |
| 4 | W | 206 | ARG | NE-CZ-NH1 | 6.95 | 123.77 | 120.30 |
| 2 | B | 150 | TYR | CB-CG-CD1 | -6.95 | 116.83 | 121.00 |
| 4 | 5 | 79 | TRP | CE2-CD2-CG | -6.95 | 101.74 | 107.30 |
| 4 | 1 | 206 | ARG | NE-CZ-NH1 | 6.94 | 123.77 | 120.30 |
| 4 | W | 340 | TRP | CD1-CG-CD2 | 6.94 | 111.85 | 106.30 |
| 4 | 3 | 340 | TRP | CD1-CG-CD2 | 6.94 | 111.85 | 106.30 |
| 1 | G | 218 | LEU | CB-CG-CD1 | 6.93 | 122.78 | 111.00 |
| 4 | 9 | 79 | TRP | CE2-CD2-CG | -6.92 | 101.77 | 107.30 |
| 1 | D | 148 | ARG | NE-CZ-NH2 | -6.91 | 116.85 | 120.30 |
| 4 | V | 340 | TRP | CD1-CG-CD2 | 6.91 | 111.83 | 106.30 |
| 4 | 2 | 340 | TRP | CD1-CG-CD2 | 6.90 | 111.82 | 106.30 |
| 4 | 5 | 340 | TRP | CD1-CG-CD2 | 6.90 | 111.82 | 106.30 |
| 4 | 7 | 79 | TRP | CE2-CD2-CG | -6.90 | 101.78 | 107.30 |
| 4 | Y | 206 | ARG | NE-CZ-NH1 | 6.90 | 123.75 | 120.30 |
| 1 | D | 728 | ASN | CA-C-N | -6.89 | 102.03 | 117.20 |
| 4 | 8 | 340 | TRP | CD1-CG-CD2 | 6.89 | 111.81 | 106.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1 | G | 450 | ASP | CB-CG-OD2 | 6.89 | 124.50 | 118.30 |
| 4 | 4 | 340 | TRP | CD1-CG-CD2 | 6.89 | 111.81 | 106.30 |
| 1 | J | 728 | ASN | CA-C-N | -6.88 | 102.06 | 117.20 |
| 1 | J | 75 | ASP | N-CA-CB | 6.87 | 122.97 | 110.60 |
| 4 | Y | 340 | TRP | CD1-CG-CD2 | 6.87 | 111.79 | 106.30 |
| 1 | P | 75 | ASP | N-CA-CB | 6.86 | 122.95 | 110.60 |
| 1 | M | 148 | ARG | NE-CZ-NH2 | -6.86 | 116.87 | 120.30 |
| 1 | G | 75 | ASP | N-CA-CB | 6.85 | 122.94 | 110.60 |
| 1 | M | 728 | ASN | CA-C-N | -6.85 | 102.12 | 117.20 |
| 1 | J | 450 | ASP | CB-CG-OD2 | 6.85 | 124.47 | 118.30 |
| 1 | P | 728 | ASN | CA-C-N | -6.85 | 102.13 | 117.20 |
| 4 | Z | 340 | TRP | CD1-CG-CD2 | 6.84 | 111.77 | 106.30 |
| 1 | D | 450 | ASP | CB-CG-OD2 | 6.84 | 124.46 | 118.30 |
| 1 | A | 75 | ASP | N-CA-CB | 6.83 | 122.90 | 110.60 |
| 1 | P | 450 | ASP | CB-CG-OD2 | 6.82 | 124.44 | 118.30 |
| 1 | J | 709 | LYS | CA-C-N | 6.81 | 129.83 | 116.20 |
| 1 | G | 728 | ASN | CA-C-N | -6.81 | 102.21 | 117.20 |
| 1 | M | 75 | ASP | N-CA-CB | 6.81 | 122.86 | 110.60 |
| 1 | A | 728 | ASN | CA-C-N | -6.81 | 102.22 | 117.20 |
| 1 | G | 148 | ARG | NE-CZ-NH2 | -6.80 | 116.90 | 120.30 |
| 1 | D | 75 | ASP | N-CA-CB | 6.77 | 122.79 | 110.60 |
| 4 | 1 | 340 | TRP | CD1-CG-CD2 | 6.77 | 111.71 | 106.30 |
| 1 | P | 555 | TYR | CB-CG-CD2 | -6.76 | 116.94 | 121.00 |
| 1 | A | 450 | ASP | CB-CG-OD2 | 6.74 | 124.36 | 118.30 |
| 1 | J | 756 | THR | N-CA-CB | -6.71 | 97.56 | 110.30 |
| 1 | M | 450 | ASP | CB-CG-OD2 | 6.71 | 124.34 | 118.30 |
| 1 | G | 781 | ASP | CB-CG-OD1 | -6.68 | 112.28 | 118.30 |
| 1 | M | 219 | GLU | N-CA-C | -6.68 | 92.97 | 111.00 |
| 1 | G | 219 | GLU | N-CA-C | -6.67 | 92.99 | 111.00 |
| 1 | J | 555 | TYR | CB-CG-CD2 | -6.67 | 117.00 | 121.00 |
| 1 | J | 219 | GLU | N-CA-C | -6.67 | 93.00 | 111.00 |
| 1 | G | 756 | THR | N-CA-CB | -6.66 | 97.64 | 110.30 |
| 1 | G | 555 | TYR | CB-CG-CD2 | -6.66 | 117.01 | 121.00 |
| 1 | P | 75 | ASP | CB-CG-OD2 | 6.66 | 124.29 | 118.30 |
| 1 | P | 219 | GLU | N-CA-C | -6.65 | 93.04 | 111.00 |
| 1 | A | 781 | ASP | CB-CG-OD1 | -6.65 | 112.32 | 118.30 |
| 1 | D | 781 | ASP | CB-CG-OD1 | -6.64 | 112.32 | 118.30 |
| 1 | A | 219 | GLU | N-CA-C | -6.64 | 93.07 | 111.00 |
| 1 | P | 756 | THR | N-CA-CB | -6.63 | 97.70 | 110.30 |
| 1 | D | 75 | ASP | CB-CG-OD2 | 6.63 | 124.27 | 118.30 |
| 1 | D | 756 | THR | N-CA-CB | -6.63 | 97.71 | 110.30 |
| 1 | M | 756 | THR | N-CA-CB | -6.62 | 97.73 | 110.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1 | J | 75 | ASP | CB-CG-OD2 | 6.61 | 124.25 | 118.30 |
| 1 | M | 75 | ASP | CB-CG-OD2 | 6.60 | 124.24 | 118.30 |
| 4 | 9 | 169 | TYR | CB-CG-CD2 | -6.59 | 117.05 | 121.00 |
| 1 | A | 756 | THR | N-CA-CB | -6.58 | 97.79 | 110.30 |
| 1 | D | 219 | GLU | N-CA-C | -6.58 | 93.23 | 111.00 |
| 1 | M | 781 | ASP | CB-CG-OD1 | -6.58 | 112.38 | 118.30 |
| 4 | 1 | 169 | TYR | CB-CG-CD2 | -6.58 | 117.05 | 121.00 |
| 1 | A | 343 | PHE | CB-CG-CD1 | 6.58 | 125.41 | 120.80 |
| 4 | W | 169 | TYR | CB-CG-CD2 | -6.58 | 117.05 | 121.00 |
| 4 | 6 | 169 | TYR | CB-CG-CD2 | -6.57 | 117.06 | 121.00 |
| 4 | 1 | 283 | MET | CG-SD-CE | 6.57 | 110.71 | 100.20 |
| 4 | 9 | 283 | MET | CG-SD-CE | 6.57 | 110.71 | 100.20 |
| 1 | P | 332 | MET | CG-SD-CE | -6.57 | 89.70 | 100.20 |
| 4 | Y | 283 | MET | CG-SD-CE | 6.57 | 110.70 | 100.20 |
| 4 | W | 283 | MET | CG-SD-CE | 6.56 | 110.70 | 100.20 |
| 1 | A | 75 | ASP | CB-CG-OD2 | 6.56 | 124.20 | 118.30 |
| 4 | 6 | 283 | MET | CG-SD-CE | 6.56 | 110.69 | 100.20 |
| 4 | 3 | 283 | MET | CG-SD-CE | 6.56 | 110.69 | 100.20 |
| 1 | M | 141 | LEU | CB-CA-C | -6.56 | 97.74 | 110.20 |
| 4 | 5 | 169 | TYR | CB-CG-CD2 | -6.55 | 117.07 | 121.00 |
| 4 | X | 169 | TYR | CB-CG-CD2 | -6.55 | 117.07 | 121.00 |
| 1 | J | 141 | LEU | CB-CA-C | -6.55 | 97.76 | 110.20 |
| 4 | 4 | 196 | ARG | NE-CZ-NH1 | 6.55 | 123.57 | 120.30 |
| 1 | D | 555 | TYR | CB-CG-CD2 | -6.54 | 117.07 | 121.00 |
| 4 | 8 | 283 | MET | CG-SD-CE | 6.54 | 110.67 | 100.20 |
| 4 | Y | 169 | TYR | CB-CG-CD2 | -6.54 | 117.07 | 121.00 |
| 1 | J | 781 | ASP | CB-CG-OD1 | -6.54 | 112.41 | 118.30 |
| 1 | M | 169 | ASP | CB-CG-OD1 | -6.54 | 112.42 | 118.30 |
| 4 | 8 | 169 | TYR | CB-CG-CD2 | -6.54 | 117.08 | 121.00 |
| 4 | 7 | 283 | MET | CG-SD-CE | 6.54 | 110.66 | 100.20 |
| 1 | D | 332 | MET | CG-SD-CE | -6.53 | 89.75 | 100.20 |
| 1 | M | 332 | MET | CG-SD-CE | -6.53 | 89.75 | 100.20 |
| 4 | 4 | 169 | TYR | CB-CG-CD2 | -6.53 | 117.08 | 121.00 |
| 4 | 4 | 283 | MET | CG-SD-CE | 6.53 | 110.65 | 100.20 |
| 1 | J | 332 | MET | CG-SD-CE | -6.53 | 89.75 | 100.20 |
| 1 | P | 141 | LEU | CB-CA-C | -6.53 | 97.80 | 110.20 |
| 4 | 5 | 283 | MET | CG-SD-CE | 6.53 | 110.64 | 100.20 |
| 4 | V | 283 | MET | CG-SD-CE | 6.53 | 110.64 | 100.20 |
| 4 | X | 283 | MET | CG-SD-CE | 6.52 | 110.64 | 100.20 |
| 1 | D | 334 | THR | CA-CB-CG2 | -6.52 | 103.27 | 112.40 |
| 1 | J | 589 | ASP | CB-CG-OD1 | -6.52 | 112.43 | 118.30 |
| 4 | 9 | 196 | ARG | NE-CZ-NH1 | 6.52 | 123.56 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1 | A | 555 | TYR | CB-CG-CD2 | -6.52 | 117.09 | 121.00 |
| 1 | G | 169 | ASP | CB-CG-OD1 | -6.52 | 112.44 | 118.30 |
| 4 | 2 | 283 | MET | CG-SD-CE | 6.52 | 110.63 | 100.20 |
| 4 | 7 | 159 | VAL | CB-CA-C | -6.51 | 99.03 | 111.40 |
| 1 | P | 781 | ASP | CB-CG-OD1 | -6.51 | 112.44 | 118.30 |
| 1 | A | 332 | MET | CG-SD-CE | -6.50 | 89.79 | 100.20 |
| 4 | 1 | 159 | VAL | CB-CA-C | -6.50 | 99.04 | 111.40 |
| 4 | Z | 196 | ARG | NE-CZ-NH1 | 6.50 | 123.55 | 120.30 |
| 2 | H | 141 | PRO | N-CD-CG | -6.50 | 93.45 | 103.20 |
| 4 | Z | 283 | MET | CG-SD-CE | 6.50 | 110.59 | 100.20 |
| 1 | G | 334 | THR | CA-CB-CG2 | -6.49 | 103.31 | 112.40 |
| 1 | G | 332 | MET | CG-SD-CE | -6.49 | 89.82 | 100.20 |
| 4 | 3 | 159 | VAL | CB-CA-C | -6.49 | 99.07 | 111.40 |
| 1 | P | 589 | ASP | CB-CG-OD1 | -6.49 | 112.46 | 118.30 |
| 1 | G | 141 | LEU | CB-CA-C | -6.49 | 97.88 | 110.20 |
| 1 | M | 555 | TYR | CB-CG-CD2 | -6.49 | 117.11 | 121.00 |
| 1 | J | 169 | ASP | CB-CG-OD1 | -6.48 | 112.47 | 118.30 |
| 1 | J | 334 | THR | CA-CB-CG2 | -6.48 | 103.33 | 112.40 |
| 4 | 3 | 169 | TYR | CB-CG-CD2 | -6.48 | 117.11 | 121.00 |
| 4 | 3 | 196 | ARG | NE-CZ-NH1 | 6.48 | 123.54 | 120.30 |
| 4 | W | 159 | VAL | CB-CA-C | -6.48 | 99.09 | 111.40 |
| 4 | Y | 159 | VAL | CB-CA-C | -6.48 | 99.09 | 111.40 |
| 1 | D | 129 | TYR | CB-CG-CD2 | -6.48 | 117.11 | 121.00 |
| 1 | D | 141 | LEU | CB-CA-C | -6.48 | 97.89 | 110.20 |
| 4 | 4 | 159 | VAL | CB-CA-C | -6.48 | 99.09 | 111.40 |
| 2 | E | 141 | PRO | N-CD-CG | -6.47 | 93.49 | 103.20 |
| 1 | G | 343 | PHE | CB-CG-CD1 | 6.47 | 125.33 | 120.80 |
| 4 | 6 | 159 | VAL | CB-CA-C | -6.47 | 99.10 | 111.40 |
| 4 | 9 | 159 | VAL | CB-CA-C | -6.47 | 99.11 | 111.40 |
| 1 | A | 334 | THR | CA-CB-CG2 | -6.47 | 103.34 | 112.40 |
| 4 | 7 | 169 | TYR | CB-CG-CD2 | -6.47 | 117.12 | 121.00 |
| 4 | 2 | 196 | ARG | NE-CZ-NH1 | 6.46 | 123.53 | 120.30 |
| 1 | A | 141 | LEU | CB-CA-C | -6.46 | 97.92 | 110.20 |
| 4 | Z | 169 | TYR | CB-CG-CD2 | -6.46 | 117.12 | 121.00 |
| 4 | X | 159 | VAL | CB-CA-C | -6.46 | 99.13 | 111.40 |
| 4 | V | 159 | VAL | CB-CA-C | -6.46 | 99.14 | 111.40 |
| 4 | X | 196 | ARG | NE-CZ-NH1 | 6.45 | 123.53 | 120.30 |
| 4 | 5 | 196 | ARG | NE-CZ-NH1 | 6.45 | 123.52 | 120.30 |
| 4 | 8 | 159 | VAL | CB-CA-C | -6.45 | 99.15 | 111.40 |
| 4 | 6 | 196 | ARG | NE-CZ-NH1 | 6.45 | 123.52 | 120.30 |
| 4 | Z | 159 | VAL | CB-CA-C | -6.45 | 99.15 | 111.40 |
| 1 | P | 129 | TYR | CB-CG-CD2 | -6.44 | 117.13 | 121.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1 | M | 589 | ASP | CB-CG-OD1 | -6.44 | 112.50 | 118.30 |
| 2 | Q | 141 | PRO | N-CD-CG | -6.44 | 93.54 | 103.20 |
| 4 | V | 34 | ILE | CA-CB-CG2 | -6.44 | 98.02 | 110.90 |
| 1 | A | 169 | ASP | CB-CG-OD1 | -6.44 | 112.50 | 118.30 |
| 1 | G | 589 | ASP | CB-CG-OD1 | -6.44 | 112.51 | 118.30 |
| 1 | M | 334 | THR | CA-CB-CG2 | -6.44 | 103.39 | 112.40 |
| 4 | W | 196 | ARG | NE-CZ-NH1 | 6.44 | 123.52 | 120.30 |
| 1 | P | 334 | THR | CA-CB-CG2 | -6.43 | 103.39 | 112.40 |
| 4 | 5 | 159 | VAL | CB-CA-C | -6.43 | 99.17 | 111.40 |
| 4 | 5 | 34 | ILE | CA-CB-CG2 | -6.43 | 98.04 | 110.90 |
| 4 | 8 | 34 | ILE | CA-CB-CG2 | -6.43 | 98.04 | 110.90 |
| 4 | 2 | 159 | VAL | CB-CA-C | -6.43 | 99.19 | 111.40 |
| 4 | 6 | 34 | ILE | CA-CB-CG2 | -6.42 | 98.05 | 110.90 |
| 4 | V | 196 | ARG | NE-CZ-NH1 | 6.42 | 123.51 | 120.30 |
| 4 | Z | 34 | ILE | CA-CB-CG2 | -6.42 | 98.05 | 110.90 |
| 4 | Y | 196 | ARG | NE-CZ-NH1 | 6.42 | 123.51 | 120.30 |
| 1 | G | 75 | ASP | CB-CG-OD2 | 6.42 | 124.08 | 118.30 |
| 1 | P | 169 | ASP | CB-CG-OD1 | -6.42 | 112.52 | 118.30 |
| 2 | K | 141 | PRO | N-CD-CG | -6.42 | 93.58 | 103.20 |
| 4 | 2 | 34 | ILE | CA-CB-CG2 | -6.41 | 98.07 | 110.90 |
| 4 | 4 | 34 | ILE | CA-CB-CG2 | -6.41 | 98.07 | 110.90 |
| 4 | X | 34 | ILE | CA-CB-CG2 | -6.41 | 98.08 | 110.90 |
| 4 | 7 | 34 | ILE | CA-CB-CG2 | -6.41 | 98.09 | 110.90 |
| 1 | J | 129 | TYR | CB-CG-CD2 | -6.40 | 117.16 | 121.00 |
| 2 | N | 141 | PRO | N-CD-CG | -6.40 | 93.60 | 103.20 |
| 4 | V | 169 | TYR | CB-CG-CD2 | -6.40 | 117.16 | 121.00 |
| 4 | 7 | 196 | ARG | NE-CZ-NH1 | 6.40 | 123.50 | 120.30 |
| 4 | 9 | 34 | ILE | CA-CB-CG2 | -6.40 | 98.11 | 110.90 |
| 1 | D | 589 | ASP | CB-CG-OD1 | -6.39 | 112.55 | 118.30 |
| 1 | D | 343 | PHE | CB-CG-CD1 | 6.39 | 125.27 | 120.80 |
| 4 | 2 | 169 | TYR | CB-CG-CD2 | -6.38 | 117.17 | 121.00 |
| 1 | M | 129 | TYR | CB-CG-CD2 | -6.38 | 117.17 | 121.00 |
| 1 | A | 589 | ASP | CB-CG-OD1 | -6.37 | 112.56 | 118.30 |
| 4 | 1 | 196 | ARG | NE-CZ-NH1 | 6.37 | 123.49 | 120.30 |
| 1 | D | 169 | ASP | CB-CG-OD1 | -6.37 | 112.57 | 118.30 |
| 1 | P | 578 | HIS | N-CA-CB | 6.37 | 122.06 | 110.60 |
| 4 | W | 34 | ILE | CA-CB-CG2 | -6.36 | 98.18 | 110.90 |
| 1 | G | 590 | TYR | CB-CG-CD2 | 6.36 | 124.82 | 121.00 |
| 1 | J | 810 | ARG | NE-CZ-NH1 | 6.36 | 123.48 | 120.30 |
| 1 | P | 343 | PHE | CB-CG-CD1 | 6.36 | 125.25 | 120.80 |
| 1 | J | 343 | PHE | CB-CG-CD1 | 6.35 | 125.25 | 120.80 |
| 4 | 3 | 34 | ILE | CA-CB-CG2 | -6.35 | 98.20 | 110.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 4 | 8 | 196 | ARG | NE-CZ-NH1 | 6.35 | 123.47 | 120.30 |
| 4 | 1 | 34 | ILE | CA-CB-CG2 | -6.35 | 98.20 | 110.90 |
| 2 | B | 141 | PRO | N-CD-CG | -6.34 | 93.69 | 103.20 |
| 1 | M | 760 | PHE | CB-CG-CD2 | -6.34 | 116.36 | 120.80 |
| 4 | Y | 34 | ILE | CA-CB-CG2 | -6.34 | 98.22 | 110.90 |
| 1 | A | 341 | LEU | CB-CA-C | 6.33 | 122.23 | 110.20 |
| 1 | G | 578 | HIS | N-CA-CB | 6.33 | 122.00 | 110.60 |
| 1 | M | 343 | PHE | CB-CG-CD1 | 6.33 | 125.23 | 120.80 |
| 1 | M | 341 | LEU | CB-CA-C | 6.32 | 122.21 | 110.20 |
| 4 | X | 217 | CYS | CA-CB-SG | -6.32 | 102.63 | 114.00 |
| 4 | 5 | 217 | CYS | CA-CB-SG | -6.31 | 102.64 | 114.00 |
| 1 | G | 709 | LYS | C-N-CA | 6.31 | 135.54 | 122.30 |
| 4 | 3 | 217 | CYS | CA-CB-SG | -6.31 | 102.65 | 114.00 |
| 1 | J | 578 | HIS | N-CA-CB | 6.30 | 121.94 | 110.60 |
| 1 | P | 341 | LEU | CB-CA-C | 6.30 | 122.17 | 110.20 |
| 1 | D | 590 | TYR | CB-CG-CD2 | 6.30 | 124.78 | 121.00 |
| 4 | V | 217 | CYS | CA-CB-SG | -6.30 | 102.67 | 114.00 |
| 1 | J | 327 | ASP | CB-CG-OD2 | 6.29 | 123.97 | 118.30 |
| 4 | 1 | 217 | CYS | CA-CB-SG | -6.29 | 102.67 | 114.00 |
| 4 | Z | 217 | CYS | CA-CB-SG | -6.29 | 102.67 | 114.00 |
| 4 | 4 | 217 | CYS | CA-CB-SG | -6.29 | 102.67 | 114.00 |
| 4 | 2 | 217 | CYS | CA-CB-SG | -6.29 | 102.68 | 114.00 |
| 1 | J | 341 | LEU | CB-CA-C | 6.29 | 122.15 | 110.20 |
| 1 | A | 578 | HIS | N-CA-CB | 6.29 | 121.91 | 110.60 |
| 1 | G | 341 | LEU | CB-CA-C | 6.28 | 122.14 | 110.20 |
| 2 | Q | 129 | THR | CB-CA-C | -6.28 | 94.65 | 111.60 |
| 4 | Y | 217 | CYS | CA-CB-SG | -6.28 | 102.71 | 114.00 |
| 1 | D | 578 | HIS | N-CA-CB | 6.27 | 121.89 | 110.60 |
| 4 | 8 | 217 | CYS | CA-CB-SG | -6.27 | 102.71 | 114.00 |
| 1 | M | 578 | HIS | N-CA-CB | 6.27 | 121.88 | 110.60 |
| 4 | W | 217 | CYS | CA-CB-SG | -6.26 | 102.72 | 114.00 |
| 1 | A | 129 | TYR | CB-CG-CD2 | -6.26 | 117.24 | 121.00 |
| 1 | M | 104 | TYR | CB-CG-CD1 | -6.26 | 117.24 | 121.00 |
| 4 | 7 | 217 | CYS | CA-CB-SG | -6.25 | 102.74 | 114.00 |
| 4 | 6 | 217 | CYS | CA-CB-SG | -6.25 | 102.75 | 114.00 |
| 2 | N | 129 | THR | CB-CA-C | -6.25 | 94.73 | 111.60 |
| 1 | D | 341 | LEU | CB-CA-C | 6.25 | 122.07 | 110.20 |
| 4 | 9 | 217 | CYS | CA-CB-SG | -6.24 | 102.77 | 114.00 |
| 1 | J | 779 | ARG | NE-CZ-NH1 | 6.24 | 123.42 | 120.30 |
| 2 | K | 129 | THR | CB-CA-C | -6.24 | 94.76 | 111.60 |
| 1 | M | 327 | ASP | CB-CG-OD2 | 6.24 | 123.91 | 118.30 |
| 1 | G | 129 | TYR | CB-CG-CD2 | -6.23 | 117.26 | 121.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1 | P | 327 | ASP | CB-CG-OD2 | 6.23 | 123.90 | 118.30 |
| 2 | K | 141 | PRO | N-CA-CB | -6.21 | 95.76 | 102.60 |
| 1 | M | 779 | ARG | NE-CZ-NH1 | 6.21 | 123.41 | 120.30 |
| 1 | G | 104 | TYR | CB-CG-CD1 | -6.21 | 117.27 | 121.00 |
| 1 | M | 810 | ARG | NE-CZ-NH1 | 6.21 | 123.40 | 120.30 |
| 1 | D | 214 | MET | CG-SD-CE | 6.20 | 110.13 | 100.20 |
| 1 | A | 760 | PHE | CB-CG-CD2 | -6.20 | 116.46 | 120.80 |
| 1 | A | 590 | TYR | CB-CG-CD2 | 6.20 | 124.72 | 121.00 |
| 1 | A | 698 | ASN | CB-CA-C | -6.20 | 98.00 | 110.40 |
| 1 | D | 810 | ARG | NE-CZ-NH1 | 6.20 | 123.40 | 120.30 |
| 2 | E | 129 | THR | CB-CA-C | -6.19 | 94.88 | 111.60 |
| 1 | J | 760 | PHE | CB-CG-CD2 | -6.19 | 116.47 | 120.80 |
| 1 | P | 810 | ARG | NE-CZ-NH1 | 6.19 | 123.40 | 120.30 |
| 2 | H | 129 | THR | CB-CA-C | -6.19 | 94.88 | 111.60 |
| 1 | M | 214 | MET | CG-SD-CE | 6.18 | 110.09 | 100.20 |
| 1 | M | 698 | ASN | CB-CA-C | -6.18 | 98.05 | 110.40 |
| 4 | 1 | 259 | GLU | CA-CB-CG | 6.17 | 126.98 | 113.40 |
| 1 | A | 463 | ASP | CB-CG-OD2 | -6.17 | 112.75 | 118.30 |
| 1 | J | 214 | MET | CG-SD-CE | 6.17 | 110.08 | 100.20 |
| 2 | Q | 141 | PRO | N-CA-CB | -6.17 | 95.81 | 102.60 |
| 4 | 2 | 259 | GLU | CA-CB-CG | 6.17 | 126.97 | 113.40 |
| 1 | P | 450 | ASP | CB-CG-OD1 | -6.17 | 112.75 | 118.30 |
| 1 | P | 779 | ARG | NE-CZ-NH1 | 6.17 | 123.38 | 120.30 |
| 1 | A | 214 | MET | CG-SD-CE | 6.16 | 110.06 | 100.20 |
| 1 | J | 698 | ASN | CB-CA-C | -6.16 | 98.08 | 110.40 |
| 1 | D | 327 | ASP | CB-CG-OD2 | 6.16 | 123.84 | 118.30 |
| 4 | 9 | 259 | GLU | CA-CB-CG | 6.16 | 126.95 | 113.40 |
| 4 | V | 259 | GLU | CA-CB-CG | 6.16 | 126.95 | 113.40 |
| 4 | 4 | 259 | GLU | CA-CB-CG | 6.15 | 126.94 | 113.40 |
| 1 | G | 214 | MET | CG-SD-CE | 6.15 | 110.04 | 100.20 |
| 2 | B | 129 | THR | CB-CA-C | -6.15 | 95.00 | 111.60 |
| 4 | 7 | 259 | GLU | CA-CB-CG | 6.15 | 126.92 | 113.40 |
| 4 | Y | 259 | GLU | CA-CB-CG | 6.14 | 126.91 | 113.40 |
| 4 | W | 259 | GLU | CA-CB-CG | 6.14 | 126.91 | 113.40 |
| 4 | Z | 259 | GLU | CA-CB-CG | 6.14 | 126.91 | 113.40 |
| 1 | P | 214 | MET | CG-SD-CE | 6.14 | 110.02 | 100.20 |
| 4 | 6 | 259 | GLU | CA-CB-CG | 6.14 | 126.90 | 113.40 |
| 4 | 8 | 259 | GLU | CA-CB-CG | 6.14 | 126.90 | 113.40 |
| 1 | P | 698 | ASN | CB-CA-C | -6.13 | 98.13 | 110.40 |
| 4 | 3 | 259 | GLU | CA-CB-CG | 6.13 | 126.89 | 113.40 |
| 2 | B | 129 | THR | CA-CB-CG2 | 6.13 | 120.98 | 112.40 |
| 4 | X | 259 | GLU | CA-CB-CG | 6.13 | 126.88 | 113.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 3 | F | 58 | MET | CG-SD-CE | 6.12 | 110.00 | 100.20 |
| 1 | G | 698 | ASN | CB-CA-C | -6.12 | 98.15 | 110.40 |
| 1 | G | 760 | PHE | CB-CG-CD2 | -6.12 | 116.52 | 120.80 |
| 1 | M | 682 | THR | CA-CB-CG2 | -6.12 | 103.83 | 112.40 |
| 1 | G | 463 | ASP | CB-CG-OD2 | -6.11 | 112.80 | 118.30 |
| 3 | R | 58 | MET | CG-SD-CE | 6.11 | 109.98 | 100.20 |
| 4 | 5 | 259 | GLU | CA-CB-CG | 6.11 | 126.84 | 113.40 |
| 1 | D | 698 | ASN | CB-CA-C | -6.11 | 98.19 | 110.40 |
| 2 | E | 141 | PRO | N-CA-CB | -6.11 | 95.89 | 102.60 |
| 1 | G | 327 | ASP | CB-CG-OD2 | 6.10 | 123.79 | 118.30 |
| 1 | J | 590 | TYR | CB-CG-CD2 | 6.10 | 124.66 | 121.00 |
| 1 | G | 779 | ARG | NE-CZ-NH1 | 6.10 | 123.35 | 120.30 |
| 2 | B | 141 | PRO | N-CA-CB | -6.10 | 95.89 | 102.60 |
| 1 | A | 327 | ASP | CB-CG-OD2 | 6.09 | 123.78 | 118.30 |
| 1 | J | 463 | ASP | CB-CG-OD2 | -6.09 | 112.82 | 118.30 |
| 1 | D | 760 | PHE | CB-CG-CD2 | -6.09 | 116.54 | 120.80 |
| 1 | P | 682 | THR | CA-CB-CG2 | -6.09 | 103.88 | 112.40 |
| 3 | I | 58 | MET | CG-SD-CE | 6.09 | 109.94 | 100.20 |
| 2 | E | 129 | THR | CA-CB-CG2 | 6.09 | 120.92 | 112.40 |
| 1 | J | 752 | ASP | CB-CG-OD2 | 6.08 | 123.78 | 118.30 |
| 3 | C | 58 | MET | CG-SD-CE | 6.08 | 109.93 | 100.20 |
| 1 | A | 780 | ASP | CB-CG-OD2 | 6.08 | 123.77 | 118.30 |
| 1 | P | 104 | TYR | CB-CG-CD1 | -6.08 | 117.35 | 121.00 |
| 1 | A | 779 | ARG | NE-CZ-NH1 | 6.08 | 123.34 | 120.30 |
| 1 | P | 590 | TYR | CB-CG-CD2 | 6.08 | 124.65 | 121.00 |
| 4 | V | 349 | LEU | CA-C-N | -6.08 | 103.83 | 117.20 |
| 2 | N | 141 | PRO | N-CA-CB | -6.07 | 95.92 | 102.60 |
| 4 | 6 | 349 | LEU | CA-C-N | -6.07 | 103.84 | 117.20 |
| 1 | M | 463 | ASP | CB-CG-OD2 | -6.07 | 112.83 | 118.30 |
| 1 | P | 760 | PHE | CB-CG-CD2 | -6.07 | 116.55 | 120.80 |
| 4 | 5 | 16 | LEU | CA-CB-CG | 6.06 | 129.25 | 115.30 |
| 1 | J | 450 | ASP | CB-CG-OD1 | -6.06 | 112.84 | 118.30 |
| 1 | G | 625 | THR | CA-CB-OG1 | 6.06 | 121.72 | 109.00 |
| 4 | 2 | 349 | LEU | CA-C-N | -6.06 | 103.87 | 117.20 |
| 3 | O | 58 | MET | CG-SD-CE | 6.06 | 109.89 | 100.20 |
| 4 | Z | 16 | LEU | CA-CB-CG | 6.06 | 129.23 | 115.30 |
| 1 | M | 780 | ASP | CB-CG-OD2 | 6.06 | 123.75 | 118.30 |
| 4 | X | 16 | LEU | CA-CB-CG | 6.06 | 129.23 | 115.30 |
| 4 | 7 | 349 | LEU | CA-C-N | -6.05 | 103.88 | 117.20 |
| 4 | Z | 349 | LEU | CA-C-N | -6.05 | 103.88 | 117.20 |
| 1 | J | 104 | TYR | CB-CG-CD1 | -6.05 | 117.37 | 121.00 |
| 1 | A | 682 | THR | CA-CB-CG2 | -6.05 | 103.93 | 112.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1 | D | 779 | ARG | NE-CZ-NH1 | 6.05 | 123.33 | 120.30 |
| 2 | H | 141 | PRO | N-CA-CB | -6.05 | 95.95 | 102.60 |
| 1 | M | 590 | TYR | CB-CG-CD2 | 6.05 | 124.63 | 121.00 |
| 4 | 4 | 349 | LEU | CA-C-N | -6.05 | 103.90 | 117.20 |
| 4 | W | 16 | LEU | CA-CB-CG | 6.05 | 129.21 | 115.30 |
| 4 | V | 16 | LEU | CA-CB-CG | 6.04 | 129.20 | 115.30 |
| 4 | X | 349 | LEU | CA-C-N | -6.04 | 103.90 | 117.20 |
| 1 | G | 682 | THR | CA-CB-CG2 | -6.04 | 103.94 | 112.40 |
| 4 | 1 | 16 | LEU | CA-CB-CG | 6.04 | 129.20 | 115.30 |
| 4 | 3 | 16 | LEU | CA-CB-CG | 6.04 | 129.20 | 115.30 |
| 4 | 5 | 349 | LEU | CA-C-N | -6.04 | 103.91 | 117.20 |
| 2 | H | 129 | THR | CA-CB-CG2 | 6.04 | 120.86 | 112.40 |
| 1 | J | 682 | THR | CA-CB-CG2 | -6.04 | 103.95 | 112.40 |
| 1 | M | 752 | ASP | CB-CG-OD2 | 6.04 | 123.73 | 118.30 |
| 4 | 8 | 16 | LEU | CA-CB-CG | 6.04 | 129.19 | 115.30 |
| 1 | D | 346 | ASP | CB-CG-OD1 | 6.03 | 123.73 | 118.30 |
| 1 | P | 463 | ASP | CB-CG-OD2 | -6.03 | 112.87 | 118.30 |
| 4 | 8 | 349 | LEU | CA-C-N | -6.03 | 103.93 | 117.20 |
| 1 | D | 104 | TYR | CB-CG-CD1 | -6.03 | 117.38 | 121.00 |
| 3 | L | 58 | MET | CG-SD-CE | 6.03 | 109.85 | 100.20 |
| 4 | 7 | 16 | LEU | CA-CB-CG | 6.03 | 129.17 | 115.30 |
| 4 | 9 | 335 | ARG | NE-CZ-NH2 | -6.03 | 117.28 | 120.30 |
| 1 | D | 625 | THR | CA-CB-OG1 | 6.03 | 121.66 | 109.00 |
| 1 | G | 780 | ASP | CB-CG-OD2 | 6.03 | 123.73 | 118.30 |
| 4 | 2 | 16 | LEU | CA-CB-CG | 6.03 | 129.16 | 115.30 |
| 4 | 9 | 16 | LEU | CA-CB-CG | 6.03 | 129.16 | 115.30 |
| 1 | A | 104 | TYR | CB-CG-CD1 | -6.03 | 117.39 | 121.00 |
| 1 | M | 625 | THR | CA-CB-OG1 | 6.03 | 121.65 | 109.00 |
| 4 | 4 | 16 | LEU | CA-CB-CG | 6.03 | 129.16 | 115.30 |
| 4 | 9 | 349 | LEU | CA-C-N | -6.03 | 103.94 | 117.20 |
| 4 | 1 | 349 | LEU | CA-C-N | -6.02 | 103.95 | 117.20 |
| 1 | A | 810 | ARG | NE-CZ-NH1 | 6.02 | 123.31 | 120.30 |
| 1 | P | 665 | ARG | NE-CZ-NH2 | -6.02 | 117.29 | 120.30 |
| 4 | Y | 16 | LEU | CA-CB-CG | 6.02 | 129.14 | 115.30 |
| 1 | A | 625 | THR | CA-CB-OG1 | 6.01 | 121.63 | 109.00 |
| 1 | P | 447 | GLN | N-CA-CB | 6.01 | 121.42 | 110.60 |
| 1 | A | 447 | GLN | N-CA-CB | 6.01 | 121.42 | 110.60 |
| 1 | P | 625 | THR | CA-CB-OG1 | 6.01 | 121.63 | 109.00 |
| 1 | D | 378 | ASP | CB-CG-OD1 | -6.01 | 112.89 | 118.30 |
| 4 | W | 116 | ARG | NE-CZ-NH1 | 6.01 | 123.30 | 120.30 |
| 4 | W | 349 | LEU | CA-C-N | -6.01 | 103.98 | 117.20 |
| 1 | D | 682 | THR | CA-CB-CG2 | -6.01 | 103.99 | 112.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1 | J | 625 | THR | CA-CB-OG1 | 6.01 | 121.61 | 109.00 |
| 1 | P | 752 | ASP | CB-CG-OD2 | 6.01 | 123.70 | 118.30 |
| 4 | 3 | 349 | LEU | CA-C-N | -6.01 | 103.99 | 117.20 |
| 4 | 6 | 16 | LEU | CA-CB-CG | 6.01 | 129.11 | 115.30 |
| 1 | D | 463 | ASP | CB-CG-OD2 | -6.00 | 112.90 | 118.30 |
| 1 | G | 192 | VAL | CA-CB-CG1 | -6.00 | 101.90 | 110.90 |
| 4 | 3 | 116 | ARG | NE-CZ-NH1 | 6.00 | 123.30 | 120.30 |
| 1 | G | 810 | ARG | NE-CZ-NH1 | 6.00 | 123.30 | 120.30 |
| 1 | D | 780 | ASP | CB-CG-OD2 | 5.99 | 123.69 | 118.30 |
| 1 | G | 346 | ASP | CB-CG-OD1 | 5.99 | 123.69 | 118.30 |
| 1 | J | 447 | GLN | N-CA-CB | 5.99 | 121.39 | 110.60 |
| 1 | M | 192 | VAL | CA-CB-CG1 | -5.99 | 101.91 | 110.90 |
| 2 | K | 129 | THR | CA-CB-CG2 | 5.99 | 120.79 | 112.40 |
| 1 | J | 192 | VAL | CA-CB-CG1 | -5.99 | 101.91 | 110.90 |
| 1 | D | 754 | ASP | CB-CG-OD2 | -5.98 | 112.92 | 118.30 |
| 1 | D | 192 | VAL | CA-CB-CG1 | -5.98 | 101.93 | 110.90 |
| 4 | Y | 349 | LEU | CA-C-N | -5.98 | 104.04 | 117.20 |
| 1 | M | 450 | ASP | CB-CG-OD1 | -5.98 | 112.92 | 118.30 |
| 1 | D | 450 | ASP | CB-CG-OD1 | -5.98 | 112.92 | 118.30 |
| 1 | J | 754 | ASP | CB-CG-OD2 | -5.98 | 112.92 | 118.30 |
| 1 | G | 665 | ARG | NE-CZ-NH2 | -5.97 | 117.31 | 120.30 |
| 1 | P | 192 | VAL | CA-CB-CG1 | -5.97 | 101.94 | 110.90 |
| 1 | M | 447 | GLN | N-CA-CB | 5.97 | 121.34 | 110.60 |
| 2 | N | 129 | THR | CA-CB-CG2 | 5.97 | 120.75 | 112.40 |
| 1 | G | 809 | ARG | NE-CZ-NH2 | -5.96 | 117.32 | 120.30 |
| 1 | J | 665 | ARG | NE-CZ-NH2 | -5.96 | 117.32 | 120.30 |
| 1 | D | 447 | GLN | N-CA-CB | 5.96 | 121.32 | 110.60 |
| 1 | G | 447 | GLN | N-CA-CB | 5.95 | 121.32 | 110.60 |
| 4 | Y | 335 | ARG | NE-CZ-NH2 | -5.95 | 117.32 | 120.30 |
| 2 | Q | 129 | THR | CA-CB-CG2 | 5.93 | 120.70 | 112.40 |
| 4 | 1 | 116 | ARG | NE-CZ-NH1 | 5.93 | 123.26 | 120.30 |
| 1 | D | 471 | ASP | CB-CG-OD1 | -5.92 | 112.97 | 118.30 |
| 1 | P | 754 | ASP | CB-CG-OD2 | -5.92 | 112.97 | 118.30 |
| 4 | 1 | 79 | TRP | CG-CD2-CE3 | 5.92 | 139.23 | 133.90 |
| 4 | V | 335 | ARG | NE-CZ-NH2 | -5.92 | 117.34 | 120.30 |
| 4 | Y | 79 | TRP | CG-CD2-CE3 | 5.92 | 139.22 | 133.90 |
| 1 | A | 378 | ASP | CB-CG-OD1 | -5.91 | 112.98 | 118.30 |
| 1 | G | 339 | ASP | CB-CG-OD2 | 5.91 | 123.62 | 118.30 |
| 4 | 8 | 335 | ARG | NE-CZ-NH2 | -5.91 | 117.34 | 120.30 |
| 1 | G | 752 | ASP | CB-CG-OD2 | 5.91 | 123.62 | 118.30 |
| 4 | Z | 79 | TRP | CG-CD2-CE3 | 5.91 | 139.22 | 133.90 |
| 4 | 1 | 335 | ARG | NE-CZ-NH2 | -5.91 | 117.34 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 4 | 3 | 79 | TRP | CG-CD2-CE3 | 5.91 | 139.22 | 133.90 |
| 1 | M | 665 | ARG | NE-CZ-NH2 | -5.91 | 117.35 | 120.30 |
| 4 | X | 335 | ARG | NE-CZ-NH2 | -5.91 | 117.35 | 120.30 |
| 1 | A | 754 | ASP | CB-CG-OD2 | -5.91 | 112.98 | 118.30 |
| 1 | P | 815 | CYS | CA-CB-SG | -5.91 | 103.37 | 114.00 |
| 4 | V | 200 | PHE | CA-C-N | -5.91 | 104.21 | 117.20 |
| 1 | J | 346 | ASP | CB-CG-OD1 | 5.90 | 123.61 | 118.30 |
| 4 | 4 | 116 | ARG | NE-CZ-NH1 | 5.90 | 123.25 | 120.30 |
| 1 | M | 738 | MET | CG-SD-CE | 5.90 | 109.64 | 100.20 |
| 1 | P | 738 | MET | CG-SD-CE | 5.90 | 109.64 | 100.20 |
| 4 | 8 | 200 | PHE | CA-C-N | -5.90 | 104.22 | 117.20 |
| 4 | 2 | 79 | TRP | CG-CD2-CE3 | 5.90 | 139.21 | 133.90 |
| 1 | A | 192 | VAL | CA-CB-CG1 | -5.89 | 102.06 | 110.90 |
| 1 | D | 339 | ASP | CB-CG-OD2 | 5.89 | 123.61 | 118.30 |
| 1 | G | 754 | ASP | CB-CG-OD2 | -5.89 | 113.00 | 118.30 |
| 1 | D | 738 | MET | CG-SD-CE | 5.89 | 109.63 | 100.20 |
| 1 | J | 378 | ASP | CB-CG-OD1 | -5.89 | 113.00 | 118.30 |
| 4 | X | 254 | ARG | NE-CZ-NH1 | 5.89 | 123.25 | 120.30 |
| 4 | 5 | 200 | PHE | CA-C-N | -5.89 | 104.24 | 117.20 |
| 4 | 6 | 79 | TRP | CG-CD2-CE3 | 5.89 | 139.20 | 133.90 |
| 1 | G | 738 | MET | CG-SD-CE | 5.89 | 109.62 | 100.20 |
| 1 | P | 378 | ASP | CB-CG-OD1 | -5.89 | 113.00 | 118.30 |
| 1 | G | 450 | ASP | CB-CG-OD1 | -5.88 | 113.01 | 118.30 |
| 1 | J | 815 | CYS | CA-CB-SG | -5.88 | 103.42 | 114.00 |
| 1 | J | 780 | ASP | CB-CG-OD2 | 5.88 | 123.59 | 118.30 |
| 1 | G | 378 | ASP | CB-CG-OD1 | -5.88 | 113.01 | 118.30 |
| 4 | Z | 200 | PHE | CA-C-N | -5.88 | 104.27 | 117.20 |
| 1 | A | 738 | MET | CG-SD-CE | 5.87 | 109.60 | 100.20 |
| 4 | 8 | 79 | TRP | CG-CD2-CE3 | 5.87 | 139.19 | 133.90 |
| 1 | A | 450 | ASP | CB-CG-OD1 | -5.87 | 113.02 | 118.30 |
| 4 | 7 | 335 | ARG | NE-CZ-NH2 | -5.87 | 117.36 | 120.30 |
| 1 | M | 754 | ASP | CB-CG-OD2 | -5.87 | 113.02 | 118.30 |
| 4 | 7 | 200 | PHE | CA-C-N | -5.87 | 104.29 | 117.20 |
| 4 | 4 | 79 | TRP | CG-CD2-CE3 | 5.87 | 139.18 | 133.90 |
| 4 | 7 | 79 | TRP | CG-CD2-CE3 | 5.87 | 139.18 | 133.90 |
| 4 | W | 79 | TRP | CG-CD2-CE3 | 5.87 | 139.18 | 133.90 |
| 1 | A | 665 | ARG | NE-CZ-NH2 | -5.87 | 117.37 | 120.30 |
| 4 | 3 | 200 | PHE | CA-C-N | -5.87 | 104.30 | 117.20 |
| 4 | W | 335 | ARG | NE-CZ-NH2 | -5.86 | 117.37 | 120.30 |
| 1 | J | 339 | ASP | CB-CG-OD2 | 5.86 | 123.58 | 118.30 |
| 4 | 1 | 200 | PHE | CA-C-N | -5.86 | 104.31 | 117.20 |
| 4 | 2 | 200 | PHE | CA-C-N | -5.86 | 104.31 | 117.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 4 | X | 200 | PHE | CA-C-N | -5.86 | 104.31 | 117.20 |
| 1 | D | 556 | ASP | CB-CG-OD1 | -5.86 | 113.03 | 118.30 |
| 1 | A | 815 | CYS | CA-CB-SG | -5.86 | 103.46 | 114.00 |
| 4 | 6 | 335 | ARG | NE-CZ-NH2 | -5.86 | 117.37 | 120.30 |
| 4 | Y | 116 | ARG | NE-CZ-NH1 | 5.86 | 123.23 | 120.30 |
| 4 | 6 | 200 | PHE | CA-C-N | -5.86 | 104.32 | 117.20 |
| 1 | M | 339 | ASP | CB-CG-OD2 | 5.85 | 123.57 | 118.30 |
| 4 | 9 | 200 | PHE | CA-C-N | -5.85 | 104.32 | 117.20 |
| 1 | G | 780 | ASP | CB-CG-OD1 | -5.85 | 113.03 | 118.30 |
| 1 | P | 471 | ASP | CB-CG-OD1 | -5.85 | 113.03 | 118.30 |
| 4 | 4 | 335 | ARG | NE-CZ-NH2 | -5.85 | 117.37 | 120.30 |
| 4 | W | 200 | PHE | CA-C-N | -5.85 | 104.32 | 117.20 |
| 4 | Z | 335 | ARG | NE-CZ-NH2 | -5.85 | 117.37 | 120.30 |
| 4 | 9 | 116 | ARG | NE-CZ-NH1 | 5.85 | 123.23 | 120.30 |
| 4 | 5 | 79 | TRP | CG-CD2-CE3 | 5.85 | 139.16 | 133.90 |
| 4 | 9 | 79 | TRP | CG-CD2-CE3 | 5.85 | 139.16 | 133.90 |
| 4 | 4 | 200 | PHE | CA-C-N | -5.85 | 104.34 | 117.20 |
| 1 | P | 339 | ASP | CB-CG-OD2 | 5.84 | 123.56 | 118.30 |
| 1 | D | 809 | ARG | NE-CZ-NH2 | -5.84 | 117.38 | 120.30 |
| 1 | J | 471 | ASP | CB-CG-OD1 | -5.84 | 113.04 | 118.30 |
| 4 | Y | 200 | PHE | CA-C-N | -5.84 | 104.35 | 117.20 |
| 1 | A | 752 | ASP | CB-CG-OD2 | 5.84 | 123.56 | 118.30 |
| 1 | M | 346 | ASP | CB-CG-OD1 | 5.84 | 123.56 | 118.30 |
| 1 | P | 346 | ASP | CB-CG-OD1 | 5.84 | 123.56 | 118.30 |
| 1 | D | 665 | ARG | NE-CZ-NH2 | -5.84 | 117.38 | 120.30 |
| 1 | J | 738 | MET | CG-SD-CE | 5.84 | 109.54 | 100.20 |
| 1 | P | 556 | ASP | CB-CG-OD1 | -5.84 | 113.05 | 118.30 |
| 1 | D | 815 | CYS | CA-CB-SG | -5.83 | 103.50 | 114.00 |
| 1 | P | 780 | ASP | CB-CG-OD2 | 5.83 | 123.55 | 118.30 |
| 4 | X | 79 | TRP | CG-CD2-CE3 | 5.83 | 139.15 | 133.90 |
| 4 | X | 116 | ARG | NE-CZ-NH1 | 5.83 | 123.21 | 120.30 |
| 1 | M | 378 | ASP | CB-CG-OD1 | -5.83 | 113.06 | 118.30 |
| 4 | 2 | 116 | ARG | NE-CZ-NH1 | 5.82 | 123.21 | 120.30 |
| 1 | G | 556 | ASP | CB-CG-OD1 | -5.81 | 113.07 | 118.30 |
| 4 | V | 254 | ARG | NE-CZ-NH1 | 5.81 | 123.21 | 120.30 |
| 4 | 2 | 95 | ARG | CA-CB-CG | 5.80 | 126.16 | 113.40 |
| 4 | V | 95 | ARG | CA-CB-CG | 5.80 | 126.16 | 113.40 |
| 1 | D | 752 | ASP | CB-CG-OD2 | 5.80 | 123.52 | 118.30 |
| 4 | 1 | 95 | ARG | CA-CB-CG | 5.80 | 126.15 | 113.40 |
| 4 | 5 | 95 | ARG | CA-CB-CG | 5.80 | 126.15 | 113.40 |
| 4 | 5 | 254 | ARG | NE-CZ-NH1 | 5.80 | 123.20 | 120.30 |
| 4 | 4 | 254 | ARG | NE-CZ-NH1 | 5.79 | 123.20 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 4 | 7 | 116 | ARG | NE-CZ-NH1 | 5.79 | 123.20 | 120.30 |
| 4 | V | 79 | TRP | CG-CD2-CE3 | 5.79 | 139.12 | 133.90 |
| 4 | X | 95 | ARG | CA-CB-CG | 5.79 | 126.15 | 113.40 |
| 4 | 3 | 95 | ARG | CA-CB-CG | 5.79 | 126.14 | 113.40 |
| 4 | Z | 95 | ARG | CA-CB-CG | 5.79 | 126.14 | 113.40 |
| 4 | Z | 116 | ARG | NE-CZ-NH1 | 5.79 | 123.20 | 120.30 |
| 4 | Y | 95 | ARG | CA-CB-CG | 5.79 | 126.14 | 113.40 |
| 4 | 3 | 335 | ARG | NE-CZ-NH2 | -5.79 | 117.41 | 120.30 |
| 1 | A | 346 | ASP | CB-CG-OD1 | 5.78 | 123.50 | 118.30 |
| 4 | 3 | 254 | ARG | NE-CZ-NH1 | 5.78 | 123.19 | 120.30 |
| 1 | J | 556 | ASP | CB-CG-OD1 | -5.78 | 113.10 | 118.30 |
| 4 | 8 | 95 | ARG | CA-CB-CG | 5.78 | 126.11 | 113.40 |
| 1 | M | 815 | CYS | CA-CB-SG | -5.78 | 103.60 | 114.00 |
| 1 | M | 556 | ASP | CB-CG-OD1 | -5.77 | 113.10 | 118.30 |
| 1 | A | 471 | ASP | CB-CG-OD1 | -5.77 | 113.11 | 118.30 |
| 4 | W | 95 | ARG | CA-CB-CG | 5.77 | 126.10 | 113.40 |
| 4 | 7 | 95 | ARG | CA-CB-CG | 5.77 | 126.09 | 113.40 |
| 4 | V | 116 | ARG | NE-CZ-NH1 | 5.77 | 123.18 | 120.30 |
| 4 | 2 | 335 | ARG | NE-CZ-NH2 | -5.76 | 117.42 | 120.30 |
| 4 | 6 | 95 | ARG | CA-CB-CG | 5.76 | 126.07 | 113.40 |
| 1 | A | 339 | ASP | CB-CG-OD2 | 5.76 | 123.48 | 118.30 |
| 1 | J | 4 | ASP | CB-CG-OD2 | 5.75 | 123.48 | 118.30 |
| 4 | 9 | 254 | ARG | NE-CZ-NH1 | 5.75 | 123.18 | 120.30 |
| 1 | A | 556 | ASP | CB-CG-OD1 | -5.75 | 113.12 | 118.30 |
| 1 | D | 4 | ASP | CB-CG-OD2 | 5.75 | 123.48 | 118.30 |
| 1 | G | 471 | ASP | CB-CG-OD1 | -5.75 | 113.12 | 118.30 |
| 1 | A | 809 | ARG | NE-CZ-NH2 | -5.75 | 117.42 | 120.30 |
| 4 | 6 | 335 | ARG | CA-CB-CG | 5.75 | 126.05 | 113.40 |
| 4 | 4 | 95 | ARG | CA-CB-CG | 5.75 | 126.05 | 113.40 |
| 1 | A | 780 | ASP | CB-CG-OD1 | -5.75 | 113.13 | 118.30 |
| 1 | D | 352 | TYR | N-CA-CB | 5.75 | 120.94 | 110.60 |
| 4 | 5 | 335 | ARG | CA-CB-CG | 5.75 | 126.04 | 113.40 |
| 4 | 8 | 116 | ARG | NE-CZ-NH1 | 5.74 | 123.17 | 120.30 |
| 4 | 9 | 95 | ARG | CA-CB-CG | 5.74 | 126.04 | 113.40 |
| 4 | 1 | 335 | ARG | CA-CB-CG | 5.74 | 126.03 | 113.40 |
| 1 | P | 165 | PHE | N-CA-CB | -5.74 | 100.27 | 110.60 |
| 1 | J | 165 | PHE | N-CA-CB | -5.74 | 100.27 | 110.60 |
| 4 | Z | 254 | ARG | NE-CZ-NH1 | 5.74 | 123.17 | 120.30 |
| 1 | M | 471 | ASP | CB-CG-OD1 | -5.73 | 113.14 | 118.30 |
| 2 | H | 149 | ASP | N-CA-CB | 5.73 | 120.92 | 110.60 |
| 4 | 8 | 254 | ARG | NE-CZ-NH1 | 5.73 | 123.17 | 120.30 |
| 4 | 7 | 335 | ARG | CA-CB-CG | 5.72 | 126.00 | 113.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 4 | W | 254 | ARG | NE-CZ-NH1 | 5.72 | 123.16 | 120.30 |
| 1 | G | 165 | PHE | N-CA-CB | -5.72 | 100.30 | 110.60 |
| 1 | D | 165 | PHE | N-CA-CB | -5.72 | 100.30 | 110.60 |
| 1 | G | 4 | ASP | CB-CG-OD2 | 5.72 | 123.45 | 118.30 |
| 1 | M | 165 | PHE | N-CA-CB | -5.72 | 100.31 | 110.60 |
| 2 | B | 149 | ASP | N-CA-CB | 5.71 | 120.89 | 110.60 |
| 4 | 2 | 254 | ARG | NE-CZ-NH1 | 5.71 | 123.16 | 120.30 |
| 4 | W | 335 | ARG | CA-CB-CG | 5.71 | 125.97 | 113.40 |
| 1 | G | 815 | CYS | CA-CB-SG | -5.71 | 103.72 | 114.00 |
| 4 | 1 | 254 | ARG | NE-CZ-NH1 | 5.71 | 123.16 | 120.30 |
| 4 | 8 | 335 | ARG | CA-CB-CG | 5.71 | 125.96 | 113.40 |
| 4 | 5 | 116 | ARG | NE-CZ-NH1 | 5.71 | 123.15 | 120.30 |
| 1 | A | 4 | ASP | CB-CG-OD2 | 5.71 | 123.44 | 118.30 |
| 1 | P | 4 | ASP | CB-CG-OD2 | 5.70 | 123.43 | 118.30 |
| 1 | P | 780 | ASP | CB-CG-OD1 | -5.70 | 113.17 | 118.30 |
| 1 | P | 809 | ARG | NE-CZ-NH2 | -5.70 | 117.45 | 120.30 |
| 4 | 4 | 335 | ARG | CA-CB-CG | 5.70 | 125.94 | 113.40 |
| 4 | 9 | 335 | ARG | CA-CB-CG | 5.70 | 125.94 | 113.40 |
| 4 | 2 | 335 | ARG | CA-CB-CG | 5.70 | 125.93 | 113.40 |
| 4 | 3 | 335 | ARG | CA-CB-CG | 5.70 | 125.93 | 113.40 |
| 4 | Y | 335 | ARG | CA-CB-CG | 5.69 | 125.93 | 113.40 |
| 1 | M | 780 | ASP | CB-CG-OD1 | -5.69 | 113.18 | 118.30 |
| 1 | M | 809 | ARG | NE-CZ-NH2 | -5.69 | 117.45 | 120.30 |
| 4 | 6 | 116 | ARG | NE-CZ-NH1 | 5.69 | 123.14 | 120.30 |
| 4 | X | 335 | ARG | CA-CB-CG | 5.69 | 125.92 | 113.40 |
| 1 | A | 165 | PHE | N-CA-CB | -5.69 | 100.36 | 110.60 |
| 4 | 6 | 254 | ARG | NE-CZ-NH1 | 5.69 | 123.14 | 120.30 |
| 4 | V | 335 | ARG | CA-CB-CG | 5.69 | 125.91 | 113.40 |
| 4 | Z | 335 | ARG | CA-CB-CG | 5.68 | 125.91 | 113.40 |
| 1 | J | 780 | ASP | CB-CG-OD1 | -5.68 | 113.19 | 118.30 |
| 1 | D | 780 | ASP | CB-CG-OD1 | -5.68 | 113.19 | 118.30 |
| 4 | Y | 279 | TYR | CB-CG-CD2 | -5.67 | 117.59 | 121.00 |
| 1 | G | 352 | TYR | N-CA-CB | 5.67 | 120.81 | 110.60 |
| 1 | M | 4 | ASP | CB-CG-OD2 | 5.67 | 123.40 | 118.30 |
| 2 | Q | 149 | ASP | N-CA-CB | 5.67 | 120.81 | 110.60 |
| 4 | Y | 254 | ARG | NE-CZ-NH1 | 5.67 | 123.13 | 120.30 |
| 2 | E | 149 | ASP | N-CA-CB | 5.66 | 120.79 | 110.60 |
| 4 | 6 | 279 | TYR | CB-CG-CD2 | -5.66 | 117.61 | 121.00 |
| 1 | D | 781 | ASP | CB-CG-OD2 | 5.66 | 123.39 | 118.30 |
| 4 | 9 | 279 | TYR | CB-CG-CD2 | -5.66 | 117.61 | 121.00 |
| 2 | N | 149 | ASP | N-CA-CB | 5.65 | 120.78 | 110.60 |
| 1 | G | 693 | HIS | CA-CB-CG | -5.65 | 103.99 | 113.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 4 | 7 | 254 | ARG | NE-CZ-NH1 | 5.65 | 123.12 | 120.30 |
| 4 | 7 | 294 | TYR | CB-CG-CD2 | -5.65 | 117.61 | 121.00 |
| 1 | M | 693 | HIS | CA-CB-CG | -5.64 | 104.01 | 113.60 |
| 4 | 5 | 335 | ARG | NE-CZ-NH2 | -5.64 | 117.48 | 120.30 |
| 1 | A | 781 | ASP | CB-CG-OD2 | 5.63 | 123.37 | 118.30 |
| 1 | J | 352 | TYR | N-CA-CB | 5.63 | 120.74 | 110.60 |
| 1 | J | 809 | ARG | NE-CZ-NH2 | -5.63 | 117.48 | 120.30 |
| 1 | D | 384 | ASP | CB-CG-OD1 | -5.63 | 113.24 | 118.30 |
| 1 | D | 693 | HIS | CA-CB-CG | -5.62 | 104.04 | 113.60 |
| 4 | W | 356 | TRP | CG-CD2-CE3 | 5.62 | 138.96 | 133.90 |
| 4 | W | 279 | TYR | CB-CG-CD2 | -5.62 | 117.63 | 121.00 |
| 4 | 1 | 279 | TYR | CB-CG-CD2 | -5.62 | 117.63 | 121.00 |
| 2 | K | 149 | ASP | N-CA-CB | 5.62 | 120.71 | 110.60 |
| 1 | P | 352 | TYR | N-CA-CB | 5.61 | 120.70 | 110.60 |
| 4 | 2 | 113 | LYS | CA-CB-CG | 5.61 | 125.75 | 113.40 |
| 4 | 1 | 294 | TYR | CB-CG-CD2 | -5.61 | 117.63 | 121.00 |
| 4 | 2 | 11 | ASP | CB-CG-OD1 | 5.61 | 123.35 | 118.30 |
| 4 | V | 113 | LYS | CA-CB-CG | 5.60 | 125.72 | 113.40 |
| 4 | 3 | 294 | TYR | CB-CG-CD2 | -5.59 | 117.64 | 121.00 |
| 1 | J | 693 | HIS | CA-CB-CG | -5.59 | 104.09 | 113.60 |
| 4 | 9 | 356 | TRP | CG-CD2-CE3 | 5.59 | 138.93 | 133.90 |
| 1 | G | 781 | ASP | CB-CG-OD2 | 5.59 | 123.33 | 118.30 |
| 1 | G | 785 | GLU | O-C-N | 5.59 | 131.64 | 122.70 |
| 4 | 7 | 113 | LYS | CA-CB-CG | 5.59 | 125.69 | 113.40 |
| 1 | M | 352 | TYR | N-CA-CB | 5.58 | 120.64 | 110.60 |
| 4 | 4 | 113 | LYS | CA-CB-CG | 5.58 | 125.67 | 113.40 |
| 4 | Z | 113 | LYS | CA-CB-CG | 5.58 | 125.67 | 113.40 |
| 1 | J | 686 | MET | N-CA-CB | -5.58 | 100.57 | 110.60 |
| 1 | P | 686 | MET | N-CA-CB | -5.58 | 100.56 | 110.60 |
| 4 | 1 | 113 | LYS | CA-CB-CG | 5.58 | 125.67 | 113.40 |
| 4 | W | 294 | TYR | CB-CG-CD2 | -5.58 | 117.66 | 121.00 |
| 4 | Y | 113 | LYS | CA-CB-CG | 5.58 | 125.67 | 113.40 |
| 1 | M | 33 | ASP | CB-CG-OD2 | 5.57 | 123.31 | 118.30 |
| 1 | M | 781 | ASP | CB-CG-OD2 | 5.57 | 123.31 | 118.30 |
| 1 | P | 693 | HIS | CA-CB-CG | -5.57 | 104.13 | 113.60 |
| 4 | 3 | 254 | ARG | N-CA-CB | -5.57 | 100.58 | 110.60 |
| 4 | 9 | 113 | LYS | CA-CB-CG | 5.57 | 125.64 | 113.40 |
| 4 | 9 | 294 | TYR | CB-CG-CD2 | -5.57 | 117.66 | 121.00 |
| 4 | 3 | 113 | LYS | CA-CB-CG | 5.56 | 125.64 | 113.40 |
| 4 | Z | 356 | TRP | CG-CD2-CE3 | 5.56 | 138.91 | 133.90 |
| 1 | A | 693 | HIS | CA-CB-CG | -5.56 | 104.15 | 113.60 |
| 1 | G | 723 | ARG | NE-CZ-NH1 | 5.56 | 123.08 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 4 | 3 | 279 | TYR | CB-CG-CD2 | -5.56 | 117.66 | 121.00 |
| 1 | A | 352 | TYR | N-CA-CB | 5.56 | 120.60 | 110.60 |
| 1 | G | 320 | ILE | CB-CA-C | -5.56 | 100.48 | 111.60 |
| 4 | 8 | 113 | LYS | CA-CB-CG | 5.55 | 125.62 | 113.40 |
| 4 | X | 113 | LYS | CA-CB-CG | 5.55 | 125.61 | 113.40 |
| 4 | 7 | 279 | TYR | CB-CG-CD2 | -5.55 | 117.67 | 121.00 |
| 4 | 6 | 113 | LYS | CA-CB-CG | 5.55 | 125.60 | 113.40 |
| 1 | P | 33 | ASP | CB-CG-OD2 | 5.54 | 123.29 | 118.30 |
| 1 | D | 752 | ASP | CB-CA-C | 5.54 | 121.48 | 110.40 |
| 1 | M | 686 | MET | N-CA-CB | -5.54 | 100.63 | 110.60 |
| 1 | D | 686 | MET | N-CA-CB | -5.54 | 100.63 | 110.60 |
| 1 | D | 306 | THR | CA-CB-CG2 | -5.54 | 104.65 | 112.40 |
| 4 | W | 113 | LYS | CA-CB-CG | 5.54 | 125.58 | 113.40 |
| 1 | A | 752 | ASP | CB-CA-C | 5.54 | 121.47 | 110.40 |
| 4 | 8 | 254 | ARG | N-CA-CB | -5.54 | 100.64 | 110.60 |
| 4 | W | 254 | ARG | N-CA-CB | -5.54 | 100.64 | 110.60 |
| 4 | 1 | 356 | TRP | CG-CD2-CE3 | 5.53 | 138.88 | 133.90 |
| 4 | 5 | 113 | LYS | CA-CB-CG | 5.53 | 125.58 | 113.40 |
| 1 | G | 306 | THR | CA-CB-CG2 | -5.53 | 104.66 | 112.40 |
| 4 | 9 | 147 | ARG | NE-CZ-NH2 | -5.53 | 117.53 | 120.30 |
| 4 | X | 11 | ASP | CB-CG-OD1 | 5.53 | 123.28 | 118.30 |
| 4 | 2 | 279 | TYR | CB-CG-CD2 | -5.53 | 117.68 | 121.00 |
| 1 | M | 723 | ARG | NE-CZ-NH1 | 5.53 | 123.06 | 120.30 |
| 4 | 7 | 356 | TRP | CG-CD2-CE3 | 5.53 | 138.88 | 133.90 |
| 4 | V | 254 | ARG | N-CA-CB | -5.53 | 100.65 | 110.60 |
| 4 | Y | 254 | ARG | N-CA-CB | -5.53 | 100.65 | 110.60 |
| 1 | J | 781 | ASP | CB-CG-OD2 | 5.53 | 123.27 | 118.30 |
| 4 | 2 | 254 | ARG | N-CA-CB | -5.53 | 100.66 | 110.60 |
| 4 | Y | 294 | TYR | CB-CG-CD2 | -5.53 | 117.69 | 121.00 |
| 1 | G | 686 | MET | N-CA-CB | -5.52 | 100.66 | 110.60 |
| 4 | 8 | 356 | TRP | CG-CD2-CE3 | 5.52 | 138.87 | 133.90 |
| 4 | 2 | 356 | TRP | CG-CD2-CE3 | 5.52 | 138.87 | 133.90 |
| 1 | M | 320 | ILE | CB-CA-C | -5.52 | 100.56 | 111.60 |
| 1 | P | 343 | PHE | CB-CG-CD2 | -5.52 | 116.94 | 120.80 |
| 4 | 1 | 254 | ARG | N-CA-CB | -5.52 | 100.67 | 110.60 |
| 4 | 4 | 279 | TYR | CB-CG-CD2 | -5.52 | 117.69 | 121.00 |
| 4 | 5 | 254 | ARG | N-CA-CB | -5.51 | 100.67 | 110.60 |
| 1 | A | 686 | MET | N-CA-CB | -5.51 | 100.68 | 110.60 |
| 4 | 3 | 356 | TRP | CG-CD2-CE3 | 5.51 | 138.86 | 133.90 |
| 1 | J | 752 | ASP | CB-CA-C | 5.51 | 121.42 | 110.40 |
| 4 | 6 | 356 | TRP | CG-CD2-CE3 | 5.51 | 138.86 | 133.90 |
| 1 | P | 781 | ASP | CB-CG-OD2 | 5.51 | 123.26 | 118.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1 | J | 320 | ILE | CB-CA-C | -5.50 | 100.59 | 111.60 |
| 1 | J | 343 | PHE | CB-CG-CD2 | -5.50 | 116.95 | 120.80 |
| 4 | 4 | 254 | ARG | N-CA-CB | -5.50 | 100.69 | 110.60 |
| 1 | M | 752 | ASP | CB-CA-C | 5.50 | 121.40 | 110.40 |
| 4 | 6 | 254 | ARG | N-CA-CB | -5.50 | 100.70 | 110.60 |
| 4 | 9 | 254 | ARG | N-CA-CB | -5.50 | 100.70 | 110.60 |
| 4 | Y | 356 | TRP | CG-CD2-CE3 | 5.50 | 138.85 | 133.90 |
| 1 | G | 752 | ASP | CB-CA-C | 5.49 | 121.39 | 110.40 |
| 4 | 4 | 11 | ASP | CB-CG-OD1 | 5.49 | 123.24 | 118.30 |
| 4 | 5 | 294 | TYR | CB-CG-CD2 | -5.49 | 117.70 | 121.00 |
| 4 | 2 | 294 | TYR | CB-CG-CD2 | -5.49 | 117.71 | 121.00 |
| 4 | 7 | 254 | ARG | N-CA-CB | -5.49 | 100.72 | 110.60 |
| 4 | 3 | 11 | ASP | CB-CG-OD1 | 5.49 | 123.24 | 118.30 |
| 4 | X | 254 | ARG | N-CA-CB | -5.48 | 100.73 | 110.60 |
| 1 | P | 752 | ASP | CB-CA-C | 5.48 | 121.36 | 110.40 |
| 4 | Z | 254 | ARG | N-CA-CB | -5.48 | 100.74 | 110.60 |
| 1 | A | 306 | THR | CA-CB-CG2 | -5.48 | 104.73 | 112.40 |
| 4 | 1 | 79 | TRP | CB-CG-CD1 | -5.47 | 119.88 | 127.00 |
| 1 | J | 33 | ASP | CB-CG-OD2 | 5.47 | 123.23 | 118.30 |
| 1 | P | 320 | ILE | CB-CA-C | -5.47 | 100.65 | 111.60 |
| 1 | P | 547 | ASP | CB-CG-OD2 | 5.47 | 123.22 | 118.30 |
| 4 | 9 | 79 | TRP | CB-CG-CD1 | -5.47 | 119.89 | 127.00 |
| 1 | A | 320 | ILE | CB-CA-C | -5.47 | 100.66 | 111.60 |
| 4 | 5 | 279 | TYR | CB-CG-CD2 | -5.47 | 117.72 | 121.00 |
| 4 | 8 | 11 | ASP | CB-CG-OD1 | 5.47 | 123.22 | 118.30 |
| 4 | 8 | 294 | TYR | CB-CG-CD2 | -5.47 | 117.72 | 121.00 |
| 4 | X | 294 | TYR | CB-CG-CD2 | -5.46 | 117.72 | 121.00 |
| 1 | M | 306 | THR | CA-CB-CG2 | -5.46 | 104.75 | 112.40 |
| 4 | 4 | 79 | TRP | CB-CG-CD1 | -5.46 | 119.90 | 127.00 |
| 4 | 9 | 356 | TRP | CG-CD1-NE1 | -5.46 | 104.64 | 110.10 |
| 4 | Z | 294 | TYR | CB-CG-CD2 | -5.46 | 117.72 | 121.00 |
| 1 | D | 320 | ILE | CB-CA-C | -5.46 | 100.68 | 111.60 |
| 4 | 4 | 356 | TRP | CG-CD2-CE3 | 5.46 | 138.81 | 133.90 |
| 4 | 5 | 356 | TRP | CG-CD2-CE3 | 5.46 | 138.81 | 133.90 |
| 4 | 9 | 356 | TRP | CB-CG-CD1 | -5.46 | 119.91 | 127.00 |
| 4 | 3 | 147 | ARG | NE-CZ-NH2 | -5.45 | 117.57 | 120.30 |
| 4 | 6 | 11 | ASP | CB-CG-OD1 | 5.45 | 123.21 | 118.30 |
| 4 | 7 | 11 | ASP | CB-CG-OD1 | 5.45 | 123.21 | 118.30 |
| 4 | 9 | 11 | ASP | CB-CG-OD1 | 5.45 | 123.21 | 118.30 |
| 4 | Z | 279 | TYR | CB-CG-CD2 | -5.45 | 117.73 | 121.00 |
| 1 | M | 384 | ASP | CB-CG-OD1 | -5.45 | 113.40 | 118.30 |
| 4 | 6 | 294 | TYR | CB-CG-CD2 | -5.45 | 117.73 | 121.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 4 | 7 | 79 | TRP | CB-CG-CD1 | -5.45 | 119.92 | 127.00 |
| 4 | 5 | 79 | TRP | CB-CG-CD1 | -5.45 | 119.92 | 127.00 |
| 1 | J | 241 | ASP | CB-CG-OD2 | 5.44 | 123.20 | 118.30 |
| 4 | 1 | 147 | ARG | NE-CZ-NH2 | -5.44 | 117.58 | 120.30 |
| 4 | 3 | 356 | TRP | CB-CG-CD1 | -5.44 | 119.93 | 127.00 |
| 4 | Y | 356 | TRP | CB-CG-CD1 | -5.44 | 119.93 | 127.00 |
| 1 | A | 241 | ASP | CB-CG-OD2 | 5.44 | 123.19 | 118.30 |
| 4 | Z | 11 | ASP | CB-CG-OD1 | 5.44 | 123.19 | 118.30 |
| 1 | M | 326 | ASP | CB-CG-OD2 | 5.44 | 123.19 | 118.30 |
| 1 | A | 384 | ASP | CB-CG-OD1 | -5.43 | 113.41 | 118.30 |
| 1 | D | 241 | ASP | CB-CG-OD2 | 5.43 | 123.19 | 118.30 |
| 1 | P | 326 | ASP | CB-CG-OD2 | 5.43 | 123.19 | 118.30 |
| 1 | A | 326 | ASP | CB-CG-OD2 | 5.43 | 123.19 | 118.30 |
| 4 | 8 | 335 | ARG | NE-CZ-NH1 | 5.43 | 123.02 | 120.30 |
| 1 | P | 306 | THR | CA-CB-CG2 | -5.43 | 104.80 | 112.40 |
| 4 | 8 | 279 | TYR | CB-CG-CD2 | -5.43 | 117.74 | 121.00 |
| 1 | D | 33 | ASP | CB-CG-OD2 | 5.43 | 123.18 | 118.30 |
| 1 | G | 326 | ASP | CB-CG-OD2 | 5.43 | 123.18 | 118.30 |
| 1 | P | 384 | ASP | CB-CG-OD1 | -5.43 | 113.42 | 118.30 |
| 4 | V | 11 | ASP | CB-CG-OD1 | 5.43 | 123.18 | 118.30 |
| 1 | P | 723 | ARG | NE-CZ-NH1 | 5.42 | 123.01 | 120.30 |
| 4 | 1 | 356 | TRP | CB-CG-CD1 | -5.42 | 119.95 | 127.00 |
| 1 | M | 343 | PHE | CB-CG-CD2 | -5.42 | 117.01 | 120.80 |
| 1 | A | 723 | ARG | NE-CZ-NH1 | 5.42 | 123.01 | 120.30 |
| 1 | G | 601 | ASP | CB-CG-OD2 | 5.42 | 123.17 | 118.30 |
| 1 | J | 306 | THR | CA-CB-CG2 | -5.42 | 104.82 | 112.40 |
| 4 | W | 356 | TRP | CB-CG-CD1 | -5.42 | 119.96 | 127.00 |
| 4 | X | 356 | TRP | CB-CG-CD1 | -5.42 | 119.96 | 127.00 |
| 1 | M | 547 | ASP | CB-CG-OD2 | 5.42 | 123.17 | 118.30 |
| 4 | W | 11 | ASP | CB-CG-OD1 | 5.41 | 123.17 | 118.30 |
| 1 | J | 547 | ASP | CB-CG-OD2 | 5.41 | 123.17 | 118.30 |
| 4 | 5 | 356 | TRP | CB-CG-CD1 | -5.41 | 119.97 | 127.00 |
| 4 | 6 | 79 | TRP | CB-CG-CD1 | -5.41 | 119.97 | 127.00 |
| 4 | 1 | 251 | GLY | CA-C-N | -5.41 | 105.31 | 117.20 |
| 4 | X | 356 | TRP | CG-CD2-CE3 | 5.41 | 138.77 | 133.90 |
| 1 | A | 33 | ASP | CB-CG-OD2 | 5.41 | 123.17 | 118.30 |
| 4 | V | 335 | ARG | NE-CZ-NH1 | 5.41 | 123.00 | 120.30 |
| 4 | W | 79 | TRP | CB-CG-CD1 | -5.41 | 119.97 | 127.00 |
| 1 | M | 218 | LEU | O-C-N | 5.40 | 131.35 | 122.70 |
| 4 | 3 | 79 | TRP | CB-CG-CD1 | -5.40 | 119.98 | 127.00 |
| 4 | Y | 79 | TRP | CB-CG-CD1 | -5.40 | 119.98 | 127.00 |
| 4 | 1 | 11 | ASP | CB-CG-OD1 | 5.40 | 123.16 | 118.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1 | J | 384 | ASP | CB-CG-OD1 | -5.39 | 113.44 | 118.30 |
| 1 | P | 241 | ASP | CB-CG-OD2 | 5.39 | 123.16 | 118.30 |
| 4 | 8 | 356 | TRP | CB-CG-CD1 | -5.39 | 119.99 | 127.00 |
| 4 | V | 356 | TRP | CB-CG-CD1 | -5.39 | 119.99 | 127.00 |
| 4 | 2 | 356 | TRP | CB-CG-CD1 | -5.38 | 120.00 | 127.00 |
| 4 | 7 | 356 | TRP | CB-CG-CD1 | -5.38 | 120.00 | 127.00 |
| 4 | V | 294 | TYR | CB-CG-CD2 | -5.38 | 117.77 | 121.00 |
| 4 | W | 251 | GLY | CA-C-N | -5.38 | 105.36 | 117.20 |
| 4 | 9 | 251 | GLY | CA-C-N | -5.38 | 105.37 | 117.20 |
| 1 | A | 343 | PHE | CB-CG-CD2 | -5.38 | 117.04 | 120.80 |
| 1 | J | 326 | ASP | CB-CG-OD2 | 5.38 | 123.14 | 118.30 |
| 4 | 4 | 356 | TRP | CB-CG-CD1 | -5.38 | 120.01 | 127.00 |
| 1 | D | 547 | ASP | CB-CG-OD2 | 5.37 | 123.14 | 118.30 |
| 4 | 6 | 356 | TRP | CB-CG-CD1 | -5.37 | 120.01 | 127.00 |
| 1 | A | 601 | ASP | CB-CG-OD2 | 5.37 | 123.14 | 118.30 |
| 1 | D | 800 | ARG | NH1-CZ-NH2 | 5.37 | 125.31 | 119.40 |
| 4 | 4 | 294 | TYR | CB-CG-CD2 | -5.37 | 117.78 | 121.00 |
| 4 | V | 279 | TYR | CB-CG-CD2 | -5.37 | 117.78 | 121.00 |
| 1 | D | 326 | ASP | CB-CG-OD2 | 5.37 | 123.13 | 118.30 |
| 4 | 6 | 356 | TRP | CG-CD1-NE1 | -5.37 | 104.73 | 110.10 |
| 4 | 8 | 251 | GLY | CA-C-N | -5.37 | 105.39 | 117.20 |
| 1 | J | 800 | ARG | NH1-CZ-NH2 | 5.37 | 125.30 | 119.40 |
| 4 | Z | 356 | TRP | CB-CG-CD1 | -5.37 | 120.03 | 127.00 |
| 2 | B | 136 | MET | CG-SD-CE | 5.36 | 108.78 | 100.20 |
| 1 | D | 343 | PHE | CB-CG-CD2 | -5.36 | 117.05 | 120.80 |
| 2 | K | 136 | MET | CG-SD-CE | 5.36 | 108.78 | 100.20 |
| 1 | A | 686 | MET | CG-SD-CE | -5.36 | 91.62 | 100.20 |
| 1 | D | 723 | ARG | NE-CZ-NH1 | 5.36 | 122.98 | 120.30 |
| 4 | 7 | 251 | GLY | CA-C-N | -5.36 | 105.41 | 117.20 |
| 4 | 8 | 79 | TRP | CB-CG-CD1 | -5.36 | 120.03 | 127.00 |
| 4 | V | 79 | TRP | CB-CG-CD1 | -5.36 | 120.03 | 127.00 |
| 4 | Y | 11 | ASP | CB-CG-OD1 | 5.36 | 123.12 | 118.30 |
| 4 | Y | 147 | ARG | NE-CZ-NH2 | -5.36 | 117.62 | 120.30 |
| 4 | Y | 251 | GLY | CA-C-N | -5.36 | 105.41 | 117.20 |
| 1 | M | 686 | MET | CG-SD-CE | -5.36 | 91.63 | 100.20 |
| 4 | Z | 79 | TRP | CB-CG-CD1 | -5.36 | 120.03 | 127.00 |
| 4 | 4 | 251 | GLY | CA-C-N | -5.36 | 105.41 | 117.20 |
| 1 | G | 218 | LEU | O-C-N | 5.35 | 131.26 | 122.70 |
| 1 | G | 241 | ASP | CB-CG-OD2 | 5.35 | 123.12 | 118.30 |
| 4 | 3 | 251 | GLY | CA-C-N | -5.35 | 105.43 | 117.20 |
| 4 | 5 | 251 | GLY | CA-C-N | -5.35 | 105.44 | 117.20 |
| 4 | X | 176 | MET | CG-SD-CE | 5.35 | 108.75 | 100.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1 | P | 686 | MET | CG-SD-CE | -5.34 | 91.65 | 100.20 |
| 4 | 7 | 147 | ARG | NE-CZ-NH2 | -5.34 | 117.63 | 120.30 |
| 4 | X | 147 | ARG | NE-CZ-NH2 | -5.34 | 117.63 | 120.30 |
| 4 | V | 176 | MET | CG-SD-CE | 5.34 | 108.75 | 100.20 |
| 1 | J | 218 | LEU | O-C-N | 5.34 | 131.25 | 122.70 |
| 2 | Q | 136 | MET | CG-SD-CE | 5.34 | 108.75 | 100.20 |
| 4 | 2 | 79 | TRP | CB-CG-CD1 | -5.34 | 120.06 | 127.00 |
| 4 | X | 279 | TYR | CB-CG-CD2 | -5.34 | 117.80 | 121.00 |
| 1 | P | 218 | LEU | O-C-N | 5.34 | 131.24 | 122.70 |
| 4 | 1 | 356 | TRP | CG-CD1-NE1 | -5.34 | 104.76 | 110.10 |
| 4 | 3 | 356 | TRP | CG-CD1-NE1 | -5.34 | 104.76 | 110.10 |
| 1 | D | 125 | THR | CA-CB-CG2 | -5.34 | 104.93 | 112.40 |
| 4 | 4 | 147 | ARG | NE-CZ-NH2 | -5.34 | 117.63 | 120.30 |
| 4 | 5 | 356 | TRP | CG-CD1-NE1 | -5.34 | 104.76 | 110.10 |
| 1 | J | 686 | MET | CG-SD-CE | -5.33 | 91.67 | 100.20 |
| 4 | 5 | 11 | ASP | CB-CG-OD1 | 5.33 | 123.10 | 118.30 |
| 4 | 6 | 251 | GLY | CA-C-N | -5.33 | 105.47 | 117.20 |
| 4 | Z | 176 | MET | CG-SD-CE | 5.33 | 108.73 | 100.20 |
| 1 | G | 343 | PHE | CB-CG-CD2 | -5.33 | 117.07 | 120.80 |
| 4 | 2 | 147 | ARG | NE-CZ-NH2 | -5.33 | 117.63 | 120.30 |
| 4 | Y | 356 | TRP | CG-CD1-NE1 | -5.33 | 104.77 | 110.10 |
| 1 | G | 33 | ASP | CB-CG-OD2 | 5.33 | 123.10 | 118.30 |
| 1 | G | 686 | MET | CG-SD-CE | -5.33 | 91.67 | 100.20 |
| 4 | 8 | 176 | MET | CG-SD-CE | 5.33 | 108.73 | 100.20 |
| 4 | 9 | 62 | ARG | NE-CZ-NH1 | 5.33 | 122.97 | 120.30 |
| 1 | G | 125 | THR | CA-CB-CG2 | -5.33 | 104.94 | 112.40 |
| 4 | V | 356 | TRP | CG-CD2-CE3 | 5.33 | 138.69 | 133.90 |
| 1 | M | 241 | ASP | CB-CG-OD2 | 5.33 | 123.09 | 118.30 |
| 2 | N | 136 | MET | CG-SD-CE | 5.33 | 108.72 | 100.20 |
| 4 | X | 62 | ARG | NE-CZ-NH1 | 5.33 | 122.96 | 120.30 |
| 4 | X | 251 | GLY | CA-C-N | -5.33 | 105.48 | 117.20 |
| 1 | A | 760 | PHE | CB-CG-CD1 | 5.32 | 124.53 | 120.80 |
| 4 | 4 | 176 | MET | CG-SD-CE | 5.32 | 108.72 | 100.20 |
| 4 | X | 79 | TRP | CB-CG-CD1 | -5.32 | 120.08 | 127.00 |
| 1 | G | 384 | ASP | CB-CG-OD1 | -5.32 | 113.51 | 118.30 |
| 4 | 8 | 356 | TRP | CG-CD1-NE1 | -5.32 | 104.78 | 110.10 |
| 4 | 2 | 176 | MET | CG-SD-CE | 5.31 | 108.70 | 100.20 |
| 4 | 9 | 335 | ARG | NE-CZ-NH1 | 5.31 | 122.96 | 120.30 |
| 4 | V | 147 | ARG | NE-CZ-NH2 | -5.31 | 117.64 | 120.30 |
| 4 | X | 356 | TRP | CG-CD1-NE1 | -5.31 | 104.79 | 110.10 |
| 4 | W | 356 | TRP | CG-CD1-NE1 | -5.31 | 104.79 | 110.10 |
| 1 | G | 354 | LEU | CB-CG-CD2 | -5.31 | 101.97 | 111.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 4 | 7 | 176 | MET | CG-SD-CE | 5.31 | 108.69 | 100.20 |
| 4 | 7 | 356 | TRP | CG-CD1-NE1 | -5.31 | 104.79 | 110.10 |
| 4 | W | 147 | ARG | NE-CZ-NH2 | -5.31 | 117.65 | 120.30 |
| 4 | 2 | 251 | GLY | CA-C-N | -5.31 | 105.52 | 117.20 |
| 1 | J | 125 | THR | CA-CB-CG2 | -5.30 | 104.98 | 112.40 |
| 1 | D | 660 | LEU | CB-CG-CD2 | 5.30 | 120.01 | 111.00 |
| 1 | J | 4 | ASP | CB-CG-OD1 | -5.30 | 113.53 | 118.30 |
| 1 | M | 170 | ARG | NE-CZ-NH1 | 5.30 | 122.95 | 120.30 |
| 1 | M | 800 | ARG | NH1-CZ-NH2 | 5.30 | 125.23 | 119.40 |
| 1 | P | 800 | ARG | NH1-CZ-NH2 | 5.30 | 125.23 | 119.40 |
| 4 | Z | 251 | GLY | CA-C-N | -5.30 | 105.54 | 117.20 |
| 1 | A | 354 | LEU | CB-CG-CD2 | -5.30 | 102.00 | 111.00 |
| 2 | E | 136 | MET | CG-SD-CE | 5.30 | 108.67 | 100.20 |
| 4 | 4 | 356 | TRP | CG-CD1-NE1 | -5.30 | 104.80 | 110.10 |
| 2 | H | 136 | MET | CG-SD-CE | 5.29 | 108.67 | 100.20 |
| 4 | V | 251 | GLY | CA-C-N | -5.29 | 105.55 | 117.20 |
| 4 | Y | 176 | MET | CG-SD-CE | 5.29 | 108.67 | 100.20 |
| 1 | P | 4 | ASP | CB-CG-OD1 | -5.29 | 113.54 | 118.30 |
| 4 | Z | 147 | ARG | NE-CZ-NH2 | -5.29 | 117.66 | 120.30 |
| 1 | A | 125 | THR | CA-CB-CG2 | -5.29 | 105.00 | 112.40 |
| 1 | P | 125 | THR | CA-CB-CG2 | -5.29 | 105.00 | 112.40 |
| 4 | 2 | 356 | TRP | CG-CD1-NE1 | -5.29 | 104.81 | 110.10 |
| 1 | M | 601 | ASP | CB-CG-OD2 | 5.28 | 123.06 | 118.30 |
| 1 | P | 660 | LEU | CB-CG-CD2 | 5.28 | 119.98 | 111.00 |
| 1 | A | 547 | ASP | CB-CG-OD2 | 5.28 | 123.05 | 118.30 |
| 4 | 3 | 176 | MET | CG-SD-CE | 5.28 | 108.65 | 100.20 |
| 4 | V | 337 | TYR | CB-CG-CD1 | -5.28 | 117.83 | 121.00 |
| 4 | Z | 335 | ARG | NE-CZ-NH1 | 5.28 | 122.94 | 120.30 |
| 1 | M | 760 | PHE | CB-CG-CD1 | 5.28 | 124.49 | 120.80 |
| 4 | 6 | 147 | ARG | NE-CZ-NH2 | -5.28 | 117.66 | 120.30 |
| 1 | J | 170 | ARG | NE-CZ-NH1 | 5.28 | 122.94 | 120.30 |
| 4 | V | 356 | TRP | CG-CD1-NE1 | -5.28 | 104.82 | 110.10 |
| 4 | W | 62 | ARG | NE-CZ-NH1 | 5.28 | 122.94 | 120.30 |
| 1 | G | 660 | LEU | CB-CG-CD2 | 5.27 | 119.97 | 111.00 |
| 1 | A | 800 | ARG | NH1-CZ-NH2 | 5.27 | 125.20 | 119.40 |
| 1 | D | 354 | LEU | CB-CG-CD2 | -5.27 | 102.04 | 111.00 |
| 4 | 6 | 176 | MET | CG-SD-CE | 5.27 | 108.63 | 100.20 |
| 1 | J | 660 | LEU | CB-CG-CD2 | 5.27 | 119.95 | 111.00 |
| 4 | 9 | 176 | MET | CG-SD-CE | 5.27 | 108.63 | 100.20 |
| 1 | D | 686 | MET | CG-SD-CE | -5.26 | 91.78 | 100.20 |
| 1 | P | 170 | ARG | NE-CZ-NH1 | 5.26 | 122.93 | 120.30 |
| 4 | Z | 356 | TRP | CG-CD1-NE1 | -5.26 | 104.84 | 110.10 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1 | G | 800 | ARG | NH1-CZ-NH2 | 5.25 | 125.18 | 119.40 |
| 4 | 1 | 176 | MET | CG-SD-CE | 5.25 | 108.60 | 100.20 |
| 1 | J | 601 | ASP | CB-CG-OD2 | 5.25 | 123.03 | 118.30 |
| 1 | J | 723 | ARG | NE-CZ-NH1 | 5.25 | 122.92 | 120.30 |
| 1 | D | 601 | ASP | CB-CG-OD2 | 5.25 | 123.02 | 118.30 |
| 4 | W | 176 | MET | CG-SD-CE | 5.25 | 108.60 | 100.20 |
| 1 | A | 660 | LEU | CB-CG-CD2 | 5.24 | 119.92 | 111.00 |
| 4 | 1 | 91 | TYR | CB-CG-CD2 | -5.24 | 117.85 | 121.00 |
| 4 | 6 | 91 | TYR | CB-CG-CD2 | -5.24 | 117.85 | 121.00 |
| 4 | X | 335 | ARG | NE-CZ-NH1 | 5.24 | 122.92 | 120.30 |
| 1 | M | 660 | LEU | CB-CG-CD2 | 5.24 | 119.91 | 111.00 |
| 4 | 5 | 337 | TYR | CB-CG-CD1 | -5.24 | 117.86 | 121.00 |
| 4 | 5 | 176 | MET | CG-SD-CE | 5.24 | 108.58 | 100.20 |
| 1 | D | 4 | ASP | CB-CG-OD1 | -5.24 | 113.59 | 118.30 |
| 1 | M | 125 | THR | CA-CB-CG2 | -5.24 | 105.07 | 112.40 |
| 1 | M | 4 | ASP | CB-CG-OD1 | -5.23 | 113.59 | 118.30 |
| 1 | M | 354 | LEU | CB-CG-CD2 | -5.23 | 102.11 | 111.00 |
| 4 | 6 | 53 | TYR | CB-CG-CD1 | -5.23 | 117.86 | 121.00 |
| 1 | J | 354 | LEU | CB-CG-CD2 | -5.23 | 102.11 | 111.00 |
| 4 | Y | 53 | TYR | CB-CG-CD1 | -5.23 | 117.86 | 121.00 |
| 4 | 6 | 335 | ARG | NE-CZ-NH1 | 5.23 | 122.91 | 120.30 |
| 4 | Z | 337 | TYR | CB-CG-CD1 | -5.23 | 117.86 | 121.00 |
| 4 | 8 | 147 | ARG | NE-CZ-NH2 | -5.23 | 117.69 | 120.30 |
| 4 | W | 91 | TYR | CB-CG-CD2 | -5.22 | 117.87 | 121.00 |
| 1 | G | 760 | PHE | CB-CG-CD1 | 5.22 | 124.45 | 120.80 |
| 1 | D | 760 | PHE | CB-CG-CD1 | 5.21 | 124.45 | 120.80 |
| 1 | J | 346 | ASP | N-CA-CB | -5.21 | 101.22 | 110.60 |
| 1 | M | 346 | ASP | N-CA-CB | -5.21 | 101.21 | 110.60 |
| 1 | P | 354 | LEU | CB-CG-CD2 | -5.21 | 102.15 | 111.00 |
| 4 | 1 | 62 | ARG | NE-CZ-NH1 | 5.21 | 122.90 | 120.30 |
| 1 | G | 547 | ASP | CB-CG-OD2 | 5.20 | 122.98 | 118.30 |
| 4 | 2 | 335 | ARG | NE-CZ-NH1 | 5.20 | 122.90 | 120.30 |
| 4 | 4 | 337 | TYR | CB-CG-CD1 | -5.20 | 117.88 | 121.00 |
| 1 | A | 170 | ARG | NE-CZ-NH1 | 5.20 | 122.90 | 120.30 |
| 4 | 3 | 62 | ARG | NE-CZ-NH1 | 5.20 | 122.90 | 120.30 |
| 4 | 5 | 147 | ARG | NE-CZ-NH2 | -5.20 | 117.70 | 120.30 |
| 1 | D | 218 | LEU | O-C-N | 5.20 | 131.01 | 122.70 |
| 4 | W | 290 | ARG | CA-C-N | 5.20 | 128.63 | 117.20 |
| 1 | J | 760 | PHE | CB-CG-CD1 | 5.19 | 124.44 | 120.80 |
| 4 | 8 | 337 | TYR | CB-CG-CD1 | -5.19 | 117.89 | 121.00 |
| 1 | A | 218 | LEU | O-C-N | 5.19 | 131.00 | 122.70 |
| 4 | 9 | 290 | ARG | CA-C-N | 5.19 | 128.62 | 117.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1 | P | 760 | PHE | CB-CG-CD1 | 5.19 | 124.43 | 120.80 |
| 1 | A | 346 | ASP | N-CA-CB | -5.19 | 101.27 | 110.60 |
| 1 | G | 555 | TYR | CB-CG-CD1 | 5.18 | 124.11 | 121.00 |
| 1 | D | 346 | ASP | N-CA-CB | -5.18 | 101.27 | 110.60 |
| 4 | 5 | 91 | TYR | CB-CG-CD2 | -5.18 | 117.89 | 121.00 |
| 1 | G | 346 | ASP | N-CA-CB | -5.18 | 101.28 | 110.60 |
| 4 | 7 | 290 | ARG | CA-C-N | 5.18 | 128.59 | 117.20 |
| 4 | 6 | 290 | ARG | CA-C-N | 5.17 | 128.58 | 117.20 |
| 4 | Y | 290 | ARG | CA-C-N | 5.17 | 128.58 | 117.20 |
| 4 | 4 | 290 | ARG | CA-C-N | 5.17 | 128.58 | 117.20 |
| 4 | 7 | 53 | TYR | CB-CG-CD1 | -5.17 | 117.90 | 121.00 |
| 4 | 9 | 53 | TYR | CB-CG-CD1 | -5.17 | 117.90 | 121.00 |
| 4 | W | 335 | ARG | NE-CZ-NH1 | 5.17 | 122.88 | 120.30 |
| 4 | 1 | 335 | ARG | NE-CZ-NH1 | 5.17 | 122.88 | 120.30 |
| 4 | 8 | 290 | ARG | CA-C-N | 5.16 | 128.56 | 117.20 |
| 4 | Z | 290 | ARG | CA-C-N | 5.16 | 128.56 | 117.20 |
| 1 | P | 601 | ASP | CB-CG-OD2 | 5.16 | 122.94 | 118.30 |
| 4 | 1 | 290 | ARG | CA-C-N | 5.16 | 128.55 | 117.20 |
| 4 | 5 | 290 | ARG | CA-C-N | 5.16 | 128.55 | 117.20 |
| 4 | 7 | 337 | TYR | CB-CG-CD1 | -5.16 | 117.91 | 121.00 |
| 4 | W | 53 | TYR | CB-CG-CD1 | -5.16 | 117.91 | 121.00 |
| 1 | A | 90 | ASP | CB-CG-OD1 | -5.16 | 113.66 | 118.30 |
| 1 | P | 346 | ASP | N-CA-CB | -5.16 | 101.32 | 110.60 |
| 4 | 5 | 62 | ARG | NE-CZ-NH1 | 5.16 | 122.88 | 120.30 |
| 4 | 2 | 337 | TYR | CB-CG-CD1 | -5.15 | 117.91 | 121.00 |
| 4 | 4 | 335 | ARG | NE-CZ-NH1 | 5.15 | 122.88 | 120.30 |
| 4 | 3 | 337 | TYR | CB-CG-CD1 | -5.15 | 117.91 | 121.00 |
| 4 | 4 | 91 | TYR | CB-CG-CD2 | -5.15 | 117.91 | 121.00 |
| 4 | X | 337 | TYR | CB-CG-CD1 | -5.15 | 117.91 | 121.00 |
| 4 | 2 | 290 | ARG | CA-C-N | 5.15 | 128.52 | 117.20 |
| 4 | 3 | 290 | ARG | CA-C-N | 5.15 | 128.52 | 117.20 |
| 1 | G | 4 | ASP | CB-CG-OD1 | -5.14 | 113.67 | 118.30 |
| 1 | A | 576 | GLU | CA-CB-CG | -5.14 | 102.09 | 113.40 |
| 4 | 1 | 53 | TYR | CB-CG-CD1 | -5.14 | 117.92 | 121.00 |
| 4 | X | 290 | ARG | CA-C-N | 5.14 | 128.51 | 117.20 |
| 4 | Y | 335 | ARG | NE-CZ-NH1 | 5.14 | 122.87 | 120.30 |
| 1 | G | 170 | ARG | NE-CZ-NH1 | 5.14 | 122.87 | 120.30 |
| 4 | V | 290 | ARG | CA-C-N | 5.14 | 128.50 | 117.20 |
| 4 | 9 | 91 | TYR | CB-CG-CD2 | -5.13 | 117.92 | 121.00 |
| 1 | J | 555 | TYR | CB-CG-CD1 | 5.13 | 124.08 | 121.00 |
| 4 | 7 | 335 | ARG | NE-CZ-NH1 | 5.13 | 122.86 | 120.30 |
| 1 | P | 160 | ASP | CB-CG-OD2 | -5.12 | 113.69 | 118.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1 | A | 628 | GLY | O-C-N | -5.12 | 114.51 | 122.70 |
| 1 | M | 628 | GLY | O-C-N | -5.12 | 114.51 | 122.70 |
| 4 | X | 91 | TYR | CB-CG-CD2 | -5.12 | 117.93 | 121.00 |
| 4 | Y | 62 | ARG | NE-CZ-NH1 | 5.12 | 122.86 | 120.30 |
| 1 | D | 576 | GLU | CA-CB-CG | -5.12 | 102.14 | 113.40 |
| 1 | P | 555 | TYR | CB-CG-CD1 | 5.12 | 124.07 | 121.00 |
| 1 | A | 160 | ASP | CB-CG-OD2 | -5.12 | 113.70 | 118.30 |
| 4 | 3 | 86 | TRP | CG-CD1-NE1 | -5.12 | 104.98 | 110.10 |
| 1 | D | 82 | PRO | N-CA-CB | 5.11 | 109.44 | 103.30 |
| 1 | M | 82 | PRO | N-CA-CB | 5.11 | 109.44 | 103.30 |
| 1 | G | 576 | GLU | CA-CB-CG | -5.11 | 102.15 | 113.40 |
| 4 | W | 337 | TYR | CB-CG-CD1 | -5.11 | 117.93 | 121.00 |
| 1 | D | 218 | LEU | CA-CB-CG | 5.11 | 127.05 | 115.30 |
| 1 | J | 160 | ASP | CB-CG-OD2 | -5.11 | 113.70 | 118.30 |
| 4 | Z | 91 | TYR | CB-CG-CD2 | -5.11 | 117.93 | 121.00 |
| 1 | D | 621 | LEU | CA-CB-CG | -5.11 | 103.55 | 115.30 |
| 1 | J | 301 | ASP | CB-CG-OD2 | 5.11 | 122.90 | 118.30 |
| 4 | 4 | 191 | LYS | CA-C-N | 5.11 | 128.44 | 117.20 |
| 4 | 7 | 191 | LYS | CA-C-N | 5.11 | 128.44 | 117.20 |
| 4 | Z | 62 | ARG | NE-CZ-NH1 | 5.11 | 122.85 | 120.30 |
| 4 | 9 | 62 | ARG | CA-CB-CG | 5.11 | 124.63 | 113.40 |
| 1 | M | 160 | ASP | CB-CG-OD2 | -5.10 | 113.71 | 118.30 |
| 4 | 5 | 335 | ARG | NE-CZ-NH1 | 5.10 | 122.85 | 120.30 |
| 4 | 6 | 62 | ARG | CA-CB-CG | 5.10 | 124.63 | 113.40 |
| 4 | 7 | 91 | TYR | CB-CG-CD2 | -5.10 | 117.94 | 121.00 |
| 4 | Z | 62 | ARG | CA-CB-CG | 5.10 | 124.63 | 113.40 |
| 1 | G | 628 | GLY | O-C-N | -5.10 | 114.54 | 122.70 |
| 1 | J | 739 | ASP | N-CA-CB | 5.10 | 119.78 | 110.60 |
| 4 | W | 62 | ARG | CA-CB-CG | 5.10 | 124.61 | 113.40 |
| 1 | M | 576 | GLU | CA-CB-CG | -5.10 | 102.19 | 113.40 |
| 1 | A | 555 | TYR | CB-CG-CD1 | 5.09 | 124.06 | 121.00 |
| 1 | P | 628 | GLY | O-C-N | -5.09 | 114.55 | 122.70 |
| 4 | V | 62 | ARG | NE-CZ-NH1 | 5.09 | 122.85 | 120.30 |
| 4 | Y | 91 | TYR | CB-CG-CD2 | -5.09 | 117.94 | 121.00 |
| 4 | 3 | 62 | ARG | CA-CB-CG | 5.09 | 124.61 | 113.40 |
| 4 | 1 | 62 | ARG | CA-CB-CG | 5.09 | 124.60 | 113.40 |
| 4 | 8 | 86 | TRP | CG-CD1-NE1 | -5.09 | 105.01 | 110.10 |
| 4 | 3 | 91 | TYR | CB-CG-CD2 | -5.09 | 117.95 | 121.00 |
| 4 | 9 | 191 | LYS | CA-C-N | 5.09 | 128.39 | 117.20 |
| 4 | 8 | 62 | ARG | CA-CB-CG | 5.09 | 124.59 | 113.40 |
| 4 | Y | 62 | ARG | CA-CB-CG | 5.09 | 124.59 | 113.40 |
| 1 | D | 628 | GLY | O-C-N | -5.08 | 114.56 | 122.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 4 | 4 | 62 | ARG | CA-CB-CG | 5.08 | 124.59 | 113.40 |
| 1 | P | 621 | LEU | CA-CB-CG | -5.08 | 103.61 | 115.30 |
| 4 | 4 | 53 | TYR | CB-CG-CD1 | -5.08 | 117.95 | 121.00 |
| 4 | 7 | 62 | ARG | CA-CB-CG | 5.08 | 124.58 | 113.40 |
| 4 | X | 62 | ARG | CA-CB-CG | 5.08 | 124.58 | 113.40 |
| 4 | 2 | 91 | TYR | CB-CG-CD2 | -5.08 | 117.95 | 121.00 |
| 4 | 5 | 62 | ARG | CA-CB-CG | 5.08 | 124.58 | 113.40 |
| 4 | 2 | 62 | ARG | CA-CB-CG | 5.08 | 124.58 | 113.40 |
| 1 | P | 576 | GLU | CA-CB-CG | -5.08 | 102.23 | 113.40 |
| 1 | A | 218 | LEU | CA-CB-CG | 5.08 | 126.98 | 115.30 |
| 4 | V | 53 | TYR | CB-CG-CD1 | -5.08 | 117.95 | 121.00 |
| 1 | J | 218 | LEU | CA-CB-CG | 5.08 | 126.97 | 115.30 |
| 1 | A | 621 | LEU | CA-CB-CG | -5.07 | 103.63 | 115.30 |
| 4 | 6 | 191 | LYS | CA-C-N | 5.07 | 128.36 | 117.20 |
| 1 | D | 160 | ASP | CB-CG-OD2 | -5.07 | 113.73 | 118.30 |
| 1 | J | 621 | LEU | CA-CB-CG | -5.07 | 103.64 | 115.30 |
| 4 | 1 | 191 | LYS | CA-C-N | 5.07 | 128.35 | 117.20 |
| 4 | 6 | 337 | TYR | CB-CG-CD1 | -5.07 | 117.96 | 121.00 |
| 4 | 5 | 86 | TRP | CG-CD1-NE1 | -5.07 | 105.03 | 110.10 |
| 4 | V | 62 | ARG | CA-CB-CG | 5.07 | 124.55 | 113.40 |
| 1 | P | 82 | PRO | N-CA-CB | 5.07 | 109.38 | 103.30 |
| 4 | X | 191 | LYS | CA-C-N | 5.07 | 128.35 | 117.20 |
| 1 | A | 4 | ASP | CB-CG-OD1 | -5.07 | 113.74 | 118.30 |
| 4 | 1 | 86 | TRP | CG-CD1-NE1 | -5.07 | 105.03 | 110.10 |
| 4 | Z | 191 | LYS | CA-C-N | 5.06 | 128.34 | 117.20 |
| 1 | G | 90 | ASP | CB-CG-OD1 | -5.06 | 113.74 | 118.30 |
| 1 | P | 90 | ASP | CB-CG-OD1 | -5.06 | 113.74 | 118.30 |
| 4 | 2 | 191 | LYS | CA-C-N | 5.06 | 128.34 | 117.20 |
| 1 | M | 218 | LEU | CA-CB-CG | 5.06 | 126.94 | 115.30 |
| 4 | Y | 191 | LYS | CA-C-N | 5.06 | 128.33 | 117.20 |
| 1 | G | 621 | LEU | CA-CB-CG | -5.06 | 103.67 | 115.30 |
| 4 | W | 191 | LYS | CA-C-N | 5.06 | 128.33 | 117.20 |
| 1 | P | 218 | LEU | CA-CB-CG | 5.06 | 126.93 | 115.30 |
| 1 | P | 301 | ASP | CB-CG-OD2 | 5.06 | 122.85 | 118.30 |
| 4 | 1 | 337 | TYR | CB-CG-CD1 | -5.06 | 117.97 | 121.00 |
| 1 | D | 555 | TYR | CB-CG-CD1 | 5.05 | 124.03 | 121.00 |
| 1 | J | 576 | GLU | CA-CB-CG | -5.05 | 102.28 | 113.40 |
| 4 | 2 | 86 | TRP | CG-CD1-NE1 | -5.05 | 105.05 | 110.10 |
| 4 | W | 86 | TRP | CG-CD1-NE1 | -5.05 | 105.05 | 110.10 |
| 4 | Y | 337 | TYR | CB-CG-CD1 | -5.05 | 117.97 | 121.00 |
| 1 | J | 628 | GLY | O-C-N | -5.05 | 114.62 | 122.70 |
| 4 | 3 | 191 | LYS | CA-C-N | 5.05 | 128.31 | 117.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 4 | 5 | 191 | LYS | CA-C-N | 5.05 | 128.31 | 117.20 |
| 4 | V | 86 | TRP | CG-CD1-NE1 | -5.05 | 105.05 | 110.10 |
| 1 | A | 235 | ALA | N-CA-CB | -5.05 | 103.04 | 110.10 |
| 1 | M | 301 | ASP | CB-CG-OD2 | 5.05 | 122.84 | 118.30 |
| 4 | 8 | 191 | LYS | CA-C-N | 5.04 | 128.30 | 117.20 |
| 4 | V | 191 | LYS | CA-C-N | 5.04 | 128.29 | 117.20 |
| 1 | J | 90 | ASP | CB-CG-OD1 | -5.04 | 113.76 | 118.30 |
| 1 | D | 739 | ASP | N-CA-CB | 5.04 | 119.67 | 110.60 |
| 1 | G | 160 | ASP | CB-CG-OD2 | -5.04 | 113.77 | 118.30 |
| 1 | M | 739 | ASP | CA-CB-CG | -5.04 | 102.32 | 113.40 |
| 1 | J | 82 | PRO | N-CA-CB | 5.04 | 109.34 | 103.30 |
| 1 | A | 82 | PRO | N-CA-CB | 5.03 | 109.34 | 103.30 |
| 1 | M | 621 | LEU | CA-CB-CG | -5.03 | 103.72 | 115.30 |
| 1 | A | 739 | ASP | CA-CB-CG | -5.03 | 102.33 | 113.40 |
| 1 | G | 218 | LEU | CA-CB-CG | 5.03 | 126.87 | 115.30 |
| 1 | D | 463 | ASP | CB-CG-OD1 | 5.03 | 122.83 | 118.30 |
| 4 | 8 | 91 | TYR | CB-CG-CD2 | -5.03 | 117.98 | 121.00 |
| 1 | P | 235 | ALA | N-CA-CB | -5.02 | 103.07 | 110.10 |
| 1 | G | 739 | ASP | CA-CB-CG | -5.02 | 102.35 | 113.40 |
| 4 | 5 | 53 | TYR | CB-CG-CD1 | -5.02 | 117.99 | 121.00 |
| 4 | Z | 86 | TRP | CG-CD1-NE1 | -5.02 | 105.08 | 110.10 |
| 2 | H | 129 | THR | N-CA-CB | 5.02 | 119.83 | 110.30 |
| 1 | D | 90 | ASP | CB-CG-OD1 | -5.01 | 113.79 | 118.30 |
| 1 | P | 739 | ASP | N-CA-CB | 5.01 | 119.62 | 110.60 |
| 1 | J | 235 | ALA | N-CA-CB | -5.01 | 103.09 | 110.10 |
| 4 | 9 | 86 | TRP | CG-CD1-NE1 | -5.01 | 105.09 | 110.10 |
| 4 | 6 | 62 | ARG | NE-CZ-NH1 | 5.01 | 122.80 | 120.30 |
| 1 | P | 274 | ARG | NE-CZ-NH2 | -5.00 | 117.80 | 120.30 |
| 4 | 2 | 53 | TYR | CB-CG-CD1 | -5.00 | 118.00 | 121.00 |
| 4 | 3 | 335 | ARG | NE-CZ-NH1 | 5.00 | 122.80 | 120.30 |

All (6) chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 1 | A | 648 | THR | CB |
| 1 | D | 648 | THR | CB |
| 1 | G | 648 | THR | CB |
| 1 | J | 648 | THR | CB |
| 1 | M | 648 | THR | CB |
| 1 | P | 648 | THR | CB |

All (72) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|-------------------|
| 4 | 1 | 62 | ARG | Sidechain |
| 4 | 2 | 62 | ARG | Sidechain |
| 4 | 3 | 62 | ARG | Sidechain |
| 4 | 4 | 62 | ARG | Sidechain |
| 4 | 5 | 62 | ARG | Sidechain |
| 4 | 6 | 62 | ARG | Sidechain |
| 4 | 7 | 62 | ARG | Sidechain |
| 4 | 8 | 62 | ARG | Sidechain |
| 4 | 9 | 62 | ARG | Sidechain |
| 1 | A | 623 | PHE | Sidechain |
| 1 | A | 637 | LYS | Mainchain |
| 1 | A | 649 | VAL | Mainchain |
| 1 | A | 98 | HIS | Mainchain |
| 2 | B | 150 | TYR | Sidechain |
| 2 | B | 155 | TYR | Mainchain |
| 2 | B | 22 | THR | Mainchain |
| 3 | C | 75 | ALA | Mainchain |
| 3 | C | 85 | GLU | Mainchain |
| 1 | D | 623 | PHE | Sidechain |
| 1 | D | 637 | LYS | Mainchain |
| 1 | D | 649 | VAL | Mainchain |
| 1 | D | 98 | HIS | Mainchain |
| 2 | E | 150 | TYR | Sidechain |
| 2 | E | 155 | TYR | Mainchain |
| 2 | E | 22 | THR | Mainchain |
| 3 | F | 75 | ALA | Mainchain |
| 3 | F | 85 | GLU | Mainchain |
| 1 | G | 623 | PHE | Sidechain |
| 1 | G | 637 | LYS | Mainchain |
| 1 | G | 649 | VAL | Mainchain |
| 1 | G | 98 | HIS | Mainchain |
| 2 | H | 150 | TYR | Sidechain |
| 2 | H | 155 | TYR | Mainchain |
| 2 | H | 22 | THR | Mainchain |
| 3 | I | 75 | ALA | Mainchain |
| 3 | I | 85 | GLU | Mainchain |
| 1 | J | 623 | PHE | Sidechain |
| 1 | J | 637 | LYS | Mainchain |
| 1 | J | 649 | VAL | Mainchain |
| 1 | J | 709 | LYS | Peptide,Mainchain |
| 1 | J | 98 | HIS | Mainchain |
| 2 | K | 150 | TYR | Sidechain |
| 2 | K | 155 | TYR | Mainchain |

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| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|-------------------|
| 2 | K | 22 | THR | Mainchain |
| 3 | L | 75 | ALA | Mainchain |
| 3 | L | 85 | GLU | Mainchain |
| 1 | M | 623 | PHE | Sidechain |
| 1 | M | 637 | LYS | Mainchain |
| 1 | M | 649 | VAL | Mainchain |
| 1 | M | 98 | HIS | Mainchain |
| 2 | N | 150 | TYR | Sidechain |
| 2 | N | 155 | TYR | Mainchain |
| 2 | N | 22 | THR | Mainchain |
| 3 | O | 75 | ALA | Mainchain |
| 3 | O | 85 | GLU | Mainchain |
| 1 | P | 623 | PHE | Sidechain |
| 1 | P | 637 | LYS | Mainchain |
| 1 | P | 649 | VAL | Mainchain |
| 1 | P | 785 | GLU | Peptide,Mainchain |
| 1 | P | 98 | HIS | Mainchain |
| 2 | Q | 150 | TYR | Sidechain |
| 2 | Q | 155 | TYR | Mainchain |
| 2 | Q | 22 | THR | Mainchain |
| 3 | R | 75 | ALA | Mainchain |
| 3 | R | 85 | GLU | Mainchain |
| 4 | V | 62 | ARG | Sidechain |
| 4 | W | 62 | ARG | Sidechain |
| 4 | X | 62 | ARG | Sidechain |
| 4 | Y | 62 | ARG | Sidechain |
| 4 | Z | 62 | ARG | Sidechain |

5.2 Too-close contacts [i](#)

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | A | 6797 | 0 | 6756 | 1513 | 0 |
| 1 | D | 6797 | 0 | 6756 | 1419 | 0 |
| 1 | G | 6797 | 0 | 6764 | 1560 | 0 |
| 1 | J | 6797 | 0 | 6755 | 1414 | 0 |
| 1 | M | 6797 | 0 | 6769 | 1360 | 0 |
| 1 | P | 6797 | 0 | 6766 | 1424 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 2 | B | 1127 | 0 | 1085 | 248 | 0 |
| 2 | E | 1127 | 0 | 1086 | 266 | 0 |
| 2 | H | 1127 | 0 | 1088 | 300 | 0 |
| 2 | K | 1127 | 0 | 1088 | 271 | 0 |
| 2 | N | 1127 | 0 | 1088 | 248 | 0 |
| 2 | Q | 1127 | 0 | 1088 | 250 | 0 |
| 3 | C | 1123 | 0 | 1083 | 194 | 0 |
| 3 | F | 1123 | 0 | 1083 | 173 | 0 |
| 3 | I | 1123 | 0 | 1083 | 185 | 0 |
| 3 | L | 1123 | 0 | 1083 | 158 | 0 |
| 3 | O | 1123 | 0 | 1084 | 183 | 0 |
| 3 | R | 1123 | 0 | 1084 | 189 | 0 |
| 4 | 1 | 2906 | 0 | 2856 | 418 | 0 |
| 4 | 2 | 2906 | 0 | 2860 | 207 | 0 |
| 4 | 3 | 2906 | 0 | 2863 | 169 | 0 |
| 4 | 4 | 2906 | 0 | 2863 | 179 | 0 |
| 4 | 5 | 2906 | 0 | 2865 | 94 | 0 |
| 4 | 6 | 2906 | 0 | 2865 | 99 | 0 |
| 4 | 7 | 2906 | 0 | 2866 | 74 | 0 |
| 4 | 8 | 2906 | 0 | 2857 | 315 | 0 |
| 4 | 9 | 2906 | 0 | 2855 | 344 | 0 |
| 4 | V | 2906 | 0 | 2851 | 379 | 0 |
| 4 | W | 2906 | 0 | 2851 | 395 | 0 |
| 4 | X | 2906 | 0 | 2863 | 179 | 0 |
| 4 | Y | 2906 | 0 | 2863 | 193 | 0 |
| 4 | Z | 2906 | 0 | 2855 | 380 | 0 |
| All | All | 94966 | 0 | 93622 | 11072 | 0 |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 59.

All (11072) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:N:144:VAL:HG13 | 2:N:153:ILE:CD1 | 1.22 | 1.68 |
| 1:J:797:PHE:CE1 | 3:L:146:ILE:HG23 | 1.24 | 1.68 |
| 1:A:831:TRP:CZ3 | 2:B:50:THR:HG21 | 1.27 | 1.67 |
| 1:A:753:VAL:HG12 | 1:A:775:LEU:CG | 1.22 | 1.66 |
| 4:2:287:ILE:CG2 | 4:4:202:THR:HB | 1.23 | 1.66 |
| 1:M:795:ARG:HH21 | 3:O:116:GLU:CB | 1.06 | 1.64 |
| 1:M:836:PHE:CE1 | 2:N:159:HIS:HA | 1.34 | 1.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:E:144:VAL:HG13 | 2:E:153:ILE:CG1 | 1.18 | 1.63 |
| 1:G:757:GLN:HG3 | 1:G:776:GLU:CG | 1.18 | 1.62 |
| 2:B:144:VAL:HG13 | 2:B:153:ILE:CG1 | 1.17 | 1.61 |
| 1:G:757:GLN:CG | 1:G:776:GLU:HG2 | 1.14 | 1.61 |
| 1:G:831:TRP:CH2 | 2:H:47:LEU:HD21 | 1.31 | 1.61 |
| 1:G:538:GLU:CA | 4:V:349:LEU:CD1 | 1.79 | 1.61 |
| 2:E:144:VAL:HG13 | 2:E:153:ILE:CD1 | 1.21 | 1.60 |
| 1:M:725:ARG:HE | 1:M:733:PRO:CB | 1.09 | 1.60 |
| 1:A:538:GLU:CA | 4:8:349:LEU:CD1 | 1.78 | 1.60 |
| 2:H:144:VAL:HG13 | 2:H:153:ILE:CD1 | 1.22 | 1.60 |
| 4:2:287:ILE:HG23 | 4:4:202:THR:CB | 1.26 | 1.60 |
| 1:D:797:PHE:CE2 | 3:F:126:LEU:HD22 | 1.28 | 1.59 |
| 2:Q:144:VAL:HG13 | 2:Q:153:ILE:CD1 | 1.22 | 1.59 |
| 1:A:505:MLY:CB | 1:A:762:HIS:HD2 | 1.06 | 1.59 |
| 2:N:144:VAL:HG13 | 2:N:153:ILE:CG1 | 1.17 | 1.59 |
| 2:Q:111:SER:HB2 | 2:Q:148:VAL:C | 1.23 | 1.59 |
| 1:D:538:GLU:CA | 4:9:349:LEU:CD1 | 1.78 | 1.59 |
| 1:D:725:ARG:HE | 1:D:733:PRO:CB | 1.09 | 1.59 |
| 1:J:538:GLU:CA | 4:W:349:LEU:CD1 | 1.79 | 1.59 |
| 2:K:144:VAL:HG13 | 2:K:153:ILE:CG1 | 1.17 | 1.59 |
| 1:P:783:LEU:HG | 1:P:786:ILE:CD1 | 1.28 | 1.58 |
| 1:G:725:ARG:HE | 1:G:733:PRO:CB | 1.09 | 1.58 |
| 1:M:538:GLU:CA | 4:Z:349:LEU:CD1 | 1.79 | 1.58 |
| 1:J:818:TYR:CE1 | 2:K:127:ARG:NH2 | 1.72 | 1.58 |
| 1:P:538:GLU:CA | 4:1:349:LEU:CD1 | 1.79 | 1.58 |
| 2:B:144:VAL:HG13 | 2:B:153:ILE:CD1 | 1.22 | 1.57 |
| 2:K:144:VAL:HG13 | 2:K:153:ILE:CD1 | 1.22 | 1.57 |
| 1:M:206:LYS:CD | 1:M:217:THR:HG23 | 1.28 | 1.57 |
| 1:A:725:ARG:HE | 1:A:733:PRO:CB | 1.09 | 1.57 |
| 1:P:795:ARG:HH21 | 3:R:116:GLU:CB | 1.08 | 1.57 |
| 2:Q:144:VAL:HG13 | 2:Q:153:ILE:CG1 | 1.17 | 1.57 |
| 1:D:834:LEU:HD11 | 2:E:54:MET:CG | 1.22 | 1.57 |
| 1:J:725:ARG:HE | 1:J:733:PRO:CB | 1.09 | 1.57 |
| 4:2:287:ILE:CG1 | 4:4:203:THR:N | 1.67 | 1.57 |
| 1:P:725:ARG:HE | 1:P:733:PRO:CB | 1.09 | 1.56 |
| 1:A:795:ARG:HB3 | 3:C:35:ARG:CZ | 1.34 | 1.56 |
| 1:G:84:MLY:CG | 1:G:723:ARG:HD2 | 1.10 | 1.56 |
| 1:J:736:GLN:HA | 1:J:743:ALA:CB | 1.34 | 1.56 |
| 1:J:797:PHE:CZ | 3:L:146:ILE:CD1 | 1.82 | 1.56 |
| 1:P:206:LYS:CD | 1:P:217:THR:HG23 | 1.28 | 1.56 |
| 1:D:798:LEU:CD1 | 3:F:126:LEU:HD11 | 1.22 | 1.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:H:144:VAL:HG13 | 2:H:153:ILE:CG1 | 1.17 | 1.55 |
| 1:J:818:TYR:CZ | 2:K:127:ARG:NH2 | 1.69 | 1.55 |
| 1:P:836:PHE:CE1 | 2:Q:159:HIS:HA | 1.36 | 1.55 |
| 1:D:834:LEU:CD1 | 2:E:54:MET:HG3 | 1.13 | 1.55 |
| 1:A:206:LYS:CD | 1:A:217:THR:HG23 | 1.28 | 1.55 |
| 1:A:736:GLN:HA | 1:A:743:ALA:CB | 1.35 | 1.55 |
| 1:P:641:LYS:HG3 | 1:P:647:GLN:CG | 1.36 | 1.55 |
| 1:A:530:MET:HG2 | 4:8:354:GLN:CB | 1.35 | 1.55 |
| 1:D:641:LYS:HG3 | 1:D:647:GLN:CG | 1.36 | 1.55 |
| 1:G:206:LYS:CD | 1:G:217:THR:HG23 | 1.28 | 1.55 |
| 1:J:641:LYS:HG3 | 1:J:647:GLN:CG | 1.37 | 1.55 |
| 1:M:530:MET:HG2 | 4:Z:354:GLN:CB | 1.36 | 1.55 |
| 1:J:798:LEU:HD11 | 3:L:126:LEU:CD1 | 1.37 | 1.55 |
| 1:D:798:LEU:HD11 | 3:F:126:LEU:CD1 | 1.31 | 1.54 |
| 1:D:206:LYS:CD | 1:D:217:THR:HG23 | 1.28 | 1.54 |
| 1:D:799:MET:SD | 3:F:32:ASP:HB3 | 1.46 | 1.54 |
| 1:J:838:ILE:HD11 | 2:K:54:MET:CE | 1.31 | 1.54 |
| 1:M:641:LYS:HG3 | 1:M:647:GLN:CG | 1.36 | 1.54 |
| 4:1:243:PRO:CB | 4:Y:291:LYS:HE3 | 1.33 | 1.53 |
| 1:J:206:LYS:CD | 1:J:217:THR:HG23 | 1.28 | 1.53 |
| 2:E:111:SER:HB2 | 2:E:148:VAL:C | 1.23 | 1.53 |
| 1:D:834:LEU:CG | 2:E:54:MET:HG3 | 1.34 | 1.53 |
| 1:A:834:LEU:HD21 | 2:B:54:MET:CE | 1.09 | 1.52 |
| 1:D:792:ALA:CB | 3:F:42:THR:HG22 | 1.39 | 1.52 |
| 2:K:111:SER:HB2 | 2:K:148:VAL:C | 1.23 | 1.52 |
| 2:Q:117:LEU:HD12 | 2:Q:147:ASN:CG | 1.30 | 1.52 |
| 1:A:799:MET:SD | 3:C:32:ASP:HB3 | 1.47 | 1.52 |
| 1:G:792:ALA:HB2 | 3:I:42:THR:CG2 | 1.04 | 1.52 |
| 1:J:530:MET:HG2 | 4:W:354:GLN:CB | 1.36 | 1.52 |
| 1:D:792:ALA:HB2 | 3:F:42:THR:CG2 | 1.33 | 1.52 |
| 1:D:838:ILE:HD12 | 2:E:54:MET:SD | 1.50 | 1.52 |
| 1:G:530:MET:HG2 | 4:V:354:GLN:CB | 1.36 | 1.52 |
| 1:M:736:GLN:HA | 1:M:743:ALA:CB | 1.35 | 1.52 |
| 1:P:838:ILE:HD11 | 2:Q:54:MET:CE | 1.39 | 1.52 |
| 4:1:247:VAL:CG2 | 4:Y:324:THR:HG22 | 1.35 | 1.52 |
| 1:A:641:LYS:HG3 | 1:A:647:GLN:CG | 1.37 | 1.52 |
| 1:G:792:ALA:CB | 3:I:42:THR:HG22 | 1.10 | 1.52 |
| 1:J:206:LYS:HD3 | 1:J:217:THR:CG2 | 1.40 | 1.52 |
| 1:J:505:MLY:HD2 | 1:J:762:HIS:CE1 | 1.44 | 1.52 |
| 2:N:111:SER:HB2 | 2:N:148:VAL:C | 1.22 | 1.52 |
| 1:G:736:GLN:HA | 1:G:743:ALA:CB | 1.35 | 1.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:P:818:TYR:CE1 | 2:Q:127:ARG:NH2 | 1.78 | 1.51 |
| 1:D:797:PHE:CD1 | 3:F:146:ILE:HG23 | 1.44 | 1.51 |
| 2:K:117:LEU:HD12 | 2:K:147:ASN:CG | 1.30 | 1.51 |
| 2:B:111:SER:HB2 | 2:B:148:VAL:C | 1.23 | 1.51 |
| 1:D:736:GLN:HA | 1:D:743:ALA:CB | 1.35 | 1.51 |
| 1:P:530:MET:HG2 | 4:1:354:GLN:CB | 1.36 | 1.51 |
| 1:D:206:LYS:HD3 | 1:D:217:THR:CG2 | 1.40 | 1.50 |
| 1:D:530:MET:HG2 | 4:9:354:GLN:CB | 1.35 | 1.50 |
| 1:A:206:LYS:HD3 | 1:A:217:THR:CG2 | 1.40 | 1.50 |
| 2:H:111:SER:HB2 | 2:H:148:VAL:C | 1.23 | 1.50 |
| 1:P:736:GLN:HA | 1:P:743:ALA:CB | 1.35 | 1.50 |
| 4:3:290:ARG:NH2 | 4:5:202:THR:CG2 | 1.71 | 1.50 |
| 1:G:791:GLN:NE2 | 3:I:115:GLY:HA3 | 1.18 | 1.50 |
| 2:N:117:LEU:HD12 | 2:N:147:ASN:CG | 1.30 | 1.50 |
| 1:P:769:ALA:C | 1:P:771:LEU:H | 1.13 | 1.49 |
| 1:P:206:LYS:HD3 | 1:P:217:THR:CG2 | 1.40 | 1.49 |
| 1:A:721:LYS:HG3 | 1:A:736:GLN:CG | 1.15 | 1.49 |
| 2:B:117:LEU:HD12 | 2:B:147:ASN:CB | 1.42 | 1.49 |
| 1:M:838:ILE:HD11 | 2:N:54:MET:CE | 1.40 | 1.49 |
| 4:W:324:THR:CG2 | 4:Y:247:VAL:H | 1.25 | 1.49 |
| 4:X:287:ILE:CB | 4:Z:205:GLU:HG3 | 1.23 | 1.49 |
| 1:G:797:PHE:CE2 | 3:I:126:LEU:HD22 | 1.46 | 1.49 |
| 1:J:84:MLY:HH11 | 1:J:720:PHE:CD1 | 1.46 | 1.49 |
| 1:M:206:LYS:HD3 | 1:M:217:THR:CG2 | 1.40 | 1.49 |
| 2:E:117:LEU:HD12 | 2:E:147:ASN:CG | 1.30 | 1.48 |
| 2:E:117:LEU:HD12 | 2:E:147:ASN:CB | 1.41 | 1.48 |
| 1:G:556:ASP:CG | 4:X:47:MET:CE | 1.76 | 1.48 |
| 1:G:641:LYS:HG3 | 1:G:647:GLN:CG | 1.37 | 1.48 |
| 1:P:641:LYS:CG | 1:P:647:GLN:NE2 | 1.77 | 1.48 |
| 1:J:641:LYS:CG | 1:J:647:GLN:NE2 | 1.77 | 1.48 |
| 1:P:798:LEU:HD11 | 3:R:126:LEU:CD2 | 1.41 | 1.48 |
| 1:A:753:VAL:CG1 | 1:A:775:LEU:HG | 1.38 | 1.48 |
| 1:J:797:PHE:CZ | 3:L:146:ILE:HD12 | 0.96 | 1.48 |
| 1:A:831:TRP:CZ3 | 2:B:50:THR:CG2 | 1.92 | 1.48 |
| 1:G:721:LYS:HG3 | 1:G:736:GLN:CG | 1.15 | 1.48 |
| 1:M:818:TYR:CE1 | 2:N:127:ARG:NH2 | 1.82 | 1.48 |
| 2:N:117:LEU:HD12 | 2:N:147:ASN:CB | 1.41 | 1.48 |
| 4:2:287:ILE:HG12 | 4:4:202:THR:C | 1.29 | 1.48 |
| 1:M:721:LYS:HG3 | 1:M:736:GLN:CG | 1.15 | 1.47 |
| 1:A:505:MLY:HB3 | 1:A:762:HIS:CD2 | 1.46 | 1.47 |
| 1:A:831:TRP:CH2 | 2:B:50:THR:HB | 1.49 | 1.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:641:LYS:CG | 1:D:647:GLN:NE2 | 1.77 | 1.47 |
| 1:D:834:LEU:CD1 | 2:E:54:MET:CG | 1.80 | 1.47 |
| 2:H:117:LEU:HD12 | 2:H:147:ASN:CB | 1.42 | 1.47 |
| 1:P:795:ARG:NH2 | 3:R:116:GLU:HB3 | 1.23 | 1.47 |
| 1:P:821:ARG:NH2 | 2:Q:127:ARG:HG2 | 1.16 | 1.47 |
| 1:G:206:LYS:HD3 | 1:G:217:THR:CG2 | 1.40 | 1.47 |
| 1:G:755:HIS:H | 1:G:779:ARG:CZ | 1.27 | 1.47 |
| 1:G:831:TRP:CH2 | 2:H:47:LEU:CD2 | 1.98 | 1.47 |
| 1:G:84:MLY:HB3 | 1:G:723:ARG:NE | 1.28 | 1.46 |
| 2:Q:117:LEU:HD12 | 2:Q:147:ASN:CB | 1.41 | 1.46 |
| 1:G:641:LYS:CG | 1:G:647:GLN:NE2 | 1.77 | 1.46 |
| 1:D:818:TYR:HB2 | 2:E:90:GLY:CA | 1.46 | 1.46 |
| 1:A:641:LYS:CG | 1:A:647:GLN:NE2 | 1.76 | 1.46 |
| 1:J:84:MLY:CH2 | 1:J:720:PHE:HA | 1.46 | 1.46 |
| 2:K:117:LEU:HD12 | 2:K:147:ASN:CB | 1.41 | 1.46 |
| 1:G:505:MLY:HH23 | 1:G:762:HIS:NE2 | 1.16 | 1.45 |
| 1:G:538:GLU:C | 4:V:349:LEU:CD1 | 1.84 | 1.45 |
| 1:G:641:LYS:CD | 1:G:647:GLN:CD | 1.85 | 1.45 |
| 1:P:641:LYS:CD | 1:P:647:GLN:CD | 1.85 | 1.45 |
| 2:B:117:LEU:HD12 | 2:B:147:ASN:CG | 1.30 | 1.45 |
| 1:G:818:TYR:CZ | 2:H:127:ARG:NH2 | 1.84 | 1.45 |
| 1:M:799:MET:SD | 3:O:32:ASP:HB3 | 1.55 | 1.45 |
| 1:A:797:PHE:CE1 | 3:C:146:ILE:HA | 1.49 | 1.45 |
| 1:M:641:LYS:CD | 1:M:647:GLN:CD | 1.85 | 1.45 |
| 1:M:538:GLU:C | 4:Z:349:LEU:CD1 | 1.84 | 1.45 |
| 1:A:819:ASN:ND2 | 2:B:91:ALA:CA | 1.77 | 1.45 |
| 1:J:538:GLU:C | 4:W:349:LEU:CD1 | 1.84 | 1.44 |
| 1:P:505:MLY:CH2 | 1:P:762:HIS:HD1 | 1.23 | 1.44 |
| 4:X:287:ILE:HB | 4:Z:205:GLU:CG | 0.99 | 1.44 |
| 1:G:795:ARG:NE | 3:I:116:GLU:HB3 | 1.32 | 1.44 |
| 1:M:798:LEU:CD1 | 3:O:126:LEU:HD21 | 1.48 | 1.44 |
| 1:D:538:GLU:C | 4:9:349:LEU:CD1 | 1.84 | 1.44 |
| 1:D:641:LYS:CD | 1:D:647:GLN:CD | 1.85 | 1.44 |
| 1:D:795:ARG:HB3 | 3:F:35:ARG:NH1 | 1.30 | 1.44 |
| 1:M:641:LYS:CG | 1:M:647:GLN:NE2 | 1.77 | 1.44 |
| 1:P:819:ASN:CG | 2:Q:92:ASP:HB2 | 1.28 | 1.44 |
| 1:P:546:THR:CG2 | 4:3:46:GLY:O | 1.66 | 1.43 |
| 1:A:641:LYS:CD | 1:A:647:GLN:CD | 1.85 | 1.43 |
| 1:A:813:ILE:CG2 | 2:B:127:ARG:HD2 | 1.45 | 1.43 |
| 1:D:799:MET:SD | 3:F:32:ASP:CB | 2.04 | 1.43 |
| 2:H:117:LEU:HD12 | 2:H:147:ASN:CG | 1.30 | 1.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:641:LYS:CD | 1:J:647:GLN:CD | 1.85 | 1.43 |
| 1:G:819:ASN:ND2 | 2:H:92:ASP:HB2 | 1.20 | 1.43 |
| 1:P:721:LYS:HG3 | 1:P:736:GLN:CG | 1.15 | 1.43 |
| 1:A:149:GLN:CG | 1:A:719:ASP:OD1 | 1.65 | 1.43 |
| 1:G:567:LYS:NZ | 4:X:92:ASN:HD22 | 1.17 | 1.43 |
| 1:J:817:GLN:HG2 | 2:K:127:ARG:CB | 1.49 | 1.43 |
| 1:M:798:LEU:HD11 | 3:O:126:LEU:CD2 | 1.46 | 1.42 |
| 1:P:538:GLU:C | 4:1:349:LEU:CD1 | 1.84 | 1.42 |
| 1:P:736:GLN:N | 1:P:743:ALA:HB1 | 1.35 | 1.42 |
| 1:P:795:ARG:HG2 | 3:R:118:MET:CE | 1.50 | 1.42 |
| 1:A:831:TRP:HH2 | 2:B:50:THR:CB | 1.28 | 1.42 |
| 4:2:203:THR:CG2 | 4:Z:287:ILE:HB | 1.48 | 1.41 |
| 1:J:798:LEU:CD1 | 3:L:126:LEU:HD11 | 1.50 | 1.41 |
| 4:2:287:ILE:HG12 | 4:4:202:THR:CA | 1.51 | 1.41 |
| 1:D:736:GLN:N | 1:D:743:ALA:HB1 | 1.35 | 1.41 |
| 1:G:733:PRO:O | 1:G:737:PHE:CD1 | 1.74 | 1.41 |
| 1:A:819:ASN:HD21 | 2:B:91:ALA:C | 0.88 | 1.41 |
| 2:E:144:VAL:CG1 | 2:E:153:ILE:CD1 | 1.99 | 1.41 |
| 2:N:144:VAL:CG1 | 2:N:153:ILE:CD1 | 1.99 | 1.41 |
| 1:P:97:LEU:CD2 | 1:P:712:PRO:HB3 | 1.50 | 1.41 |
| 1:A:733:PRO:O | 1:A:737:PHE:CD1 | 1.73 | 1.40 |
| 1:D:838:ILE:CD1 | 2:E:54:MET:CE | 1.96 | 1.40 |
| 1:M:795:ARG:NH2 | 3:O:116:GLU:HB3 | 1.25 | 1.40 |
| 1:A:149:GLN:NE2 | 1:A:718:ALA:HB3 | 1.34 | 1.40 |
| 1:M:821:ARG:NH2 | 2:N:127:ARG:HG2 | 1.15 | 1.40 |
| 1:G:530:MET:CG | 4:V:354:GLN:HB2 | 1.51 | 1.40 |
| 1:P:537:GLU:O | 4:1:349:LEU:CD1 | 1.70 | 1.40 |
| 1:A:538:GLU:C | 4:8:349:LEU:CD1 | 1.84 | 1.40 |
| 1:A:795:ARG:NH2 | 3:C:116:GLU:CD | 1.70 | 1.40 |
| 1:D:818:TYR:CB | 2:E:90:GLY:HA3 | 1.49 | 1.40 |
| 1:J:537:GLU:O | 4:W:349:LEU:CD1 | 1.70 | 1.40 |
| 1:J:733:PRO:O | 1:J:737:PHE:CD1 | 1.73 | 1.40 |
| 1:P:546:THR:OG1 | 4:3:46:GLY:CA | 1.64 | 1.40 |
| 2:Q:144:VAL:CG1 | 2:Q:153:ILE:CD1 | 1.99 | 1.40 |
| 1:A:149:GLN:OE1 | 1:A:716:LEU:CD2 | 1.69 | 1.40 |
| 1:G:218:LEU:CB | 1:G:221:GLN:HG3 | 1.51 | 1.40 |
| 1:J:721:LYS:CG | 1:J:736:GLN:CG | 1.97 | 1.40 |
| 1:A:149:GLN:HB3 | 1:A:719:ASP:N | 1.33 | 1.39 |
| 1:A:218:LEU:CB | 1:A:221:GLN:HG3 | 1.52 | 1.39 |
| 1:A:736:GLN:CA | 1:A:743:ALA:CB | 2.00 | 1.39 |
| 1:D:797:PHE:HE2 | 3:F:126:LEU:CD2 | 1.33 | 1.39 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:J:84:MLY:HH11 | 1:J:720:PHE:CE1 | 1.56 | 1.39 |
| 4:4:288:ASP:CG | 4:6:203:THR:CG2 | 1.90 | 1.39 |
| 1:A:537:GLU:O | 4:8:349:LEU:CD1 | 1.70 | 1.39 |
| 1:D:733:PRO:O | 1:D:737:PHE:CD1 | 1.74 | 1.39 |
| 1:G:736:GLN:N | 1:G:743:ALA:HB1 | 1.34 | 1.39 |
| 4:2:287:ILE:CG2 | 4:4:202:THR:CB | 1.87 | 1.39 |
| 1:A:530:MET:CG | 4:8:354:GLN:HB2 | 1.50 | 1.39 |
| 2:B:144:VAL:CG1 | 2:B:153:ILE:CD1 | 1.99 | 1.39 |
| 1:D:202:SER:HA | 1:D:207:LYS:CE | 1.51 | 1.39 |
| 1:D:530:MET:CG | 4:9:354:GLN:HB2 | 1.50 | 1.39 |
| 1:G:84:MLY:HG2 | 1:G:723:ARG:CD | 1.49 | 1.39 |
| 1:M:733:PRO:O | 1:M:737:PHE:CD1 | 1.73 | 1.39 |
| 1:J:202:SER:HA | 1:J:207:LYS:CE | 1.51 | 1.39 |
| 1:J:821:ARG:NH2 | 2:K:127:ARG:HG2 | 1.37 | 1.39 |
| 1:M:537:GLU:O | 4:Z:349:LEU:CD1 | 1.70 | 1.39 |
| 1:J:218:LEU:CB | 1:J:221:GLN:HG3 | 1.52 | 1.39 |
| 1:P:733:PRO:O | 1:P:737:PHE:CD1 | 1.73 | 1.39 |
| 1:A:202:SER:HA | 1:A:207:LYS:CE | 1.51 | 1.38 |
| 1:A:736:GLN:CA | 1:A:743:ALA:HB1 | 1.53 | 1.38 |
| 1:J:736:GLN:CA | 1:J:743:ALA:CB | 2.00 | 1.38 |
| 1:M:202:SER:HA | 1:M:207:LYS:CE | 1.51 | 1.38 |
| 1:P:530:MET:CG | 4:1:354:GLN:HB2 | 1.51 | 1.38 |
| 1:D:736:GLN:CA | 1:D:743:ALA:CB | 2.00 | 1.38 |
| 1:G:736:GLN:CA | 1:G:743:ALA:CB | 2.00 | 1.38 |
| 1:J:534:SER:O | 4:W:351:THR:CG2 | 1.64 | 1.38 |
| 1:A:795:ARG:HB3 | 3:C:35:ARG:NH1 | 1.34 | 1.38 |
| 2:B:144:VAL:CG1 | 2:B:153:ILE:HG12 | 1.54 | 1.38 |
| 1:D:736:GLN:CA | 1:D:743:ALA:HB1 | 1.53 | 1.38 |
| 1:G:736:GLN:CA | 1:G:743:ALA:HB1 | 1.53 | 1.38 |
| 1:M:736:GLN:CA | 1:M:743:ALA:HB1 | 1.53 | 1.38 |
| 1:A:799:MET:SD | 3:C:32:ASP:CB | 2.11 | 1.38 |
| 1:D:218:LEU:CB | 1:D:221:GLN:HG3 | 1.52 | 1.38 |
| 1:G:202:SER:HA | 1:G:207:LYS:CE | 1.51 | 1.38 |
| 1:J:797:PHE:CD1 | 3:L:146:ILE:HG23 | 1.57 | 1.38 |
| 1:P:798:LEU:CD1 | 3:R:126:LEU:HD21 | 1.53 | 1.38 |
| 1:A:797:PHE:CZ | 3:C:146:ILE:HD13 | 1.57 | 1.38 |
| 1:A:819:ASN:ND2 | 2:B:90:GLY:O | 1.57 | 1.38 |
| 1:A:834:LEU:CD2 | 2:B:54:MET:CE | 1.96 | 1.38 |
| 1:G:537:GLU:O | 4:V:349:LEU:CD1 | 1.71 | 1.38 |
| 1:G:819:ASN:CA | 2:H:90:GLY:O | 1.70 | 1.38 |
| 1:P:218:LEU:CB | 1:P:221:GLN:HG3 | 1.52 | 1.38 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:K:144:VAL:CG1 | 2:K:153:ILE:CD1 | 1.99 | 1.37 |
| 4:2:202:THR:CG2 | 4:Z:290:ARG:HH21 | 1.34 | 1.38 |
| 1:J:530:MET:CG | 4:W:354:GLN:HB2 | 1.51 | 1.37 |
| 1:P:736:GLN:CA | 1:P:743:ALA:CB | 2.00 | 1.37 |
| 1:P:783:LEU:CG | 1:P:786:ILE:HD11 | 1.53 | 1.37 |
| 1:P:819:ASN:ND2 | 2:Q:92:ASP:HB2 | 1.39 | 1.37 |
| 1:D:641:LYS:HG3 | 1:D:647:GLN:CD | 1.45 | 1.37 |
| 1:M:218:LEU:CB | 1:M:221:GLN:HG3 | 1.52 | 1.37 |
| 1:M:530:MET:CG | 4:Z:354:GLN:HB2 | 1.51 | 1.37 |
| 1:P:534:SER:O | 4:1:351:THR:CG2 | 1.64 | 1.37 |
| 4:1:287:ILE:HB | 4:3:203:THR:CG2 | 1.54 | 1.37 |
| 1:D:831:TRP:CZ3 | 2:E:34:ILE:HG23 | 1.57 | 1.37 |
| 2:Q:144:VAL:CG1 | 2:Q:153:ILE:HG12 | 1.54 | 1.37 |
| 4:2:203:THR:HG22 | 4:Z:287:ILE:CB | 1.53 | 1.37 |
| 1:A:505:MLY:CG | 1:A:762:HIS:HD2 | 1.38 | 1.37 |
| 1:G:795:ARG:HE | 3:I:116:GLU:CB | 1.37 | 1.37 |
| 2:H:144:VAL:CG1 | 2:H:153:ILE:CD1 | 1.99 | 1.37 |
| 4:3:290:ARG:CZ | 4:5:202:THR:HG21 | 1.52 | 1.37 |
| 1:D:537:GLU:O | 4:9:349:LEU:CD1 | 1.70 | 1.36 |
| 1:G:553:MLY:CH1 | 4:X:45:VAL:HG11 | 1.55 | 1.36 |
| 2:K:117:LEU:HB2 | 2:K:147:ASN:ND2 | 1.39 | 1.36 |
| 1:P:721:LYS:CG | 1:P:736:GLN:CG | 1.97 | 1.36 |
| 1:P:806:MET:C | 1:P:807:VAL:N | 1.78 | 1.36 |
| 1:A:831:TRP:CH2 | 2:B:50:THR:CB | 2.04 | 1.36 |
| 1:D:795:ARG:CB | 3:F:35:ARG:NH1 | 1.88 | 1.36 |
| 1:G:642:LYS:HG3 | 4:V:23:GLY:N | 1.39 | 1.36 |
| 1:G:792:ALA:HB2 | 3:I:42:THR:CB | 1.53 | 1.36 |
| 1:G:795:ARG:HG2 | 3:I:118:MET:CE | 1.54 | 1.36 |
| 1:J:710:GLY:CA | 1:J:772:LEU:HD22 | 1.53 | 1.36 |
| 1:M:736:GLN:CA | 1:M:743:ALA:CB | 2.00 | 1.36 |
| 1:P:641:LYS:HG3 | 1:P:647:GLN:CD | 1.45 | 1.36 |
| 1:A:642:LYS:HG3 | 4:8:23:GLY:N | 1.40 | 1.36 |
| 1:D:534:SER:O | 4:9:351:THR:CG2 | 1.64 | 1.36 |
| 1:A:795:ARG:CB | 3:C:35:ARG:NH1 | 1.87 | 1.36 |
| 1:D:727:LEU:CD1 | 1:D:782:MLY:HD3 | 1.54 | 1.36 |
| 1:J:641:LYS:CG | 1:J:647:GLN:CD | 1.93 | 1.36 |
| 1:J:642:LYS:HG3 | 4:W:23:GLY:N | 1.40 | 1.36 |
| 1:M:831:TRP:HH2 | 2:N:47:LEU:CD2 | 1.37 | 1.36 |
| 1:D:649:VAL:O | 1:D:649:VAL:CG1 | 1.74 | 1.36 |
| 2:K:144:VAL:CG1 | 2:K:153:ILE:HG12 | 1.54 | 1.36 |
| 1:P:202:SER:HA | 1:P:207:LYS:CE | 1.51 | 1.36 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:P:736:GLN:CA | 1:P:743:ALA:HB1 | 1.53 | 1.36 |
| 1:P:793:ARG:HH11 | 3:R:40:ASN:ND2 | 1.21 | 1.36 |
| 4:4:288:ASP:OD2 | 4:6:203:THR:CG2 | 1.72 | 1.36 |
| 1:A:641:LYS:HG3 | 1:A:647:GLN:CD | 1.46 | 1.35 |
| 1:D:641:LYS:CG | 1:D:647:GLN:CD | 1.93 | 1.35 |
| 1:D:831:TRP:CH2 | 2:E:47:LEU:HA | 1.61 | 1.35 |
| 2:N:117:LEU:HB2 | 2:N:147:ASN:ND2 | 1.40 | 1.35 |
| 1:A:641:LYS:CG | 1:A:647:GLN:CD | 1.93 | 1.35 |
| 1:A:736:GLN:N | 1:A:743:ALA:HB1 | 1.35 | 1.35 |
| 1:A:831:TRP:CH2 | 2:B:50:THR:CG2 | 2.08 | 1.35 |
| 2:E:117:LEU:HB2 | 2:E:147:ASN:ND2 | 1.40 | 1.35 |
| 1:G:797:PHE:CD1 | 3:I:146:ILE:HG23 | 1.61 | 1.35 |
| 1:M:736:GLN:N | 1:M:743:ALA:HB1 | 1.35 | 1.35 |
| 1:P:649:VAL:CG1 | 1:P:649:VAL:O | 1.74 | 1.35 |
| 1:D:538:GLU:CA | 4:9:349:LEU:HD12 | 0.87 | 1.35 |
| 2:H:144:VAL:CG1 | 2:H:153:ILE:HG12 | 1.54 | 1.35 |
| 1:J:649:VAL:O | 1:J:649:VAL:CG1 | 1.74 | 1.35 |
| 1:J:736:GLN:CA | 1:J:743:ALA:HB1 | 1.53 | 1.35 |
| 1:P:538:GLU:CA | 4:1:349:LEU:HD12 | 0.88 | 1.35 |
| 1:D:642:LYS:HG3 | 4:9:23:GLY:N | 1.40 | 1.35 |
| 1:G:505:MLY:HH23 | 1:G:762:HIS:ND1 | 1.34 | 1.35 |
| 2:H:117:LEU:CD1 | 2:H:147:ASN:OD1 | 1.74 | 1.35 |
| 1:J:538:GLU:CA | 4:W:349:LEU:HD12 | 0.88 | 1.35 |
| 1:J:797:PHE:HZ | 3:L:146:ILE:CD1 | 1.19 | 1.35 |
| 1:P:642:LYS:HG3 | 4:1:23:GLY:N | 1.40 | 1.35 |
| 1:A:530:MET:HA | 4:8:354:GLN:CG | 1.56 | 1.35 |
| 1:D:795:ARG:HB3 | 3:F:35:ARG:CZ | 1.54 | 1.35 |
| 1:D:799:MET:CE | 3:F:32:ASP:HB3 | 1.54 | 1.35 |
| 1:J:736:GLN:N | 1:J:743:ALA:HB1 | 1.35 | 1.35 |
| 2:N:117:LEU:CD1 | 2:N:147:ASN:OD1 | 1.74 | 1.35 |
| 1:P:795:ARG:CD | 3:R:43:ASN:OD1 | 1.74 | 1.35 |
| 1:A:534:SER:O | 4:8:351:THR:CG2 | 1.64 | 1.34 |
| 1:G:641:LYS:CG | 1:G:647:GLN:CD | 1.93 | 1.34 |
| 1:M:538:GLU:CA | 4:Z:349:LEU:HD12 | 0.88 | 1.34 |
| 2:B:117:LEU:CD1 | 2:B:147:ASN:OD1 | 1.74 | 1.34 |
| 1:D:721:LYS:HG3 | 1:D:736:GLN:CG | 1.15 | 1.34 |
| 2:E:117:LEU:CD1 | 2:E:147:ASN:OD1 | 1.74 | 1.34 |
| 2:E:144:VAL:CG1 | 2:E:153:ILE:CG1 | 2.03 | 1.34 |
| 1:M:795:ARG:HB3 | 3:O:35:ARG:NH2 | 1.39 | 1.34 |
| 2:E:144:VAL:CG1 | 2:E:153:ILE:HG12 | 1.54 | 1.34 |
| 1:J:629:GLU:HA | 1:J:643:GLY:O | 1.17 | 1.34 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:721:LYS:HG3 | 1:J:736:GLN:CG | 1.15 | 1.34 |
| 1:J:831:TRP:CH2 | 2:K:47:LEU:CD2 | 2.11 | 1.34 |
| 1:M:819:ASN:CG | 2:N:92:ASP:HB2 | 1.24 | 1.34 |
| 1:A:538:GLU:CA | 4:8:349:LEU:HD12 | 0.87 | 1.34 |
| 1:D:831:TRP:CZ2 | 2:E:47:LEU:CD2 | 2.11 | 1.34 |
| 1:M:649:VAL:O | 1:M:649:VAL:CG1 | 1.74 | 1.34 |
| 1:P:783:LEU:HA | 1:P:786:ILE:CG1 | 1.54 | 1.34 |
| 1:A:649:VAL:O | 1:A:649:VAL:CG1 | 1.74 | 1.34 |
| 1:D:727:LEU:HD12 | 1:D:782:MLY:CE | 1.55 | 1.34 |
| 1:G:538:GLU:CA | 4:V:349:LEU:HD12 | 0.88 | 1.34 |
| 1:G:721:LYS:CG | 1:G:736:GLN:CG | 1.97 | 1.34 |
| 2:N:144:VAL:CG1 | 2:N:153:ILE:HG12 | 1.54 | 1.34 |
| 4:1:290:ARG:HH21 | 4:3:202:THR:CG2 | 1.41 | 1.34 |
| 1:G:534:SER:O | 4:V:351:THR:CG2 | 1.64 | 1.33 |
| 1:G:629:GLU:HA | 1:G:643:GLY:O | 1.17 | 1.33 |
| 2:K:117:LEU:CD1 | 2:K:147:ASN:OD1 | 1.74 | 1.33 |
| 1:M:819:ASN:ND2 | 2:N:92:ASP:HB2 | 1.43 | 1.33 |
| 1:A:499:GLU:OE1 | 1:A:766:PHE:CZ | 1.80 | 1.33 |
| 1:A:629:GLU:HA | 1:A:643:GLY:O | 1.17 | 1.33 |
| 1:G:753:VAL:HA | 1:G:780:ASP:OD1 | 1.20 | 1.33 |
| 1:M:530:MET:HA | 4:Z:354:GLN:CG | 1.56 | 1.33 |
| 1:P:819:ASN:OD1 | 2:Q:92:ASP:N | 1.58 | 1.33 |
| 1:A:85:TYR:OH | 1:A:772:LEU:CD2 | 1.75 | 1.33 |
| 1:J:710:GLY:HA2 | 1:J:772:LEU:CD2 | 1.57 | 1.33 |
| 1:M:641:LYS:CG | 1:M:647:GLN:CD | 1.93 | 1.33 |
| 1:M:795:ARG:HG2 | 3:O:118:MET:CE | 1.57 | 1.33 |
| 4:2:202:THR:HG22 | 4:Z:290:ARG:NH2 | 1.43 | 1.33 |
| 1:A:721:LYS:CG | 1:A:736:GLN:CG | 1.97 | 1.33 |
| 1:D:530:MET:HA | 4:9:354:GLN:CG | 1.56 | 1.33 |
| 1:D:629:GLU:HA | 1:D:643:GLY:O | 1.17 | 1.33 |
| 1:G:649:VAL:O | 1:G:649:VAL:CG1 | 1.74 | 1.33 |
| 1:G:819:ASN:CG | 2:H:92:ASP:HB2 | 1.31 | 1.33 |
| 1:J:530:MET:HA | 4:W:354:GLN:CG | 1.56 | 1.33 |
| 1:M:795:ARG:NH2 | 3:O:116:GLU:CB | 1.83 | 1.33 |
| 1:A:819:ASN:CG | 2:B:91:ALA:HA | 1.45 | 1.33 |
| 1:G:28:GLN:HB3 | 1:G:723:ARG:NH1 | 1.44 | 1.33 |
| 1:P:795:ARG:HB3 | 3:R:35:ARG:NH2 | 1.40 | 1.33 |
| 1:A:635:GLY:CA | 4:8:334:GLU:HG2 | 1.59 | 1.32 |
| 1:J:635:GLY:CA | 4:W:334:GLU:HG2 | 1.59 | 1.32 |
| 1:M:642:LYS:HG3 | 4:Z:23:GLY:N | 1.40 | 1.32 |
| 1:P:721:LYS:CG | 1:P:736:GLN:CD | 1.98 | 1.32 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:117:LEU:HB2 | 2:B:147:ASN:ND2 | 1.39 | 1.32 |
| 1:G:754:ASP:CB | 1:G:776:GLU:OE2 | 1.77 | 1.32 |
| 2:H:117:LEU:HB2 | 2:H:147:ASN:ND2 | 1.40 | 1.32 |
| 1:J:506:GLU:OE2 | 1:J:761:GLY:HA2 | 1.21 | 1.32 |
| 2:Q:117:LEU:CD1 | 2:Q:147:ASN:OD1 | 1.74 | 1.32 |
| 4:1:287:ILE:CB | 4:3:203:THR:HG22 | 1.57 | 1.32 |
| 1:A:792:ALA:HB2 | 3:C:42:THR:CG2 | 1.57 | 1.32 |
| 2:B:144:VAL:CG1 | 2:B:153:ILE:CG1 | 2.03 | 1.32 |
| 1:G:530:MET:HA | 4:V:354:GLN:CG | 1.57 | 1.32 |
| 1:P:641:LYS:CG | 1:P:647:GLN:CD | 1.93 | 1.32 |
| 4:1:202:THR:CB | 4:Y:286:ASP:OD1 | 1.75 | 1.32 |
| 1:D:635:GLY:CA | 4:9:334:GLU:HG2 | 1.59 | 1.32 |
| 1:G:721:LYS:CG | 1:G:736:GLN:CD | 1.98 | 1.32 |
| 1:J:641:LYS:HG3 | 1:J:647:GLN:CD | 1.45 | 1.32 |
| 1:P:530:MET:HA | 4:1:354:GLN:CG | 1.56 | 1.32 |
| 1:A:725:ARG:NE | 1:A:733:PRO:HB3 | 0.99 | 1.32 |
| 2:B:114:LYS:CA | 2:B:146:GLY:O | 1.76 | 1.32 |
| 1:G:635:GLY:CA | 4:V:334:GLU:HG2 | 1.59 | 1.32 |
| 1:G:754:ASP:CB | 1:G:776:GLU:CD | 1.96 | 1.32 |
| 2:H:114:LYS:CA | 2:H:146:GLY:O | 1.76 | 1.32 |
| 1:J:94:MET:O | 1:J:713:SER:CB | 1.75 | 1.32 |
| 1:J:831:TRP:CH2 | 2:K:47:LEU:HD21 | 1.65 | 1.32 |
| 1:P:793:ARG:NH1 | 3:R:40:ASN:HD22 | 1.25 | 1.32 |
| 2:Q:117:LEU:HB2 | 2:Q:147:ASN:ND2 | 1.40 | 1.32 |
| 2:K:121:LEU:O | 2:K:128:PHE:CB | 1.78 | 1.31 |
| 1:M:635:GLY:CA | 4:Z:334:GLU:HG2 | 1.59 | 1.31 |
| 2:E:114:LYS:CA | 2:E:146:GLY:O | 1.76 | 1.31 |
| 1:J:557:GLU:CA | 4:Y:47:MET:HA | 1.09 | 1.31 |
| 1:M:721:LYS:CG | 1:M:736:GLN:CD | 1.98 | 1.31 |
| 1:M:725:ARG:NE | 1:M:733:PRO:HB3 | 1.00 | 1.31 |
| 1:P:831:TRP:HH2 | 2:Q:47:LEU:CD2 | 1.42 | 1.31 |
| 4:1:247:VAL:HG22 | 4:Y:324:THR:CG2 | 1.59 | 1.31 |
| 1:G:725:ARG:NE | 1:G:733:PRO:HB3 | 0.99 | 1.31 |
| 1:G:753:VAL:O | 1:G:779:ARG:NH1 | 1.62 | 1.31 |
| 2:H:144:VAL:CG1 | 2:H:153:ILE:CG1 | 2.03 | 1.31 |
| 1:A:721:LYS:CG | 1:A:736:GLN:CD | 1.98 | 1.31 |
| 1:D:725:ARG:NE | 1:D:733:PRO:HB3 | 1.00 | 1.31 |
| 1:G:97:LEU:CD2 | 1:G:712:PRO:HB3 | 1.60 | 1.31 |
| 1:J:725:ARG:NE | 1:J:733:PRO:HB3 | 1.00 | 1.31 |
| 2:K:114:LYS:CA | 2:K:146:GLY:O | 1.76 | 1.31 |
| 1:M:549:SER:N | 4:2:47:MET:O | 1.59 | 1.31 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:799:MET:SD | 3:O:32:ASP:CB | 2.18 | 1.31 |
| 1:P:721:LYS:HG2 | 1:P:736:GLN:OE1 | 1.29 | 1.31 |
| 4:2:287:ILE:HG12 | 4:4:203:THR:N | 1.25 | 1.31 |
| 1:J:788:THR:O | 3:L:42:THR:HG21 | 1.21 | 1.31 |
| 1:J:819:ASN:ND2 | 2:K:92:ASP:HB2 | 1.44 | 1.31 |
| 1:J:836:PHE:CE1 | 2:K:159:HIS:HA | 1.64 | 1.31 |
| 4:2:287:ILE:CB | 4:4:202:THR:HB | 1.60 | 1.31 |
| 2:B:121:LEU:O | 2:B:128:PHE:CB | 1.79 | 1.30 |
| 2:E:121:LEU:O | 2:E:128:PHE:CB | 1.79 | 1.30 |
| 1:G:795:ARG:CA | 3:I:118:MET:HE1 | 1.60 | 1.30 |
| 1:M:534:SER:O | 4:Z:351:THR:CG2 | 1.64 | 1.30 |
| 1:M:735:GLY:O | 1:M:743:ALA:HB2 | 1.29 | 1.30 |
| 2:N:114:LYS:CA | 2:N:146:GLY:O | 1.76 | 1.30 |
| 1:P:635:GLY:CA | 4:1:334:GLU:HG2 | 1.59 | 1.30 |
| 4:2:202:THR:CG2 | 4:Z:290:ARG:NH2 | 1.93 | 1.30 |
| 1:A:791:GLN:NE2 | 3:C:116:GLU:H | 1.26 | 1.30 |
| 1:G:735:GLY:O | 1:G:743:ALA:HB2 | 1.29 | 1.30 |
| 1:G:821:ARG:NH2 | 2:H:127:ARG:HG2 | 1.45 | 1.30 |
| 2:H:121:LEU:O | 2:H:128:PHE:CB | 1.79 | 1.30 |
| 1:M:721:LYS:CG | 1:M:736:GLN:CG | 1.97 | 1.30 |
| 1:G:757:GLN:HG2 | 1:G:776:GLU:OE2 | 1.17 | 1.30 |
| 1:P:769:ALA:C | 1:P:771:LEU:N | 1.85 | 1.30 |
| 2:Q:114:LYS:CA | 2:Q:146:GLY:O | 1.76 | 1.30 |
| 1:A:707:CYS:O | 1:A:714:ARG:NH2 | 1.61 | 1.30 |
| 1:D:713:SER:H | 1:D:771:LEU:CD2 | 1.43 | 1.30 |
| 1:G:97:LEU:HD23 | 1:G:712:PRO:CB | 1.61 | 1.30 |
| 1:G:721:LYS:HG2 | 1:G:736:GLN:OE1 | 1.29 | 1.30 |
| 1:J:797:PHE:CE1 | 3:L:146:ILE:CG2 | 2.15 | 1.30 |
| 1:M:641:LYS:HG3 | 1:M:647:GLN:CD | 1.46 | 1.30 |
| 1:P:599:ASN:HA | 1:P:649:VAL:CB | 1.60 | 1.30 |
| 1:A:819:ASN:ND2 | 2:B:91:ALA:C | 1.72 | 1.30 |
| 1:G:801:VAL:HG21 | 3:I:126:LEU:CD2 | 1.62 | 1.30 |
| 1:M:629:GLU:HA | 1:M:643:GLY:O | 1.17 | 1.30 |
| 1:P:725:ARG:NE | 1:P:733:PRO:HB3 | 1.00 | 1.30 |
| 1:P:798:LEU:CD2 | 3:R:126:LEU:HD11 | 1.61 | 1.30 |
| 1:D:814:PHE:HA | 2:E:127:ARG:NH1 | 1.44 | 1.29 |
| 1:G:641:LYS:HG3 | 1:G:647:GLN:CD | 1.45 | 1.29 |
| 1:J:735:GLY:O | 1:J:743:ALA:HB2 | 1.30 | 1.29 |
| 1:A:599:ASN:HA | 1:A:649:VAL:CB | 1.60 | 1.29 |
| 1:A:800:ARG:HH22 | 3:C:40:ASN:ND2 | 1.27 | 1.29 |
| 1:D:791:GLN:OE1 | 3:F:116:GLU:HG3 | 1.19 | 1.29 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:735:GLY:C | 1:G:743:ALA:CB | 2.01 | 1.29 |
| 1:M:783:LEU:HA | 1:M:786:ILE:CG1 | 1.62 | 1.29 |
| 2:N:121:LEU:O | 2:N:128:PHE:CB | 1.78 | 1.29 |
| 1:D:721:LYS:CG | 1:D:736:GLN:CD | 1.98 | 1.29 |
| 1:G:599:ASN:HA | 1:G:649:VAL:CB | 1.60 | 1.29 |
| 1:M:538:GLU:O | 4:Z:349:LEU:CD1 | 1.78 | 1.29 |
| 1:P:629:GLU:HA | 1:P:643:GLY:O | 1.17 | 1.29 |
| 1:P:817:GLN:CG | 2:Q:127:ARG:HD2 | 1.61 | 1.29 |
| 1:A:538:GLU:C | 4:8:349:LEU:HD12 | 1.48 | 1.29 |
| 1:A:735:GLY:C | 1:A:743:ALA:CB | 2.01 | 1.29 |
| 1:J:721:LYS:CG | 1:J:736:GLN:CD | 1.98 | 1.29 |
| 1:P:798:LEU:CD1 | 3:R:126:LEU:HD11 | 1.60 | 1.29 |
| 1:D:599:ASN:HA | 1:D:649:VAL:CB | 1.60 | 1.29 |
| 1:G:503:TYR:OH | 1:G:711:PHE:HD2 | 1.02 | 1.29 |
| 1:J:537:GLU:C | 4:W:349:LEU:HD13 | 1.52 | 1.29 |
| 1:M:795:ARG:NH2 | 3:O:116:GLU:CG | 1.94 | 1.29 |
| 1:M:795:ARG:CD | 3:O:43:ASN:OD1 | 1.79 | 1.29 |
| 1:P:735:GLY:C | 1:P:743:ALA:CB | 2.01 | 1.29 |
| 1:G:755:HIS:ND1 | 1:G:779:ARG:NH1 | 1.80 | 1.28 |
| 1:J:599:ASN:HA | 1:J:649:VAL:CB | 1.60 | 1.28 |
| 1:J:819:ASN:HA | 2:K:90:GLY:O | 1.19 | 1.28 |
| 1:M:599:ASN:HA | 1:M:649:VAL:CB | 1.60 | 1.28 |
| 1:M:735:GLY:C | 1:M:743:ALA:CB | 2.01 | 1.28 |
| 1:P:798:LEU:HD11 | 3:R:126:LEU:CD1 | 1.63 | 1.28 |
| 1:A:505:MLY:CG | 1:A:762:HIS:CD2 | 2.13 | 1.28 |
| 1:G:795:ARG:NH2 | 3:I:116:GLU:HG2 | 1.45 | 1.28 |
| 1:G:838:ILE:HD11 | 2:H:54:MET:CE | 1.63 | 1.28 |
| 1:M:534:SER:O | 4:Z:351:THR:CA | 1.82 | 1.28 |
| 1:M:821:ARG:NH2 | 2:N:127:ARG:CG | 1.95 | 1.28 |
| 4:W:324:THR:HG21 | 4:Y:247:VAL:N | 0.98 | 1.28 |
| 1:J:817:GLN:CG | 2:K:127:ARG:HD2 | 1.63 | 1.28 |
| 1:A:534:SER:O | 4:8:351:THR:CA | 1.81 | 1.28 |
| 1:A:537:GLU:C | 4:8:349:LEU:HD13 | 1.52 | 1.28 |
| 1:D:838:ILE:HD12 | 2:E:54:MET:CE | 1.60 | 1.28 |
| 1:G:552:ASN:O | 4:X:47:MET:SD | 1.91 | 1.28 |
| 1:D:538:GLU:O | 4:9:349:LEU:CD1 | 1.78 | 1.28 |
| 1:D:721:LYS:CG | 1:D:736:GLN:CG | 1.97 | 1.28 |
| 1:D:735:GLY:C | 1:D:743:ALA:CB | 2.01 | 1.28 |
| 1:G:84:MLY:CD | 1:G:723:ARG:HD2 | 1.62 | 1.28 |
| 1:P:538:GLU:C | 4:1:349:LEU:HD12 | 1.48 | 1.28 |
| 4:W:325:MET:SD | 4:Y:244:ASP:HB2 | 1.72 | 1.28 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:721:LYS:HG3 | 1:A:736:GLN:CD | 1.53 | 1.27 |
| 1:D:537:GLU:C | 4:9:349:LEU:HD13 | 1.52 | 1.27 |
| 1:D:735:GLY:O | 1:D:743:ALA:HB2 | 1.29 | 1.27 |
| 1:G:94:MET:O | 1:G:713:SER:HB3 | 1.15 | 1.27 |
| 1:G:792:ALA:CB | 3:I:42:THR:CG2 | 1.79 | 1.27 |
| 4:1:166:TYR:CE2 | 4:3:64:ILE:HG21 | 1.68 | 1.27 |
| 2:K:144:VAL:CG1 | 2:K:153:ILE:CG1 | 2.03 | 1.27 |
| 1:M:817:GLN:CG | 2:N:127:ARG:HD2 | 1.63 | 1.27 |
| 2:Q:121:LEU:O | 2:Q:128:PHE:CB | 1.79 | 1.27 |
| 1:A:721:LYS:CG | 1:A:736:GLN:OE1 | 1.82 | 1.27 |
| 1:A:735:GLY:O | 1:A:743:ALA:HB2 | 1.29 | 1.27 |
| 1:A:819:ASN:HD21 | 2:B:91:ALA:CA | 1.37 | 1.27 |
| 1:G:752:ASP:O | 1:G:780:ASP:HA | 1.33 | 1.27 |
| 1:G:819:ASN:CG | 2:H:92:ASP:CB | 2.00 | 1.27 |
| 1:P:537:GLU:C | 4:1:349:LEU:HD13 | 1.52 | 1.27 |
| 1:P:735:GLY:O | 1:P:743:ALA:HB2 | 1.29 | 1.27 |
| 4:1:243:PRO:HB2 | 4:Y:291:LYS:CE | 1.64 | 1.27 |
| 1:A:797:PHE:CZ | 3:C:146:ILE:CD1 | 2.16 | 1.27 |
| 1:A:93:MET:CE | 1:A:715:VAL:HA | 1.65 | 1.26 |
| 1:G:97:LEU:CD2 | 1:G:712:PRO:CB | 2.13 | 1.26 |
| 1:G:538:GLU:O | 4:V:349:LEU:CD1 | 1.78 | 1.26 |
| 1:J:538:GLU:O | 4:W:349:LEU:CD1 | 1.78 | 1.26 |
| 1:J:733:PRO:O | 1:J:737:PHE:HD1 | 0.93 | 1.26 |
| 1:J:735:GLY:C | 1:J:743:ALA:CB | 2.01 | 1.26 |
| 1:M:721:LYS:CG | 1:M:736:GLN:OE1 | 1.82 | 1.26 |
| 4:1:243:PRO:CB | 4:Y:291:LYS:CE | 2.14 | 1.26 |
| 1:G:534:SER:O | 4:V:351:THR:CA | 1.82 | 1.26 |
| 1:J:721:LYS:CG | 1:J:736:GLN:OE1 | 1.83 | 1.26 |
| 1:P:792:ALA:HB2 | 3:R:42:THR:CG2 | 1.64 | 1.26 |
| 1:A:149:GLN:HB2 | 1:A:718:ALA:CB | 1.65 | 1.26 |
| 1:M:733:PRO:O | 1:M:737:PHE:HD1 | 0.93 | 1.26 |
| 1:M:831:TRP:CH2 | 2:N:47:LEU:CD2 | 2.17 | 1.26 |
| 1:P:721:LYS:CG | 1:P:736:GLN:OE1 | 1.83 | 1.26 |
| 1:D:534:SER:O | 4:9:351:THR:CA | 1.82 | 1.26 |
| 1:M:537:GLU:C | 4:Z:349:LEU:HD13 | 1.52 | 1.26 |
| 1:P:538:GLU:O | 4:1:349:LEU:CD1 | 1.78 | 1.26 |
| 1:P:733:PRO:O | 1:P:737:PHE:HD1 | 0.92 | 1.26 |
| 1:A:721:LYS:HG2 | 1:A:736:GLN:OE1 | 1.29 | 1.26 |
| 1:J:534:SER:O | 4:W:351:THR:CA | 1.82 | 1.26 |
| 1:J:721:LYS:HG2 | 1:J:736:GLN:OE1 | 1.29 | 1.26 |
| 1:P:534:SER:O | 4:1:351:THR:CA | 1.82 | 1.26 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:P:546:THR:OG1 | 4:3:46:GLY:C | 1.71 | 1.26 |
| 1:A:795:ARG:CZ | 3:C:116:GLU:OE2 | 1.81 | 1.25 |
| 1:G:818:TYR:CE1 | 2:H:127:ARG:NH2 | 2.03 | 1.25 |
| 4:1:290:ARG:NH2 | 4:3:202:THR:HG22 | 1.50 | 1.25 |
| 1:A:501:GLU:HG2 | 1:A:762:HIS:ND1 | 1.48 | 1.25 |
| 1:J:215:GLN:N | 1:J:340:ILE:HG12 | 1.19 | 1.25 |
| 1:A:630:ALA:O | 4:8:25:ASP:OD2 | 1.53 | 1.25 |
| 1:A:795:ARG:CD | 3:C:43:ASN:OD1 | 1.83 | 1.25 |
| 1:A:795:ARG:CD | 3:C:35:ARG:HH12 | 1.49 | 1.25 |
| 1:A:799:MET:CE | 3:C:32:ASP:HB3 | 1.65 | 1.25 |
| 1:A:813:ILE:HG22 | 2:B:127:ARG:CD | 1.67 | 1.25 |
| 1:A:836:PHE:CE1 | 2:B:159:HIS:HB2 | 1.71 | 1.25 |
| 1:G:28:GLN:CB | 1:G:723:ARG:HH12 | 1.47 | 1.25 |
| 1:G:537:GLU:C | 4:V:349:LEU:HD13 | 1.53 | 1.25 |
| 1:G:791:GLN:HE22 | 3:I:115:GLY:CA | 1.48 | 1.25 |
| 1:P:721:LYS:HG3 | 1:P:736:GLN:CD | 1.54 | 1.25 |
| 1:P:821:ARG:NH2 | 2:Q:127:ARG:CG | 1.99 | 1.25 |
| 1:D:721:LYS:CG | 1:D:736:GLN:OE1 | 1.82 | 1.25 |
| 1:D:769:ALA:O | 1:D:774:LEU:CD1 | 1.84 | 1.25 |
| 1:G:800:ARG:NH2 | 3:I:40:ASN:OD1 | 1.69 | 1.25 |
| 1:M:630:ALA:O | 4:Z:25:ASP:OD2 | 1.52 | 1.25 |
| 2:N:117:LEU:CD1 | 2:N:147:ASN:CG | 2.05 | 1.25 |
| 1:P:783:LEU:CG | 1:P:786:ILE:CD1 | 2.12 | 1.25 |
| 1:P:798:LEU:HD11 | 3:R:126:LEU:CG | 1.64 | 1.25 |
| 1:A:538:GLU:O | 4:8:349:LEU:CD1 | 1.78 | 1.25 |
| 1:A:733:PRO:O | 1:A:737:PHE:HD1 | 0.93 | 1.25 |
| 4:2:287:ILE:CB | 4:4:203:THR:N | 2.00 | 1.25 |
| 4:4:288:ASP:OD2 | 4:6:203:THR:HG21 | 1.14 | 1.25 |
| 1:A:641:LYS:CG | 1:A:647:GLN:CG | 2.16 | 1.24 |
| 1:D:831:TRP:CZ2 | 2:E:47:LEU:HD23 | 1.72 | 1.24 |
| 1:J:829:TRP:CZ3 | 2:K:87:LYS:NZ | 2.04 | 1.24 |
| 1:M:800:ARG:NH2 | 3:O:40:ASN:OD1 | 1.67 | 1.24 |
| 1:P:546:THR:HG21 | 4:3:46:GLY:O | 1.22 | 1.24 |
| 1:P:831:TRP:CH2 | 2:Q:47:LEU:CD2 | 2.19 | 1.24 |
| 1:G:641:LYS:CG | 1:G:647:GLN:CG | 2.16 | 1.24 |
| 1:M:721:LYS:HG3 | 1:M:736:GLN:CD | 1.53 | 1.24 |
| 1:P:93:MET:SD | 1:P:714:ARG:O | 1.94 | 1.24 |
| 1:P:630:ALA:O | 4:1:25:ASP:OD2 | 1.52 | 1.24 |
| 1:D:721:LYS:HG3 | 1:D:736:GLN:CD | 1.54 | 1.24 |
| 1:D:815:CYS:SG | 2:E:92:ASP:HB2 | 1.76 | 1.24 |
| 1:G:733:PRO:O | 1:G:737:PHE:HD1 | 0.93 | 1.24 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:641:LYS:CD | 1:J:647:GLN:NE2 | 1.99 | 1.24 |
| 1:P:795:ARG:CG | 3:R:118:MET:HE3 | 1.68 | 1.24 |
| 4:V:324:THR:HG21 | 4:X:247:VAL:N | 1.49 | 1.24 |
| 1:J:817:GLN:HB3 | 2:K:127:ARG:CD | 1.66 | 1.24 |
| 4:X:287:ILE:CG1 | 4:Z:205:GLU:HG3 | 1.67 | 1.24 |
| 1:A:149:GLN:NE2 | 1:A:718:ALA:CB | 1.99 | 1.24 |
| 1:A:149:GLN:CD | 1:A:716:LEU:HD23 | 1.58 | 1.24 |
| 1:D:813:ILE:HD13 | 2:E:128:PHE:CE1 | 1.73 | 1.24 |
| 1:D:838:ILE:CD1 | 2:E:54:MET:SD | 2.25 | 1.24 |
| 1:G:641:LYS:CD | 1:G:647:GLN:NE2 | 1.99 | 1.24 |
| 1:G:831:TRP:CZ2 | 2:H:47:LEU:HD21 | 1.71 | 1.24 |
| 4:W:324:THR:CG2 | 4:Y:247:VAL:N | 1.89 | 1.24 |
| 1:D:646:PHE:CE2 | 1:D:652:LEU:HD11 | 1.73 | 1.23 |
| 2:E:117:LEU:CD1 | 2:E:147:ASN:CG | 2.05 | 1.23 |
| 1:G:795:ARG:NH2 | 3:I:116:GLU:CG | 1.99 | 1.23 |
| 2:E:121:LEU:C | 2:E:128:PHE:CB | 2.07 | 1.23 |
| 1:G:783:LEU:O | 1:G:787:ILE:N | 1.71 | 1.23 |
| 1:G:817:GLN:OE1 | 2:H:127:ARG:HD2 | 1.36 | 1.23 |
| 1:M:646:PHE:CE2 | 1:M:652:LEU:HD11 | 1.73 | 1.23 |
| 2:Q:144:VAL:CG1 | 2:Q:153:ILE:CG1 | 2.03 | 1.23 |
| 4:3:322:PRO:HB3 | 4:5:244:ASP:OD2 | 1.39 | 1.23 |
| 4:9:322:PRO:CB | 4:W:244:ASP:OD2 | 1.86 | 1.23 |
| 1:A:93:MET:HE2 | 1:A:715:VAL:CA | 1.68 | 1.23 |
| 4:V:325:MET:SD | 4:X:244:ASP:HB2 | 1.77 | 1.23 |
| 2:B:121:LEU:C | 2:B:128:PHE:CB | 2.07 | 1.23 |
| 1:D:721:LYS:HG2 | 1:D:736:GLN:OE1 | 1.29 | 1.23 |
| 1:J:629:GLU:CA | 1:J:643:GLY:O | 1.87 | 1.23 |
| 1:J:646:PHE:CE2 | 1:J:652:LEU:HD11 | 1.73 | 1.23 |
| 1:J:817:GLN:CB | 2:K:127:ARG:HD2 | 1.69 | 1.23 |
| 1:M:798:LEU:HD11 | 3:O:126:LEU:CG | 1.69 | 1.23 |
| 1:M:819:ASN:CA | 2:N:90:GLY:O | 1.87 | 1.23 |
| 1:P:629:GLU:CA | 1:P:643:GLY:O | 1.87 | 1.23 |
| 1:P:641:LYS:CD | 1:P:647:GLN:NE2 | 1.99 | 1.23 |
| 1:P:795:ARG:NH2 | 3:R:116:GLU:CG | 1.99 | 1.23 |
| 2:Q:117:LEU:CD1 | 2:Q:147:ASN:CG | 2.05 | 1.23 |
| 4:2:288:ASP:OD2 | 4:4:203:THR:HG21 | 1.32 | 1.23 |
| 1:A:646:PHE:CE2 | 1:A:652:LEU:HD11 | 1.73 | 1.23 |
| 1:A:836:PHE:CZ | 2:B:160:GLY:N | 2.06 | 1.23 |
| 2:B:117:LEU:HD12 | 2:B:147:ASN:OD1 | 1.32 | 1.23 |
| 2:B:117:LEU:CD1 | 2:B:147:ASN:CG | 2.05 | 1.23 |
| 1:D:641:LYS:CD | 1:D:647:GLN:NE2 | 1.99 | 1.23 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:733:PRO:O | 1:D:737:PHE:HD1 | 0.93 | 1.23 |
| 1:J:756:THR:HG21 | 1:J:776:GLU:O | 1.38 | 1.23 |
| 2:K:121:LEU:C | 2:K:128:PHE:CB | 2.07 | 1.23 |
| 1:P:534:SER:O | 4:1:351:THR:CB | 1.87 | 1.23 |
| 1:D:215:GLN:N | 1:D:340:ILE:HG12 | 1.20 | 1.22 |
| 1:D:641:LYS:CG | 1:D:647:GLN:CG | 2.15 | 1.22 |
| 1:G:721:LYS:CG | 1:G:736:GLN:OE1 | 1.83 | 1.22 |
| 2:H:121:LEU:C | 2:H:128:PHE:CB | 2.07 | 1.22 |
| 1:J:534:SER:O | 4:W:351:THR:CB | 1.88 | 1.22 |
| 1:M:215:GLN:N | 1:M:340:ILE:CG1 | 2.02 | 1.22 |
| 1:M:538:GLU:O | 4:Z:349:LEU:HD11 | 1.35 | 1.22 |
| 2:N:121:LEU:C | 2:N:128:PHE:CB | 2.07 | 1.22 |
| 2:N:144:VAL:CG1 | 2:N:153:ILE:CG1 | 2.03 | 1.22 |
| 1:P:646:PHE:CE2 | 1:P:652:LEU:HD11 | 1.73 | 1.22 |
| 1:G:215:GLN:N | 1:G:340:ILE:CG1 | 2.02 | 1.22 |
| 1:J:819:ASN:CG | 2:K:92:ASP:HB2 | 1.59 | 1.22 |
| 4:8:322:PRO:CB | 4:V:244:ASP:OD2 | 1.86 | 1.22 |
| 1:J:756:THR:HG22 | 1:J:776:GLU:CB | 1.67 | 1.22 |
| 2:K:144:VAL:CG1 | 2:K:153:ILE:HD11 | 1.65 | 1.22 |
| 1:D:727:LEU:HD12 | 1:D:782:MLY:CD | 1.64 | 1.22 |
| 1:J:215:GLN:N | 1:J:340:ILE:CG1 | 2.02 | 1.22 |
| 1:J:538:GLU:C | 4:W:349:LEU:HD12 | 1.48 | 1.22 |
| 1:J:721:LYS:HG3 | 1:J:736:GLN:CD | 1.54 | 1.22 |
| 1:A:641:LYS:CD | 1:A:647:GLN:NE2 | 1.99 | 1.22 |
| 1:A:534:SER:O | 4:8:351:THR:CB | 1.87 | 1.21 |
| 1:D:641:LYS:CG | 1:D:647:GLN:HG3 | 1.71 | 1.21 |
| 2:E:144:VAL:CG1 | 2:E:153:ILE:HD11 | 1.64 | 1.21 |
| 1:G:567:LYS:NZ | 4:X:92:ASN:ND2 | 1.86 | 1.21 |
| 1:G:646:PHE:CE2 | 1:G:652:LEU:HD11 | 1.73 | 1.21 |
| 1:G:707:CYS:SG | 1:G:714:ARG:NH2 | 2.13 | 1.21 |
| 1:G:769:ALA:CB | 1:G:770:GLY:HA2 | 1.69 | 1.21 |
| 1:M:641:LYS:CD | 1:M:647:GLN:NE2 | 1.99 | 1.21 |
| 1:M:721:LYS:HG2 | 1:M:736:GLN:OE1 | 1.29 | 1.21 |
| 1:P:641:LYS:CG | 1:P:647:GLN:CG | 2.16 | 1.21 |
| 4:8:322:PRO:HB2 | 4:V:244:ASP:OD2 | 1.39 | 1.21 |
| 1:M:629:GLU:CA | 1:M:643:GLY:O | 1.87 | 1.21 |
| 1:P:641:LYS:CG | 1:P:647:GLN:HG3 | 1.71 | 1.21 |
| 4:2:288:ASP:CG | 4:4:203:THR:HG21 | 1.59 | 1.21 |
| 1:A:149:GLN:HG3 | 1:A:719:ASP:OD1 | 1.20 | 1.21 |
| 1:A:502:GLU:CA | 1:A:761:GLY:HA3 | 1.70 | 1.21 |
| 1:D:823:PHE:HE1 | 2:E:160:GLY:CA | 1.52 | 1.21 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:538:GLU:C | 4:V:349:LEU:HD12 | 1.48 | 1.21 |
| 1:G:721:LYS:HG3 | 1:G:736:GLN:CD | 1.54 | 1.21 |
| 2:K:117:LEU:CD1 | 2:K:147:ASN:CG | 2.05 | 1.21 |
| 1:M:836:PHE:CZ | 2:N:160:GLY:N | 2.08 | 1.21 |
| 4:1:287:ILE:CG2 | 4:3:203:THR:HG22 | 1.69 | 1.21 |
| 4:4:288:ASP:CG | 4:6:203:THR:HG23 | 1.47 | 1.21 |
| 4:7:322:PRO:CB | 4:9:244:ASP:OD2 | 1.86 | 1.21 |
| 1:A:215:GLN:N | 1:A:340:ILE:CG1 | 2.02 | 1.21 |
| 1:A:768:MLY:CB | 1:A:771:LEU:HB2 | 1.69 | 1.21 |
| 2:B:144:VAL:CG1 | 2:B:153:ILE:HD11 | 1.65 | 1.21 |
| 1:D:215:GLN:N | 1:D:340:ILE:CG1 | 2.02 | 1.21 |
| 1:D:629:GLU:CA | 1:D:643:GLY:O | 1.87 | 1.21 |
| 1:G:557:GLU:CB | 4:X:46:GLY:O | 1.86 | 1.21 |
| 1:G:797:PHE:CE1 | 3:I:146:ILE:HG23 | 1.76 | 1.21 |
| 2:K:117:LEU:HD12 | 2:K:147:ASN:OD1 | 1.33 | 1.21 |
| 1:M:534:SER:O | 4:Z:351:THR:CB | 1.88 | 1.21 |
| 1:M:538:GLU:C | 4:Z:349:LEU:HD12 | 1.48 | 1.21 |
| 1:P:215:GLN:N | 1:P:340:ILE:CG1 | 2.02 | 1.21 |
| 4:2:288:ASP:CG | 4:4:203:THR:CG2 | 2.09 | 1.21 |
| 1:A:797:PHE:CD1 | 3:C:146:ILE:O | 1.93 | 1.21 |
| 1:D:630:ALA:O | 4:9:25:ASP:OD2 | 1.52 | 1.21 |
| 1:G:534:SER:O | 4:V:351:THR:CB | 1.88 | 1.21 |
| 1:G:797:PHE:CZ | 3:I:126:LEU:HD22 | 1.75 | 1.21 |
| 1:J:630:ALA:O | 4:W:25:ASP:OD2 | 1.52 | 1.21 |
| 1:J:820:VAL:HG11 | 2:K:136:MET:CE | 1.69 | 1.21 |
| 1:M:798:LEU:CD1 | 3:O:126:LEU:HD11 | 1.68 | 1.21 |
| 4:1:202:THR:HB | 4:Y:286:ASP:OD1 | 1.06 | 1.21 |
| 1:A:629:GLU:CA | 1:A:643:GLY:O | 1.87 | 1.20 |
| 1:A:818:TYR:HB2 | 2:B:90:GLY:CA | 1.71 | 1.20 |
| 1:D:534:SER:O | 4:9:351:THR:CB | 1.87 | 1.20 |
| 1:G:629:GLU:CA | 1:G:643:GLY:O | 1.87 | 1.20 |
| 1:J:505:MLY:CD | 1:J:762:HIS:CE1 | 2.24 | 1.20 |
| 1:P:215:GLN:N | 1:P:340:ILE:HG12 | 1.19 | 1.20 |
| 1:J:557:GLU:HA | 4:Y:47:MET:C | 1.62 | 1.20 |
| 1:J:641:LYS:CG | 1:J:647:GLN:HG3 | 1.71 | 1.20 |
| 1:M:641:LYS:CG | 1:M:647:GLN:HG3 | 1.71 | 1.20 |
| 1:P:538:GLU:O | 4:1:349:LEU:HD11 | 1.35 | 1.20 |
| 1:P:796:GLY:HA2 | 3:R:35:ARG:HD3 | 1.22 | 1.20 |
| 4:2:287:ILE:CG1 | 4:4:202:THR:CA | 2.19 | 1.20 |
| 1:A:791:GLN:OE1 | 3:C:116:GLU:HG3 | 1.38 | 1.20 |
| 1:G:641:LYS:CG | 1:G:647:GLN:HG3 | 1.71 | 1.20 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:793:ARG:HH11 | 3:O:40:ASN:ND2 | 1.40 | 1.20 |
| 4:1:290:ARG:HH21 | 4:3:202:THR:HG21 | 1.05 | 1.20 |
| 4:9:322:PRO:HB2 | 4:W:244:ASP:OD2 | 1.39 | 1.20 |
| 2:B:117:LEU:CD1 | 2:B:147:ASN:CB | 2.19 | 1.20 |
| 2:Q:117:LEU:CD1 | 2:Q:147:ASN:CB | 2.19 | 1.20 |
| 4:1:244:ASP:OD2 | 4:Y:325:MET:SD | 1.99 | 1.20 |
| 4:1:247:VAL:CG2 | 4:Y:324:THR:CG2 | 2.16 | 1.20 |
| 1:A:798:LEU:HD11 | 3:C:126:LEU:CD2 | 1.72 | 1.20 |
| 1:D:800:ARG:NH2 | 3:F:40:ASN:ND2 | 1.89 | 1.20 |
| 2:E:117:LEU:CD1 | 2:E:147:ASN:CB | 2.19 | 1.20 |
| 1:M:836:PHE:CE1 | 2:N:159:HIS:CA | 2.25 | 1.20 |
| 1:P:538:GLU:OE2 | 4:1:355:MET:CE | 1.90 | 1.20 |
| 1:P:793:ARG:NH1 | 3:R:40:ASN:ND2 | 1.82 | 1.20 |
| 2:Q:121:LEU:C | 2:Q:128:PHE:CB | 2.07 | 1.20 |
| 1:A:709:LYS:C | 1:A:710:GLY:HA3 | 1.60 | 1.19 |
| 1:A:735:GLY:O | 1:A:743:ALA:CB | 1.91 | 1.19 |
| 1:G:557:GLU:HA | 4:X:48:GLY:N | 1.13 | 1.19 |
| 1:G:819:ASN:ND2 | 2:H:92:ASP:CB | 2.05 | 1.19 |
| 2:H:144:VAL:CG1 | 2:H:153:ILE:HD11 | 1.64 | 1.19 |
| 1:A:641:LYS:CG | 1:A:647:GLN:HG3 | 1.71 | 1.19 |
| 1:A:768:MLY:HB3 | 1:A:771:LEU:CB | 1.72 | 1.19 |
| 1:D:727:LEU:CD1 | 1:D:782:MLY:CE | 2.15 | 1.19 |
| 1:D:831:TRP:CZ2 | 2:E:47:LEU:HA | 1.75 | 1.19 |
| 1:G:538:GLU:OE2 | 4:V:355:MET:CE | 1.90 | 1.19 |
| 1:J:756:THR:HG21 | 1:J:776:GLU:C | 1.60 | 1.19 |
| 1:M:538:GLU:OE2 | 4:Z:355:MET:CE | 1.90 | 1.19 |
| 4:7:322:PRO:HB2 | 4:9:244:ASP:OD2 | 1.39 | 1.19 |
| 1:A:797:PHE:CE2 | 3:C:146:ILE:HD12 | 1.77 | 1.19 |
| 1:G:530:MET:HE2 | 4:V:354:GLN:CG | 1.72 | 1.19 |
| 1:G:735:GLY:O | 1:G:743:ALA:CB | 1.91 | 1.19 |
| 2:H:117:LEU:CD1 | 2:H:147:ASN:CB | 2.20 | 1.19 |
| 1:M:795:ARG:CG | 3:O:118:MET:HE3 | 1.70 | 1.19 |
| 1:P:829:TRP:CZ3 | 2:Q:87:LYS:NZ | 2.10 | 1.19 |
| 1:A:97:LEU:HD23 | 1:A:712:PRO:HB3 | 1.22 | 1.19 |
| 1:G:556:ASP:CG | 4:X:47:MET:HE3 | 1.48 | 1.19 |
| 1:J:819:ASN:OD1 | 2:K:92:ASP:N | 1.75 | 1.19 |
| 1:M:783:LEU:HG | 1:M:786:ILE:CD1 | 1.71 | 1.19 |
| 1:P:836:PHE:CZ | 2:Q:160:GLY:N | 2.09 | 1.19 |
| 2:B:54:MET:HA | 2:H:21:GLU:OE1 | 1.41 | 1.18 |
| 1:D:538:GLU:O | 4:9:349:LEU:HD11 | 1.35 | 1.18 |
| 1:D:538:GLU:OE2 | 4:9:355:MET:CE | 1.90 | 1.18 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:553:MLY:HG3 | 4:X:45:VAL:O | 1.01 | 1.18 |
| 1:J:639:GLY:CA | 4:W:345:ILE:HA | 1.73 | 1.18 |
| 1:J:641:LYS:CG | 1:J:647:GLN:CG | 2.16 | 1.18 |
| 2:K:117:LEU:CD1 | 2:K:147:ASN:CB | 2.19 | 1.18 |
| 1:M:641:LYS:CG | 1:M:647:GLN:CG | 2.16 | 1.18 |
| 1:D:557:GLU:H | 4:W:48:GLY:CA | 1.56 | 1.18 |
| 1:D:727:LEU:HD12 | 1:D:782:MLY:NZ | 1.33 | 1.18 |
| 1:D:769:ALA:O | 1:D:774:LEU:HD13 | 1.02 | 1.18 |
| 2:H:117:LEU:CD1 | 2:H:147:ASN:CG | 2.05 | 1.18 |
| 1:J:641:LYS:CB | 1:J:647:GLN:NE2 | 2.07 | 1.18 |
| 1:J:721:LYS:HA | 1:J:736:GLN:NE2 | 1.58 | 1.18 |
| 1:A:538:GLU:OE2 | 4:8:355:MET:CE | 1.91 | 1.18 |
| 1:A:795:ARG:HD2 | 3:C:35:ARG:HH12 | 1.02 | 1.18 |
| 2:N:117:LEU:CD1 | 2:N:147:ASN:CB | 2.19 | 1.18 |
| 1:P:735:GLY:O | 1:P:743:ALA:CB | 1.91 | 1.18 |
| 2:Q:117:LEU:HD12 | 2:Q:147:ASN:OD1 | 1.33 | 1.18 |
| 1:A:557:GLU:H | 4:V:48:GLY:CA | 1.56 | 1.18 |
| 1:A:819:ASN:ND2 | 2:B:92:ASP:N | 1.90 | 1.18 |
| 1:G:817:GLN:CD | 2:H:127:ARG:HD2 | 1.64 | 1.18 |
| 1:G:818:TYR:OH | 2:H:127:ARG:NH2 | 1.64 | 1.18 |
| 1:J:739:ASP:HB3 | 1:J:742:LYS:HB3 | 1.21 | 1.18 |
| 1:J:817:GLN:CG | 2:K:127:ARG:HB2 | 1.71 | 1.18 |
| 1:M:215:GLN:N | 1:M:340:ILE:HG12 | 1.20 | 1.18 |
| 1:M:783:LEU:CA | 1:M:786:ILE:HG13 | 1.72 | 1.18 |
| 2:N:144:VAL:CG1 | 2:N:153:ILE:HD11 | 1.64 | 1.18 |
| 1:P:530:MET:HE2 | 4:1:354:GLN:CG | 1.73 | 1.18 |
| 1:A:641:LYS:CB | 1:A:647:GLN:NE2 | 2.07 | 1.18 |
| 1:J:84:MLY:CH1 | 1:J:720:PHE:CD1 | 2.26 | 1.18 |
| 4:8:290:ARG:NH2 | 4:V:202:THR:HG23 | 1.59 | 1.18 |
| 4:W:325:MET:HE2 | 4:Y:244:ASP:OD2 | 1.40 | 1.18 |
| 1:A:149:GLN:CB | 1:A:719:ASP:N | 2.07 | 1.17 |
| 1:A:721:LYS:HA | 1:A:736:GLN:NE2 | 1.58 | 1.17 |
| 1:G:753:VAL:CA | 1:G:780:ASP:OD1 | 1.91 | 1.17 |
| 1:M:721:LYS:HA | 1:M:736:GLN:NE2 | 1.59 | 1.17 |
| 1:P:819:ASN:HA | 2:Q:90:GLY:O | 1.00 | 1.17 |
| 1:G:791:GLN:NE2 | 3:I:115:GLY:CA | 2.02 | 1.17 |
| 1:J:538:GLU:OE2 | 4:W:355:MET:CE | 1.90 | 1.17 |
| 1:A:97:LEU:CD2 | 1:A:712:PRO:HB3 | 1.73 | 1.17 |
| 1:G:538:GLU:HA | 4:V:349:LEU:CD1 | 1.55 | 1.17 |
| 1:G:795:ARG:CZ | 3:I:116:GLU:CD | 2.13 | 1.17 |
| 1:J:94:MET:C | 1:J:713:SER:HB3 | 1.63 | 1.17 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:N:117:LEU:HD12 | 2:N:147:ASN:OD1 | 1.33 | 1.17 |
| 1:A:538:GLU:HA | 4:8:349:LEU:CD1 | 1.54 | 1.17 |
| 1:A:736:GLN:N | 1:A:743:ALA:CB | 2.05 | 1.17 |
| 1:A:739:ASP:HB3 | 1:A:742:LYS:HB3 | 1.22 | 1.17 |
| 1:D:553:MLY:CE | 4:W:45:VAL:HA | 1.52 | 1.17 |
| 1:D:797:PHE:CE2 | 3:F:126:LEU:CD2 | 2.14 | 1.17 |
| 1:J:84:MLY:HH21 | 1:J:720:PHE:CA | 1.74 | 1.17 |
| 1:M:201:ALA:O | 1:M:202:SER:HB3 | 1.35 | 1.17 |
| 1:P:641:LYS:CB | 1:P:647:GLN:NE2 | 2.07 | 1.17 |
| 1:P:721:LYS:HA | 1:P:736:GLN:NE2 | 1.58 | 1.17 |
| 1:P:836:PHE:CE1 | 2:Q:159:HIS:CA | 2.26 | 1.17 |
| 2:Q:144:VAL:CG1 | 2:Q:153:ILE:HD11 | 1.65 | 1.17 |
| 4:1:202:THR:HB | 4:Y:286:ASP:CG | 1.46 | 1.17 |
| 1:G:641:LYS:CB | 1:G:647:GLN:NE2 | 2.07 | 1.17 |
| 1:G:641:LYS:CE | 4:V:348:SER:O | 1.93 | 1.17 |
| 1:G:795:ARG:CG | 3:I:118:MET:HE1 | 1.72 | 1.17 |
| 1:J:201:ALA:O | 1:J:202:SER:CB | 1.92 | 1.17 |
| 1:M:641:LYS:HG3 | 1:M:647:GLN:HG3 | 1.20 | 1.17 |
| 1:M:641:LYS:CE | 4:Z:348:SER:O | 1.93 | 1.17 |
| 1:M:829:TRP:CZ3 | 2:N:87:LYS:NZ | 2.13 | 1.17 |
| 1:A:641:LYS:CE | 4:8:348:SER:O | 1.93 | 1.16 |
| 1:A:797:PHE:CE1 | 3:C:146:ILE:CA | 2.27 | 1.16 |
| 1:D:641:LYS:HD2 | 1:D:647:GLN:NE2 | 1.59 | 1.16 |
| 1:D:795:ARG:NH2 | 3:F:116:GLU:CD | 1.98 | 1.16 |
| 1:M:215:GLN:HA | 1:M:340:ILE:CG2 | 1.76 | 1.16 |
| 1:M:538:GLU:HA | 4:Z:349:LEU:CD1 | 1.55 | 1.16 |
| 1:M:642:LYS:CG | 4:Z:23:GLY:N | 2.08 | 1.16 |
| 4:1:290:ARG:NH2 | 4:3:202:THR:CG2 | 2.04 | 1.16 |
| 1:A:640:LYS:HB3 | 1:A:645:SER:OG | 1.46 | 1.16 |
| 1:A:721:LYS:HG3 | 1:A:736:GLN:HG2 | 1.25 | 1.16 |
| 1:A:800:ARG:HB3 | 3:C:149:VAL:HG22 | 1.20 | 1.16 |
| 1:D:639:GLY:CA | 4:9:345:ILE:HA | 1.73 | 1.16 |
| 1:D:641:LYS:CB | 1:D:647:GLN:NE2 | 2.07 | 1.16 |
| 1:D:721:LYS:HA | 1:D:736:GLN:NE2 | 1.58 | 1.16 |
| 1:D:831:TRP:CZ3 | 2:E:34:ILE:CG2 | 2.28 | 1.16 |
| 1:G:215:GLN:HA | 1:G:340:ILE:CG2 | 1.76 | 1.16 |
| 1:G:553:MLY:HE2 | 4:X:45:VAL:CB | 1.75 | 1.16 |
| 1:G:553:MLY:CE | 4:X:45:VAL:CB | 2.22 | 1.16 |
| 4:2:43:VAL:O | 4:Z:167:GLU:OE1 | 1.60 | 1.16 |
| 4:X:288:ASP:HB2 | 4:Z:204:ALA:CB | 1.67 | 1.16 |
| 1:A:215:GLN:HA | 1:A:340:ILE:CG2 | 1.76 | 1.16 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:641:LYS:CE | 4:9:348:SER:O | 1.93 | 1.16 |
| 2:H:117:LEU:CD1 | 2:H:147:ASN:HB3 | 1.76 | 1.16 |
| 1:M:795:ARG:NH2 | 3:O:116:GLU:CD | 1.98 | 1.16 |
| 1:M:819:ASN:CG | 2:N:92:ASP:CB | 2.11 | 1.16 |
| 1:M:836:PHE:CE2 | 2:N:160:GLY:N | 2.14 | 1.16 |
| 1:P:783:LEU:CA | 1:P:786:ILE:HG13 | 1.74 | 1.16 |
| 4:9:290:ARG:NH2 | 4:W:202:THR:HG23 | 1.59 | 1.16 |
| 1:A:798:LEU:HD11 | 3:C:126:LEU:HD21 | 1.21 | 1.16 |
| 1:D:201:ALA:O | 1:D:202:SER:HB3 | 1.36 | 1.16 |
| 1:G:642:LYS:CG | 4:V:23:GLY:N | 2.08 | 1.16 |
| 1:J:530:MET:HE2 | 4:W:354:GLN:CG | 1.75 | 1.16 |
| 1:J:538:GLU:O | 4:W:349:LEU:HD11 | 1.35 | 1.16 |
| 1:J:641:LYS:HD2 | 1:J:647:GLN:NE2 | 1.59 | 1.16 |
| 1:M:641:LYS:HD2 | 1:M:647:GLN:NE2 | 1.59 | 1.16 |
| 1:P:795:ARG:NH2 | 3:R:116:GLU:CB | 1.83 | 1.16 |
| 4:2:64:ILE:HG21 | 4:Z:166:TYR:CE2 | 1.79 | 1.16 |
| 1:D:642:LYS:CG | 4:9:23:GLY:N | 2.08 | 1.16 |
| 1:G:640:LYS:HB3 | 1:G:645:SER:OG | 1.46 | 1.16 |
| 1:G:795:ARG:HA | 3:I:118:MET:HE1 | 1.23 | 1.16 |
| 1:J:642:LYS:CG | 4:W:23:GLY:N | 2.08 | 1.16 |
| 1:J:818:TYR:CE1 | 2:K:127:ARG:CZ | 2.28 | 1.16 |
| 1:J:838:ILE:HD11 | 2:K:54:MET:HE3 | 1.19 | 1.16 |
| 1:M:641:LYS:CB | 1:M:647:GLN:NE2 | 2.07 | 1.16 |
| 1:M:649:VAL:HA | 1:M:649:VAL:CG2 | 1.76 | 1.16 |
| 1:M:806:MET:C | 1:M:807:VAL:N | 1.99 | 1.16 |
| 1:P:641:LYS:CE | 4:1:348:SER:O | 1.93 | 1.16 |
| 1:D:530:MET:HE2 | 4:9:354:GLN:HG2 | 1.26 | 1.15 |
| 1:D:640:LYS:HB3 | 1:D:645:SER:OG | 1.45 | 1.15 |
| 1:D:823:PHE:CE1 | 2:E:160:GLY:CA | 2.29 | 1.15 |
| 2:E:117:LEU:CD1 | 2:E:147:ASN:HB3 | 1.76 | 1.15 |
| 1:G:641:LYS:HD2 | 1:G:647:GLN:NE2 | 1.59 | 1.15 |
| 1:J:735:GLY:O | 1:J:743:ALA:CB | 1.91 | 1.15 |
| 1:J:817:GLN:CD | 2:K:127:ARG:HD2 | 1.64 | 1.15 |
| 1:M:709:LYS:C | 1:M:710:GLY:N | 1.99 | 1.15 |
| 1:A:95:THR:OG1 | 1:A:769:ALA:C | 1.84 | 1.15 |
| 1:A:800:ARG:NH2 | 3:C:40:ASN:HD21 | 1.42 | 1.15 |
| 1:D:727:LEU:CG | 1:D:782:MLY:CE | 2.22 | 1.15 |
| 1:G:641:LYS:HG3 | 1:G:647:GLN:HG3 | 1.20 | 1.15 |
| 1:G:721:LYS:HA | 1:G:736:GLN:NE2 | 1.58 | 1.15 |
| 1:M:218:LEU:HB2 | 1:M:221:GLN:HG3 | 1.17 | 1.15 |
| 1:P:641:LYS:HD2 | 1:P:647:GLN:NE2 | 1.59 | 1.15 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:542:PHE:HA | 4:8:143:TYR:CE1 | 1.82 | 1.15 |
| 1:A:791:GLN:HE22 | 3:C:116:GLU:N | 1.42 | 1.15 |
| 1:A:799:MET:SD | 3:C:32:ASP:CA | 2.34 | 1.15 |
| 1:D:215:GLN:HA | 1:D:340:ILE:CG2 | 1.76 | 1.15 |
| 1:G:796:GLY:HA2 | 3:I:35:ARG:HD3 | 1.25 | 1.15 |
| 1:J:640:LYS:HB3 | 1:J:645:SER:OG | 1.45 | 1.15 |
| 1:J:641:LYS:CE | 4:W:348:SER:O | 1.93 | 1.15 |
| 1:P:639:GLY:HA3 | 4:1:344:SER:O | 1.46 | 1.15 |
| 1:D:542:PHE:HA | 4:9:143:TYR:CE1 | 1.82 | 1.15 |
| 1:G:639:GLY:CA | 4:V:345:ILE:HA | 1.73 | 1.15 |
| 2:N:111:SER:CA | 2:N:148:VAL:O | 1.95 | 1.15 |
| 1:P:642:LYS:CG | 4:1:23:GLY:N | 2.08 | 1.15 |
| 1:P:819:ASN:CG | 2:Q:92:ASP:CB | 2.14 | 1.15 |
| 1:P:819:ASN:CA | 2:Q:90:GLY:O | 1.93 | 1.15 |
| 4:W:325:MET:SD | 4:Y:244:ASP:CB | 2.35 | 1.15 |
| 1:D:735:GLY:O | 1:D:743:ALA:CB | 1.91 | 1.15 |
| 1:G:542:PHE:HA | 4:V:143:TYR:CE1 | 1.82 | 1.15 |
| 1:J:538:GLU:OE2 | 4:W:355:MET:HE1 | 1.44 | 1.15 |
| 1:J:542:PHE:HA | 4:W:143:TYR:CE1 | 1.82 | 1.15 |
| 1:M:735:GLY:O | 1:M:743:ALA:CB | 1.91 | 1.15 |
| 1:P:640:LYS:HB3 | 1:P:645:SER:OG | 1.45 | 1.15 |
| 4:V:325:MET:SD | 4:X:244:ASP:CB | 2.33 | 1.15 |
| 1:A:639:GLY:HA2 | 4:8:345:ILE:HA | 1.26 | 1.14 |
| 1:A:641:LYS:NZ | 4:8:348:SER:O | 1.80 | 1.14 |
| 1:D:649:VAL:HA | 1:D:649:VAL:CG2 | 1.76 | 1.14 |
| 1:G:508:ILE:HD11 | 1:G:759:ALA:CB | 1.76 | 1.14 |
| 1:G:639:GLY:HA3 | 4:V:344:SER:O | 1.47 | 1.14 |
| 2:H:111:SER:CA | 2:H:148:VAL:O | 1.95 | 1.14 |
| 1:J:639:GLY:HA3 | 4:W:344:SER:O | 1.46 | 1.14 |
| 1:J:831:TRP:HH2 | 2:K:47:LEU:CD2 | 1.54 | 1.14 |
| 1:M:542:PHE:HA | 4:Z:143:TYR:CE1 | 1.82 | 1.14 |
| 2:N:112:ILE:O | 2:N:147:ASN:O | 1.66 | 1.14 |
| 2:N:117:LEU:CD1 | 2:N:147:ASN:HB3 | 1.76 | 1.14 |
| 2:Q:112:ILE:O | 2:Q:147:ASN:O | 1.66 | 1.14 |
| 4:7:290:ARG:NH2 | 4:9:202:THR:HG23 | 1.59 | 1.14 |
| 2:B:111:SER:CA | 2:B:148:VAL:O | 1.95 | 1.14 |
| 1:D:538:GLU:OE2 | 4:9:355:MET:HE1 | 1.44 | 1.14 |
| 1:D:797:PHE:CE1 | 3:F:146:ILE:HA | 1.81 | 1.14 |
| 1:G:649:VAL:HA | 1:G:649:VAL:CG2 | 1.76 | 1.14 |
| 1:G:797:PHE:CE2 | 3:I:126:LEU:CD2 | 2.29 | 1.14 |
| 1:J:557:GLU:HA | 4:Y:47:MET:CA | 1.48 | 1.14 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:639:GLY:HA2 | 4:W:345:ILE:HA | 1.26 | 1.14 |
| 1:J:754:ASP:CA | 1:J:780:ASP:OD2 | 1.95 | 1.14 |
| 1:P:538:GLU:C | 4:1:349:LEU:HD11 | 1.54 | 1.14 |
| 1:P:736:GLN:N | 1:P:743:ALA:CB | 2.05 | 1.14 |
| 1:A:639:GLY:HA3 | 4:8:344:SER:O | 1.47 | 1.14 |
| 2:E:111:SER:CA | 2:E:148:VAL:O | 1.95 | 1.14 |
| 2:E:121:LEU:CA | 2:E:128:PHE:HB3 | 1.77 | 1.14 |
| 2:H:112:ILE:O | 2:H:147:ASN:O | 1.65 | 1.14 |
| 2:H:117:LEU:HD12 | 2:H:147:ASN:OD1 | 1.32 | 1.14 |
| 1:J:649:VAL:HA | 1:J:649:VAL:CG2 | 1.76 | 1.14 |
| 1:J:756:THR:CG2 | 1:J:776:GLU:CA | 2.25 | 1.14 |
| 1:P:93:MET:CG | 1:P:714:ARG:O | 1.96 | 1.14 |
| 1:P:201:ALA:O | 1:P:202:SER:HB3 | 1.36 | 1.14 |
| 1:P:542:PHE:HA | 4:1:143:TYR:CE1 | 1.82 | 1.14 |
| 1:P:792:ALA:CB | 3:R:42:THR:HG22 | 1.77 | 1.14 |
| 1:P:799:MET:SD | 3:R:32:ASP:HB3 | 1.88 | 1.14 |
| 1:A:93:MET:HE1 | 1:A:715:VAL:HG13 | 1.16 | 1.14 |
| 1:A:649:VAL:HA | 1:A:649:VAL:CG2 | 1.76 | 1.14 |
| 1:A:795:ARG:HD3 | 3:C:43:ASN:OD1 | 1.47 | 1.14 |
| 1:G:755:HIS:N | 1:G:779:ARG:CZ | 2.10 | 1.14 |
| 2:K:121:LEU:CA | 2:K:128:PHE:HB3 | 1.78 | 1.14 |
| 1:M:639:GLY:HA3 | 4:Z:344:SER:O | 1.46 | 1.14 |
| 1:P:783:LEU:HA | 1:P:786:ILE:CD1 | 1.78 | 1.14 |
| 1:A:538:GLU:OE2 | 4:8:355:MET:HE1 | 1.46 | 1.14 |
| 1:D:538:GLU:C | 4:9:349:LEU:HD12 | 1.48 | 1.14 |
| 1:D:800:ARG:NH2 | 3:F:40:ASN:HD21 | 1.43 | 1.14 |
| 2:E:111:SER:CB | 2:E:148:VAL:C | 1.93 | 1.14 |
| 2:E:112:ILE:O | 2:E:147:ASN:O | 1.65 | 1.14 |
| 1:J:215:GLN:HA | 1:J:340:ILE:CG2 | 1.75 | 1.14 |
| 2:K:117:LEU:CD1 | 2:K:147:ASN:HB3 | 1.76 | 1.14 |
| 1:P:201:ALA:O | 1:P:202:SER:CB | 1.92 | 1.14 |
| 1:P:215:GLN:HA | 1:P:340:ILE:CG2 | 1.75 | 1.14 |
| 1:P:641:LYS:NZ | 4:1:348:SER:O | 1.80 | 1.14 |
| 1:A:642:LYS:CG | 4:8:23:GLY:N | 2.09 | 1.13 |
| 1:D:641:LYS:NZ | 4:9:348:SER:O | 1.80 | 1.13 |
| 1:D:799:MET:SD | 3:F:32:ASP:CA | 2.35 | 1.13 |
| 1:G:557:GLU:HB3 | 4:X:46:GLY:O | 0.99 | 1.13 |
| 1:M:640:LYS:HB3 | 1:M:645:SER:OG | 1.46 | 1.13 |
| 1:P:546:THR:CG2 | 4:3:46:GLY:C | 2.16 | 1.13 |
| 1:P:546:THR:OG1 | 4:3:46:GLY:N | 1.79 | 1.13 |
| 1:P:639:GLY:HA2 | 4:1:345:ILE:HA | 1.26 | 1.13 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:P:649:VAL:CG2 | 1:P:649:VAL:HA | 1.76 | 1.13 |
| 2:Q:121:LEU:CA | 2:Q:128:PHE:HB3 | 1.78 | 1.13 |
| 1:D:599:ASN:OD1 | 1:D:649:VAL:CB | 1.96 | 1.13 |
| 1:G:553:MLY:CE | 4:X:45:VAL:HG11 | 1.53 | 1.13 |
| 1:G:801:VAL:HG21 | 3:I:126:LEU:HD23 | 1.14 | 1.13 |
| 1:G:831:TRP:HE1 | 2:H:67:MET:HB3 | 1.05 | 1.13 |
| 1:J:97:LEU:HD23 | 1:J:712:PRO:HB3 | 1.28 | 1.13 |
| 2:K:111:SER:CA | 2:K:148:VAL:O | 1.95 | 1.13 |
| 1:M:795:ARG:HB3 | 3:O:35:ARG:CZ | 1.76 | 1.13 |
| 1:M:799:MET:SD | 3:O:32:ASP:CG | 2.27 | 1.13 |
| 1:A:553:MLY:CE | 4:V:45:VAL:HA | 1.52 | 1.13 |
| 1:A:641:LYS:HD2 | 1:A:647:GLN:NE2 | 1.59 | 1.13 |
| 1:D:800:ARG:HH22 | 3:F:40:ASN:ND2 | 1.45 | 1.13 |
| 1:D:831:TRP:HZ2 | 2:E:47:LEU:CB | 1.60 | 1.13 |
| 1:G:635:GLY:HA2 | 4:V:334:GLU:HG2 | 1.16 | 1.13 |
| 1:G:721:LYS:HG3 | 1:G:736:GLN:HG2 | 1.25 | 1.13 |
| 1:G:795:ARG:HH21 | 3:I:116:GLU:CG | 1.59 | 1.13 |
| 1:M:641:LYS:NZ | 4:Z:348:SER:O | 1.80 | 1.13 |
| 2:N:121:LEU:CA | 2:N:128:PHE:HB3 | 1.77 | 1.13 |
| 4:3:290:ARG:NH2 | 4:5:202:THR:HG23 | 1.41 | 1.13 |
| 1:A:218:LEU:HB2 | 1:A:221:GLN:HG3 | 1.17 | 1.13 |
| 1:A:505:MLY:HG2 | 1:A:762:HIS:CD2 | 1.83 | 1.13 |
| 1:A:541:MET:C | 4:8:143:TYR:OH | 1.87 | 1.13 |
| 1:A:599:ASN:OD1 | 1:A:649:VAL:CB | 1.96 | 1.13 |
| 1:D:538:GLU:C | 4:9:349:LEU:HD11 | 1.54 | 1.13 |
| 1:D:834:LEU:HD21 | 2:E:54:MET:HE2 | 1.30 | 1.13 |
| 1:G:218:LEU:HB2 | 1:G:221:GLN:HG3 | 1.17 | 1.13 |
| 1:J:641:LYS:NZ | 4:W:348:SER:O | 1.80 | 1.13 |
| 1:M:721:LYS:HG3 | 1:M:736:GLN:HG2 | 1.25 | 1.13 |
| 1:P:599:ASN:OD1 | 1:P:649:VAL:CB | 1.96 | 1.13 |
| 1:P:639:GLY:CA | 4:1:345:ILE:HA | 1.73 | 1.13 |
| 2:Q:111:SER:CA | 2:Q:148:VAL:O | 1.95 | 1.13 |
| 2:Q:117:LEU:CD1 | 2:Q:147:ASN:HB3 | 1.75 | 1.13 |
| 1:D:201:ALA:O | 1:D:202:SER:CB | 1.92 | 1.13 |
| 1:D:639:GLY:HA3 | 4:9:344:SER:O | 1.47 | 1.13 |
| 1:G:201:ALA:O | 1:G:202:SER:CB | 1.92 | 1.13 |
| 1:G:557:GLU:CA | 4:X:48:GLY:N | 1.99 | 1.12 |
| 1:G:599:ASN:OD1 | 1:G:649:VAL:CB | 1.96 | 1.12 |
| 1:G:641:LYS:CE | 1:G:647:GLN:OE1 | 1.97 | 1.12 |
| 1:G:831:TRP:CZ2 | 2:H:47:LEU:CD2 | 2.29 | 1.12 |
| 2:H:121:LEU:CA | 2:H:128:PHE:HB3 | 1.77 | 1.13 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:838:ILE:CD1 | 2:K:54:MET:CE | 2.26 | 1.13 |
| 1:M:541:MET:C | 4:Z:143:TYR:OH | 1.87 | 1.12 |
| 1:M:599:ASN:OD1 | 1:M:649:VAL:CB | 1.96 | 1.12 |
| 1:M:831:TRP:CH2 | 2:N:47:LEU:HD22 | 1.82 | 1.13 |
| 1:J:541:MET:C | 4:W:143:TYR:OH | 1.87 | 1.12 |
| 1:M:838:ILE:HD11 | 2:N:54:MET:HE1 | 1.13 | 1.12 |
| 1:P:93:MET:HG2 | 1:P:714:ARG:O | 1.49 | 1.12 |
| 1:P:541:MET:C | 4:1:143:TYR:OH | 1.87 | 1.13 |
| 1:A:635:GLY:HA2 | 4:8:334:GLU:HG2 | 1.16 | 1.12 |
| 1:D:218:LEU:HB2 | 1:D:221:GLN:HG3 | 1.17 | 1.12 |
| 1:P:530:MET:HE2 | 4:1:354:GLN:HG2 | 1.13 | 1.12 |
| 3:R:48:LYS:C | 3:R:52:ASN:ND2 | 2.03 | 1.12 |
| 4:2:203:THR:H | 4:Z:287:ILE:HG12 | 1.07 | 1.12 |
| 4:2:287:ILE:HG23 | 4:4:202:THR:OG1 | 1.48 | 1.12 |
| 1:D:541:MET:C | 4:9:143:TYR:OH | 1.87 | 1.12 |
| 1:G:541:MET:C | 4:V:143:TYR:OH | 1.87 | 1.12 |
| 1:G:553:MLY:CE | 4:X:45:VAL:HG12 | 1.68 | 1.12 |
| 1:J:599:ASN:OD1 | 1:J:649:VAL:CB | 1.96 | 1.12 |
| 1:J:756:THR:HG22 | 1:J:776:GLU:CD | 1.67 | 1.12 |
| 1:D:641:LYS:CE | 1:D:647:GLN:OE1 | 1.97 | 1.12 |
| 1:G:736:GLN:N | 1:G:743:ALA:CB | 2.04 | 1.12 |
| 1:G:754:ASP:HB3 | 1:G:776:GLU:OE2 | 0.95 | 1.12 |
| 1:J:530:MET:HE2 | 4:W:354:GLN:HG2 | 1.16 | 1.12 |
| 1:J:641:LYS:CE | 1:J:647:GLN:OE1 | 1.97 | 1.12 |
| 1:A:791:GLN:NE2 | 3:C:116:GLU:N | 1.97 | 1.12 |
| 1:D:553:MLY:HB3 | 4:W:46:GLY:CA | 1.51 | 1.12 |
| 1:G:818:TYR:CE1 | 2:H:127:ARG:CZ | 2.32 | 1.12 |
| 1:J:218:LEU:HB2 | 1:J:221:GLN:HG3 | 1.17 | 1.12 |
| 1:J:721:LYS:HG3 | 1:J:736:GLN:HG2 | 1.25 | 1.12 |
| 1:M:817:GLN:HB3 | 2:N:127:ARG:HH11 | 1.13 | 1.12 |
| 2:N:111:SER:HB3 | 2:N:148:VAL:O | 1.50 | 1.12 |
| 4:1:243:PRO:HB3 | 4:Y:291:LYS:HE3 | 1.15 | 1.12 |
| 1:A:201:ALA:O | 1:A:202:SER:HB3 | 1.36 | 1.12 |
| 1:A:498:LEU:CD2 | 1:A:764:MLY:HH22 | 1.77 | 1.12 |
| 1:A:639:GLY:CA | 4:8:345:ILE:HA | 1.74 | 1.12 |
| 2:B:121:LEU:O | 2:B:128:PHE:HB2 | 0.94 | 1.12 |
| 1:D:649:VAL:HG22 | 1:D:649:VAL:HG13 | 1.21 | 1.12 |
| 1:D:727:LEU:CD1 | 1:D:782:MLY:NZ | 2.07 | 1.12 |
| 2:E:121:LEU:C | 2:E:128:PHE:HB2 | 1.67 | 1.12 |
| 3:F:48:LYS:C | 3:F:52:ASN:ND2 | 2.03 | 1.12 |
| 1:G:623:PHE:CB | 1:G:623:PHE:CG | 2.33 | 1.12 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:I:48:LYS:C | 3:I:52:ASN:ND2 | 2.03 | 1.12 |
| 1:J:623:PHE:CG | 1:J:623:PHE:CB | 2.33 | 1.12 |
| 1:M:623:PHE:CG | 1:M:623:PHE:CB | 2.33 | 1.12 |
| 1:M:795:ARG:CZ | 3:O:116:GLU:OE2 | 1.96 | 1.12 |
| 1:M:834:LEU:HD13 | 2:N:51:PHE:CE1 | 1.83 | 1.12 |
| 1:A:623:PHE:CB | 1:A:623:PHE:CG | 2.33 | 1.11 |
| 2:B:117:LEU:CD1 | 2:B:147:ASN:HB3 | 1.76 | 1.11 |
| 1:G:215:GLN:N | 1:G:340:ILE:HG12 | 1.20 | 1.11 |
| 1:G:503:TYR:CE1 | 1:G:711:PHE:CE2 | 2.37 | 1.11 |
| 1:G:530:MET:CE | 4:V:354:GLN:HG2 | 1.80 | 1.11 |
| 1:G:641:LYS:NZ | 4:V:348:SER:O | 1.80 | 1.11 |
| 1:G:739:ASP:HB3 | 1:G:742:LYS:HB3 | 1.21 | 1.11 |
| 1:G:792:ALA:HB3 | 3:I:42:THR:HG22 | 1.20 | 1.11 |
| 1:J:538:GLU:C | 4:W:349:LEU:HD11 | 1.54 | 1.11 |
| 1:J:641:LYS:HG3 | 1:J:647:GLN:HG3 | 1.21 | 1.11 |
| 1:J:649:VAL:O | 1:J:649:VAL:HG12 | 0.94 | 1.11 |
| 1:J:797:PHE:CE1 | 3:L:146:ILE:HD12 | 1.84 | 1.11 |
| 1:M:201:ALA:O | 1:M:202:SER:CB | 1.92 | 1.11 |
| 1:P:641:LYS:CE | 1:P:647:GLN:OE1 | 1.97 | 1.11 |
| 4:X:287:ILE:HG22 | 4:Z:205:GLU:OE2 | 1.48 | 1.11 |
| 1:A:215:GLN:N | 1:A:340:ILE:HG12 | 1.20 | 1.11 |
| 3:C:48:LYS:C | 3:C:52:ASN:ND2 | 2.03 | 1.11 |
| 1:D:649:VAL:O | 1:D:649:VAL:HG12 | 0.94 | 1.11 |
| 1:D:721:LYS:HG3 | 1:D:736:GLN:HG2 | 1.25 | 1.11 |
| 1:D:797:PHE:CD1 | 3:F:146:ILE:CG2 | 2.32 | 1.11 |
| 2:H:121:LEU:O | 2:H:128:PHE:HB2 | 0.94 | 1.11 |
| 1:P:508:ILE:HD11 | 1:P:759:ALA:CB | 1.79 | 1.11 |
| 4:7:290:ARG:CZ | 4:9:202:THR:HG21 | 1.81 | 1.11 |
| 1:A:641:LYS:CE | 1:A:647:GLN:CD | 2.18 | 1.11 |
| 1:A:792:ALA:CB | 3:C:42:THR:HG22 | 1.78 | 1.11 |
| 2:B:121:LEU:CA | 2:B:128:PHE:HB3 | 1.77 | 1.11 |
| 1:G:754:ASP:HB2 | 1:G:776:GLU:HA | 1.18 | 1.11 |
| 1:G:795:ARG:HA | 3:I:118:MET:CE | 1.81 | 1.11 |
| 1:J:829:TRP:CZ2 | 2:K:87:LYS:HE2 | 1.84 | 1.11 |
| 2:K:121:LEU:O | 2:K:128:PHE:HB2 | 0.94 | 1.11 |
| 1:M:641:LYS:CE | 1:M:647:GLN:OE1 | 1.97 | 1.11 |
| 1:M:798:LEU:HD11 | 3:O:126:LEU:CD1 | 1.79 | 1.11 |
| 1:P:623:PHE:CG | 1:P:623:PHE:CB | 2.33 | 1.11 |
| 1:P:649:VAL:O | 1:P:649:VAL:HG12 | 0.94 | 1.11 |
| 1:P:734:GLU:O | 1:P:738:MET:HG2 | 1.51 | 1.11 |
| 1:P:836:PHE:CE2 | 2:Q:160:GLY:N | 2.17 | 1.11 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:8:287:ILE:HG21 | 4:V:205:GLU:HG2 | 1.17 | 1.11 |
| 1:D:641:LYS:CE | 1:D:647:GLN:CD | 2.18 | 1.11 |
| 2:E:121:LEU:O | 2:E:128:PHE:HB2 | 0.94 | 1.11 |
| 1:G:752:ASP:O | 1:G:780:ASP:OD1 | 1.69 | 1.11 |
| 1:G:838:ILE:CD1 | 2:H:54:MET:CE | 2.28 | 1.11 |
| 2:H:111:SER:HB3 | 2:H:148:VAL:O | 1.49 | 1.11 |
| 1:J:201:ALA:O | 1:J:202:SER:HB3 | 1.35 | 1.11 |
| 3:L:48:LYS:C | 3:L:52:ASN:ND2 | 2.03 | 1.11 |
| 1:M:530:MET:HE2 | 4:Z:354:GLN:HG2 | 1.28 | 1.11 |
| 1:M:639:GLY:HA2 | 4:Z:345:ILE:HA | 1.26 | 1.11 |
| 1:M:639:GLY:CA | 4:Z:345:ILE:HA | 1.73 | 1.11 |
| 1:M:736:GLN:N | 1:M:743:ALA:CB | 2.05 | 1.11 |
| 1:M:792:ALA:HB2 | 3:O:42:THR:CG2 | 1.80 | 1.11 |
| 2:Q:117:LEU:HB2 | 2:Q:147:ASN:CG | 1.70 | 1.11 |
| 4:9:290:ARG:CZ | 4:W:202:THR:HG21 | 1.81 | 1.11 |
| 1:G:93:MET:HA | 1:G:714:ARG:H | 1.07 | 1.11 |
| 1:G:641:LYS:CE | 1:G:647:GLN:CD | 2.18 | 1.11 |
| 1:G:832:MET:SD | 2:H:84:PHE:HE2 | 1.72 | 1.11 |
| 1:M:530:MET:CE | 4:Z:354:GLN:HG2 | 1.80 | 1.11 |
| 4:4:287:ILE:HD13 | 4:6:203:THR:HB | 1.22 | 1.11 |
| 4:X:287:ILE:HG12 | 4:Z:201:VAL:N | 1.41 | 1.11 |
| 1:A:641:LYS:CE | 1:A:647:GLN:OE1 | 1.97 | 1.10 |
| 1:A:649:VAL:HG13 | 1:A:649:VAL:HG22 | 1.21 | 1.10 |
| 1:A:707:CYS:HA | 1:A:714:ARG:CZ | 1.80 | 1.10 |
| 2:B:112:ILE:O | 2:B:147:ASN:O | 1.65 | 1.10 |
| 2:B:117:LEU:HB2 | 2:B:147:ASN:CG | 1.71 | 1.10 |
| 1:D:727:LEU:HD11 | 1:D:782:MLY:HD3 | 1.25 | 1.10 |
| 1:D:795:ARG:CB | 3:F:35:ARG:HH12 | 1.52 | 1.10 |
| 1:G:201:ALA:O | 1:G:202:SER:HB3 | 1.36 | 1.10 |
| 1:G:649:VAL:O | 1:G:649:VAL:HG12 | 0.94 | 1.10 |
| 1:G:838:ILE:CD1 | 2:H:54:MET:HE3 | 1.79 | 1.10 |
| 1:M:649:VAL:O | 1:M:649:VAL:HG12 | 0.94 | 1.10 |
| 2:N:117:LEU:HB2 | 2:N:147:ASN:CG | 1.71 | 1.10 |
| 2:N:121:LEU:O | 2:N:128:PHE:HB2 | 0.94 | 1.10 |
| 2:N:144:VAL:HG13 | 2:N:153:ILE:HD11 | 1.21 | 1.10 |
| 1:P:649:VAL:HG22 | 1:P:649:VAL:HG13 | 1.21 | 1.10 |
| 2:Q:121:LEU:O | 2:Q:128:PHE:HB2 | 0.94 | 1.10 |
| 1:A:734:GLU:O | 1:A:738:MET:HG2 | 1.51 | 1.10 |
| 1:A:823:PHE:CE1 | 2:B:160:GLY:HA2 | 1.86 | 1.10 |
| 3:C:24:LYS:CB | 3:C:63:ILE:O | 1.99 | 1.10 |
| 1:D:635:GLY:HA2 | 4:9:334:GLU:HG2 | 1.16 | 1.10 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:P:721:LYS:HG3 | 1:P:736:GLN:HG2 | 1.25 | 1.10 |
| 1:P:798:LEU:CD1 | 3:R:126:LEU:CD1 | 2.23 | 1.10 |
| 1:A:819:ASN:OD1 | 2:B:91:ALA:HA | 1.50 | 1.10 |
| 1:D:202:SER:CA | 1:D:207:LYS:HE2 | 1.82 | 1.10 |
| 1:D:734:GLU:O | 1:D:738:MET:HG2 | 1.51 | 1.10 |
| 1:D:823:PHE:CE1 | 2:E:160:GLY:HA2 | 1.86 | 1.10 |
| 1:G:639:GLY:HA2 | 4:V:345:ILE:HA | 1.26 | 1.10 |
| 1:G:734:GLU:O | 1:G:738:MET:HG2 | 1.51 | 1.10 |
| 1:G:769:ALA:CB | 1:G:770:GLY:CA | 2.28 | 1.10 |
| 1:G:813:ILE:HG23 | 2:H:128:PHE:CZ | 1.86 | 1.10 |
| 1:J:641:LYS:CE | 1:J:647:GLN:CD | 2.18 | 1.10 |
| 1:J:649:VAL:HG22 | 1:J:649:VAL:HG13 | 1.21 | 1.10 |
| 1:J:736:GLN:N | 1:J:743:ALA:CB | 2.05 | 1.10 |
| 2:K:111:SER:CB | 2:K:148:VAL:C | 1.93 | 1.10 |
| 3:O:48:LYS:C | 3:O:52:ASN:ND2 | 2.03 | 1.10 |
| 1:P:641:LYS:CE | 1:P:647:GLN:CD | 2.18 | 1.10 |
| 1:P:798:LEU:CG | 3:R:126:LEU:HD11 | 1.82 | 1.10 |
| 1:P:834:LEU:HD13 | 2:Q:51:PHE:HE1 | 1.00 | 1.10 |
| 2:Q:111:SER:HB3 | 2:Q:148:VAL:O | 1.50 | 1.10 |
| 4:2:202:THR:HG21 | 4:Z:290:ARG:HH21 | 0.97 | 1.10 |
| 1:A:95:THR:OG1 | 1:A:769:ALA:CA | 2.00 | 1.10 |
| 1:A:649:VAL:O | 1:A:649:VAL:HG12 | 0.94 | 1.10 |
| 1:A:795:ARG:HB3 | 3:C:35:ARG:NH2 | 1.65 | 1.10 |
| 1:J:530:MET:CE | 4:W:354:GLN:HG2 | 1.80 | 1.10 |
| 1:M:734:GLU:O | 1:M:738:MET:HG2 | 1.51 | 1.10 |
| 1:P:641:LYS:HE3 | 1:P:647:GLN:OE1 | 1.50 | 1.10 |
| 1:P:739:ASP:HB3 | 1:P:742:LYS:HB3 | 1.21 | 1.10 |
| 4:2:203:THR:N | 4:Z:287:ILE:HG12 | 1.67 | 1.10 |
| 1:D:530:MET:CE | 4:9:354:GLN:HG2 | 1.80 | 1.10 |
| 1:G:538:GLU:C | 4:V:349:LEU:HD11 | 1.54 | 1.10 |
| 1:G:769:ALA:HB3 | 1:G:770:GLY:CA | 1.82 | 1.10 |
| 1:J:635:GLY:HA2 | 4:W:334:GLU:HG2 | 1.16 | 1.10 |
| 1:M:202:SER:CA | 1:M:207:LYS:HE2 | 1.82 | 1.10 |
| 1:M:641:LYS:CE | 1:M:647:GLN:CD | 2.18 | 1.10 |
| 1:M:739:ASP:HB3 | 1:M:742:LYS:HB3 | 1.22 | 1.10 |
| 1:P:797:PHE:CZ | 3:R:146:ILE:HD13 | 1.87 | 1.10 |
| 3:R:24:LYS:CB | 3:R:63:ILE:O | 1.99 | 1.10 |
| 1:A:530:MET:CE | 4:8:354:GLN:HG2 | 1.80 | 1.09 |
| 1:D:623:PHE:CB | 1:D:623:PHE:CG | 2.33 | 1.09 |
| 2:E:117:LEU:HB2 | 2:E:147:ASN:CG | 1.71 | 1.09 |
| 1:G:754:ASP:HB2 | 1:G:776:GLU:CD | 1.64 | 1.09 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:757:GLN:OE1 | 1:G:772:LEU:O | 1.69 | 1.09 |
| 1:J:202:SER:CA | 1:J:207:LYS:HE2 | 1.82 | 1.09 |
| 1:J:641:LYS:HE3 | 1:J:647:GLN:OE1 | 1.50 | 1.09 |
| 1:M:571:ALA:O | 1:M:572:LYS:HG3 | 1.52 | 1.09 |
| 1:M:649:VAL:HG22 | 1:M:649:VAL:HG13 | 1.21 | 1.09 |
| 1:P:834:LEU:HD13 | 2:Q:51:PHE:CE1 | 1.86 | 1.09 |
| 2:Q:121:LEU:C | 2:Q:128:PHE:HB2 | 1.67 | 1.09 |
| 4:4:322:PRO:HB3 | 4:6:244:ASP:CG | 1.72 | 1.09 |
| 4:X:288:ASP:HB2 | 4:Z:204:ALA:HB3 | 1.12 | 1.09 |
| 1:D:831:TRP:CE2 | 2:E:47:LEU:HD22 | 1.86 | 1.09 |
| 2:H:111:SER:CB | 2:H:148:VAL:C | 1.93 | 1.09 |
| 2:H:117:LEU:HB2 | 2:H:147:ASN:CG | 1.70 | 1.09 |
| 2:K:117:LEU:HB2 | 2:K:147:ASN:CG | 1.70 | 1.09 |
| 3:L:24:LYS:CB | 3:L:63:ILE:O | 1.99 | 1.09 |
| 1:M:819:ASN:HA | 2:N:90:GLY:O | 0.94 | 1.09 |
| 1:P:202:SER:CA | 1:P:207:LYS:HE2 | 1.82 | 1.09 |
| 1:P:530:MET:CE | 4:1:354:GLN:HG2 | 1.80 | 1.09 |
| 4:1:244:ASP:N | 4:Y:291:LYS:HD2 | 1.66 | 1.09 |
| 4:8:290:ARG:CZ | 4:V:202:THR:HG21 | 1.81 | 1.09 |
| 1:A:795:ARG:NE | 3:C:43:ASN:OD1 | 1.84 | 1.09 |
| 1:A:819:ASN:ND2 | 2:B:90:GLY:C | 2.05 | 1.09 |
| 1:D:576:GLU:HG2 | 1:D:577:ALA:N | 1.66 | 1.09 |
| 1:G:757:GLN:CG | 1:G:776:GLU:OE2 | 2.01 | 1.09 |
| 1:G:830:PRO:HB3 | 2:H:67:MET:HE1 | 1.29 | 1.09 |
| 3:I:24:LYS:CB | 3:I:63:ILE:O | 1.99 | 1.09 |
| 1:J:571:ALA:O | 1:J:572:LYS:HG3 | 1.52 | 1.09 |
| 1:J:734:GLU:O | 1:J:738:MET:HG2 | 1.51 | 1.09 |
| 1:J:817:GLN:HB3 | 2:K:127:ARG:HD3 | 1.33 | 1.09 |
| 2:K:121:LEU:C | 2:K:128:PHE:HB2 | 1.67 | 1.09 |
| 1:P:218:LEU:HB2 | 1:P:221:GLN:HG3 | 1.17 | 1.09 |
| 1:P:795:ARG:HD2 | 3:R:43:ASN:OD1 | 1.42 | 1.09 |
| 1:A:498:LEU:HD21 | 1:A:764:MLY:HH22 | 1.33 | 1.09 |
| 2:E:117:LEU:HD12 | 2:E:147:ASN:OD1 | 1.32 | 1.09 |
| 3:F:24:LYS:CB | 3:F:63:ILE:O | 1.99 | 1.09 |
| 1:M:638:GLY:CA | 4:Z:341:ILE:O | 2.01 | 1.09 |
| 1:M:783:LEU:HG | 1:M:786:ILE:HD12 | 1.10 | 1.09 |
| 1:M:785:GLU:C | 1:M:786:ILE:N | 2.05 | 1.09 |
| 3:O:24:LYS:CB | 3:O:63:ILE:O | 1.99 | 1.09 |
| 1:P:93:MET:O | 1:P:713:SER:HB3 | 1.50 | 1.09 |
| 1:P:571:ALA:O | 1:P:572:LYS:HG3 | 1.52 | 1.09 |
| 1:P:721:LYS:HA | 1:P:736:GLN:CD | 1.73 | 1.09 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:530:MET:HE2 | 4:V:354:GLN:HG2 | 1.13 | 1.09 |
| 1:G:721:LYS:HA | 1:G:736:GLN:CD | 1.73 | 1.09 |
| 1:J:834:LEU:CD1 | 2:K:51:PHE:HE1 | 1.66 | 1.09 |
| 2:K:112:ILE:O | 2:K:147:ASN:O | 1.65 | 1.09 |
| 1:M:721:LYS:HA | 1:M:736:GLN:CD | 1.73 | 1.09 |
| 2:N:121:LEU:C | 2:N:128:PHE:HB2 | 1.67 | 1.09 |
| 1:P:783:LEU:HG | 1:P:786:ILE:HD12 | 1.31 | 1.09 |
| 4:2:203:THR:HG22 | 4:Z:287:ILE:CG2 | 1.83 | 1.09 |
| 4:2:287:ILE:HD13 | 4:4:203:THR:HB | 1.10 | 1.09 |
| 4:3:288:ASP:H | 4:5:203:THR:HG22 | 1.17 | 1.09 |
| 1:A:202:SER:CA | 1:A:207:LYS:HE2 | 1.82 | 1.08 |
| 1:D:739:ASP:HB3 | 1:D:742:LYS:HB3 | 1.21 | 1.08 |
| 1:D:769:ALA:C | 1:D:774:LEU:HB2 | 1.73 | 1.08 |
| 1:G:202:SER:CA | 1:G:207:LYS:HE2 | 1.82 | 1.08 |
| 1:G:571:ALA:O | 1:G:572:LYS:HG3 | 1.52 | 1.08 |
| 1:G:649:VAL:HG22 | 1:G:649:VAL:HG13 | 1.21 | 1.08 |
| 1:J:796:GLY:HA2 | 3:L:35:ARG:CD | 1.81 | 1.08 |
| 1:P:538:GLU:HA | 4:1:349:LEU:CD1 | 1.55 | 1.08 |
| 1:P:829:TRP:CZ2 | 2:Q:87:LYS:HE2 | 1.88 | 1.08 |
| 1:A:571:ALA:O | 1:A:572:LYS:HG3 | 1.52 | 1.08 |
| 1:A:638:GLY:CA | 4:8:341:ILE:O | 2.01 | 1.08 |
| 1:A:800:ARG:NH2 | 3:C:40:ASN:ND2 | 1.97 | 1.08 |
| 1:G:641:LYS:HE3 | 1:G:647:GLN:OE1 | 1.50 | 1.08 |
| 1:M:643:GLY:O | 1:M:644:SER:OG | 1.70 | 1.08 |
| 1:M:798:LEU:CD2 | 3:O:126:LEU:HD11 | 1.83 | 1.08 |
| 1:A:201:ALA:O | 1:A:202:SER:CB | 1.92 | 1.08 |
| 1:A:538:GLU:O | 4:8:349:LEU:HD11 | 1.35 | 1.08 |
| 1:D:538:GLU:HA | 4:9:349:LEU:CD1 | 1.55 | 1.08 |
| 1:D:643:GLY:O | 1:D:644:SER:OG | 1.70 | 1.08 |
| 1:G:643:GLY:O | 1:G:644:SER:OG | 1.70 | 1.08 |
| 1:J:538:GLU:HA | 4:W:349:LEU:CD1 | 1.55 | 1.08 |
| 4:1:246:GLN:HA | 4:Y:324:THR:CB | 1.84 | 1.08 |
| 1:A:641:LYS:HE3 | 1:A:647:GLN:OE1 | 1.50 | 1.08 |
| 1:D:721:LYS:HA | 1:D:736:GLN:CD | 1.73 | 1.08 |
| 1:D:838:ILE:CD1 | 2:E:54:MET:HE1 | 1.74 | 1.08 |
| 2:E:111:SER:CB | 2:E:148:VAL:O | 0.78 | 1.08 |
| 1:J:576:GLU:HG2 | 1:J:577:ALA:N | 1.66 | 1.08 |
| 1:M:736:GLN:HA | 1:M:743:ALA:HB3 | 1.35 | 1.08 |
| 1:A:149:GLN:HB2 | 1:A:718:ALA:HB3 | 1.12 | 1.08 |
| 1:D:72:VAL:HG13 | 1:D:76:GLN:HB3 | 1.36 | 1.08 |
| 1:G:641:LYS:HB2 | 1:G:647:GLN:NE2 | 1.68 | 1.08 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:721:LYS:HA | 1:J:736:GLN:CD | 1.73 | 1.08 |
| 1:M:529:PRO:HB3 | 4:Z:353:GLN:OE1 | 1.53 | 1.08 |
| 1:M:538:GLU:C | 4:Z:349:LEU:HD11 | 1.54 | 1.08 |
| 1:M:635:GLY:HA2 | 4:Z:334:GLU:HG2 | 1.16 | 1.08 |
| 1:P:643:GLY:O | 1:P:644:SER:OG | 1.70 | 1.08 |
| 2:Q:111:SER:CB | 2:Q:148:VAL:O | 0.78 | 1.08 |
| 4:2:287:ILE:HB | 4:4:203:THR:HG22 | 1.32 | 1.08 |
| 4:3:324:THR:CB | 4:5:243:PRO:O | 2.01 | 1.08 |
| 1:A:499:GLU:OE1 | 1:A:766:PHE:HZ | 1.16 | 1.07 |
| 1:A:736:GLN:HA | 1:A:743:ALA:HB3 | 1.35 | 1.07 |
| 1:A:798:LEU:CD1 | 3:C:126:LEU:HD21 | 1.83 | 1.07 |
| 2:B:111:SER:OG | 2:B:148:VAL:O | 1.71 | 1.07 |
| 1:D:541:MET:SD | 4:9:345:ILE:O | 2.12 | 1.07 |
| 1:D:639:GLY:HA2 | 4:9:345:ILE:HA | 1.26 | 1.07 |
| 1:D:813:ILE:HD13 | 2:E:128:PHE:HE1 | 0.91 | 1.07 |
| 1:G:538:GLU:OE2 | 4:V:355:MET:HE1 | 1.52 | 1.07 |
| 1:G:638:GLY:CA | 4:V:341:ILE:O | 2.02 | 1.07 |
| 2:H:111:SER:CB | 2:H:148:VAL:O | 0.78 | 1.07 |
| 1:J:638:GLY:CA | 4:W:341:ILE:O | 2.01 | 1.07 |
| 1:J:641:LYS:HD2 | 1:J:647:GLN:CD | 1.70 | 1.07 |
| 1:J:757:GLN:NE2 | 1:J:777:GLU:N | 2.02 | 1.07 |
| 1:P:409:GLY:N | 1:P:636:LYS:HG3 | 1.70 | 1.07 |
| 1:P:529:PRO:HB3 | 4:1:353:GLN:OE1 | 1.53 | 1.07 |
| 1:P:798:LEU:CD1 | 3:R:126:LEU:CD2 | 2.18 | 1.07 |
| 4:3:290:ARG:CZ | 4:5:202:THR:CG2 | 2.20 | 1.07 |
| 4:7:287:ILE:HG21 | 4:9:205:GLU:HG2 | 1.18 | 1.07 |
| 1:A:97:LEU:CD2 | 1:A:712:PRO:CB | 2.33 | 1.07 |
| 1:A:501:GLU:HG2 | 1:A:762:HIS:HD1 | 0.91 | 1.07 |
| 1:A:709:LYS:O | 1:A:710:GLY:CA | 2.02 | 1.07 |
| 2:B:111:SER:CB | 2:B:148:VAL:O | 0.78 | 1.07 |
| 1:D:713:SER:N | 1:D:771:LEU:HD22 | 1.57 | 1.07 |
| 1:G:409:GLY:N | 1:G:636:LYS:HG3 | 1.69 | 1.07 |
| 2:N:111:SER:CB | 2:N:148:VAL:O | 0.78 | 1.07 |
| 1:A:72:VAL:HG13 | 1:A:76:GLN:HB3 | 1.36 | 1.07 |
| 1:A:149:GLN:HE21 | 1:A:718:ALA:CB | 1.62 | 1.07 |
| 1:A:502:GLU:HA | 1:A:761:GLY:HA3 | 1.29 | 1.07 |
| 1:A:538:GLU:C | 4:8:349:LEU:HD11 | 1.54 | 1.07 |
| 1:A:721:LYS:HA | 1:A:736:GLN:CD | 1.73 | 1.07 |
| 1:D:409:GLY:N | 1:D:636:LYS:HG3 | 1.70 | 1.07 |
| 1:D:727:LEU:HG | 1:D:782:MLY:HE2 | 1.14 | 1.07 |
| 2:E:121:LEU:C | 2:E:128:PHE:HB3 | 1.72 | 1.07 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:H:121:LEU:C | 2:H:128:PHE:HB2 | 1.67 | 1.07 |
| 1:J:792:ALA:HA | 3:L:42:THR:HA | 1.30 | 1.07 |
| 1:J:817:GLN:CG | 2:K:127:ARG:CD | 2.32 | 1.07 |
| 2:K:111:SER:CB | 2:K:148:VAL:O | 0.78 | 1.07 |
| 1:M:409:GLY:N | 1:M:636:LYS:HG3 | 1.69 | 1.07 |
| 1:D:834:LEU:HG | 2:E:54:MET:HG3 | 1.29 | 1.07 |
| 1:G:538:GLU:O | 4:V:349:LEU:HD11 | 1.35 | 1.07 |
| 1:G:736:GLN:HA | 1:G:743:ALA:HB3 | 1.35 | 1.07 |
| 1:J:529:PRO:HB3 | 4:W:353:GLN:OE1 | 1.53 | 1.07 |
| 1:J:643:GLY:O | 1:J:644:SER:OG | 1.70 | 1.07 |
| 1:J:813:ILE:HG23 | 2:K:128:PHE:CE1 | 1.90 | 1.07 |
| 1:M:793:ARG:NH1 | 3:O:40:ASN:HD22 | 1.51 | 1.07 |
| 1:P:638:GLY:CA | 4:1:341:ILE:O | 2.01 | 1.07 |
| 2:Q:144:VAL:HG13 | 2:Q:153:ILE:HD11 | 1.22 | 1.07 |
| 4:3:322:PRO:HB3 | 4:5:244:ASP:CG | 1.75 | 1.07 |
| 4:X:287:ILE:CG1 | 4:Z:201:VAL:H | 1.60 | 1.07 |
| 1:A:541:MET:SD | 4:8:345:ILE:O | 2.12 | 1.07 |
| 1:A:643:GLY:O | 1:A:644:SER:OG | 1.70 | 1.07 |
| 1:D:641:LYS:HB2 | 1:D:647:GLN:NE2 | 1.68 | 1.07 |
| 1:D:641:LYS:HE3 | 1:D:647:GLN:OE1 | 1.50 | 1.07 |
| 1:D:713:SER:H | 1:D:771:LEU:HD22 | 0.97 | 1.07 |
| 1:D:726:VAL:HG12 | 1:D:785:GLU:HG2 | 1.34 | 1.07 |
| 1:J:541:MET:SD | 4:W:345:ILE:O | 2.13 | 1.07 |
| 1:J:791:GLN:CD | 3:L:116:GLU:HG3 | 1.74 | 1.07 |
| 1:J:831:TRP:HE1 | 2:K:67:MET:HB3 | 1.20 | 1.07 |
| 1:M:541:MET:SD | 4:Z:345:ILE:O | 2.13 | 1.07 |
| 1:P:72:VAL:HG13 | 1:P:76:GLN:HB3 | 1.37 | 1.07 |
| 1:P:641:LYS:HD2 | 1:P:647:GLN:CD | 1.70 | 1.07 |
| 1:P:736:GLN:HA | 1:P:743:ALA:HB3 | 1.35 | 1.07 |
| 1:P:783:LEU:HA | 1:P:786:ILE:HG13 | 1.09 | 1.07 |
| 2:Q:111:SER:CB | 2:Q:148:VAL:C | 1.93 | 1.07 |
| 4:1:3:ASP:HA | 4:1:6:THR:HB | 1.36 | 1.07 |
| 4:W:324:THR:HG21 | 4:Y:246:GLN:C | 1.61 | 1.07 |
| 1:A:530:MET:HE2 | 4:8:354:GLN:HG2 | 1.35 | 1.06 |
| 1:A:542:PHE:CG | 4:8:143:TYR:HE1 | 1.73 | 1.06 |
| 1:J:567:LYS:NZ | 4:Y:92:ASN:HD22 | 1.50 | 1.06 |
| 2:K:111:SER:OG | 2:K:148:VAL:O | 1.71 | 1.06 |
| 4:W:3:ASP:HA | 4:W:6:THR:HB | 1.36 | 1.06 |
| 2:B:121:LEU:C | 2:B:128:PHE:HB2 | 1.67 | 1.06 |
| 1:D:542:PHE:CG | 4:9:143:TYR:HE1 | 1.73 | 1.06 |
| 1:D:571:ALA:O | 1:D:572:LYS:HG3 | 1.52 | 1.06 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:795:ARG:HB3 | 3:F:35:ARG:NH2 | 1.69 | 1.06 |
| 1:G:557:GLU:HB3 | 4:X:46:GLY:C | 1.76 | 1.06 |
| 2:H:111:SER:OG | 2:H:148:VAL:O | 1.71 | 1.06 |
| 1:J:409:GLY:N | 1:J:636:LYS:HG3 | 1.69 | 1.06 |
| 1:J:756:THR:C | 1:J:776:GLU:OE1 | 1.93 | 1.06 |
| 1:M:538:GLU:OE2 | 4:Z:355:MET:HE1 | 1.52 | 1.06 |
| 1:M:793:ARG:NH1 | 3:O:40:ASN:ND2 | 2.02 | 1.06 |
| 1:P:538:GLU:OE2 | 4:1:355:MET:HE1 | 1.55 | 1.06 |
| 1:P:549:SER:HB2 | 4:3:43:VAL:HG21 | 1.35 | 1.06 |
| 1:P:838:ILE:CD1 | 2:Q:54:MET:CE | 2.34 | 1.06 |
| 4:2:202:THR:HB | 4:Z:287:ILE:HG23 | 1.37 | 1.06 |
| 2:B:114:LYS:HA | 2:B:146:GLY:O | 0.89 | 1.06 |
| 1:G:553:MLY:HE2 | 4:X:45:VAL:HB | 1.09 | 1.06 |
| 2:H:114:LYS:HA | 2:H:146:GLY:O | 0.89 | 1.06 |
| 1:J:635:GLY:HA3 | 4:W:341:ILE:HD13 | 1.36 | 1.06 |
| 1:J:736:GLN:HA | 1:J:743:ALA:HB3 | 1.35 | 1.06 |
| 1:J:834:LEU:CD1 | 2:K:51:PHE:CE1 | 2.38 | 1.06 |
| 1:M:641:LYS:HB2 | 1:M:647:GLN:NE2 | 1.68 | 1.06 |
| 1:P:541:MET:SD | 4:1:345:ILE:O | 2.13 | 1.06 |
| 4:9:287:ILE:HG21 | 4:W:205:GLU:HG2 | 1.17 | 1.06 |
| 1:A:502:GLU:CG | 1:A:761:GLY:HA3 | 1.85 | 1.06 |
| 1:A:831:TRP:CH2 | 2:B:50:THR:HG21 | 1.79 | 1.06 |
| 1:D:635:GLY:HA3 | 4:9:341:ILE:HD13 | 1.37 | 1.06 |
| 1:D:800:ARG:NH2 | 3:F:40:ASN:CG | 2.09 | 1.06 |
| 2:E:111:SER:OG | 2:E:148:VAL:O | 1.71 | 1.06 |
| 2:E:163:ALA:HA | 2:K:21:GLU:HB3 | 1.36 | 1.06 |
| 1:M:72:VAL:HG13 | 1:M:76:GLN:HB3 | 1.36 | 1.06 |
| 4:W:325:MET:CE | 4:Y:244:ASP:OD2 | 2.04 | 1.06 |
| 1:D:638:GLY:CA | 4:9:341:ILE:O | 2.02 | 1.06 |
| 1:G:541:MET:SD | 4:V:345:ILE:O | 2.13 | 1.06 |
| 1:M:34:ALA:HB3 | 1:M:777:GLU:OE2 | 1.53 | 1.06 |
| 1:M:641:LYS:HE3 | 1:M:647:GLN:OE1 | 1.50 | 1.06 |
| 1:P:795:ARG:HB3 | 3:R:35:ARG:CZ | 1.83 | 1.06 |
| 1:P:795:ARG:CG | 3:R:118:MET:CE | 2.31 | 1.06 |
| 1:A:85:TYR:OH | 1:A:772:LEU:HD23 | 0.90 | 1.05 |
| 1:A:409:GLY:N | 1:A:636:LYS:HG3 | 1.69 | 1.05 |
| 1:A:641:LYS:HE3 | 4:8:348:SER:O | 1.56 | 1.05 |
| 2:B:140:PHE:O | 2:B:141:PRO:O | 1.74 | 1.05 |
| 2:B:144:VAL:HG11 | 2:B:153:ILE:HG12 | 1.38 | 1.05 |
| 1:D:530:MET:HE2 | 4:9:354:GLN:CG | 1.86 | 1.05 |
| 1:D:797:PHE:HE1 | 3:F:146:ILE:HA | 1.01 | 1.05 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:815:CYS:SG | 2:E:92:ASP:CB | 2.44 | 1.05 |
| 2:E:111:SER:HB3 | 2:E:148:VAL:O | 1.49 | 1.05 |
| 2:E:114:LYS:HA | 2:E:146:GLY:O | 0.89 | 1.05 |
| 1:G:754:ASP:CB | 1:G:776:GLU:HA | 1.86 | 1.05 |
| 1:J:756:THR:HG21 | 1:J:776:GLU:CA | 1.83 | 1.05 |
| 2:K:114:LYS:HA | 2:K:146:GLY:O | 0.89 | 1.05 |
| 1:P:635:GLY:HA2 | 4:1:334:GLU:HG2 | 1.16 | 1.05 |
| 1:P:834:LEU:CD1 | 2:Q:51:PHE:HE1 | 1.69 | 1.05 |
| 2:Q:121:LEU:C | 2:Q:128:PHE:HB3 | 1.72 | 1.05 |
| 1:A:638:GLY:HA2 | 4:8:341:ILE:O | 1.57 | 1.05 |
| 1:A:709:LYS:O | 1:A:710:GLY:HA3 | 1.57 | 1.05 |
| 1:A:800:ARG:NH2 | 3:C:40:ASN:OD1 | 1.89 | 1.05 |
| 2:B:111:SER:HB3 | 2:B:148:VAL:O | 1.49 | 1.05 |
| 1:J:542:PHE:CG | 4:W:143:TYR:HE1 | 1.73 | 1.05 |
| 1:M:838:ILE:CD1 | 2:N:54:MET:CE | 2.33 | 1.05 |
| 1:D:506:GLU:HG3 | 1:D:764:MLY:HE3 | 1.37 | 1.05 |
| 1:D:529:PRO:HB3 | 4:9:353:GLN:OE1 | 1.53 | 1.05 |
| 1:D:641:LYS:HE3 | 1:D:647:GLN:CD | 1.77 | 1.05 |
| 1:D:767:PHE:C | 1:D:771:LEU:HD11 | 1.73 | 1.05 |
| 1:G:707:CYS:SG | 1:G:714:ARG:CZ | 2.44 | 1.05 |
| 1:M:797:PHE:CD1 | 3:O:149:VAL:CG1 | 2.40 | 1.05 |
| 1:M:834:LEU:HD13 | 2:N:51:PHE:HE1 | 0.96 | 1.05 |
| 1:P:530:MET:CA | 4:1:354:GLN:HG3 | 1.87 | 1.05 |
| 1:P:838:ILE:HD11 | 2:Q:54:MET:HE1 | 1.07 | 1.05 |
| 2:Q:114:LYS:HA | 2:Q:146:GLY:O | 0.89 | 1.05 |
| 2:Q:140:PHE:O | 2:Q:141:PRO:O | 1.75 | 1.05 |
| 2:Q:144:VAL:HG11 | 2:Q:153:ILE:HG12 | 1.38 | 1.05 |
| 4:8:3:ASP:HA | 4:8:6:THR:HB | 1.36 | 1.05 |
| 1:D:530:MET:CA | 4:9:354:GLN:HG3 | 1.87 | 1.05 |
| 1:D:819:ASN:ND2 | 2:E:90:GLY:O | 1.87 | 1.05 |
| 1:G:553:MLY:HH13 | 4:X:45:VAL:HG11 | 1.37 | 1.05 |
| 2:H:140:PHE:O | 2:H:141:PRO:O | 1.75 | 1.05 |
| 1:J:834:LEU:HD13 | 2:K:51:PHE:CE1 | 1.90 | 1.05 |
| 1:M:635:GLY:HA3 | 4:Z:341:ILE:HD13 | 1.37 | 1.05 |
| 1:M:796:GLY:HA2 | 3:O:35:ARG:HD3 | 1.39 | 1.05 |
| 2:N:111:SER:OG | 2:N:148:VAL:O | 1.71 | 1.05 |
| 2:N:140:PHE:O | 2:N:141:PRO:O | 1.75 | 1.05 |
| 1:P:769:ALA:C | 1:P:770:GLY:N | 2.09 | 1.05 |
| 1:P:831:TRP:CH2 | 2:Q:47:LEU:HD22 | 1.89 | 1.05 |
| 4:3:322:PRO:HB2 | 4:5:244:ASP:CB | 1.85 | 1.05 |
| 1:A:149:GLN:CB | 1:A:718:ALA:HB3 | 1.87 | 1.05 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:638:GLY:HA2 | 4:9:341:ILE:O | 1.57 | 1.05 |
| 2:E:121:LEU:HG | 2:E:128:PHE:CA | 1.59 | 1.05 |
| 1:G:94:MET:O | 1:G:713:SER:CB | 2.04 | 1.05 |
| 1:G:529:PRO:HB3 | 4:V:353:GLN:OE1 | 1.53 | 1.05 |
| 1:G:556:ASP:OD1 | 4:X:47:MET:HE3 | 1.55 | 1.05 |
| 1:J:641:LYS:HB2 | 1:J:647:GLN:NE2 | 1.68 | 1.05 |
| 1:M:834:LEU:CD1 | 2:N:51:PHE:HE1 | 1.69 | 1.05 |
| 4:9:3:ASP:HA | 4:9:6:THR:HB | 1.36 | 1.05 |
| 1:G:641:LYS:HE3 | 4:V:348:SER:O | 1.56 | 1.04 |
| 1:J:641:LYS:HE3 | 1:J:647:GLN:CD | 1.77 | 1.04 |
| 1:M:641:LYS:HE3 | 1:M:647:GLN:CD | 1.77 | 1.04 |
| 1:P:635:GLY:HA3 | 4:1:341:ILE:HD13 | 1.37 | 1.04 |
| 1:A:529:PRO:HB3 | 4:8:353:GLN:OE1 | 1.53 | 1.04 |
| 1:D:814:PHE:CA | 2:E:127:ARG:NH1 | 2.17 | 1.04 |
| 1:G:795:ARG:HG2 | 3:I:118:MET:HE2 | 1.39 | 1.04 |
| 2:H:121:LEU:C | 2:H:128:PHE:HB3 | 1.72 | 1.04 |
| 1:J:639:GLY:HA3 | 4:W:344:SER:C | 1.78 | 1.04 |
| 1:J:793:ARG:NH1 | 3:L:40:ASN:HD22 | 1.54 | 1.04 |
| 1:P:542:PHE:CG | 4:1:143:TYR:HE1 | 1.73 | 1.04 |
| 2:Q:111:SER:OG | 2:Q:148:VAL:O | 1.71 | 1.04 |
| 4:V:324:THR:HG21 | 4:X:246:GLN:C | 1.70 | 1.04 |
| 1:A:795:ARG:HH21 | 3:C:116:GLU:CB | 1.70 | 1.04 |
| 1:D:599:ASN:HA | 1:D:649:VAL:HB | 1.05 | 1.04 |
| 1:D:641:LYS:HD2 | 1:D:647:GLN:CD | 1.70 | 1.04 |
| 1:D:736:GLN:N | 1:D:743:ALA:CB | 2.05 | 1.04 |
| 1:G:769:ALA:HB3 | 1:G:770:GLY:HA2 | 1.34 | 1.04 |
| 1:J:754:ASP:CB | 1:J:780:ASP:OD2 | 2.05 | 1.04 |
| 2:K:111:SER:HB3 | 2:K:148:VAL:O | 1.50 | 1.04 |
| 2:N:114:LYS:HA | 2:N:146:GLY:O | 0.89 | 1.04 |
| 1:P:546:THR:HG23 | 4:3:46:GLY:O | 1.56 | 1.04 |
| 1:P:641:LYS:HG3 | 1:P:647:GLN:HG3 | 1.20 | 1.04 |
| 4:7:290:ARG:CZ | 4:9:202:THR:CG2 | 2.36 | 1.04 |
| 4:V:3:ASP:HA | 4:V:6:THR:HB | 1.36 | 1.04 |
| 1:A:576:GLU:HG2 | 1:A:577:ALA:N | 1.66 | 1.04 |
| 1:A:834:LEU:CD2 | 2:B:54:MET:HE3 | 1.66 | 1.04 |
| 1:G:821:ARG:HH22 | 2:H:127:ARG:HG2 | 0.92 | 1.04 |
| 1:J:819:ASN:CA | 2:K:90:GLY:O | 2.05 | 1.04 |
| 1:M:542:PHE:CG | 4:Z:143:TYR:HE1 | 1.73 | 1.04 |
| 4:1:287:ILE:HG12 | 4:3:203:THR:H | 1.18 | 1.04 |
| 4:9:290:ARG:CZ | 4:W:202:THR:CG2 | 2.36 | 1.04 |
| 1:A:837:MLY:HH21 | 2:H:20:ASP:HA | 1.36 | 1.04 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:639:GLY:HA3 | 4:9:344:SER:C | 1.78 | 1.04 |
| 1:D:795:ARG:HG2 | 3:F:118:MET:CE | 1.88 | 1.04 |
| 1:D:831:TRP:CZ2 | 2:E:47:LEU:CA | 2.39 | 1.04 |
| 1:G:84:MLY:HD3 | 1:G:723:ARG:HD3 | 1.39 | 1.04 |
| 1:G:641:LYS:HE3 | 1:G:647:GLN:CD | 1.77 | 1.04 |
| 1:J:72:VAL:HG13 | 1:J:76:GLN:HB3 | 1.37 | 1.04 |
| 1:J:638:GLY:HA2 | 4:W:341:ILE:O | 1.57 | 1.04 |
| 1:J:641:LYS:CG | 4:W:348:SER:HB2 | 1.86 | 1.04 |
| 3:L:49:ILE:CA | 3:L:52:ASN:HD22 | 1.71 | 1.04 |
| 1:M:829:TRP:CZ2 | 2:N:87:LYS:HE2 | 1.92 | 1.04 |
| 4:1:243:PRO:HB2 | 4:Y:291:LYS:CD | 1.87 | 1.04 |
| 1:A:530:MET:CA | 4:8:354:GLN:HG3 | 1.86 | 1.03 |
| 1:A:635:GLY:HA3 | 4:8:341:ILE:HD13 | 1.37 | 1.03 |
| 1:A:795:ARG:CB | 3:C:35:ARG:CZ | 2.28 | 1.03 |
| 1:D:800:ARG:NH2 | 3:F:40:ASN:OD1 | 1.90 | 1.03 |
| 3:F:49:ILE:HA | 3:F:52:ASN:HD22 | 1.23 | 1.03 |
| 1:G:542:PHE:CG | 4:V:143:TYR:HE1 | 1.74 | 1.03 |
| 1:G:635:GLY:HA3 | 4:V:341:ILE:HD13 | 1.37 | 1.03 |
| 1:G:638:GLY:HA2 | 4:V:341:ILE:O | 1.58 | 1.03 |
| 1:G:829:TRP:CZ3 | 2:H:84:PHE:CE1 | 2.45 | 1.03 |
| 3:I:49:ILE:CA | 3:I:52:ASN:HD22 | 1.71 | 1.03 |
| 1:J:530:MET:CA | 4:W:354:GLN:HG3 | 1.87 | 1.03 |
| 1:J:641:LYS:HE3 | 4:W:348:SER:O | 1.55 | 1.03 |
| 2:N:149:ASP:OD2 | 2:N:150:TYR:N | 1.91 | 1.03 |
| 3:O:49:ILE:CA | 3:O:52:ASN:HD22 | 1.71 | 1.03 |
| 1:P:529:PRO:C | 4:1:354:GLN:HB3 | 1.77 | 1.03 |
| 1:P:641:LYS:HE3 | 1:P:647:GLN:CD | 1.77 | 1.03 |
| 4:6:3:ASP:HA | 4:6:6:THR:HB | 1.36 | 1.03 |
| 1:A:641:LYS:HG3 | 1:A:647:GLN:HG3 | 1.21 | 1.03 |
| 1:A:753:VAL:HG12 | 1:A:775:LEU:CD2 | 1.87 | 1.03 |
| 1:A:798:LEU:HD11 | 3:C:126:LEU:CD1 | 1.87 | 1.03 |
| 1:G:530:MET:CA | 4:V:354:GLN:HG3 | 1.87 | 1.03 |
| 1:G:552:ASN:O | 4:X:47:MET:CE | 2.05 | 1.03 |
| 2:H:149:ASP:OD2 | 2:H:150:TYR:N | 1.91 | 1.03 |
| 1:J:599:ASN:HA | 1:J:649:VAL:HB | 1.05 | 1.03 |
| 1:M:529:PRO:C | 4:Z:354:GLN:HB3 | 1.77 | 1.03 |
| 1:M:530:MET:HE2 | 4:Z:354:GLN:CG | 1.88 | 1.03 |
| 1:M:530:MET:CA | 4:Z:354:GLN:HG3 | 1.87 | 1.03 |
| 1:P:97:LEU:HD22 | 1:P:712:PRO:HB3 | 1.04 | 1.03 |
| 1:P:639:GLY:HA3 | 4:1:344:SER:C | 1.78 | 1.03 |
| 1:P:786:ILE:HB | 1:P:787:ILE:N | 1.73 | 1.03 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:P:838:ILE:CD1 | 2:Q:54:MET:HE1 | 1.89 | 1.03 |
| 4:3:3:ASP:HA | 4:3:6:THR:HB | 1.36 | 1.03 |
| 4:Y:3:ASP:HA | 4:Y:6:THR:HB | 1.36 | 1.03 |
| 1:A:202:SER:CA | 1:A:207:LYS:CE | 2.36 | 1.03 |
| 1:A:641:LYS:HE3 | 1:A:647:GLN:CD | 1.77 | 1.03 |
| 1:G:730:SER:OG | 3:I:113:THR:HG21 | 1.57 | 1.03 |
| 1:G:795:ARG:HH21 | 3:I:116:GLU:HG2 | 0.98 | 1.03 |
| 2:H:144:VAL:HG11 | 2:H:153:ILE:HG12 | 1.38 | 1.03 |
| 2:K:149:ASP:OD2 | 2:K:150:TYR:N | 1.91 | 1.03 |
| 1:P:769:ALA:O | 1:P:771:LEU:CB | 2.05 | 1.03 |
| 3:R:49:ILE:CA | 3:R:52:ASN:HD22 | 1.71 | 1.03 |
| 4:2:3:ASP:HA | 4:2:6:THR:HB | 1.36 | 1.03 |
| 1:A:641:LYS:HB2 | 1:A:647:GLN:NE2 | 1.68 | 1.03 |
| 3:C:49:ILE:HA | 3:C:52:ASN:HD22 | 1.22 | 1.03 |
| 1:D:830:PRO:HG2 | 2:E:67:MET:CE | 1.89 | 1.03 |
| 2:E:140:PHE:O | 2:E:141:PRO:O | 1.74 | 1.03 |
| 1:G:757:GLN:CG | 1:G:776:GLU:CG | 1.95 | 1.03 |
| 2:H:144:VAL:HG13 | 2:H:153:ILE:HD11 | 1.22 | 1.03 |
| 2:K:140:PHE:O | 2:K:141:PRO:O | 1.75 | 1.03 |
| 1:M:638:GLY:HA2 | 4:Z:341:ILE:O | 1.57 | 1.03 |
| 1:M:639:GLY:HA3 | 4:Z:344:SER:C | 1.78 | 1.03 |
| 1:M:641:LYS:HE3 | 4:Z:348:SER:O | 1.56 | 1.03 |
| 1:P:206:LYS:HD2 | 1:P:217:THR:HG23 | 1.41 | 1.03 |
| 2:B:121:LEU:C | 2:B:128:PHE:HB3 | 1.72 | 1.03 |
| 1:D:639:GLY:N | 4:9:345:ILE:N | 1.94 | 1.03 |
| 2:E:149:ASP:OD2 | 2:E:150:TYR:N | 1.91 | 1.03 |
| 3:F:49:ILE:CA | 3:F:52:ASN:HD22 | 1.70 | 1.03 |
| 1:G:826:VAL:HG21 | 2:H:88:LEU:HD21 | 1.40 | 1.03 |
| 1:J:95:THR:HA | 1:J:713:SER:OG | 1.58 | 1.03 |
| 1:J:818:TYR:OH | 2:K:127:ARG:NH2 | 1.91 | 1.03 |
| 4:1:243:PRO:HB2 | 4:Y:291:LYS:HE3 | 1.06 | 1.03 |
| 4:2:288:ASP:OD2 | 4:4:203:THR:CG2 | 2.06 | 1.03 |
| 4:4:3:ASP:HA | 4:4:6:THR:HB | 1.36 | 1.03 |
| 4:5:3:ASP:HA | 4:5:6:THR:HB | 1.36 | 1.03 |
| 4:8:290:ARG:CZ | 4:V:202:THR:CG2 | 2.36 | 1.03 |
| 1:A:795:ARG:HD2 | 3:C:35:ARG:NH1 | 1.73 | 1.02 |
| 2:B:144:VAL:HG13 | 2:B:153:ILE:HD11 | 1.22 | 1.02 |
| 3:C:24:LYS:HG2 | 3:C:63:ILE:O | 1.59 | 1.02 |
| 1:D:506:GLU:CG | 1:D:764:MLY:HE3 | 1.89 | 1.02 |
| 2:E:150:TYR:O | 2:E:151:LYS:CB | 2.06 | 1.02 |
| 1:G:503:TYR:CZ | 1:G:711:PHE:CD2 | 2.46 | 1.02 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:576:GLU:HG2 | 1:G:577:ALA:N | 1.66 | 1.02 |
| 1:J:56:GLU:HB2 | 1:J:59:MLY:HB3 | 1.40 | 1.02 |
| 1:P:641:LYS:HB2 | 1:P:647:GLN:NE2 | 1.68 | 1.02 |
| 2:Q:121:LEU:HG | 2:Q:128:PHE:CA | 1.60 | 1.02 |
| 4:3:324:THR:CG2 | 4:5:244:ASP:O | 1.97 | 1.02 |
| 1:D:557:GLU:N | 4:W:48:GLY:CA | 2.12 | 1.02 |
| 1:D:838:ILE:HD13 | 2:E:54:MET:CE | 1.80 | 1.02 |
| 1:J:813:ILE:CG2 | 2:K:128:PHE:CE1 | 2.42 | 1.02 |
| 2:K:150:TYR:O | 2:K:151:LYS:CB | 2.07 | 1.02 |
| 1:M:202:SER:CA | 1:M:207:LYS:CE | 2.36 | 1.02 |
| 1:M:549:SER:CA | 4:2:47:MET:O | 2.06 | 1.02 |
| 2:N:144:VAL:HG11 | 2:N:153:ILE:HG12 | 1.38 | 1.02 |
| 1:P:546:THR:CB | 4:3:46:GLY:C | 2.27 | 1.02 |
| 1:P:795:ARG:NH2 | 3:R:116:GLU:CD | 2.11 | 1.02 |
| 1:A:795:ARG:NH2 | 3:C:116:GLU:CG | 2.22 | 1.02 |
| 1:D:529:PRO:C | 4:9:354:GLN:HB3 | 1.78 | 1.02 |
| 1:D:646:PHE:HE2 | 1:D:652:LEU:HD21 | 1.24 | 1.02 |
| 1:G:72:VAL:HG13 | 1:G:76:GLN:HB3 | 1.36 | 1.02 |
| 1:G:769:ALA:CB | 1:G:770:GLY:N | 2.21 | 1.02 |
| 1:G:819:ASN:HA | 2:H:90:GLY:O | 0.86 | 1.02 |
| 1:J:639:GLY:N | 4:W:345:ILE:N | 1.94 | 1.02 |
| 2:K:121:LEU:C | 2:K:128:PHE:HB3 | 1.72 | 1.02 |
| 1:P:599:ASN:HA | 1:P:649:VAL:HB | 1.05 | 1.02 |
| 1:P:638:GLY:HA2 | 4:1:341:ILE:O | 1.57 | 1.02 |
| 1:P:639:GLY:N | 4:1:345:ILE:N | 1.94 | 1.02 |
| 1:P:797:PHE:HE2 | 3:R:126:LEU:HD22 | 1.25 | 1.02 |
| 4:3:324:THR:HG21 | 4:5:244:ASP:O | 1.59 | 1.02 |
| 1:A:56:GLU:HB2 | 1:A:59:MLY:HB3 | 1.40 | 1.02 |
| 1:A:639:GLY:HA3 | 4:8:344:SER:C | 1.78 | 1.02 |
| 1:D:541:MET:HB3 | 4:9:143:TYR:OH | 1.60 | 1.02 |
| 1:D:641:LYS:HG3 | 1:D:647:GLN:HG3 | 1.20 | 1.02 |
| 1:D:641:LYS:HE3 | 4:9:348:SER:O | 1.55 | 1.02 |
| 1:D:736:GLN:HA | 1:D:743:ALA:HB3 | 1.35 | 1.02 |
| 1:G:795:ARG:CB | 3:I:118:MET:HE1 | 1.88 | 1.02 |
| 1:J:94:MET:O | 1:J:713:SER:HB3 | 0.84 | 1.02 |
| 2:Q:149:ASP:OD2 | 2:Q:150:TYR:N | 1.91 | 1.02 |
| 1:A:819:ASN:HD21 | 2:B:92:ASP:N | 1.52 | 1.02 |
| 3:C:24:LYS:CG | 3:C:63:ILE:O | 2.08 | 1.02 |
| 3:C:49:ILE:CA | 3:C:52:ASN:HD22 | 1.70 | 1.02 |
| 1:D:795:ARG:CZ | 3:F:116:GLU:CD | 2.27 | 1.02 |
| 1:D:823:PHE:HE1 | 2:E:160:GLY:HA3 | 1.25 | 1.02 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:G:642:LYS:HG3 | 4:V:23:GLY:H | 0.85 | 1.02 |
| 1:J:529:PRO:C | 4:W:354:GLN:HB3 | 1.78 | 1.02 |
| 1:J:642:LYS:HG3 | 4:W:23:GLY:H | 0.86 | 1.02 |
| 1:J:838:ILE:CD1 | 2:K:54:MET:HE1 | 1.85 | 1.02 |
| 3:O:24:LYS:HG2 | 3:O:63:ILE:O | 1.59 | 1.02 |
| 1:P:642:LYS:HG3 | 4:1:23:GLY:H | 0.86 | 1.02 |
| 1:P:796:GLY:HA2 | 3:R:35:ARG:CD | 1.89 | 1.02 |
| 4:4:288:ASP:CG | 4:6:203:THR:HG21 | 1.64 | 1.02 |
| 4:7:3:ASP:HA | 4:7:6:THR:HB | 1.36 | 1.02 |
| 4:X:3:ASP:HA | 4:X:6:THR:HB | 1.36 | 1.02 |
| 2:B:149:ASP:OD2 | 2:B:150:TYR:N | 1.91 | 1.01 |
| 1:D:599:ASN:CA | 1:D:649:VAL:HB | 1.89 | 1.01 |
| 1:D:724:TYR:HA | 1:D:782:MLY:HD2 | 1.39 | 1.01 |
| 3:F:24:LYS:CG | 3:F:63:ILE:O | 2.08 | 1.01 |
| 3:F:24:LYS:HG2 | 3:F:63:ILE:O | 1.59 | 1.01 |
| 1:G:202:SER:CA | 1:G:207:LYS:CE | 2.36 | 1.01 |
| 1:G:599:ASN:CA | 1:G:649:VAL:HB | 1.89 | 1.01 |
| 1:J:506:GLU:OE2 | 1:J:761:GLY:CA | 2.07 | 1.01 |
| 1:J:599:ASN:CA | 1:J:649:VAL:HB | 1.89 | 1.01 |
| 1:J:817:GLN:CB | 2:K:127:ARG:CD | 2.31 | 1.01 |
| 3:L:24:LYS:HG2 | 3:L:63:ILE:O | 1.59 | 1.01 |
| 1:M:206:LYS:HD2 | 1:M:217:THR:HG23 | 1.41 | 1.01 |
| 1:M:599:ASN:HA | 1:M:649:VAL:HB | 1.05 | 1.01 |
| 3:R:24:LYS:HG2 | 3:R:63:ILE:O | 1.60 | 1.01 |
| 4:2:203:THR:N | 4:Z:287:ILE:HG21 | 1.75 | 1.01 |
| 4:8:290:ARG:NH2 | 4:V:202:THR:CG2 | 2.23 | 1.01 |
| 4:Z:3:ASP:HA | 4:Z:6:THR:HB | 1.36 | 1.01 |
| 1:A:28:GLN:HE22 | 1:A:723:ARG:HH21 | 1.05 | 1.01 |
| 1:A:502:GLU:HG3 | 1:A:761:GLY:N | 1.73 | 1.01 |
| 1:A:541:MET:HB3 | 4:8:143:TYR:OH | 1.60 | 1.01 |
| 1:D:642:LYS:HD3 | 4:9:340:TRP:CZ3 | 1.96 | 1.01 |
| 1:D:795:ARG:CZ | 3:F:116:GLU:OE2 | 2.07 | 1.01 |
| 1:G:557:GLU:CB | 4:X:46:GLY:C | 2.26 | 1.01 |
| 1:J:534:SER:O | 4:W:351:THR:HA | 1.60 | 1.01 |
| 1:J:576:GLU:HG2 | 1:J:577:ALA:H | 0.85 | 1.01 |
| 1:J:642:LYS:HD3 | 4:W:340:TRP:CH2 | 1.96 | 1.01 |
| 1:M:641:LYS:HD2 | 1:M:647:GLN:CD | 1.70 | 1.01 |
| 1:M:642:LYS:HG3 | 4:Z:23:GLY:H | 0.86 | 1.01 |
| 1:M:797:PHE:HE2 | 3:O:126:LEU:HD22 | 1.16 | 1.01 |
| 1:P:642:LYS:HD3 | 4:1:340:TRP:CH2 | 1.96 | 1.01 |
| 4:4:288:ASP:N | 4:6:203:THR:HG22 | 1.75 | 1.01 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:553:MLY:HG2 | 4:V:44:MET:O | 1.59 | 1.01 |
| 1:A:641:LYS:HE3 | 1:A:647:GLN:HB2 | 1.42 | 1.01 |
| 1:D:206:LYS:HD2 | 1:D:217:THR:HG23 | 1.41 | 1.01 |
| 1:D:534:SER:O | 4:9:351:THR:HA | 1.60 | 1.01 |
| 3:F:48:LYS:O | 3:F:52:ASN:ND2 | 1.94 | 1.01 |
| 1:G:599:ASN:HA | 1:G:649:VAL:HB | 1.05 | 1.01 |
| 3:I:48:LYS:O | 3:I:52:ASN:ND2 | 1.94 | 1.01 |
| 1:J:817:GLN:HG2 | 2:K:127:ARG:HB2 | 1.05 | 1.01 |
| 1:J:821:ARG:HH22 | 2:K:127:ARG:HG2 | 1.21 | 1.01 |
| 2:K:121:LEU:HG | 2:K:128:PHE:CA | 1.59 | 1.01 |
| 1:M:534:SER:O | 4:Z:351:THR:HA | 1.59 | 1.01 |
| 1:P:93:MET:O | 1:P:713:SER:CB | 2.08 | 1.01 |
| 1:P:202:SER:CA | 1:P:207:LYS:CE | 2.36 | 1.01 |
| 1:P:534:SER:C | 4:1:351:THR:HA | 1.81 | 1.01 |
| 1:P:541:MET:HB3 | 4:1:143:TYR:OH | 1.59 | 1.01 |
| 1:P:805:ALA:HA | 1:P:808:GLU:HB2 | 1.40 | 1.01 |
| 1:P:831:TRP:HH2 | 2:Q:47:LEU:HD21 | 1.21 | 1.01 |
| 3:R:49:ILE:HA | 3:R:52:ASN:HD22 | 1.23 | 1.01 |
| 4:7:287:ILE:HB | 4:9:204:ALA:H | 1.26 | 1.01 |
| 1:A:98:HIS:HB3 | 1:A:100:PRO:HD2 | 1.42 | 1.01 |
| 1:A:642:LYS:HG3 | 4:8:23:GLY:H | 0.87 | 1.01 |
| 1:A:642:LYS:HD3 | 4:8:340:TRP:CH2 | 1.95 | 1.01 |
| 1:A:642:LYS:HD3 | 4:8:340:TRP:CZ3 | 1.95 | 1.01 |
| 1:A:798:LEU:CD1 | 3:C:126:LEU:HD11 | 1.90 | 1.01 |
| 1:A:818:TYR:CB | 2:B:90:GLY:HA3 | 1.91 | 1.01 |
| 1:D:56:GLU:HB2 | 1:D:59:MLY:HB3 | 1.40 | 1.01 |
| 1:D:553:MLY:HG2 | 4:W:44:MET:O | 1.59 | 1.01 |
| 1:G:206:LYS:HD2 | 1:G:217:THR:HG23 | 1.41 | 1.01 |
| 3:I:24:LYS:CG | 3:I:63:ILE:O | 2.08 | 1.01 |
| 2:K:144:VAL:HG11 | 2:K:153:ILE:HG12 | 1.38 | 1.01 |
| 1:M:534:SER:C | 4:Z:351:THR:HA | 1.81 | 1.01 |
| 1:M:541:MET:HB3 | 4:Z:143:TYR:OH | 1.60 | 1.01 |
| 1:P:549:SER:HA | 4:3:43:VAL:HG11 | 1.39 | 1.01 |
| 1:P:798:LEU:HD12 | 3:R:126:LEU:HD21 | 1.40 | 1.01 |
| 1:P:817:GLN:HB3 | 2:Q:127:ARG:HH11 | 1.20 | 1.01 |
| 4:1:245:GLY:HA3 | 4:Y:324:THR:O | 1.58 | 1.01 |
| 1:A:553:MLY:CB | 4:V:46:GLY:CA | 2.32 | 1.01 |
| 1:A:599:ASN:CA | 1:A:649:VAL:HB | 1.89 | 1.01 |
| 2:B:121:LEU:CB | 2:B:128:PHE:HB3 | 1.69 | 1.01 |
| 1:G:84:MLY:CD | 1:G:723:ARG:CD | 2.28 | 1.01 |
| 1:G:148:ARG:NH2 | 1:G:764:MLY:HH21 | 1.76 | 1.01 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:206:LYS:CD | 1:G:217:THR:CG2 | 2.16 | 1.01 |
| 1:J:28:GLN:OE1 | 1:J:723:ARG:HG2 | 1.60 | 1.01 |
| 1:J:541:MET:HB3 | 4:W:143:TYR:OH | 1.59 | 1.01 |
| 1:J:820:VAL:HG11 | 2:K:136:MET:HE3 | 1.02 | 1.01 |
| 3:L:24:LYS:CG | 3:L:63:ILE:O | 2.08 | 1.01 |
| 1:M:641:LYS:CG | 4:Z:348:SER:HB2 | 1.87 | 1.01 |
| 1:M:641:LYS:HE3 | 1:M:647:GLN:HB2 | 1.42 | 1.01 |
| 1:M:795:ARG:HD2 | 3:O:43:ASN:OD1 | 1.57 | 1.01 |
| 4:1:287:ILE:HB | 4:3:203:THR:HG22 | 1.08 | 1.01 |
| 4:9:290:ARG:NH2 | 4:W:202:THR:CG2 | 2.23 | 1.01 |
| 1:A:505:MLY:HB2 | 1:A:761:GLY:HA2 | 1.42 | 1.00 |
| 1:A:599:ASN:HA | 1:A:649:VAL:HB | 1.06 | 1.00 |
| 1:D:642:LYS:HD3 | 4:9:340:TRP:CH2 | 1.96 | 1.00 |
| 1:G:98:HIS:HB3 | 1:G:100:PRO:HD2 | 1.42 | 1.00 |
| 1:G:541:MET:HB3 | 4:V:143:TYR:OH | 1.60 | 1.00 |
| 2:H:150:TYR:O | 2:H:151:LYS:CB | 2.07 | 1.00 |
| 1:J:505:MLY:HD2 | 1:J:762:HIS:ND1 | 1.76 | 1.00 |
| 1:M:98:HIS:HB3 | 1:M:100:PRO:HD2 | 1.42 | 1.00 |
| 1:M:642:LYS:HD3 | 4:Z:340:TRP:CZ3 | 1.96 | 1.00 |
| 1:P:56:GLU:HB2 | 1:P:59:MLY:HB3 | 1.40 | 1.00 |
| 1:P:576:GLU:HG2 | 1:P:577:ALA:H | 0.85 | 1.00 |
| 1:P:805:ALA:O | 1:P:809:ARG:N | 1.92 | 1.00 |
| 1:P:806:MET:CA | 1:P:807:VAL:N | 2.24 | 1.00 |
| 4:2:322:PRO:HB3 | 4:4:244:ASP:CB | 1.90 | 1.00 |
| 1:A:795:ARG:HH21 | 3:C:116:GLU:HB3 | 1.21 | 1.00 |
| 3:C:48:LYS:O | 3:C:52:ASN:ND2 | 1.94 | 1.00 |
| 2:E:144:VAL:HG11 | 2:E:153:ILE:HG12 | 1.38 | 1.00 |
| 1:G:529:PRO:C | 4:V:354:GLN:HB3 | 1.79 | 1.00 |
| 1:G:639:GLY:HA3 | 4:V:344:SER:C | 1.78 | 1.00 |
| 1:G:641:LYS:HE3 | 1:G:647:GLN:HB2 | 1.42 | 1.00 |
| 3:I:49:ILE:HA | 3:I:52:ASN:HD22 | 1.23 | 1.00 |
| 1:J:215:GLN:CA | 1:J:340:ILE:HG23 | 1.92 | 1.00 |
| 1:J:534:SER:C | 4:W:351:THR:HA | 1.81 | 1.00 |
| 1:J:642:LYS:HD3 | 4:W:340:TRP:CZ3 | 1.96 | 1.00 |
| 1:J:646:PHE:HE2 | 1:J:652:LEU:HD21 | 1.24 | 1.00 |
| 3:L:49:ILE:HA | 3:L:52:ASN:HD22 | 1.23 | 1.00 |
| 1:M:174:SER:HB3 | 1:M:667:THR:HG21 | 1.44 | 1.00 |
| 1:M:838:ILE:HD11 | 2:N:54:MET:HE3 | 1.40 | 1.00 |
| 2:N:121:LEU:C | 2:N:128:PHE:HB3 | 1.71 | 1.00 |
| 1:P:546:THR:HG21 | 4:3:46:GLY:C | 1.78 | 1.00 |
| 4:2:287:ILE:CG2 | 4:4:202:THR:OG1 | 2.03 | 1.00 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:534:SER:C | 4:8:351:THR:HA | 1.81 | 1.00 |
| 1:D:534:SER:O | 4:9:351:THR:HG23 | 1.13 | 1.00 |
| 1:D:534:SER:C | 4:9:351:THR:HA | 1.81 | 1.00 |
| 1:G:56:GLU:HB2 | 1:G:59:MLY:HB3 | 1.40 | 1.00 |
| 1:G:84:MLY:HD3 | 1:G:723:ARG:CD | 1.90 | 1.00 |
| 1:G:508:ILE:CD1 | 1:G:759:ALA:HB2 | 1.90 | 1.00 |
| 1:G:829:TRP:HZ3 | 2:H:84:PHE:CZ | 1.78 | 1.00 |
| 1:J:817:GLN:OE1 | 2:K:127:ARG:HD2 | 1.61 | 1.00 |
| 1:M:56:GLU:HB2 | 1:M:59:MLY:HB3 | 1.40 | 1.00 |
| 1:M:95:THR:OG1 | 1:M:770:GLY:N | 1.95 | 1.00 |
| 1:M:576:GLU:HG2 | 1:M:577:ALA:H | 0.85 | 1.00 |
| 1:M:599:ASN:CA | 1:M:649:VAL:HB | 1.89 | 1.00 |
| 2:N:150:TYR:O | 2:N:151:LYS:CB | 2.06 | 1.00 |
| 3:O:24:LYS:CG | 3:O:63:ILE:O | 2.08 | 1.00 |
| 3:O:48:LYS:O | 3:O:52:ASN:ND2 | 1.94 | 1.00 |
| 1:P:599:ASN:CA | 1:P:649:VAL:HB | 1.89 | 1.00 |
| 1:P:641:LYS:HE3 | 1:P:647:GLN:HB2 | 1.43 | 1.00 |
| 1:P:818:TYR:CE1 | 2:Q:127:ARG:CZ | 2.44 | 1.00 |
| 2:Q:150:TYR:O | 2:Q:151:LYS:CB | 2.07 | 1.00 |
| 3:R:24:LYS:CG | 3:R:63:ILE:O | 2.08 | 1.00 |
| 4:W:291:LYS:HD2 | 4:Y:243:PRO:HB2 | 1.41 | 1.00 |
| 1:A:831:TRP:CZ3 | 2:B:50:THR:HG22 | 1.96 | 1.00 |
| 1:D:727:LEU:HD11 | 1:D:782:MLY:CD | 1.81 | 1.00 |
| 1:G:796:GLY:HA2 | 3:I:35:ARG:CD | 1.91 | 1.00 |
| 1:J:98:HIS:HB3 | 1:J:100:PRO:HD2 | 1.42 | 1.00 |
| 1:J:641:LYS:HE3 | 1:J:647:GLN:HB2 | 1.43 | 1.00 |
| 1:M:798:LEU:HD12 | 3:O:126:LEU:HD21 | 1.40 | 1.00 |
| 1:P:798:LEU:HD21 | 3:R:126:LEU:CD1 | 1.91 | 1.00 |
| 4:X:287:ILE:N | 4:Z:202:THR:OG1 | 1.95 | 1.00 |
| 1:D:642:LYS:HG3 | 4:9:23:GLY:H | 0.86 | 1.00 |
| 1:D:831:TRP:CZ2 | 2:E:47:LEU:HD22 | 1.88 | 1.00 |
| 1:P:206:LYS:CD | 1:P:217:THR:CG2 | 2.16 | 1.00 |
| 1:P:641:LYS:CG | 4:1:348:SER:HB2 | 1.86 | 1.00 |
| 1:P:641:LYS:HE3 | 1:P:647:GLN:CB | 1.91 | 1.00 |
| 4:3:324:THR:HB | 4:5:243:PRO:O | 1.14 | 1.00 |
| 4:7:290:ARG:NH2 | 4:9:202:THR:CG2 | 2.23 | 1.00 |
| 1:A:553:MLY:HB3 | 4:V:46:GLY:CA | 1.51 | 1.00 |
| 1:D:218:LEU:CA | 1:D:221:GLN:HG3 | 1.91 | 1.00 |
| 1:D:641:LYS:HE3 | 1:D:647:GLN:HB2 | 1.43 | 1.00 |
| 1:G:821:ARG:HH22 | 2:H:127:ARG:CG | 1.73 | 1.00 |
| 1:M:641:LYS:HE3 | 1:M:647:GLN:CB | 1.91 | 1.00 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:642:LYS:HD3 | 4:Z:340:TRP:CH2 | 1.95 | 1.00 |
| 1:M:792:ALA:CB | 3:O:42:THR:HG22 | 1.92 | 1.00 |
| 1:M:798:LEU:CD1 | 3:O:126:LEU:CD2 | 2.21 | 1.00 |
| 1:P:218:LEU:CA | 1:P:221:GLN:HG3 | 1.91 | 1.00 |
| 1:P:799:MET:SD | 3:R:32:ASP:CB | 2.49 | 1.00 |
| 3:R:48:LYS:O | 3:R:52:ASN:ND2 | 1.94 | 1.00 |
| 4:2:203:THR:H | 4:Z:287:ILE:CG1 | 1.74 | 1.00 |
| 1:A:797:PHE:HE2 | 3:C:126:LEU:HD22 | 1.21 | 1.00 |
| 1:D:202:SER:CA | 1:D:207:LYS:CE | 2.36 | 1.00 |
| 1:G:503:TYR:CE1 | 1:G:711:PHE:CD2 | 2.47 | 1.00 |
| 1:G:642:LYS:HD3 | 4:V:340:TRP:CH2 | 1.96 | 1.00 |
| 1:G:792:ALA:HB2 | 3:I:42:THR:CA | 1.91 | 1.00 |
| 1:P:646:PHE:HE2 | 1:P:652:LEU:HD21 | 1.24 | 1.00 |
| 1:P:817:GLN:CB | 2:Q:127:ARG:HD2 | 1.90 | 1.00 |
| 4:9:322:PRO:HB3 | 4:W:244:ASP:OD2 | 1.62 | 1.00 |
| 1:A:174:SER:HB3 | 1:A:667:THR:HG21 | 1.44 | 0.99 |
| 1:D:576:GLU:HG2 | 1:D:577:ALA:H | 0.85 | 0.99 |
| 1:G:642:LYS:HD3 | 4:V:340:TRP:CZ3 | 1.96 | 0.99 |
| 1:J:576:GLU:CG | 1:J:577:ALA:H | 1.75 | 0.99 |
| 1:J:756:THR:CG2 | 1:J:776:GLU:HA | 1.92 | 0.99 |
| 2:N:139:ALA:O | 2:N:141:PRO:HD3 | 1.62 | 0.99 |
| 1:P:642:LYS:HD3 | 4:I:340:TRP:CZ3 | 1.96 | 0.99 |
| 1:P:818:TYR:CZ | 2:Q:127:ARG:NH2 | 2.11 | 0.99 |
| 4:3:287:ILE:HD13 | 4:5:203:THR:HB | 1.42 | 0.99 |
| 4:7:322:PRO:HB3 | 4:9:244:ASP:OD2 | 1.62 | 0.99 |
| 1:A:641:LYS:CD | 4:8:348:SER:HB2 | 1.92 | 0.99 |
| 1:G:641:LYS:HE3 | 1:G:647:GLN:CB | 1.91 | 0.99 |
| 1:J:202:SER:CA | 1:J:207:LYS:CE | 2.36 | 0.99 |
| 4:V:324:THR:CG2 | 4:X:247:VAL:N | 2.24 | 0.99 |
| 1:A:502:GLU:CG | 1:A:761:GLY:CA | 2.40 | 0.99 |
| 1:A:505:MLY:HB3 | 1:A:762:HIS:H | 1.23 | 0.99 |
| 1:A:612:GLN:HE22 | 1:A:627:GLY:CA | 1.75 | 0.99 |
| 1:D:576:GLU:CG | 1:D:577:ALA:H | 1.75 | 0.99 |
| 1:J:553:MLY:HE3 | 4:Y:45:VAL:CG1 | 1.92 | 0.99 |
| 1:M:798:LEU:CD1 | 3:O:126:LEU:CD1 | 2.36 | 0.99 |
| 2:N:121:LEU:HG | 2:N:128:PHE:CA | 1.59 | 0.99 |
| 2:N:149:ASP:OD2 | 2:N:150:TYR:O | 1.80 | 0.99 |
| 1:P:795:ARG:CZ | 3:R:116:GLU:OE2 | 2.10 | 0.99 |
| 1:P:798:LEU:HD21 | 3:R:126:LEU:HD11 | 1.43 | 0.99 |
| 1:A:206:LYS:HD2 | 1:A:217:THR:HG23 | 1.41 | 0.99 |
| 1:A:218:LEU:CA | 1:A:221:GLN:HG3 | 1.91 | 0.99 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:576:GLU:CG | 1:A:577:ALA:H | 1.75 | 0.99 |
| 1:A:641:LYS:HE3 | 1:A:647:GLN:CB | 1.91 | 0.99 |
| 2:B:150:TYR:O | 2:B:151:LYS:CB | 2.07 | 0.99 |
| 1:D:834:LEU:HD11 | 2:E:54:MET:HG2 | 1.00 | 0.99 |
| 1:G:576:GLU:HG2 | 1:G:577:ALA:H | 0.85 | 0.99 |
| 1:J:831:TRP:HH2 | 2:K:47:LEU:HD21 | 0.98 | 0.99 |
| 2:K:139:ALA:O | 2:K:141:PRO:HD3 | 1.62 | 0.99 |
| 4:9:286:ASP:OD1 | 4:W:203:THR:HG22 | 1.62 | 0.99 |
| 1:A:529:PRO:C | 4:8:354:GLN:HB3 | 1.78 | 0.99 |
| 1:A:576:GLU:HG2 | 1:A:577:ALA:H | 0.85 | 0.99 |
| 1:D:612:GLN:HE22 | 1:D:627:GLY:CA | 1.76 | 0.99 |
| 1:D:639:GLY:CA | 4:9:345:ILE:CA | 2.40 | 0.99 |
| 1:G:530:MET:CE | 4:V:354:GLN:CG | 2.40 | 0.99 |
| 1:J:218:LEU:CA | 1:J:221:GLN:HG3 | 1.91 | 0.99 |
| 1:P:612:GLN:HE22 | 1:P:627:GLY:CA | 1.76 | 0.99 |
| 2:B:112:ILE:O | 2:B:147:ASN:C | 2.01 | 0.99 |
| 1:D:649:VAL:CG1 | 1:D:649:VAL:HG22 | 1.92 | 0.99 |
| 1:D:713:SER:N | 1:D:771:LEU:CD2 | 2.08 | 0.99 |
| 1:G:534:SER:C | 4:V:351:THR:HA | 1.82 | 0.99 |
| 1:M:218:LEU:CA | 1:M:221:GLN:HG3 | 1.91 | 0.99 |
| 2:N:150:TYR:C | 2:N:151:LYS:HG3 | 1.83 | 0.99 |
| 2:B:139:ALA:O | 2:B:141:PRO:HD3 | 1.63 | 0.99 |
| 1:D:215:GLN:CA | 1:D:340:ILE:HG23 | 1.92 | 0.99 |
| 1:D:641:LYS:HE3 | 1:D:647:GLN:CB | 1.91 | 0.99 |
| 2:E:149:ASP:OD2 | 2:E:150:TYR:O | 1.81 | 0.99 |
| 1:G:612:GLN:HE22 | 1:G:627:GLY:CA | 1.75 | 0.99 |
| 1:G:769:ALA:HB1 | 1:G:770:GLY:HA2 | 1.41 | 0.99 |
| 1:J:639:GLY:CA | 4:W:345:ILE:CA | 2.40 | 0.99 |
| 2:K:149:ASP:OD2 | 2:K:150:TYR:O | 1.80 | 0.99 |
| 1:M:639:GLY:CA | 4:Z:345:ILE:CA | 2.40 | 0.99 |
| 1:P:215:GLN:CA | 1:P:340:ILE:HG23 | 1.92 | 0.99 |
| 1:A:93:MET:HE1 | 1:A:715:VAL:CG1 | 1.92 | 0.99 |
| 1:A:754:ASP:OD2 | 1:A:778:MET:CE | 2.11 | 0.99 |
| 2:B:111:SER:CB | 2:B:148:VAL:C | 1.93 | 0.99 |
| 1:D:797:PHE:CE1 | 3:F:146:ILE:HG23 | 1.96 | 0.99 |
| 1:G:28:GLN:HB3 | 1:G:723:ARG:HH12 | 0.85 | 0.99 |
| 1:G:174:SER:HB3 | 1:G:667:THR:HG21 | 1.44 | 0.99 |
| 2:H:149:ASP:OD2 | 2:H:150:TYR:O | 1.80 | 0.99 |
| 1:J:820:VAL:CG1 | 2:K:136:MET:HE3 | 1.93 | 0.99 |
| 1:M:797:PHE:HE2 | 3:O:126:LEU:CD2 | 1.76 | 0.99 |
| 1:P:641:LYS:HE3 | 4:1:348:SER:O | 1.55 | 0.99 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:797:PHE:HE1 | 3:C:146:ILE:HA | 1.19 | 0.99 |
| 1:D:727:LEU:CG | 1:D:782:MLY:HE2 | 1.71 | 0.99 |
| 1:G:795:ARG:CA | 3:I:118:MET:CE | 2.37 | 0.99 |
| 1:J:649:VAL:CG1 | 1:J:649:VAL:HG22 | 1.92 | 0.99 |
| 2:K:117:LEU:CB | 2:K:147:ASN:CG | 2.32 | 0.99 |
| 1:M:576:GLU:CG | 1:M:577:ALA:H | 1.75 | 0.99 |
| 1:M:612:GLN:HE22 | 1:M:627:GLY:CA | 1.76 | 0.99 |
| 3:O:49:ILE:HA | 3:O:52:ASN:HD22 | 1.23 | 0.99 |
| 1:P:795:ARG:CB | 3:R:35:ARG:NH1 | 2.26 | 0.99 |
| 4:8:287:ILE:HB | 4:V:204:ALA:H | 1.25 | 0.99 |
| 1:A:502:GLU:HA | 1:A:761:GLY:CA | 1.93 | 0.99 |
| 1:A:797:PHE:CE2 | 3:C:146:ILE:CD1 | 2.43 | 0.99 |
| 2:E:139:ALA:O | 2:E:141:PRO:HD3 | 1.62 | 0.99 |
| 1:G:218:LEU:CA | 1:G:221:GLN:HG3 | 1.91 | 0.99 |
| 1:J:641:LYS:HE3 | 1:J:647:GLN:CB | 1.91 | 0.99 |
| 1:M:215:GLN:CA | 1:M:340:ILE:HG23 | 1.92 | 0.99 |
| 1:M:782:MLY:O | 1:M:786:ILE:HG12 | 1.63 | 0.99 |
| 4:2:287:ILE:HD13 | 4:4:203:THR:CB | 1.93 | 0.99 |
| 4:X:287:ILE:CG2 | 4:Z:205:GLU:OE2 | 1.90 | 0.99 |
| 1:A:502:GLU:OE2 | 1:A:761:GLY:N | 1.77 | 0.98 |
| 1:A:534:SER:O | 4:8:351:THR:HA | 1.59 | 0.98 |
| 1:D:725:ARG:C | 1:D:782:MLY:HH22 | 1.81 | 0.98 |
| 1:G:829:TRP:HZ3 | 2:H:84:PHE:CE1 | 1.81 | 0.98 |
| 1:J:206:LYS:HD2 | 1:J:217:THR:HG23 | 1.41 | 0.98 |
| 1:J:795:ARG:C | 3:L:35:ARG:CZ | 2.31 | 0.98 |
| 1:J:834:LEU:HD13 | 2:K:51:PHE:HE1 | 1.25 | 0.98 |
| 2:K:150:TYR:C | 2:K:151:LYS:HG3 | 1.83 | 0.98 |
| 1:P:534:SER:O | 4:1:351:THR:HA | 1.60 | 0.98 |
| 4:8:322:PRO:HB3 | 4:V:244:ASP:OD2 | 1.62 | 0.98 |
| 1:D:791:GLN:OE1 | 3:F:116:GLU:CG | 2.10 | 0.98 |
| 2:E:141:PRO:HB2 | 2:E:142:PRO:HD2 | 1.44 | 0.98 |
| 1:G:215:GLN:CA | 1:G:340:ILE:HG23 | 1.92 | 0.98 |
| 3:L:48:LYS:O | 3:L:52:ASN:ND2 | 1.94 | 0.98 |
| 1:P:649:VAL:CG1 | 1:P:649:VAL:HG22 | 1.92 | 0.98 |
| 4:9:287:ILE:HB | 4:W:204:ALA:H | 1.25 | 0.98 |
| 1:A:93:MET:SD | 1:A:715:VAL:HG22 | 2.02 | 0.98 |
| 1:D:506:GLU:CG | 1:D:764:MLY:CE | 2.40 | 0.98 |
| 1:G:838:ILE:HD11 | 2:H:54:MET:HE1 | 1.46 | 0.98 |
| 3:I:24:LYS:HG2 | 3:I:63:ILE:O | 1.60 | 0.98 |
| 1:J:756:THR:HG22 | 1:J:776:GLU:CG | 1.92 | 0.98 |
| 1:P:98:HIS:HB3 | 1:P:100:PRO:HD2 | 1.42 | 0.98 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:P:786:ILE:CB | 1:P:787:ILE:N | 2.26 | 0.98 |
| 2:B:117:LEU:CB | 2:B:147:ASN:CG | 2.32 | 0.98 |
| 1:D:98:HIS:HB3 | 1:D:100:PRO:HD2 | 1.42 | 0.98 |
| 1:D:712:PRO:HG2 | 1:D:771:LEU:HB2 | 1.44 | 0.98 |
| 1:G:503:TYR:OH | 1:G:711:PHE:CD2 | 1.85 | 0.98 |
| 1:P:799:MET:SD | 3:R:32:ASP:CG | 2.42 | 0.98 |
| 2:Q:149:ASP:OD2 | 2:Q:150:TYR:O | 1.80 | 0.98 |
| 1:A:557:GLU:N | 4:V:48:GLY:CA | 2.12 | 0.98 |
| 1:A:639:GLY:CA | 4:8:345:ILE:CA | 2.41 | 0.98 |
| 1:A:795:ARG:HH21 | 3:C:116:GLU:CG | 1.75 | 0.98 |
| 1:A:836:PHE:HZ | 2:B:160:GLY:H | 0.98 | 0.98 |
| 1:G:576:GLU:CG | 1:G:577:ALA:H | 1.75 | 0.98 |
| 2:K:121:LEU:CB | 2:K:128:PHE:HB3 | 1.68 | 0.98 |
| 2:N:130:PRO:O | 2:N:133:ILE:N | 1.96 | 0.98 |
| 1:P:639:GLY:CA | 4:1:345:ILE:CA | 2.40 | 0.98 |
| 1:P:838:ILE:HD11 | 2:Q:54:MET:HE3 | 1.42 | 0.98 |
| 1:A:530:MET:CE | 4:8:354:GLN:CG | 2.41 | 0.98 |
| 1:J:84:MLY:CH1 | 1:J:720:PHE:CE1 | 2.44 | 0.98 |
| 4:1:201:VAL:N | 4:Y:287:ILE:HG12 | 1.78 | 0.98 |
| 1:G:830:PRO:CB | 2:H:67:MET:HE1 | 1.94 | 0.98 |
| 2:H:139:ALA:O | 2:H:141:PRO:HD3 | 1.62 | 0.98 |
| 1:J:612:GLN:HE22 | 1:J:627:GLY:CA | 1.76 | 0.98 |
| 1:J:797:PHE:CE2 | 3:L:126:LEU:HD22 | 1.98 | 0.98 |
| 1:J:820:VAL:CG1 | 2:K:136:MET:CE | 2.42 | 0.98 |
| 1:P:576:GLU:HG2 | 1:P:577:ALA:N | 1.66 | 0.98 |
| 1:P:820:VAL:HG11 | 2:Q:136:MET:HE3 | 1.42 | 0.98 |
| 2:Q:117:LEU:CB | 2:Q:147:ASN:CG | 2.32 | 0.98 |
| 2:Q:130:PRO:O | 2:Q:133:ILE:N | 1.96 | 0.98 |
| 1:A:215:GLN:CA | 1:A:340:ILE:HG23 | 1.92 | 0.98 |
| 1:A:639:GLY:N | 4:8:345:ILE:N | 1.94 | 0.98 |
| 2:B:149:ASP:OD2 | 2:B:150:TYR:O | 1.80 | 0.98 |
| 1:G:784:ALA:O | 1:G:788:THR:N | 1.96 | 0.98 |
| 1:J:795:ARG:NE | 3:L:116:GLU:OE2 | 1.96 | 0.98 |
| 1:J:797:PHE:CE1 | 3:L:146:ILE:CD1 | 2.43 | 0.98 |
| 1:M:530:MET:CE | 4:Z:354:GLN:CG | 2.40 | 0.98 |
| 2:N:112:ILE:O | 2:N:147:ASN:C | 2.01 | 0.98 |
| 4:4:322:PRO:CB | 4:6:244:ASP:CB | 2.41 | 0.98 |
| 1:A:642:LYS:HD2 | 4:8:24:ASP:O | 1.64 | 0.98 |
| 1:D:831:TRP:CH2 | 2:E:34:ILE:HG23 | 1.97 | 0.98 |
| 1:D:831:TRP:HZ3 | 2:E:34:ILE:HG23 | 1.24 | 0.98 |
| 1:M:838:ILE:CD1 | 2:N:54:MET:HE1 | 1.92 | 0.98 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:P:97:LEU:CD2 | 1:P:712:PRO:CB | 2.41 | 0.98 |
| 2:Q:139:ALA:O | 2:Q:141:PRO:HD3 | 1.62 | 0.98 |
| 2:Q:141:PRO:HB2 | 2:Q:142:PRO:HD2 | 1.44 | 0.98 |
| 4:W:286:ASP:OD2 | 4:Y:203:THR:HG22 | 1.61 | 0.98 |
| 1:A:813:ILE:CG2 | 2:B:127:ARG:CD | 2.33 | 0.98 |
| 2:B:150:TYR:C | 2:B:151:LYS:HG3 | 1.83 | 0.98 |
| 2:E:117:LEU:CB | 2:E:147:ASN:CG | 2.32 | 0.98 |
| 1:G:646:PHE:HE2 | 1:G:652:LEU:HD21 | 1.24 | 0.98 |
| 1:G:649:VAL:CG1 | 1:G:649:VAL:HG22 | 1.92 | 0.98 |
| 1:G:829:TRP:CZ3 | 2:H:87:LYS:NZ | 2.30 | 0.98 |
| 2:K:141:PRO:HB2 | 2:K:142:PRO:HD2 | 1.44 | 0.98 |
| 4:7:286:ASP:OD1 | 4:9:203:THR:HG22 | 1.62 | 0.98 |
| 1:A:641:LYS:CG | 4:8:348:SER:HB2 | 1.87 | 0.97 |
| 2:H:112:ILE:O | 2:H:147:ASN:C | 2.02 | 0.97 |
| 1:M:649:VAL:CG1 | 1:M:649:VAL:HG22 | 1.92 | 0.97 |
| 1:P:795:ARG:CZ | 3:R:116:GLU:HB3 | 1.94 | 0.97 |
| 4:1:287:ILE:HG12 | 4:3:203:THR:N | 1.79 | 0.97 |
| 3:C:46:ILE:O | 3:C:50:LEU:HG | 1.64 | 0.97 |
| 1:D:542:PHE:CG | 4:9:143:TYR:CE1 | 2.52 | 0.97 |
| 1:M:785:GLU:O | 1:M:789:ALA:CB | 2.12 | 0.97 |
| 1:P:829:TRP:CH2 | 2:Q:87:LYS:NZ | 2.32 | 0.97 |
| 4:2:287:ILE:CG1 | 4:4:202:THR:HA | 1.93 | 0.97 |
| 4:2:324:THR:OG1 | 4:4:244:ASP:CA | 2.12 | 0.97 |
| 1:D:218:LEU:CA | 1:D:221:GLN:CG | 2.42 | 0.97 |
| 1:D:530:MET:CE | 4:9:354:GLN:CG | 2.40 | 0.97 |
| 2:E:121:LEU:CB | 2:E:128:PHE:HB3 | 1.69 | 0.97 |
| 1:G:639:GLY:CA | 4:V:345:ILE:CA | 2.40 | 0.97 |
| 2:H:117:LEU:CB | 2:H:147:ASN:CG | 2.32 | 0.97 |
| 3:I:52:ASN:HB2 | 3:I:53:PRO:HD3 | 1.46 | 0.97 |
| 3:L:46:ILE:O | 3:L:50:LEU:HG | 1.64 | 0.97 |
| 1:M:792:ALA:HB2 | 3:O:42:THR:HG22 | 0.99 | 0.97 |
| 1:P:576:GLU:CG | 1:P:577:ALA:H | 1.75 | 0.97 |
| 1:A:707:CYS:HA | 1:A:714:ARG:NH2 | 1.78 | 0.97 |
| 3:F:52:ASN:HB2 | 3:F:53:PRO:HD3 | 1.46 | 0.97 |
| 1:G:639:GLY:N | 4:V:345:ILE:N | 1.94 | 0.97 |
| 2:H:150:TYR:C | 2:H:151:LYS:HG3 | 1.83 | 0.97 |
| 1:J:635:GLY:HA3 | 4:W:334:GLU:HG2 | 1.47 | 0.97 |
| 2:N:117:LEU:CB | 2:N:147:ASN:CG | 2.32 | 0.97 |
| 1:P:174:SER:HB3 | 1:P:667:THR:HG21 | 1.44 | 0.97 |
| 2:Q:117:LEU:HD13 | 2:Q:147:ASN:OD1 | 1.64 | 0.97 |
| 4:X:288:ASP:CB | 4:Z:204:ALA:CB | 2.41 | 0.97 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:218:LEU:CA | 1:A:221:GLN:CG | 2.42 | 0.97 |
| 2:B:130:PRO:O | 2:B:133:ILE:N | 1.97 | 0.97 |
| 1:D:823:PHE:CE1 | 2:E:160:GLY:HA3 | 1.94 | 0.97 |
| 2:E:112:ILE:O | 2:E:147:ASN:C | 2.01 | 0.97 |
| 1:G:84:MLY:HA | 1:G:723:ARG:CZ | 1.94 | 0.97 |
| 1:J:542:PHE:CG | 4:W:143:TYR:CE1 | 2.53 | 0.97 |
| 1:M:795:ARG:CB | 3:O:35:ARG:NH1 | 2.27 | 0.97 |
| 3:O:46:ILE:O | 3:O:50:LEU:HG | 1.64 | 0.97 |
| 1:P:508:ILE:HD11 | 1:P:759:ALA:HB1 | 1.45 | 0.97 |
| 4:V:325:MET:HE2 | 4:X:244:ASP:OD2 | 1.64 | 0.97 |
| 1:J:797:PHE:CD1 | 3:L:146:ILE:CG2 | 2.39 | 0.97 |
| 1:P:797:PHE:CE2 | 3:R:146:ILE:HD12 | 1.98 | 0.97 |
| 1:P:797:PHE:CD1 | 3:R:149:VAL:CG1 | 2.47 | 0.97 |
| 1:P:798:LEU:CD2 | 3:R:126:LEU:CD1 | 2.42 | 0.97 |
| 1:A:800:ARG:NH2 | 3:C:40:ASN:CG | 2.17 | 0.97 |
| 1:D:507:GLY:HA3 | 1:D:762:HIS:CG | 1.99 | 0.97 |
| 1:D:553:MLY:CB | 4:W:46:GLY:CA | 2.32 | 0.97 |
| 1:D:736:GLN:CA | 1:D:743:ALA:HB2 | 1.95 | 0.97 |
| 1:D:799:MET:SD | 3:F:32:ASP:HA | 2.05 | 0.97 |
| 2:E:130:PRO:O | 2:E:133:ILE:N | 1.96 | 0.97 |
| 1:M:549:SER:HB2 | 4:2:43:VAL:HG21 | 1.45 | 0.97 |
| 1:M:649:VAL:CG2 | 1:M:649:VAL:CA | 2.43 | 0.97 |
| 1:M:805:ALA:O | 1:M:809:ARG:HB2 | 1.65 | 0.97 |
| 1:M:831:TRP:HH2 | 2:N:47:LEU:HD21 | 1.24 | 0.97 |
| 1:A:92:ALA:O | 1:A:713:SER:HA | 1.65 | 0.97 |
| 1:A:93:MET:HG2 | 1:A:715:VAL:HG22 | 1.46 | 0.97 |
| 1:A:642:LYS:HG2 | 4:8:21:PHE:O | 1.65 | 0.97 |
| 1:D:635:GLY:HA3 | 4:9:334:GLU:HG2 | 1.47 | 0.97 |
| 1:G:649:VAL:CG2 | 1:G:649:VAL:CA | 2.43 | 0.97 |
| 1:G:813:ILE:CG2 | 2:H:128:PHE:CE1 | 2.47 | 0.97 |
| 1:J:84:MLY:HH21 | 1:J:720:PHE:HA | 0.99 | 0.97 |
| 1:J:218:LEU:CA | 1:J:221:GLN:CG | 2.42 | 0.97 |
| 1:J:649:VAL:CG2 | 1:J:649:VAL:CA | 2.42 | 0.97 |
| 1:M:206:LYS:CD | 1:M:217:THR:CG2 | 2.16 | 0.97 |
| 2:N:141:PRO:HB2 | 2:N:142:PRO:HD2 | 1.44 | 0.97 |
| 1:P:149:GLN:OE1 | 1:P:763:THR:HG21 | 1.65 | 0.97 |
| 1:P:537:GLU:C | 4:1:349:LEU:CD1 | 2.21 | 0.97 |
| 1:A:149:GLN:HB3 | 1:A:719:ASP:CA | 1.94 | 0.97 |
| 1:A:542:PHE:CG | 4:8:143:TYR:CE1 | 2.52 | 0.97 |
| 1:A:791:GLN:CD | 3:C:116:GLU:H | 1.66 | 0.97 |
| 2:B:141:PRO:HB2 | 2:B:142:PRO:HD2 | 1.44 | 0.97 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:C:52:ASN:HB2 | 3:C:53:PRO:HD3 | 1.45 | 0.97 |
| 2:E:150:TYR:C | 2:E:151:LYS:HG3 | 1.83 | 0.97 |
| 1:G:769:ALA:O | 1:G:773:GLY:CA | 2.12 | 0.97 |
| 2:H:141:PRO:HB2 | 2:H:142:PRO:HD2 | 1.44 | 0.97 |
| 1:M:542:PHE:CG | 4:Z:143:TYR:CE1 | 2.53 | 0.97 |
| 1:M:797:PHE:CE2 | 3:O:126:LEU:HD22 | 1.99 | 0.97 |
| 2:Q:112:ILE:O | 2:Q:147:ASN:C | 2.02 | 0.97 |
| 1:A:649:VAL:CG1 | 1:A:649:VAL:HG22 | 1.92 | 0.97 |
| 1:D:649:VAL:CG2 | 1:D:649:VAL:CA | 2.42 | 0.97 |
| 1:D:831:TRP:CD1 | 2:E:51:PHE:HZ | 1.81 | 0.97 |
| 1:G:553:MLY:HH12 | 4:X:45:VAL:HG21 | 1.47 | 0.97 |
| 2:Q:121:LEU:HG | 2:Q:128:PHE:HA | 1.47 | 0.97 |
| 1:A:649:VAL:CG2 | 1:A:649:VAL:CA | 2.43 | 0.96 |
| 1:D:831:TRP:CH2 | 2:E:47:LEU:HD23 | 1.98 | 0.96 |
| 2:E:144:VAL:HG13 | 2:E:153:ILE:HG12 | 1.14 | 0.96 |
| 1:G:553:MLY:CE | 4:X:45:VAL:HB | 1.91 | 0.96 |
| 1:G:708:ARG:HA | 1:G:712:PRO:HG3 | 1.43 | 0.96 |
| 1:G:754:ASP:HB2 | 1:G:776:GLU:CA | 1.94 | 0.96 |
| 1:M:642:LYS:HD2 | 4:Z:24:ASP:O | 1.65 | 0.96 |
| 2:N:121:LEU:HG | 2:N:128:PHE:HA | 1.47 | 0.96 |
| 1:P:642:LYS:HD2 | 4:1:24:ASP:O | 1.65 | 0.96 |
| 1:P:642:LYS:HG2 | 4:1:21:PHE:O | 1.65 | 0.96 |
| 1:P:649:VAL:CG2 | 1:P:649:VAL:CA | 2.42 | 0.96 |
| 4:2:287:ILE:CG2 | 4:4:204:ALA:H | 1.78 | 0.96 |
| 1:A:798:LEU:HD11 | 3:C:126:LEU:HD11 | 1.41 | 0.96 |
| 1:G:542:PHE:CG | 4:V:143:TYR:CE1 | 2.53 | 0.96 |
| 1:M:646:PHE:HE2 | 1:M:652:LEU:HD21 | 1.24 | 0.96 |
| 1:P:817:GLN:CD | 2:Q:127:ARG:HD2 | 1.84 | 0.96 |
| 4:4:288:ASP:H | 4:6:203:THR:HG22 | 1.29 | 0.96 |
| 1:A:93:MET:CG | 1:A:715:VAL:HG22 | 1.94 | 0.96 |
| 1:D:174:SER:HB3 | 1:D:667:THR:HG21 | 1.44 | 0.96 |
| 1:G:218:LEU:CA | 1:G:221:GLN:CG | 2.42 | 0.96 |
| 1:G:534:SER:O | 4:V:351:THR:HA | 1.60 | 0.96 |
| 1:G:792:ALA:CB | 3:I:42:THR:CA | 2.44 | 0.96 |
| 1:G:829:TRP:CZ3 | 2:H:84:PHE:CZ | 2.54 | 0.96 |
| 1:J:838:ILE:HD11 | 2:K:54:MET:HE1 | 1.00 | 0.96 |
| 1:M:576:GLU:HG2 | 1:M:577:ALA:N | 1.66 | 0.96 |
| 1:P:542:PHE:CG | 4:1:143:TYR:CE1 | 2.53 | 0.96 |
| 1:P:817:GLN:HG2 | 2:Q:127:ARG:HB2 | 1.45 | 0.96 |
| 1:A:149:GLN:CB | 1:A:719:ASP:OD1 | 2.12 | 0.96 |
| 1:A:541:MET:N | 4:8:349:LEU:HD21 | 1.80 | 0.96 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:736:GLN:CA | 1:A:743:ALA:HB2 | 1.95 | 0.96 |
| 1:D:795:ARG:HB2 | 3:F:35:ARG:NH1 | 1.80 | 0.96 |
| 2:H:130:PRO:O | 2:H:133:ILE:N | 1.97 | 0.96 |
| 1:J:736:GLN:CA | 1:J:743:ALA:HB2 | 1.95 | 0.96 |
| 1:J:756:THR:CG2 | 1:J:776:GLU:CB | 2.43 | 0.96 |
| 2:K:150:TYR:O | 2:K:151:LYS:HG3 | 1.65 | 0.96 |
| 1:M:642:LYS:HG2 | 4:Z:21:PHE:O | 1.65 | 0.96 |
| 1:P:530:MET:CE | 4:1:354:GLN:CG | 2.40 | 0.96 |
| 1:P:797:PHE:CE1 | 3:R:146:ILE:HA | 2.00 | 0.96 |
| 4:1:287:ILE:HG21 | 4:3:203:THR:N | 1.78 | 0.96 |
| 4:8:286:ASP:OD1 | 4:V:203:THR:HG22 | 1.62 | 0.96 |
| 1:A:537:GLU:C | 4:8:349:LEU:CD1 | 2.20 | 0.96 |
| 1:D:637:LYS:NZ | 4:9:141:SER:O | 1.99 | 0.96 |
| 1:J:174:SER:HB3 | 1:J:667:THR:HG21 | 1.44 | 0.96 |
| 1:J:756:THR:HG22 | 1:J:776:GLU:CA | 1.93 | 0.96 |
| 1:M:797:PHE:CZ | 3:O:146:ILE:HD13 | 2.00 | 0.96 |
| 1:M:818:TYR:CZ | 2:N:127:ARG:NH2 | 2.18 | 0.96 |
| 1:M:829:TRP:CH2 | 2:N:87:LYS:NZ | 2.34 | 0.96 |
| 1:P:641:LYS:HG3 | 1:P:647:GLN:NE2 | 1.59 | 0.96 |
| 2:Q:121:LEU:CB | 2:Q:128:PHE:HB3 | 1.68 | 0.96 |
| 4:4:322:PRO:HB2 | 4:6:244:ASP:CB | 1.95 | 0.96 |
| 1:A:813:ILE:HG21 | 2:B:127:ARG:HD2 | 1.46 | 0.96 |
| 3:O:52:ASN:HB2 | 3:O:53:PRO:HD3 | 1.46 | 0.96 |
| 1:A:646:PHE:HE2 | 1:A:652:LEU:HD21 | 1.24 | 0.96 |
| 1:D:649:VAL:CG1 | 1:D:649:VAL:CG2 | 2.43 | 0.96 |
| 1:G:567:LYS:HZ2 | 4:X:92:ASN:HD22 | 1.09 | 0.96 |
| 1:G:642:LYS:HG2 | 4:V:21:PHE:O | 1.65 | 0.96 |
| 1:J:836:PHE:CZ | 2:K:160:GLY:N | 2.33 | 0.96 |
| 2:K:130:PRO:O | 2:K:133:ILE:N | 1.96 | 0.96 |
| 1:A:553:MLY:HB3 | 4:V:46:GLY:HA2 | 1.47 | 0.96 |
| 2:B:121:LEU:HG | 2:B:128:PHE:CA | 1.60 | 0.96 |
| 2:K:112:ILE:O | 2:K:147:ASN:C | 2.02 | 0.96 |
| 1:P:218:LEU:CA | 1:P:221:GLN:CG | 2.42 | 0.96 |
| 1:P:819:ASN:ND2 | 2:Q:92:ASP:CB | 2.29 | 0.96 |
| 1:A:721:LYS:CA | 1:A:736:GLN:CD | 2.34 | 0.96 |
| 3:F:46:ILE:O | 3:F:50:LEU:HG | 1.65 | 0.96 |
| 1:G:148:ARG:CZ | 1:G:764:MLY:HH21 | 1.96 | 0.96 |
| 2:K:144:VAL:HG13 | 2:K:153:ILE:HD11 | 1.21 | 0.96 |
| 1:M:218:LEU:CA | 1:M:221:GLN:CG | 2.42 | 0.96 |
| 1:P:769:ALA:O | 1:P:771:LEU:N | 1.93 | 0.96 |
| 2:Q:150:TYR:C | 2:Q:151:LYS:HG3 | 1.83 | 0.96 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:R:52:ASN:HB2 | 3:R:53:PRO:HD3 | 1.46 | 0.96 |
| 4:2:322:PRO:CB | 4:4:244:ASP:CB | 2.44 | 0.96 |
| 4:4:324:THR:HG23 | 4:6:244:ASP:C | 1.86 | 0.96 |
| 1:D:813:ILE:CD1 | 2:E:128:PHE:HE1 | 1.78 | 0.96 |
| 1:D:818:TYR:CB | 2:E:90:GLY:CA | 2.23 | 0.96 |
| 1:G:543:PRO:CG | 4:V:143:TYR:O | 2.14 | 0.96 |
| 1:G:642:LYS:HD2 | 4:V:24:ASP:O | 1.65 | 0.96 |
| 2:H:150:TYR:O | 2:H:151:LYS:HG3 | 1.65 | 0.96 |
| 1:J:735:GLY:C | 1:J:743:ALA:CA | 2.35 | 0.96 |
| 1:M:735:GLY:C | 1:M:743:ALA:CA | 2.35 | 0.96 |
| 1:A:649:VAL:CG1 | 1:A:649:VAL:CG2 | 2.44 | 0.95 |
| 1:A:797:PHE:HD1 | 3:C:146:ILE:O | 1.35 | 0.95 |
| 2:B:117:LEU:HD13 | 2:B:147:ASN:OD1 | 1.64 | 0.95 |
| 1:D:642:LYS:HG2 | 4:9:21:PHE:O | 1.65 | 0.95 |
| 1:D:798:LEU:HD11 | 3:F:126:LEU:CG | 1.95 | 0.95 |
| 1:G:649:VAL:CG1 | 1:G:649:VAL:CG2 | 2.44 | 0.95 |
| 1:G:735:GLY:C | 1:G:743:ALA:CA | 2.34 | 0.95 |
| 1:J:538:GLU:HG3 | 4:W:352:PHE:N | 1.81 | 0.95 |
| 1:M:736:GLN:CA | 1:M:743:ALA:HB2 | 1.95 | 0.95 |
| 2:N:150:TYR:O | 2:N:151:LYS:HG3 | 1.65 | 0.95 |
| 4:2:287:ILE:HG12 | 4:4:202:THR:HA | 1.48 | 0.95 |
| 1:A:641:LYS:HG3 | 1:A:647:GLN:NE2 | 1.58 | 0.95 |
| 1:G:508:ILE:HD11 | 1:G:759:ALA:HB2 | 0.96 | 0.95 |
| 1:J:817:GLN:CG | 2:K:127:ARG:CB | 2.37 | 0.95 |
| 1:J:829:TRP:CH2 | 2:K:87:LYS:HE2 | 2.01 | 0.95 |
| 4:V:286:ASP:CG | 4:X:203:THR:HG22 | 1.87 | 0.95 |
| 1:A:95:THR:OG1 | 1:A:769:ALA:HA | 1.64 | 0.95 |
| 2:B:150:TYR:O | 2:B:151:LYS:HG3 | 1.65 | 0.95 |
| 1:D:721:LYS:CA | 1:D:736:GLN:CD | 2.34 | 0.95 |
| 1:J:836:PHE:HE1 | 2:K:159:HIS:HA | 1.32 | 0.95 |
| 1:M:709:LYS:N | 1:M:710:GLY:N | 2.14 | 0.95 |
| 1:M:795:ARG:HB3 | 3:O:35:ARG:HH22 | 1.16 | 0.95 |
| 1:P:635:GLY:HA3 | 4:1:334:GLU:HG2 | 1.47 | 0.95 |
| 1:A:543:PRO:CG | 4:8:143:TYR:O | 2.14 | 0.95 |
| 1:D:508:ILE:HA | 1:D:761:GLY:HA3 | 1.46 | 0.95 |
| 1:D:642:LYS:HD2 | 4:9:24:ASP:O | 1.64 | 0.95 |
| 1:G:538:GLU:HG3 | 4:V:352:PHE:N | 1.81 | 0.95 |
| 1:G:721:LYS:CA | 1:G:736:GLN:CD | 2.34 | 0.95 |
| 1:J:642:LYS:HD2 | 4:W:24:ASP:O | 1.65 | 0.95 |
| 1:J:721:LYS:CA | 1:J:736:GLN:CD | 2.34 | 0.95 |
| 1:J:783:LEU:O | 1:J:787:ILE:N | 1.99 | 0.95 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:538:GLU:HG3 | 4:Z:352:PHE:N | 1.82 | 0.95 |
| 1:M:637:LYS:NZ | 4:Z:141:SER:O | 1.99 | 0.95 |
| 1:P:637:LYS:NZ | 4:1:141:SER:O | 1.98 | 0.95 |
| 1:P:649:VAL:CG1 | 1:P:649:VAL:CG2 | 2.44 | 0.95 |
| 4:9:288:ASP:HA | 4:W:204:ALA:HB2 | 1.48 | 0.95 |
| 1:A:149:GLN:OE1 | 1:A:716:LEU:HD23 | 0.77 | 0.95 |
| 1:A:831:TRP:CZ3 | 2:B:34:ILE:HG12 | 2.01 | 0.95 |
| 1:D:538:GLU:HG3 | 4:9:352:PHE:N | 1.82 | 0.95 |
| 2:E:121:LEU:HG | 2:E:128:PHE:HA | 1.46 | 0.95 |
| 1:G:93:MET:HA | 1:G:714:ARG:N | 1.80 | 0.95 |
| 1:G:641:LYS:HG3 | 1:G:647:GLN:NE2 | 1.58 | 0.95 |
| 1:G:801:VAL:CG2 | 3:I:126:LEU:CD2 | 2.44 | 0.95 |
| 1:G:821:ARG:NH2 | 2:H:127:ARG:CG | 2.27 | 0.95 |
| 1:J:649:VAL:CG1 | 1:J:649:VAL:CG2 | 2.44 | 0.95 |
| 2:K:121:LEU:HG | 2:K:128:PHE:HA | 1.47 | 0.95 |
| 1:P:798:LEU:HD11 | 3:R:126:LEU:HD21 | 1.13 | 0.95 |
| 4:8:288:ASP:HA | 4:V:204:ALA:HB2 | 1.48 | 0.95 |
| 1:A:707:CYS:C | 1:A:714:ARG:NH2 | 2.20 | 0.95 |
| 1:A:836:PHE:HZ | 2:B:160:GLY:N | 1.53 | 0.95 |
| 1:A:836:PHE:HE1 | 2:B:159:HIS:CB | 1.79 | 0.95 |
| 1:D:538:GLU:N | 4:9:349:LEU:CD1 | 2.28 | 0.95 |
| 1:J:637:LYS:NZ | 4:W:141:SER:O | 1.99 | 0.95 |
| 1:J:642:LYS:HG2 | 4:W:21:PHE:O | 1.65 | 0.95 |
| 1:M:724:TYR:CZ | 1:M:772:LEU:HG | 2.00 | 0.95 |
| 2:N:111:SER:CB | 2:N:148:VAL:C | 1.92 | 0.95 |
| 1:P:538:GLU:N | 4:1:349:LEU:CD1 | 2.29 | 0.95 |
| 4:1:246:GLN:HA | 4:Y:324:THR:HB | 1.45 | 0.95 |
| 1:A:530:MET:HE2 | 4:8:354:GLN:CG | 1.96 | 0.95 |
| 1:A:795:ARG:CZ | 3:C:116:GLU:CD | 2.28 | 0.95 |
| 1:A:823:PHE:HE1 | 2:B:160:GLY:CA | 1.78 | 0.95 |
| 1:D:530:MET:HA | 4:9:354:GLN:HG3 | 0.96 | 0.95 |
| 1:D:797:PHE:CG | 3:F:146:ILE:HG23 | 2.01 | 0.95 |
| 2:E:117:LEU:HD13 | 2:E:147:ASN:OD1 | 1.64 | 0.95 |
| 3:I:46:ILE:O | 3:I:50:LEU:HG | 1.64 | 0.95 |
| 1:J:537:GLU:C | 4:W:349:LEU:CD1 | 2.21 | 0.95 |
| 1:J:813:ILE:CG2 | 2:K:128:PHE:HE1 | 1.78 | 0.95 |
| 1:P:735:GLY:C | 1:P:743:ALA:CA | 2.35 | 0.95 |
| 4:7:288:ASP:HA | 4:9:204:ALA:HB2 | 1.48 | 0.95 |
| 1:A:641:LYS:HD2 | 1:A:647:GLN:CD | 1.70 | 0.95 |
| 1:G:215:GLN:HA | 1:G:340:ILE:HG23 | 0.95 | 0.95 |
| 1:G:506:GLU:OE2 | 1:G:760:PHE:HB2 | 1.67 | 0.95 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:538:GLU:N | 4:W:349:LEU:CD1 | 2.28 | 0.95 |
| 1:J:543:PRO:CG | 4:W:143:TYR:O | 2.14 | 0.95 |
| 1:M:215:GLN:HA | 1:M:340:ILE:HG23 | 0.95 | 0.95 |
| 1:P:818:TYR:HE1 | 2:Q:127:ARG:NH2 | 1.63 | 0.95 |
| 4:3:288:ASP:N | 4:5:203:THR:HG22 | 1.80 | 0.95 |
| 1:A:93:MET:CE | 1:A:715:VAL:HG13 | 1.96 | 0.95 |
| 1:A:791:GLN:HE22 | 3:C:115:GLY:CA | 1.79 | 0.95 |
| 1:A:823:PHE:CE1 | 2:B:160:GLY:CA | 2.49 | 0.95 |
| 2:K:117:LEU:HD13 | 2:K:147:ASN:OD1 | 1.64 | 0.95 |
| 1:M:541:MET:N | 4:Z:349:LEU:HD21 | 1.80 | 0.95 |
| 1:P:505:MLY:HH23 | 1:P:762:HIS:ND1 | 0.95 | 0.95 |
| 1:A:795:ARG:CG | 3:C:35:ARG:HH12 | 1.78 | 0.95 |
| 1:A:836:PHE:CE1 | 2:B:159:HIS:CB | 2.48 | 0.95 |
| 1:D:543:PRO:CG | 4:9:143:TYR:O | 2.14 | 0.95 |
| 1:D:834:LEU:CD1 | 2:E:54:MET:CB | 2.45 | 0.95 |
| 2:E:150:TYR:O | 2:E:151:LYS:HG3 | 1.65 | 0.95 |
| 1:G:505:MLY:HH21 | 1:G:762:HIS:ND1 | 1.58 | 0.95 |
| 1:G:534:SER:O | 4:V:351:THR:HG23 | 1.12 | 0.95 |
| 1:G:642:LYS:CG | 4:V:23:GLY:H | 1.76 | 0.95 |
| 1:G:752:ASP:O | 1:G:780:ASP:CA | 2.14 | 0.95 |
| 1:G:795:ARG:CB | 3:I:35:ARG:HH12 | 1.80 | 0.95 |
| 2:H:150:TYR:O | 2:H:151:LYS:CG | 2.15 | 0.95 |
| 3:L:52:ASN:HB2 | 3:L:53:PRO:HD3 | 1.46 | 0.95 |
| 1:M:538:GLU:N | 4:Z:349:LEU:CD1 | 2.29 | 0.95 |
| 1:M:649:VAL:CG1 | 1:M:649:VAL:CG2 | 2.44 | 0.95 |
| 1:P:543:PRO:CG | 4:1:143:TYR:O | 2.14 | 0.95 |
| 1:P:721:LYS:CA | 1:P:736:GLN:CD | 2.34 | 0.95 |
| 1:A:538:GLU:HG3 | 4:8:352:PHE:N | 1.82 | 0.94 |
| 2:B:150:TYR:O | 2:B:151:LYS:CG | 2.15 | 0.94 |
| 1:G:530:MET:HA | 4:V:354:GLN:HG3 | 0.97 | 0.94 |
| 1:G:637:LYS:NZ | 4:V:141:SER:O | 1.99 | 0.94 |
| 1:M:543:PRO:CG | 4:Z:143:TYR:O | 2.14 | 0.94 |
| 1:A:735:GLY:C | 1:A:743:ALA:CA | 2.34 | 0.94 |
| 2:B:150:TYR:O | 2:B:151:LYS:HB2 | 1.67 | 0.94 |
| 1:D:541:MET:N | 4:9:349:LEU:HD21 | 1.80 | 0.94 |
| 1:J:530:MET:CE | 4:W:354:GLN:CG | 2.41 | 0.94 |
| 1:J:546:THR:HG22 | 1:J:548:THR:H | 1.32 | 0.94 |
| 1:M:721:LYS:CA | 1:M:736:GLN:CD | 2.34 | 0.94 |
| 1:P:546:THR:HG22 | 1:P:548:THR:H | 1.32 | 0.94 |
| 1:A:530:MET:HA | 4:8:354:GLN:HG3 | 0.96 | 0.94 |
| 1:A:813:ILE:HG22 | 2:B:127:ARG:HD2 | 0.96 | 0.94 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:530:MET:CA | 4:9:354:GLN:CG | 2.44 | 0.94 |
| 1:G:538:GLU:N | 4:V:349:LEU:CD1 | 2.29 | 0.94 |
| 1:M:836:PHE:CE2 | 2:N:160:GLY:CA | 2.50 | 0.94 |
| 1:P:502:GLU:OE2 | 1:P:761:GLY:HA3 | 1.67 | 0.94 |
| 1:P:795:ARG:HB2 | 3:R:35:ARG:NH1 | 1.81 | 0.94 |
| 2:Q:150:TYR:O | 2:Q:151:LYS:HG3 | 1.66 | 0.94 |
| 1:A:768:MLY:HG2 | 1:A:771:LEU:HD13 | 1.45 | 0.94 |
| 1:A:834:LEU:CD2 | 2:B:54:MET:HE2 | 1.97 | 0.94 |
| 1:M:635:GLY:HA3 | 4:Z:334:GLU:HG2 | 1.47 | 0.94 |
| 1:M:817:GLN:CD | 2:N:127:ARG:HD2 | 1.87 | 0.94 |
| 1:M:818:TYR:CE1 | 2:N:127:ARG:CZ | 2.49 | 0.94 |
| 1:P:538:GLU:HG3 | 4:1:352:PHE:N | 1.82 | 0.94 |
| 3:R:46:ILE:O | 3:R:50:LEU:HG | 1.64 | 0.94 |
| 1:A:538:GLU:N | 4:8:349:LEU:CD1 | 2.28 | 0.94 |
| 1:A:836:PHE:HE1 | 2:B:159:HIS:HB2 | 1.22 | 0.94 |
| 1:D:206:LYS:CD | 1:D:217:THR:CG2 | 2.16 | 0.94 |
| 1:G:84:MLY:HB3 | 1:G:723:ARG:HE | 1.14 | 0.94 |
| 1:G:541:MET:N | 4:V:349:LEU:HD21 | 1.80 | 0.94 |
| 1:J:97:LEU:HD23 | 1:J:712:PRO:CB | 1.97 | 0.94 |
| 1:J:795:ARG:C | 3:L:35:ARG:NH2 | 2.21 | 0.94 |
| 4:2:288:ASP:CG | 4:4:203:THR:HG23 | 1.86 | 0.94 |
| 1:A:149:GLN:CG | 1:A:719:ASP:H | 1.78 | 0.94 |
| 2:B:121:LEU:HG | 2:B:128:PHE:HA | 1.47 | 0.94 |
| 1:D:735:GLY:C | 1:D:743:ALA:CA | 2.35 | 0.94 |
| 1:D:767:PHE:O | 1:D:771:LEU:HD11 | 1.68 | 0.94 |
| 1:D:831:TRP:CZ2 | 2:E:47:LEU:CB | 2.51 | 0.94 |
| 2:K:150:TYR:O | 2:K:151:LYS:CG | 2.15 | 0.94 |
| 1:P:791:GLN:HE22 | 3:R:115:GLY:HA3 | 1.30 | 0.94 |
| 2:Q:150:TYR:O | 2:Q:151:LYS:CG | 2.16 | 0.94 |
| 1:A:819:ASN:ND2 | 2:B:91:ALA:N | 2.15 | 0.94 |
| 1:G:641:LYS:HD2 | 1:G:647:GLN:CD | 1.70 | 0.94 |
| 1:J:84:MLY:HH23 | 1:J:720:PHE:HA | 1.50 | 0.94 |
| 1:J:206:LYS:CD | 1:J:217:THR:CG2 | 2.16 | 0.94 |
| 1:J:530:MET:HA | 4:W:354:GLN:HG3 | 0.96 | 0.94 |
| 4:2:287:ILE:HB | 4:4:203:THR:N | 1.82 | 0.94 |
| 1:A:637:LYS:NZ | 4:8:141:SER:O | 1.99 | 0.94 |
| 1:D:553:MLY:HB3 | 4:W:46:GLY:HA2 | 1.47 | 0.94 |
| 1:G:612:GLN:NE2 | 1:G:627:GLY:CA | 2.31 | 0.94 |
| 1:G:752:ASP:C | 1:G:780:ASP:OD1 | 2.05 | 0.94 |
| 1:G:795:ARG:CG | 3:I:118:MET:CE | 2.38 | 0.94 |
| 2:H:121:LEU:HG | 2:H:128:PHE:HA | 1.47 | 0.94 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:817:GLN:CB | 2:N:127:ARG:HD2 | 1.97 | 0.94 |
| 1:M:836:PHE:CE2 | 2:N:160:GLY:HA3 | 2.02 | 0.94 |
| 1:P:97:LEU:HD22 | 1:P:712:PRO:CB | 1.97 | 0.94 |
| 1:P:541:MET:N | 4:1:349:LEU:HD21 | 1.80 | 0.94 |
| 1:G:537:GLU:C | 4:V:349:LEU:CD1 | 2.21 | 0.94 |
| 1:P:215:GLN:HA | 1:P:340:ILE:HG23 | 0.95 | 0.94 |
| 1:D:838:ILE:CD1 | 2:E:54:MET:HE3 | 1.98 | 0.94 |
| 2:E:150:TYR:O | 2:E:151:LYS:CG | 2.15 | 0.94 |
| 2:H:117:LEU:HD13 | 2:H:147:ASN:OD1 | 1.64 | 0.94 |
| 1:J:97:LEU:CD2 | 1:J:712:PRO:CB | 2.46 | 0.94 |
| 1:J:612:GLN:NE2 | 1:J:627:GLY:HA3 | 1.83 | 0.94 |
| 1:D:546:THR:HG22 | 1:D:548:THR:H | 1.32 | 0.93 |
| 1:J:530:MET:CA | 4:W:354:GLN:CG | 2.45 | 0.93 |
| 1:M:546:THR:HG22 | 1:M:548:THR:H | 1.32 | 0.93 |
| 1:P:218:LEU:CB | 1:P:221:GLN:CG | 2.46 | 0.93 |
| 1:A:557:GLU:H | 4:V:48:GLY:HA2 | 1.32 | 0.93 |
| 1:A:635:GLY:HA3 | 4:8:334:GLU:HG2 | 1.47 | 0.93 |
| 1:D:612:GLN:NE2 | 1:D:627:GLY:HA3 | 1.83 | 0.93 |
| 2:K:144:VAL:HG13 | 2:K:153:ILE:HG12 | 1.14 | 0.93 |
| 1:M:612:GLN:NE2 | 1:M:627:GLY:CA | 2.31 | 0.93 |
| 2:N:150:TYR:O | 2:N:151:LYS:CG | 2.15 | 0.93 |
| 4:3:322:PRO:CB | 4:5:244:ASP:CG | 2.37 | 0.93 |
| 1:M:530:MET:HA | 4:Z:354:GLN:HG3 | 0.96 | 0.93 |
| 4:2:287:ILE:CD1 | 4:4:203:THR:HB | 1.98 | 0.93 |
| 1:A:499:GLU:OE1 | 1:A:766:PHE:CE2 | 2.22 | 0.93 |
| 1:A:505:MLY:CA | 1:A:762:HIS:CD2 | 2.52 | 0.93 |
| 1:A:612:GLN:NE2 | 1:A:627:GLY:HA3 | 1.83 | 0.93 |
| 1:G:546:THR:HG22 | 1:G:548:THR:H | 1.32 | 0.93 |
| 1:J:756:THR:CA | 1:J:776:GLU:OE1 | 2.16 | 0.93 |
| 1:P:709:LYS:N | 1:P:710:GLY:N | 2.15 | 0.93 |
| 1:P:797:PHE:CZ | 3:R:146:ILE:CD1 | 2.52 | 0.93 |
| 1:P:831:TRP:CH2 | 2:Q:47:LEU:HD21 | 1.96 | 0.93 |
| 1:A:818:TYR:HB2 | 2:B:90:GLY:HA3 | 0.95 | 0.93 |
| 1:D:838:ILE:HD13 | 2:E:54:MET:HE1 | 1.39 | 0.93 |
| 1:G:505:MLY:HH23 | 1:G:762:HIS:CD2 | 2.02 | 0.93 |
| 1:G:788:THR:O | 3:I:42:THR:HG21 | 1.69 | 0.93 |
| 2:K:150:TYR:O | 2:K:151:LYS:HB2 | 1.67 | 0.93 |
| 1:P:534:SER:O | 4:1:351:THR:HG23 | 1.13 | 0.93 |
| 1:P:612:GLN:NE2 | 1:P:627:GLY:HA3 | 1.83 | 0.93 |
| 1:D:798:LEU:HD13 | 3:F:126:LEU:HD11 | 1.49 | 0.93 |
| 1:G:503:TYR:CZ | 1:G:711:PHE:HD2 | 1.86 | 0.93 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:795:ARG:HB2 | 3:I:35:ARG:HH12 | 1.32 | 0.93 |
| 1:P:834:LEU:CD1 | 2:Q:51:PHE:CE1 | 2.48 | 0.93 |
| 1:A:753:VAL:CG1 | 1:A:775:LEU:CD2 | 2.44 | 0.93 |
| 1:D:215:GLN:HA | 1:D:340:ILE:HG23 | 0.95 | 0.93 |
| 1:G:505:MLY:HH21 | 1:G:762:HIS:CE1 | 1.48 | 0.93 |
| 1:J:642:LYS:CB | 4:W:21:PHE:O | 2.17 | 0.93 |
| 1:M:639:GLY:N | 4:Z:345:ILE:N | 1.94 | 0.93 |
| 1:P:629:GLU:CB | 1:P:643:GLY:O | 2.17 | 0.93 |
| 1:D:831:TRP:NE1 | 2:E:67:MET:SD | 2.42 | 0.93 |
| 1:G:28:GLN:HB3 | 1:G:723:ARG:CZ | 1.97 | 0.93 |
| 1:J:642:LYS:CG | 4:W:23:GLY:H | 1.77 | 0.93 |
| 1:J:796:GLY:HA2 | 3:L:35:ARG:HD3 | 1.49 | 0.93 |
| 1:M:548:THR:HG21 | 4:2:47:MET:CG | 1.97 | 0.93 |
| 1:M:642:LYS:CB | 4:Z:21:PHE:O | 2.17 | 0.93 |
| 1:P:530:MET:CA | 4:1:354:GLN:CG | 2.45 | 0.93 |
| 1:P:642:LYS:CB | 4:1:21:PHE:O | 2.17 | 0.93 |
| 1:P:836:PHE:CE2 | 2:Q:160:GLY:CA | 2.52 | 0.93 |
| 4:2:288:ASP:N | 4:4:203:THR:HG22 | 1.82 | 0.93 |
| 1:A:546:THR:HG22 | 1:A:548:THR:H | 1.32 | 0.93 |
| 1:D:648:THR:HG21 | 1:D:651:ALA:HB2 | 1.50 | 0.93 |
| 1:G:757:GLN:CG | 1:G:776:GLU:CD | 2.36 | 0.93 |
| 1:J:541:MET:N | 4:W:349:LEU:HD21 | 1.80 | 0.93 |
| 1:A:538:GLU:N | 4:8:351:THR:H | 1.67 | 0.93 |
| 1:A:612:GLN:NE2 | 1:A:627:GLY:CA | 2.31 | 0.93 |
| 1:A:642:LYS:CG | 4:8:23:GLY:H | 1.77 | 0.93 |
| 1:D:506:GLU:HG3 | 1:D:764:MLY:CE | 1.98 | 0.93 |
| 1:G:97:LEU:CD2 | 1:G:712:PRO:HB2 | 1.95 | 0.93 |
| 1:G:635:GLY:HA3 | 4:V:334:GLU:HG2 | 1.47 | 0.93 |
| 1:G:739:ASP:HB3 | 1:G:742:LYS:CB | 1.99 | 0.93 |
| 1:J:739:ASP:HB3 | 1:J:742:LYS:CB | 1.98 | 0.93 |
| 2:K:149:ASP:CG | 2:K:150:TYR:H | 1.73 | 0.93 |
| 1:M:548:THR:HG21 | 4:2:47:MET:HG3 | 1.51 | 0.93 |
| 1:M:818:TYR:HE1 | 2:N:127:ARG:NH2 | 1.64 | 0.93 |
| 1:P:530:MET:HA | 4:1:354:GLN:HG3 | 0.96 | 0.93 |
| 1:P:612:GLN:NE2 | 1:P:627:GLY:CA | 2.31 | 0.93 |
| 1:P:836:PHE:CE2 | 2:Q:160:GLY:HA3 | 2.03 | 0.93 |
| 1:D:629:GLU:CB | 1:D:643:GLY:O | 2.17 | 0.92 |
| 1:M:798:LEU:HD11 | 3:O:126:LEU:HD21 | 1.02 | 0.92 |
| 1:M:834:LEU:CD1 | 2:N:51:PHE:CE1 | 2.48 | 0.92 |
| 2:N:150:TYR:O | 2:N:151:LYS:HB2 | 1.67 | 0.92 |
| 4:V:325:MET:CE | 4:X:244:ASP:CG | 2.37 | 0.92 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:642:LYS:CB | 4:9:21:PHE:O | 2.17 | 0.92 |
| 1:G:813:ILE:CG2 | 2:H:128:PHE:CZ | 2.52 | 0.92 |
| 2:H:121:LEU:HG | 2:H:128:PHE:CA | 1.60 | 0.92 |
| 2:N:121:LEU:CB | 2:N:128:PHE:HB3 | 1.69 | 0.92 |
| 1:P:549:SER:N | 4:3:47:MET:O | 2.02 | 0.92 |
| 1:A:797:PHE:HZ | 3:C:146:ILE:HD13 | 1.25 | 0.92 |
| 1:D:641:LYS:HG3 | 1:D:647:GLN:NE2 | 1.59 | 0.92 |
| 2:E:150:TYR:O | 2:E:151:LYS:HB2 | 1.67 | 0.92 |
| 1:J:215:GLN:HA | 1:J:340:ILE:HG23 | 0.95 | 0.92 |
| 1:D:799:MET:HE1 | 3:F:32:ASP:HB3 | 1.49 | 0.92 |
| 1:D:819:ASN:CB | 2:E:90:GLY:O | 2.18 | 0.92 |
| 1:G:506:GLU:CD | 1:G:760:PHE:O | 2.08 | 0.92 |
| 1:G:736:GLN:CA | 1:G:743:ALA:HB2 | 1.95 | 0.92 |
| 1:G:754:ASP:CA | 1:G:776:GLU:OE1 | 2.18 | 0.92 |
| 1:M:530:MET:CA | 4:Z:354:GLN:CG | 2.44 | 0.92 |
| 1:P:817:GLN:HB3 | 2:Q:127:ARG:CD | 1.99 | 0.92 |
| 4:I:244:ASP:N | 4:Y:291:LYS:CD | 2.31 | 0.92 |
| 4:4:287:ILE:HD13 | 4:6:203:THR:CB | 1.92 | 0.92 |
| 1:A:636:LYS:HD2 | 4:8:332:PRO:HB3 | 1.51 | 0.92 |
| 1:D:612:GLN:NE2 | 1:D:627:GLY:CA | 2.31 | 0.92 |
| 1:D:641:LYS:HE3 | 1:D:647:GLN:CG | 2.00 | 0.92 |
| 1:D:739:ASP:HB3 | 1:D:742:LYS:CB | 1.98 | 0.92 |
| 1:J:638:GLY:HA3 | 4:W:341:ILE:O | 1.70 | 0.92 |
| 1:M:612:GLN:NE2 | 1:M:627:GLY:HA3 | 1.83 | 0.92 |
| 1:M:785:GLU:O | 1:M:789:ALA:HB2 | 1.69 | 0.92 |
| 1:P:638:GLY:HA3 | 4:I:341:ILE:O | 1.70 | 0.92 |
| 4:W:286:ASP:OD1 | 4:Y:202:THR:HB | 1.69 | 0.92 |
| 1:A:213:LYS:HA | 1:A:220:ASP:CG | 1.90 | 0.92 |
| 1:A:530:MET:CA | 4:8:354:GLN:CG | 2.44 | 0.92 |
| 1:D:795:ARG:HG2 | 3:F:118:MET:HE3 | 1.52 | 0.92 |
| 1:G:642:LYS:CB | 4:V:21:PHE:O | 2.17 | 0.92 |
| 1:J:553:MLY:HE3 | 4:Y:45:VAL:HG11 | 1.47 | 0.92 |
| 2:N:117:LEU:HD13 | 2:N:147:ASN:OD1 | 1.64 | 0.92 |
| 1:P:642:LYS:CG | 4:I:23:GLY:H | 1.77 | 0.92 |
| 1:D:831:TRP:HH2 | 2:E:47:LEU:HA | 1.20 | 0.92 |
| 1:G:278:GLN:HG2 | 1:G:317:GLU:HB2 | 1.52 | 0.92 |
| 1:G:629:GLU:CB | 1:G:643:GLY:O | 2.17 | 0.92 |
| 1:J:629:GLU:CB | 1:J:643:GLY:O | 2.17 | 0.92 |
| 1:M:648:THR:HG21 | 1:M:651:ALA:HB2 | 1.50 | 0.92 |
| 1:M:739:ASP:HB3 | 1:M:742:LYS:CB | 1.99 | 0.92 |
| 1:P:739:ASP:HB3 | 1:P:742:LYS:CB | 1.98 | 0.92 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:2:287:ILE:CG1 | 4:4:202:THR:HB | 2.00 | 0.92 |
| 4:W:325:MET:CE | 4:Y:244:ASP:CG | 2.37 | 0.92 |
| 1:D:537:GLU:C | 4:9:349:LEU:CD1 | 2.20 | 0.92 |
| 1:D:831:TRP:HZ2 | 2:E:47:LEU:HB3 | 1.35 | 0.92 |
| 1:G:28:GLN:O | 1:G:723:ARG:NH2 | 2.03 | 0.92 |
| 1:G:537:GLU:O | 4:V:349:LEU:HD13 | 0.74 | 0.92 |
| 1:M:817:GLN:HG2 | 2:N:127:ARG:HD2 | 1.50 | 0.92 |
| 2:N:121:LEU:CA | 2:N:128:PHE:CB | 2.46 | 0.92 |
| 1:A:799:MET:SD | 3:C:32:ASP:HA | 2.08 | 0.92 |
| 1:D:798:LEU:CD1 | 3:F:126:LEU:CD1 | 2.10 | 0.92 |
| 2:E:121:LEU:CA | 2:E:128:PHE:CB | 2.46 | 0.92 |
| 1:G:530:MET:CA | 4:V:354:GLN:CG | 2.45 | 0.92 |
| 1:G:836:PHE:CE1 | 2:H:159:HIS:HA | 2.05 | 0.92 |
| 1:J:215:GLN:H | 1:J:340:ILE:CG1 | 1.72 | 0.92 |
| 1:J:641:LYS:HE3 | 1:J:647:GLN:CG | 2.00 | 0.92 |
| 1:J:795:ARG:NH2 | 3:L:116:GLU:OE1 | 2.03 | 0.92 |
| 1:M:785:GLU:C | 1:M:786:ILE:HA | 1.89 | 0.92 |
| 1:P:735:GLY:C | 1:P:743:ALA:HA | 1.91 | 0.92 |
| 4:I:246:GLN:HA | 4:Y:324:THR:OG1 | 1.70 | 0.92 |
| 1:A:629:GLU:CB | 1:A:643:GLY:O | 2.17 | 0.92 |
| 1:G:218:LEU:CB | 1:G:221:GLN:CG | 2.46 | 0.92 |
| 1:G:567:LYS:HZ1 | 4:X:92:ASN:HD22 | 1.14 | 0.92 |
| 1:G:612:GLN:NE2 | 1:G:627:GLY:HA3 | 1.83 | 0.92 |
| 1:G:636:LYS:HD2 | 4:V:332:PRO:HB3 | 1.52 | 0.92 |
| 1:J:756:THR:CG2 | 1:J:776:GLU:CD | 2.38 | 0.92 |
| 1:M:820:VAL:HG11 | 2:N:136:MET:HE3 | 1.50 | 0.92 |
| 1:P:538:GLU:N | 4:I:351:THR:H | 1.67 | 0.92 |
| 1:P:641:LYS:HE3 | 1:P:647:GLN:CG | 2.00 | 0.92 |
| 1:A:218:LEU:CB | 1:A:221:GLN:CG | 2.46 | 0.91 |
| 1:A:795:ARG:CZ | 3:C:43:ASN:OD1 | 2.14 | 0.91 |
| 1:D:218:LEU:HA | 1:D:221:GLN:CG | 2.01 | 0.91 |
| 1:D:537:GLU:O | 4:9:349:LEU:HD13 | 0.74 | 0.91 |
| 1:D:636:LYS:HD2 | 4:9:332:PRO:HB3 | 1.52 | 0.91 |
| 1:D:814:PHE:HA | 2:E:127:ARG:HH11 | 1.17 | 0.91 |
| 1:J:793:ARG:HH11 | 3:L:40:ASN:HD22 | 1.06 | 0.91 |
| 1:M:735:GLY:C | 1:M:743:ALA:HA | 1.91 | 0.91 |
| 1:M:783:LEU:HA | 1:M:786:ILE:HG13 | 0.92 | 0.91 |
| 1:P:736:GLN:HA | 1:P:743:ALA:HB2 | 1.51 | 0.91 |
| 1:P:783:LEU:HG | 1:P:786:ILE:HD11 | 0.93 | 0.91 |
| 1:A:537:GLU:O | 4:8:349:LEU:HD13 | 0.74 | 0.91 |
| 1:A:642:LYS:CB | 4:8:21:PHE:O | 2.17 | 0.91 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:727:LEU:HG | 1:D:782:MLY:CE | 1.88 | 0.91 |
| 1:D:834:LEU:HD12 | 2:E:54:MET:HG3 | 1.52 | 0.91 |
| 1:G:648:THR:HG21 | 1:G:651:ALA:HB2 | 1.50 | 0.91 |
| 1:G:735:GLY:C | 1:G:743:ALA:HA | 1.90 | 0.91 |
| 1:J:218:LEU:HA | 1:J:221:GLN:CG | 2.01 | 0.91 |
| 1:M:218:LEU:HA | 1:M:221:GLN:CG | 2.00 | 0.91 |
| 1:M:538:GLU:N | 4:Z:351:THR:H | 1.67 | 0.91 |
| 1:M:629:GLU:CB | 1:M:643:GLY:O | 2.17 | 0.91 |
| 2:Q:150:TYR:O | 2:Q:151:LYS:HB2 | 1.67 | 0.91 |
| 4:2:203:THR:HG22 | 4:Z:287:ILE:HB | 0.94 | 0.91 |
| 1:A:215:GLN:HA | 1:A:340:ILE:HG23 | 0.96 | 0.91 |
| 1:A:278:GLN:HG2 | 1:A:317:GLU:HB2 | 1.52 | 0.91 |
| 1:A:502:GLU:HG3 | 1:A:761:GLY:CA | 1.98 | 0.91 |
| 1:A:823:PHE:HE1 | 2:B:160:GLY:HA2 | 1.30 | 0.91 |
| 1:G:838:ILE:HD12 | 2:H:54:MET:HE3 | 1.51 | 0.91 |
| 1:J:537:GLU:O | 4:W:349:LEU:HD13 | 0.74 | 0.91 |
| 1:J:612:GLN:NE2 | 1:J:627:GLY:CA | 2.31 | 0.91 |
| 1:J:636:LYS:HD2 | 4:W:332:PRO:HB3 | 1.52 | 0.91 |
| 1:J:710:GLY:HA2 | 1:J:772:LEU:HD22 | 0.93 | 0.91 |
| 1:M:213:LYS:HA | 1:M:220:ASP:CG | 1.90 | 0.91 |
| 4:2:287:ILE:CG1 | 4:4:202:THR:CB | 2.48 | 0.91 |
| 4:4:322:PRO:HB2 | 4:6:244:ASP:HB3 | 1.49 | 0.91 |
| 1:A:791:GLN:HE22 | 3:C:115:GLY:HA3 | 1.32 | 0.91 |
| 1:D:213:LYS:HA | 1:D:220:ASP:CG | 1.90 | 0.91 |
| 1:D:735:GLY:C | 1:D:743:ALA:HA | 1.91 | 0.91 |
| 2:E:149:ASP:CG | 2:E:150:TYR:H | 1.73 | 0.91 |
| 1:G:213:LYS:HA | 1:G:220:ASP:CG | 1.90 | 0.91 |
| 1:J:213:LYS:HA | 1:J:220:ASP:CG | 1.90 | 0.91 |
| 1:J:542:PHE:HA | 4:W:143:TYR:HE1 | 1.34 | 0.91 |
| 1:J:788:THR:O | 3:L:42:THR:CG2 | 2.14 | 0.91 |
| 1:M:278:GLN:HG2 | 1:M:317:GLU:HB2 | 1.52 | 0.91 |
| 1:M:649:VAL:CG1 | 1:M:649:VAL:C | 2.38 | 0.91 |
| 1:A:739:ASP:HB3 | 1:A:742:LYS:CB | 1.99 | 0.91 |
| 1:G:791:GLN:HE21 | 3:I:115:GLY:HA3 | 1.20 | 0.91 |
| 3:I:62:ALA:O | 3:I:63:ILE:CG1 | 2.19 | 0.91 |
| 1:J:149:GLN:OE1 | 1:J:763:THR:HG21 | 1.70 | 0.91 |
| 1:J:538:GLU:N | 4:W:351:THR:H | 1.68 | 0.91 |
| 1:M:636:LYS:HD2 | 4:Z:332:PRO:HB3 | 1.52 | 0.91 |
| 1:M:641:LYS:HE3 | 1:M:647:GLN:CG | 2.00 | 0.91 |
| 1:P:649:VAL:CG1 | 1:P:649:VAL:C | 2.38 | 0.91 |
| 1:P:709:LYS:C | 1:P:710:GLY:N | 2.24 | 0.91 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:549:SER:C | 4:V:46:GLY:HA3 | 1.90 | 0.91 |
| 1:A:550:PHE:HA | 4:V:46:GLY:CA | 2.00 | 0.91 |
| 1:A:819:ASN:CG | 2:B:91:ALA:CA | 2.21 | 0.91 |
| 1:D:649:VAL:CB | 1:D:649:VAL:CG2 | 2.49 | 0.91 |
| 1:D:800:ARG:HH21 | 3:F:40:ASN:CG | 1.70 | 0.91 |
| 1:J:648:THR:HG21 | 1:J:651:ALA:HB2 | 1.50 | 0.91 |
| 1:J:735:GLY:C | 1:J:743:ALA:HA | 1.91 | 0.91 |
| 1:P:278:GLN:HG2 | 1:P:317:GLU:HB2 | 1.52 | 0.91 |
| 2:Q:149:ASP:CG | 2:Q:150:TYR:H | 1.72 | 0.91 |
| 1:D:218:LEU:CB | 1:D:221:GLN:CG | 2.46 | 0.91 |
| 1:D:550:PHE:HA | 4:W:46:GLY:CA | 2.00 | 0.91 |
| 1:J:756:THR:CG2 | 1:J:776:GLU:OE1 | 2.19 | 0.91 |
| 1:M:795:ARG:CG | 3:O:118:MET:CE | 2.35 | 0.91 |
| 1:P:795:ARG:HB3 | 3:R:35:ARG:HH22 | 1.09 | 0.91 |
| 1:A:206:LYS:CD | 1:A:217:THR:CG2 | 2.16 | 0.91 |
| 1:A:502:GLU:CD | 1:A:761:GLY:CA | 2.31 | 0.91 |
| 1:A:735:GLY:C | 1:A:743:ALA:HA | 1.91 | 0.91 |
| 1:D:538:GLU:N | 4:9:349:LEU:HD12 | 1.86 | 0.91 |
| 1:D:638:GLY:HA3 | 4:9:341:ILE:O | 1.70 | 0.91 |
| 1:D:724:TYR:HA | 1:D:782:MLY:CD | 2.00 | 0.91 |
| 2:E:144:VAL:HG13 | 2:E:153:ILE:HD11 | 1.21 | 0.91 |
| 1:G:538:GLU:N | 4:V:351:THR:H | 1.68 | 0.91 |
| 1:M:537:GLU:C | 4:Z:349:LEU:CD1 | 2.21 | 0.91 |
| 1:A:95:THR:HG1 | 1:A:769:ALA:C | 1.73 | 0.91 |
| 1:A:218:LEU:HA | 1:A:221:GLN:CG | 2.01 | 0.91 |
| 1:A:544:LYS:HD2 | 4:8:147:ARG:HB3 | 1.53 | 0.91 |
| 1:A:641:LYS:HE3 | 1:A:647:GLN:CG | 2.00 | 0.91 |
| 1:A:709:LYS:C | 1:A:710:GLY:CA | 2.39 | 0.91 |
| 1:D:534:SER:HA | 4:9:350:SER:O | 1.71 | 0.91 |
| 1:J:544:LYS:HD2 | 4:W:147:ARG:HB3 | 1.53 | 0.91 |
| 1:J:557:GLU:HA | 4:Y:47:MET:HA | 1.04 | 0.91 |
| 1:J:649:VAL:CB | 1:J:649:VAL:CG2 | 2.49 | 0.91 |
| 1:M:218:LEU:CB | 1:M:221:GLN:CG | 2.46 | 0.91 |
| 1:M:537:GLU:O | 4:Z:349:LEU:HD13 | 0.74 | 0.91 |
| 1:P:649:VAL:CB | 1:P:649:VAL:CG2 | 2.49 | 0.91 |
| 1:P:783:LEU:C | 1:P:786:ILE:HG13 | 1.91 | 0.91 |
| 1:P:819:ASN:OD1 | 2:Q:92:ASP:CB | 2.16 | 0.91 |
| 2:Q:137:TRP:HA | 2:Q:145:ALA:HB2 | 1.53 | 0.91 |
| 1:A:649:VAL:CG1 | 1:A:649:VAL:C | 2.38 | 0.91 |
| 1:D:544:LYS:HD2 | 4:9:147:ARG:HB3 | 1.53 | 0.91 |
| 1:G:792:ALA:CB | 3:I:42:THR:HG23 | 2.01 | 0.91 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:649:VAL:CG1 | 1:J:649:VAL:C | 2.38 | 0.91 |
| 1:P:97:LEU:HD21 | 1:P:712:PRO:HB3 | 1.50 | 0.91 |
| 4:V:286:ASP:OD2 | 4:X:203:THR:HG22 | 1.70 | 0.91 |
| 1:D:538:GLU:N | 4:9:351:THR:H | 1.68 | 0.90 |
| 1:D:649:VAL:CG1 | 1:D:649:VAL:C | 2.38 | 0.90 |
| 1:G:218:LEU:HA | 1:G:221:GLN:CG | 2.01 | 0.90 |
| 1:G:649:VAL:CG1 | 1:G:649:VAL:C | 2.39 | 0.90 |
| 3:I:62:ALA:O | 3:I:63:ILE:HG12 | 1.71 | 0.90 |
| 1:J:278:GLN:HG2 | 1:J:317:GLU:HB2 | 1.52 | 0.90 |
| 1:M:795:ARG:CB | 3:O:35:ARG:CZ | 2.49 | 0.90 |
| 1:P:538:GLU:N | 4:1:349:LEU:HD12 | 1.86 | 0.90 |
| 1:P:735:GLY:O | 1:P:743:ALA:CA | 2.19 | 0.90 |
| 1:A:97:LEU:HD23 | 1:A:712:PRO:CB | 1.99 | 0.90 |
| 1:A:215:GLN:H | 1:A:340:ILE:CG1 | 1.73 | 0.90 |
| 1:A:553:MLY:HE2 | 4:V:45:VAL:HA | 1.53 | 0.90 |
| 1:A:648:THR:HG21 | 1:A:651:ALA:HB2 | 1.50 | 0.90 |
| 1:A:735:GLY:O | 1:A:743:ALA:CA | 2.19 | 0.90 |
| 1:G:410:ASN:OD1 | 4:V:334:GLU:C | 2.09 | 0.90 |
| 1:J:97:LEU:CD2 | 1:J:712:PRO:HB3 | 2.02 | 0.90 |
| 1:J:410:ASN:OD1 | 4:W:334:GLU:C | 2.10 | 0.90 |
| 1:J:817:GLN:CD | 2:K:127:ARG:CD | 2.40 | 0.90 |
| 1:M:795:ARG:CZ | 3:O:116:GLU:HB3 | 2.01 | 0.90 |
| 1:P:537:GLU:O | 4:1:349:LEU:HD13 | 0.73 | 0.90 |
| 1:P:544:LYS:HD2 | 4:1:147:ARG:HB3 | 1.53 | 0.90 |
| 1:D:557:GLU:H | 4:W:48:GLY:HA2 | 1.32 | 0.90 |
| 1:D:834:LEU:HD21 | 2:E:54:MET:CE | 2.00 | 0.90 |
| 1:J:505:MLY:HG3 | 1:J:762:HIS:CE1 | 2.05 | 0.90 |
| 1:M:538:GLU:N | 4:Z:349:LEU:HD12 | 1.86 | 0.90 |
| 1:P:792:ALA:HB2 | 3:R:42:THR:HG22 | 0.93 | 0.90 |
| 1:P:817:GLN:CG | 2:Q:127:ARG:CD | 2.48 | 0.90 |
| 4:V:324:THR:CG2 | 4:X:247:VAL:H | 1.84 | 0.90 |
| 1:A:649:VAL:CG2 | 1:A:649:VAL:HG13 | 2.02 | 0.90 |
| 1:D:542:PHE:HA | 4:9:143:TYR:HE1 | 1.34 | 0.90 |
| 1:D:815:CYS:SG | 2:E:92:ASP:CG | 2.49 | 0.90 |
| 1:J:641:LYS:HG3 | 1:J:647:GLN:NE2 | 1.59 | 0.90 |
| 1:M:544:LYS:HD2 | 4:Z:147:ARG:HB3 | 1.53 | 0.90 |
| 1:P:213:LYS:HA | 1:P:220:ASP:CG | 1.90 | 0.90 |
| 1:D:410:ASN:OD1 | 4:9:334:GLU:C | 2.10 | 0.90 |
| 1:D:549:SER:C | 4:W:46:GLY:HA3 | 1.90 | 0.90 |
| 1:D:834:LEU:CG | 2:E:54:MET:CG | 2.27 | 0.90 |
| 3:F:62:ALA:O | 3:F:63:ILE:HG12 | 1.71 | 0.90 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:795:ARG:HD3 | 3:O:43:ASN:OD1 | 1.67 | 0.90 |
| 1:M:819:ASN:ND2 | 2:N:92:ASP:CB | 2.31 | 0.90 |
| 3:O:62:ALA:O | 3:O:63:ILE:HG12 | 1.71 | 0.90 |
| 1:P:410:ASN:OD1 | 4:1:334:GLU:C | 2.10 | 0.90 |
| 1:P:648:THR:HG21 | 1:P:651:ALA:HB2 | 1.50 | 0.90 |
| 1:P:721:LYS:CB | 1:P:736:GLN:OE1 | 2.20 | 0.90 |
| 3:C:62:ALA:O | 3:C:63:ILE:CG1 | 2.19 | 0.90 |
| 1:D:726:VAL:HG12 | 1:D:785:GLU:CG | 2.01 | 0.90 |
| 3:L:24:LYS:HB3 | 3:L:63:ILE:O | 1.72 | 0.90 |
| 3:L:62:ALA:O | 3:L:63:ILE:CG1 | 2.19 | 0.90 |
| 1:M:410:ASN:OD1 | 4:Z:334:GLU:C | 2.10 | 0.90 |
| 1:P:538:GLU:O | 4:1:349:LEU:CG | 2.20 | 0.90 |
| 4:4:288:ASP:OD1 | 4:6:203:THR:HG23 | 1.70 | 0.90 |
| 1:A:557:GLU:H | 4:V:48:GLY:HA3 | 1.29 | 0.90 |
| 1:A:629:GLU:HG2 | 1:A:643:GLY:O | 1.72 | 0.90 |
| 1:A:800:ARG:HB3 | 3:C:149:VAL:CG2 | 2.01 | 0.90 |
| 1:D:747:LEU:HD11 | 1:D:782:MLY:HH21 | 1.53 | 0.90 |
| 3:F:62:ALA:O | 3:F:63:ILE:CG1 | 2.19 | 0.90 |
| 1:G:94:MET:C | 1:G:713:SER:HB3 | 1.92 | 0.90 |
| 1:G:544:LYS:HD2 | 4:V:147:ARG:HB3 | 1.53 | 0.90 |
| 1:G:721:LYS:CB | 1:G:736:GLN:OE1 | 2.20 | 0.90 |
| 1:J:84:MLY:CH2 | 1:J:720:PHE:CA | 2.40 | 0.90 |
| 1:J:561:LYS:HE3 | 4:Y:48:GLY:HA3 | 1.51 | 0.90 |
| 1:M:836:PHE:CZ | 2:N:160:GLY:H | 1.30 | 0.90 |
| 1:P:218:LEU:HA | 1:P:221:GLN:CG | 2.01 | 0.90 |
| 1:P:797:PHE:CE1 | 3:R:149:VAL:CG1 | 2.54 | 0.90 |
| 4:2:287:ILE:CD1 | 4:4:203:THR:N | 2.34 | 0.90 |
| 1:A:791:GLN:NE2 | 3:C:115:GLY:HA3 | 1.87 | 0.90 |
| 1:A:831:TRP:HH2 | 2:B:50:THR:HB | 0.86 | 0.90 |
| 1:D:630:ALA:O | 4:9:25:ASP:CG | 2.09 | 0.90 |
| 1:D:735:GLY:O | 1:D:743:ALA:CA | 2.19 | 0.90 |
| 1:D:818:TYR:HB3 | 2:E:90:GLY:N | 1.85 | 0.90 |
| 1:G:649:VAL:CG2 | 1:G:649:VAL:HG13 | 2.02 | 0.90 |
| 1:J:629:GLU:HG2 | 1:J:643:GLY:O | 1.72 | 0.90 |
| 3:R:62:ALA:O | 3:R:63:ILE:CG1 | 2.19 | 0.90 |
| 4:1:246:GLN:CA | 4:Y:324:THR:HB | 2.01 | 0.90 |
| 4:1:247:VAL:HG23 | 4:Y:324:THR:CG2 | 1.99 | 0.90 |
| 4:1:287:ILE:HG23 | 4:3:202:THR:HB | 1.53 | 0.90 |
| 1:G:826:VAL:HG21 | 2:H:88:LEU:CD2 | 2.01 | 0.90 |
| 3:L:62:ALA:O | 3:L:63:ILE:HG12 | 1.72 | 0.90 |
| 1:M:735:GLY:O | 1:M:743:ALA:CA | 2.19 | 0.90 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:P:93:MET:O | 1:P:713:SER:HA | 1.72 | 0.90 |
| 1:P:641:LYS:CD | 1:P:647:GLN:OE1 | 2.17 | 0.90 |
| 1:A:800:ARG:CB | 3:C:149:VAL:HG22 | 2.02 | 0.90 |
| 1:D:278:GLN:HG2 | 1:D:317:GLU:HB2 | 1.52 | 0.90 |
| 1:D:507:GLY:O | 1:D:761:GLY:CA | 2.19 | 0.90 |
| 1:D:708:ARG:C | 1:D:710:GLY:N | 2.25 | 0.90 |
| 1:G:641:LYS:HE3 | 1:G:647:GLN:CG | 2.00 | 0.90 |
| 1:J:735:GLY:O | 1:J:743:ALA:CA | 2.19 | 0.90 |
| 1:J:821:ARG:NH2 | 2:K:127:ARG:CG | 2.31 | 0.90 |
| 1:M:829:TRP:CH2 | 2:N:87:LYS:HE2 | 2.06 | 0.90 |
| 3:R:24:LYS:HB3 | 3:R:63:ILE:O | 1.72 | 0.90 |
| 1:A:550:PHE:CA | 4:V:46:GLY:HA3 | 2.02 | 0.89 |
| 1:A:638:GLY:HA3 | 4:8:341:ILE:O | 1.70 | 0.89 |
| 1:A:797:PHE:CG | 3:C:146:ILE:HG23 | 2.06 | 0.89 |
| 3:C:62:ALA:O | 3:C:63:ILE:HG12 | 1.71 | 0.89 |
| 1:G:505:MLY:HH23 | 1:G:762:HIS:CG | 2.07 | 0.89 |
| 1:G:783:LEU:O | 1:G:787:ILE:HB | 1.70 | 0.89 |
| 1:M:769:ALA:C | 1:M:770:GLY:HA3 | 1.92 | 0.89 |
| 1:M:806:MET:N | 1:M:807:VAL:N | 2.20 | 0.89 |
| 3:O:24:LYS:HB3 | 3:O:63:ILE:O | 1.72 | 0.89 |
| 1:P:630:ALA:O | 4:1:25:ASP:CG | 2.09 | 0.89 |
| 4:2:202:THR:HB | 4:Z:287:ILE:CG2 | 2.02 | 0.89 |
| 1:A:553:MLY:CG | 4:V:44:MET:O | 2.20 | 0.89 |
| 1:A:707:CYS:CA | 1:A:714:ARG:NH2 | 2.35 | 0.89 |
| 1:A:834:LEU:HD21 | 2:B:54:MET:HE2 | 1.49 | 0.89 |
| 1:D:831:TRP:HZ2 | 2:E:47:LEU:CA | 1.79 | 0.89 |
| 1:G:754:ASP:HB3 | 1:G:776:GLU:CD | 1.74 | 0.89 |
| 2:H:150:TYR:O | 2:H:151:LYS:HB2 | 1.67 | 0.89 |
| 1:J:218:LEU:CB | 1:J:221:GLN:CG | 2.46 | 0.89 |
| 1:J:538:GLU:O | 4:W:349:LEU:CG | 2.20 | 0.89 |
| 1:J:630:ALA:O | 4:W:25:ASP:CG | 2.09 | 0.89 |
| 1:M:638:GLY:HA3 | 4:Z:341:ILE:O | 1.70 | 0.89 |
| 3:O:62:ALA:O | 3:O:63:ILE:CG1 | 2.19 | 0.89 |
| 1:A:530:MET:N | 4:8:354:GLN:HB3 | 1.87 | 0.89 |
| 1:A:649:VAL:CB | 1:A:649:VAL:CG2 | 2.50 | 0.89 |
| 1:D:834:LEU:HD12 | 2:E:54:MET:CB | 2.02 | 0.89 |
| 1:G:538:GLU:N | 4:V:349:LEU:HD12 | 1.87 | 0.89 |
| 1:G:629:GLU:HG2 | 1:G:643:GLY:O | 1.72 | 0.89 |
| 1:J:534:SER:HA | 4:W:350:SER:O | 1.71 | 0.89 |
| 1:M:530:MET:N | 4:Z:354:GLN:HB3 | 1.87 | 0.89 |
| 1:M:629:GLU:HG2 | 1:M:643:GLY:O | 1.72 | 0.89 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:P:829:TRP:CH2 | 2:Q:87:LYS:HE2 | 2.06 | 0.89 |
| 1:A:149:GLN:HB3 | 1:A:718:ALA:C | 1.92 | 0.89 |
| 1:A:630:ALA:O | 4:8:25:ASP:CG | 2.10 | 0.89 |
| 1:D:507:GLY:CA | 1:D:762:HIS:CG | 2.55 | 0.89 |
| 1:D:530:MET:N | 4:9:354:GLN:HB3 | 1.87 | 0.89 |
| 1:D:629:GLU:HG2 | 1:D:643:GLY:O | 1.72 | 0.89 |
| 1:J:831:TRP:CZ2 | 2:K:47:LEU:CD2 | 2.53 | 0.89 |
| 1:P:795:ARG:CB | 3:R:35:ARG:CZ | 2.50 | 0.89 |
| 1:A:538:GLU:O | 4:8:349:LEU:CG | 2.20 | 0.89 |
| 1:A:641:LYS:HD2 | 4:8:348:SER:CB | 2.02 | 0.89 |
| 1:D:550:PHE:CA | 4:W:46:GLY:HA3 | 2.02 | 0.89 |
| 1:G:505:MLY:CE | 1:G:762:HIS:NE2 | 2.35 | 0.89 |
| 1:G:538:GLU:O | 4:V:349:LEU:CG | 2.20 | 0.89 |
| 1:G:735:GLY:O | 1:G:743:ALA:CA | 2.20 | 0.89 |
| 1:J:831:TRP:CH2 | 2:K:47:LEU:HD22 | 2.05 | 0.89 |
| 1:A:410:ASN:OD1 | 4:8:334:GLU:C | 2.10 | 0.89 |
| 1:A:635:GLY:CA | 4:8:341:ILE:HD13 | 2.03 | 0.89 |
| 1:A:815:CYS:SG | 2:B:92:ASP:HB2 | 2.12 | 0.89 |
| 1:D:215:GLN:H | 1:D:340:ILE:CG1 | 1.73 | 0.89 |
| 1:G:534:SER:HA | 4:V:350:SER:O | 1.71 | 0.89 |
| 1:G:801:VAL:CG2 | 3:I:126:LEU:HD21 | 2.03 | 0.89 |
| 2:H:149:ASP:CG | 2:H:150:TYR:H | 1.73 | 0.89 |
| 1:J:649:VAL:CG2 | 1:J:649:VAL:HG13 | 2.02 | 0.89 |
| 1:J:829:TRP:CH2 | 2:K:87:LYS:CE | 2.55 | 0.89 |
| 1:P:817:GLN:HG2 | 2:Q:127:ARG:CB | 2.03 | 0.89 |
| 1:A:149:GLN:CA | 1:A:719:ASP:OD1 | 2.20 | 0.89 |
| 1:A:215:GLN:H | 1:A:340:ILE:HG12 | 1.06 | 0.89 |
| 1:D:553:MLY:CG | 4:W:44:MET:O | 2.20 | 0.89 |
| 1:D:553:MLY:HE2 | 4:W:45:VAL:HA | 1.53 | 0.89 |
| 1:G:635:GLY:CA | 4:V:341:ILE:HD13 | 2.03 | 0.89 |
| 1:M:641:LYS:HG3 | 1:M:647:GLN:NE2 | 1.59 | 0.89 |
| 1:M:721:LYS:CB | 1:M:736:GLN:OE1 | 2.20 | 0.89 |
| 1:M:782:MLY:O | 1:M:786:ILE:CG1 | 2.20 | 0.89 |
| 1:P:826:VAL:HG21 | 2:Q:88:LEU:CD2 | 2.03 | 0.89 |
| 1:A:721:LYS:CB | 1:A:736:GLN:OE1 | 2.20 | 0.89 |
| 1:M:649:VAL:CB | 1:M:649:VAL:CG2 | 2.49 | 0.89 |
| 1:M:826:VAL:HG21 | 2:N:88:LEU:CD2 | 2.03 | 0.89 |
| 1:P:541:MET:CB | 4:1:143:TYR:OH | 2.20 | 0.89 |
| 1:P:636:LYS:HD2 | 4:1:332:PRO:HB3 | 1.52 | 0.89 |
| 1:P:649:VAL:CG2 | 1:P:649:VAL:HG13 | 2.02 | 0.89 |
| 4:2:287:ILE:HG21 | 4:4:202:THR:CB | 2.02 | 0.89 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:2:322:PRO:HB3 | 4:4:244:ASP:CG | 1.93 | 0.89 |
| 1:A:149:GLN:CD | 1:A:718:ALA:HB3 | 1.93 | 0.89 |
| 1:A:834:LEU:HD21 | 2:B:54:MET:HE3 | 0.90 | 0.89 |
| 1:A:837:MLY:HH21 | 2:H:20:ASP:CA | 2.02 | 0.89 |
| 2:B:137:TRP:HA | 2:B:145:ALA:HB2 | 1.54 | 0.89 |
| 1:D:599:ASN:OD1 | 1:D:649:VAL:HB | 1.73 | 0.89 |
| 1:D:721:LYS:CB | 1:D:736:GLN:OE1 | 2.20 | 0.89 |
| 1:D:831:TRP:CD1 | 2:E:67:MET:SD | 2.65 | 0.89 |
| 1:G:649:VAL:CB | 1:G:649:VAL:CG2 | 2.50 | 0.89 |
| 2:H:137:TRP:HA | 2:H:145:ALA:HB2 | 1.54 | 0.89 |
| 1:J:530:MET:N | 4:W:354:GLN:HB3 | 1.88 | 0.89 |
| 1:J:819:ASN:CG | 2:K:92:ASP:CB | 2.40 | 0.89 |
| 2:K:137:TRP:HA | 2:K:145:ALA:HB2 | 1.54 | 0.89 |
| 2:N:137:TRP:HA | 2:N:145:ALA:HB2 | 1.53 | 0.89 |
| 1:P:736:GLN:CA | 1:P:743:ALA:HB2 | 1.95 | 0.89 |
| 1:P:795:ARG:HD3 | 3:R:43:ASN:OD1 | 1.71 | 0.89 |
| 1:G:755:HIS:HB2 | 1:G:779:ARG:NH2 | 1.88 | 0.89 |
| 1:J:642:LYS:HG2 | 4:W:22:ALA:CA | 2.03 | 0.89 |
| 1:M:795:ARG:CB | 3:O:35:ARG:NH2 | 2.33 | 0.89 |
| 1:P:534:SER:HA | 4:1:350:SER:O | 1.71 | 0.89 |
| 1:P:642:LYS:HG2 | 4:1:22:ALA:CA | 2.03 | 0.89 |
| 1:A:530:MET:HE1 | 4:8:355:MET:SD | 2.14 | 0.88 |
| 1:A:534:SER:HA | 4:8:350:SER:O | 1.71 | 0.88 |
| 1:A:541:MET:CB | 4:8:143:TYR:OH | 2.21 | 0.88 |
| 1:G:215:GLN:H | 1:G:340:ILE:HG12 | 1.06 | 0.88 |
| 1:G:829:TRP:CZ2 | 2:H:87:LYS:HE2 | 2.08 | 0.88 |
| 1:J:635:GLY:CA | 4:W:341:ILE:HD13 | 2.02 | 0.88 |
| 1:J:797:PHE:CZ | 3:L:146:ILE:HG23 | 2.07 | 0.88 |
| 1:P:530:MET:N | 4:1:354:GLN:HB3 | 1.88 | 0.88 |
| 1:P:546:THR:HB | 4:3:47:MET:O | 1.72 | 0.88 |
| 1:P:629:GLU:HG2 | 1:P:643:GLY:O | 1.72 | 0.88 |
| 1:P:797:PHE:CE1 | 3:R:149:VAL:HG12 | 2.07 | 0.88 |
| 4:1:112:PRO:HG3 | 4:2:195:GLU:O | 1.73 | 0.88 |
| 1:A:797:PHE:CE1 | 3:C:146:ILE:O | 2.25 | 0.88 |
| 1:D:642:LYS:HG2 | 4:9:22:ALA:CA | 2.04 | 0.88 |
| 1:D:649:VAL:CG2 | 1:D:649:VAL:HG13 | 2.02 | 0.88 |
| 1:D:795:ARG:NH2 | 3:F:116:GLU:CG | 2.34 | 0.88 |
| 2:E:137:TRP:HA | 2:E:145:ALA:CB | 2.04 | 0.88 |
| 1:M:538:GLU:O | 4:Z:349:LEU:CG | 2.20 | 0.88 |
| 1:M:796:GLY:HA2 | 3:O:35:ARG:CD | 2.03 | 0.88 |
| 2:N:149:ASP:CG | 2:N:150:TYR:H | 1.73 | 0.88 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:149:GLN:HG2 | 1:A:719:ASP:H | 1.36 | 0.88 |
| 1:A:798:LEU:CD2 | 3:C:126:LEU:HD11 | 2.04 | 0.88 |
| 1:D:538:GLU:O | 4:9:349:LEU:CG | 2.20 | 0.88 |
| 1:D:795:ARG:NE | 3:F:116:GLU:OE2 | 2.06 | 0.88 |
| 1:G:641:LYS:HD2 | 4:V:348:SER:CB | 2.03 | 0.88 |
| 1:M:534:SER:HA | 4:Z:350:SER:O | 1.71 | 0.88 |
| 1:P:817:GLN:HG2 | 2:Q:127:ARG:HD2 | 1.55 | 0.88 |
| 2:B:149:ASP:CG | 2:B:150:TYR:H | 1.73 | 0.88 |
| 1:D:797:PHE:CE1 | 3:F:146:ILE:CA | 2.56 | 0.88 |
| 1:G:553:MLY:NZ | 4:X:45:VAL:HG11 | 1.88 | 0.88 |
| 1:J:541:MET:CB | 4:W:143:TYR:OH | 2.20 | 0.88 |
| 1:J:641:LYS:CD | 1:J:647:GLN:OE1 | 2.17 | 0.88 |
| 1:M:541:MET:CB | 4:Z:143:TYR:OH | 2.20 | 0.88 |
| 1:M:630:ALA:O | 4:Z:25:ASP:CG | 2.09 | 0.88 |
| 1:M:649:VAL:CG2 | 1:M:649:VAL:HG13 | 2.02 | 0.88 |
| 2:Q:137:TRP:HA | 2:Q:145:ALA:CB | 2.04 | 0.88 |
| 1:A:599:ASN:OD1 | 1:A:649:VAL:HB | 1.73 | 0.88 |
| 1:A:641:LYS:CD | 1:A:647:GLN:OE1 | 2.17 | 0.88 |
| 1:A:795:ARG:NE | 3:C:116:GLU:OE2 | 2.07 | 0.88 |
| 1:G:530:MET:N | 4:V:354:GLN:HB3 | 1.88 | 0.88 |
| 1:G:798:LEU:CD2 | 3:I:118:MET:HB3 | 2.04 | 0.88 |
| 1:J:642:LYS:CG | 4:W:21:PHE:O | 2.22 | 0.88 |
| 1:M:795:ARG:CZ | 3:O:116:GLU:CD | 2.39 | 0.88 |
| 2:N:137:TRP:HA | 2:N:145:ALA:CB | 2.04 | 0.88 |
| 1:P:538:GLU:OE2 | 4:1:355:MET:HE3 | 1.72 | 0.88 |
| 1:A:754:ASP:OD2 | 1:A:778:MET:HE3 | 1.71 | 0.88 |
| 1:D:813:ILE:HG23 | 2:E:128:PHE:CZ | 2.09 | 0.88 |
| 1:J:635:GLY:HA2 | 4:W:334:GLU:CG | 2.03 | 0.88 |
| 2:B:137:TRP:HA | 2:B:145:ALA:CB | 2.04 | 0.88 |
| 2:H:144:VAL:HG13 | 2:H:153:ILE:HG12 | 1.14 | 0.88 |
| 1:J:838:ILE:CD1 | 2:K:54:MET:HE3 | 1.93 | 0.88 |
| 1:M:599:ASN:OD1 | 1:M:649:VAL:HB | 1.73 | 0.88 |
| 3:R:62:ALA:O | 3:R:63:ILE:HG12 | 1.72 | 0.88 |
| 4:4:287:ILE:CG2 | 4:6:204:ALA:H | 1.87 | 0.88 |
| 1:D:541:MET:CB | 4:9:143:TYR:OH | 2.21 | 0.88 |
| 3:I:24:LYS:HB3 | 3:I:63:ILE:O | 1.72 | 0.88 |
| 1:D:635:GLY:CA | 4:9:341:ILE:HD13 | 2.03 | 0.88 |
| 2:H:121:LEU:CB | 2:H:128:PHE:HB3 | 1.69 | 0.88 |
| 1:J:757:GLN:HA | 1:J:776:GLU:HG3 | 1.53 | 0.88 |
| 1:P:641:LYS:HD2 | 4:1:348:SER:CB | 2.03 | 0.88 |
| 2:E:137:TRP:HA | 2:E:145:ALA:HB2 | 1.54 | 0.88 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:F:24:LYS:HB3 | 3:F:63:ILE:O | 1.72 | 0.88 |
| 1:G:552:ASN:O | 4:X:47:MET:HE1 | 1.73 | 0.88 |
| 1:G:641:LYS:CD | 1:G:647:GLN:OE1 | 2.18 | 0.88 |
| 1:G:831:TRP:NE1 | 2:H:67:MET:HB3 | 1.89 | 0.88 |
| 1:J:819:ASN:CG | 2:K:90:GLY:O | 2.12 | 0.88 |
| 2:K:121:LEU:CA | 2:K:128:PHE:CB | 2.46 | 0.88 |
| 2:K:137:TRP:HA | 2:K:145:ALA:CB | 2.04 | 0.88 |
| 1:M:635:GLY:CA | 4:Z:341:ILE:HD13 | 2.02 | 0.88 |
| 1:M:797:PHE:CE1 | 3:O:149:VAL:CG1 | 2.57 | 0.88 |
| 1:A:72:VAL:CG1 | 1:A:76:GLN:HB3 | 2.05 | 0.87 |
| 1:A:635:GLY:HA2 | 4:8:334:GLU:CG | 2.03 | 0.87 |
| 1:A:642:LYS:CG | 4:8:21:PHE:O | 2.22 | 0.87 |
| 2:B:54:MET:CA | 2:H:21:GLU:OE1 | 2.22 | 0.87 |
| 1:D:641:LYS:CD | 1:D:647:GLN:OE1 | 2.17 | 0.87 |
| 1:J:721:LYS:CB | 1:J:736:GLN:OE1 | 2.20 | 0.87 |
| 1:J:829:TRP:CH2 | 2:K:87:LYS:NZ | 2.41 | 0.87 |
| 1:P:215:GLN:H | 1:P:340:ILE:CG1 | 1.72 | 0.87 |
| 1:P:791:GLN:OE1 | 3:R:116:GLU:HG3 | 1.74 | 0.87 |
| 4:2:287:ILE:HB | 4:4:203:THR:CG2 | 2.04 | 0.87 |
| 1:D:635:GLY:HA2 | 4:9:334:GLU:CG | 2.03 | 0.87 |
| 1:G:795:ARG:CZ | 3:I:116:GLU:CG | 2.48 | 0.87 |
| 2:H:137:TRP:HA | 2:H:145:ALA:CB | 2.04 | 0.87 |
| 1:J:505:MLY:CG | 1:J:762:HIS:CE1 | 2.56 | 0.87 |
| 1:M:72:VAL:CG1 | 1:M:76:GLN:HB3 | 2.04 | 0.87 |
| 1:M:836:PHE:HE1 | 2:N:159:HIS:HA | 1.05 | 0.87 |
| 4:1:167:GLU:OE1 | 4:3:43:VAL:O | 1.91 | 0.87 |
| 1:A:795:ARG:HB2 | 3:C:35:ARG:NH1 | 1.89 | 0.87 |
| 1:G:72:VAL:CG1 | 1:G:76:GLN:HB3 | 2.05 | 0.87 |
| 1:G:93:MET:CE | 1:G:764:MLY:HD3 | 2.03 | 0.87 |
| 1:G:801:VAL:HG21 | 3:I:126:LEU:HD21 | 1.55 | 0.87 |
| 1:J:646:PHE:CE2 | 1:J:652:LEU:CD1 | 2.58 | 0.87 |
| 1:P:635:GLY:CA | 4:1:341:ILE:HD13 | 2.02 | 0.87 |
| 1:P:636:LYS:H | 4:1:334:GLU:CD | 1.78 | 0.87 |
| 2:Q:121:LEU:CA | 2:Q:128:PHE:CB | 2.46 | 0.87 |
| 4:2:324:THR:HG23 | 4:4:244:ASP:HA | 1.55 | 0.87 |
| 1:A:754:ASP:OD2 | 1:A:774:LEU:HD23 | 1.74 | 0.87 |
| 1:D:755:HIS:HA | 1:D:758:TYR:CE1 | 2.10 | 0.87 |
| 1:G:505:MLY:HD2 | 1:G:762:HIS:NE2 | 1.89 | 0.87 |
| 1:J:756:THR:HG22 | 1:J:776:GLU:HB3 | 1.54 | 0.87 |
| 1:P:546:THR:OG1 | 4:3:46:GLY:HA2 | 1.74 | 0.87 |
| 1:P:646:PHE:CE2 | 1:P:652:LEU:CD1 | 2.58 | 0.87 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:84:MLY:CB | 1:G:723:ARG:CD | 2.49 | 0.87 |
| 1:G:638:GLY:HA3 | 4:V:341:ILE:O | 1.70 | 0.87 |
| 1:G:753:VAL:N | 1:G:780:ASP:OD1 | 2.08 | 0.87 |
| 1:G:817:GLN:NE2 | 2:H:127:ARG:HB2 | 1.87 | 0.87 |
| 1:J:641:LYS:HD2 | 4:W:348:SER:CB | 2.03 | 0.87 |
| 1:J:797:PHE:CE2 | 3:L:146:ILE:HD12 | 2.03 | 0.87 |
| 1:M:641:LYS:HD2 | 4:Z:348:SER:CB | 2.03 | 0.87 |
| 1:P:93:MET:C | 1:P:713:SER:HA | 1.94 | 0.87 |
| 1:P:755:HIS:HA | 1:P:758:TYR:CE1 | 2.10 | 0.87 |
| 1:P:795:ARG:CB | 3:R:35:ARG:NH2 | 2.33 | 0.87 |
| 1:A:636:LYS:H | 4:8:334:GLU:CD | 1.77 | 0.87 |
| 1:D:732:ILE:HG21 | 1:D:782:MLY:HH21 | 1.55 | 0.87 |
| 1:J:95:THR:HA | 1:J:713:SER:CB | 2.05 | 0.87 |
| 1:M:736:GLN:HA | 1:M:743:ALA:HB2 | 1.50 | 0.87 |
| 4:2:324:THR:CG2 | 4:4:244:ASP:HA | 2.05 | 0.87 |
| 1:A:649:VAL:CG1 | 1:A:649:VAL:CA | 2.53 | 0.87 |
| 1:A:707:CYS:HA | 1:A:714:ARG:NH1 | 1.90 | 0.87 |
| 1:D:642:LYS:CG | 4:9:21:PHE:O | 2.22 | 0.87 |
| 1:D:649:VAL:CG1 | 1:D:649:VAL:CA | 2.53 | 0.87 |
| 1:G:642:LYS:HG2 | 4:V:22:ALA:CA | 2.03 | 0.87 |
| 1:G:649:VAL:CG1 | 1:G:649:VAL:CA | 2.53 | 0.87 |
| 1:J:72:VAL:CG1 | 1:J:76:GLN:HB3 | 2.05 | 0.87 |
| 1:J:813:ILE:HG23 | 2:K:128:PHE:CZ | 2.09 | 0.87 |
| 1:M:642:LYS:CG | 4:Z:21:PHE:O | 2.22 | 0.87 |
| 1:M:642:LYS:HG2 | 4:Z:22:ALA:CA | 2.03 | 0.87 |
| 1:P:642:LYS:CG | 4:1:21:PHE:O | 2.22 | 0.87 |
| 1:A:530:MET:HG2 | 4:8:354:GLN:CG | 2.05 | 0.87 |
| 1:A:534:SER:O | 4:8:351:THR:HG23 | 1.13 | 0.87 |
| 1:A:736:GLN:HA | 1:A:743:ALA:HB2 | 1.51 | 0.87 |
| 1:G:541:MET:CB | 4:V:143:TYR:OH | 2.21 | 0.87 |
| 1:J:557:GLU:HA | 4:Y:48:GLY:N | 1.90 | 0.87 |
| 3:O:139:TYR:HA | 3:O:142:PHE:HB3 | 1.56 | 0.87 |
| 4:8:322:PRO:HB2 | 4:V:244:ASP:CG | 1.94 | 0.87 |
| 1:D:72:VAL:CG1 | 1:D:76:GLN:HB3 | 2.05 | 0.87 |
| 1:D:641:LYS:HD2 | 4:9:348:SER:CB | 2.03 | 0.87 |
| 1:G:556:ASP:CG | 4:X:47:MET:HE2 | 1.47 | 0.87 |
| 3:I:139:TYR:HA | 3:I:142:PHE:HB3 | 1.56 | 0.87 |
| 1:M:641:LYS:CD | 1:M:647:GLN:OE1 | 2.18 | 0.87 |
| 1:M:785:GLU:C | 1:M:786:ILE:CA | 2.42 | 0.87 |
| 1:M:795:ARG:HB2 | 3:O:35:ARG:NH1 | 1.90 | 0.87 |
| 1:P:72:VAL:CG1 | 1:P:76:GLN:HB3 | 2.05 | 0.87 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:P:646:PHE:CD2 | 1:P:652:LEU:HD11 | 2.10 | 0.87 |
| 1:P:786:ILE:O | 1:P:789:ALA:HB3 | 1.75 | 0.87 |
| 1:A:538:GLU:N | 4:8:349:LEU:HD12 | 1.86 | 0.86 |
| 2:E:163:ALA:CA | 2:K:21:GLU:HB3 | 2.05 | 0.86 |
| 1:G:530:MET:HG2 | 4:V:354:GLN:CG | 2.05 | 0.86 |
| 1:P:735:GLY:C | 1:P:743:ALA:HB2 | 1.82 | 0.86 |
| 4:2:322:PRO:CB | 4:4:244:ASP:HB3 | 2.04 | 0.86 |
| 1:D:813:ILE:HG23 | 2:E:128:PHE:CE1 | 2.09 | 0.86 |
| 1:G:503:TYR:CZ | 1:G:711:PHE:CE2 | 2.61 | 0.86 |
| 1:G:818:TYR:CZ | 2:H:127:ARG:CZ | 2.56 | 0.86 |
| 1:J:636:LYS:H | 4:W:334:GLU:CD | 1.78 | 0.86 |
| 1:J:649:VAL:CG1 | 1:J:649:VAL:CA | 2.53 | 0.86 |
| 1:M:755:HIS:HA | 1:M:758:TYR:CE1 | 2.10 | 0.86 |
| 1:M:795:ARG:HG2 | 3:O:118:MET:HE3 | 0.89 | 0.86 |
| 1:A:797:PHE:CZ | 3:C:146:ILE:HA | 2.09 | 0.86 |
| 3:C:24:LYS:HB3 | 3:C:63:ILE:O | 1.72 | 0.86 |
| 1:D:732:ILE:HG23 | 1:D:747:LEU:HB2 | 1.57 | 0.86 |
| 1:G:755:HIS:HA | 1:G:758:TYR:CE1 | 2.10 | 0.86 |
| 1:J:755:HIS:HA | 1:J:758:TYR:CE1 | 2.10 | 0.86 |
| 3:L:139:TYR:HA | 3:L:142:PHE:HB3 | 1.57 | 0.86 |
| 1:M:646:PHE:CD2 | 1:M:652:LEU:HD11 | 2.10 | 0.86 |
| 1:P:542:PHE:HA | 4:1:143:TYR:HE1 | 1.34 | 0.86 |
| 1:P:549:SER:CA | 4:3:43:VAL:HG11 | 2.04 | 0.86 |
| 4:9:322:PRO:HB2 | 4:W:244:ASP:CG | 1.94 | 0.86 |
| 4:W:286:ASP:CG | 4:Y:203:THR:HG22 | 1.96 | 0.86 |
| 1:A:646:PHE:CE2 | 1:A:652:LEU:CD1 | 2.58 | 0.86 |
| 1:A:755:HIS:HA | 1:A:758:TYR:CE1 | 2.10 | 0.86 |
| 2:E:163:ALA:O | 2:K:22:THR:N | 2.07 | 0.86 |
| 1:G:310:TYR:CZ | 1:G:320:ILE:HD11 | 2.11 | 0.86 |
| 1:J:792:ALA:CB | 3:L:42:THR:N | 2.37 | 0.86 |
| 1:P:649:VAL:CG1 | 1:P:649:VAL:CA | 2.53 | 0.86 |
| 4:7:322:PRO:HB2 | 4:9:244:ASP:CG | 1.94 | 0.86 |
| 1:A:310:TYR:CZ | 1:A:320:ILE:HD11 | 2.11 | 0.86 |
| 1:D:530:MET:HG2 | 4:9:354:GLN:CG | 2.05 | 0.86 |
| 1:D:708:ARG:HA | 1:D:710:GLY:N | 1.91 | 0.86 |
| 1:G:635:GLY:HA2 | 4:V:334:GLU:CG | 2.03 | 0.86 |
| 1:G:642:LYS:CG | 4:V:21:PHE:O | 2.22 | 0.86 |
| 1:G:757:GLN:HG2 | 1:G:776:GLU:CD | 1.95 | 0.86 |
| 1:G:818:TYR:CE1 | 2:H:127:ARG:NH1 | 2.42 | 0.86 |
| 1:M:310:TYR:CZ | 1:M:320:ILE:HD11 | 2.11 | 0.86 |
| 1:M:548:THR:HG21 | 4:2:47:MET:CB | 2.02 | 0.86 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:649:VAL:CG1 | 1:M:649:VAL:CA | 2.53 | 0.86 |
| 1:M:798:LEU:HD11 | 3:O:126:LEU:HD11 | 1.45 | 0.86 |
| 1:P:310:TYR:CZ | 1:P:320:ILE:HD11 | 2.11 | 0.86 |
| 1:P:836:PHE:HE1 | 2:Q:159:HIS:HA | 1.05 | 0.86 |
| 1:J:206:LYS:HD3 | 1:J:217:THR:CB | 2.06 | 0.86 |
| 2:K:117:LEU:CG | 2:K:147:ASN:CG | 2.44 | 0.86 |
| 1:M:206:LYS:HD3 | 1:M:217:THR:CB | 2.06 | 0.86 |
| 1:M:636:LYS:H | 4:Z:334:GLU:CD | 1.78 | 0.86 |
| 1:M:783:LEU:CG | 1:M:786:ILE:CD1 | 2.53 | 0.86 |
| 1:P:806:MET:N | 1:P:807:VAL:N | 2.23 | 0.86 |
| 4:V:286:ASP:OD1 | 4:X:203:THR:HG22 | 1.74 | 0.86 |
| 1:A:732:ILE:HG23 | 1:A:747:LEU:HB2 | 1.58 | 0.86 |
| 1:G:599:ASN:OD1 | 1:G:649:VAL:HB | 1.73 | 0.86 |
| 1:G:646:PHE:CD2 | 1:G:652:LEU:HD11 | 2.09 | 0.86 |
| 1:G:732:ILE:HG23 | 1:G:747:LEU:HB2 | 1.57 | 0.86 |
| 1:G:792:ALA:CB | 3:I:42:THR:HA | 2.06 | 0.86 |
| 1:J:646:PHE:CD2 | 1:J:652:LEU:HD11 | 2.10 | 0.86 |
| 1:M:215:GLN:H | 1:M:340:ILE:HG12 | 1.06 | 0.86 |
| 1:M:530:MET:HG2 | 4:Z:354:GLN:CG | 2.06 | 0.86 |
| 1:P:786:ILE:C | 1:P:787:ILE:N | 2.28 | 0.86 |
| 1:P:831:TRP:CZ2 | 2:Q:47:LEU:HD22 | 2.11 | 0.86 |
| 1:A:642:LYS:HG2 | 4:8:22:ALA:CA | 2.04 | 0.86 |
| 2:B:117:LEU:CG | 2:B:147:ASN:CG | 2.44 | 0.86 |
| 1:D:834:LEU:HD12 | 2:E:54:MET:CG | 2.03 | 0.86 |
| 1:G:206:LYS:HD3 | 1:G:217:THR:CB | 2.06 | 0.86 |
| 1:J:538:GLU:N | 4:W:349:LEU:HD12 | 1.86 | 0.86 |
| 4:9:287:ILE:CG2 | 4:W:205:GLU:HG2 | 2.05 | 0.86 |
| 1:A:646:PHE:CD2 | 1:A:652:LEU:HD11 | 2.09 | 0.86 |
| 1:A:791:GLN:HE22 | 3:C:115:GLY:C | 1.80 | 0.86 |
| 1:D:795:ARG:CB | 3:F:35:ARG:CZ | 2.44 | 0.86 |
| 1:D:800:ARG:O | 3:F:149:VAL:HG21 | 1.74 | 0.86 |
| 1:G:798:LEU:HD23 | 3:I:118:MET:HB3 | 1.55 | 0.86 |
| 1:J:530:MET:HG2 | 4:W:354:GLN:CG | 2.06 | 0.86 |
| 1:P:797:PHE:CE2 | 3:R:146:ILE:CD1 | 2.57 | 0.86 |
| 1:A:505:MLY:CB | 1:A:762:HIS:H | 1.88 | 0.86 |
| 1:D:830:PRO:HB2 | 2:E:51:PHE:CZ | 2.10 | 0.86 |
| 1:M:34:ALA:CB | 1:M:777:GLU:OE2 | 2.23 | 0.86 |
| 1:M:817:GLN:HG2 | 2:N:127:ARG:HB2 | 1.56 | 0.86 |
| 1:P:215:GLN:H | 1:P:340:ILE:HG12 | 1.05 | 0.86 |
| 1:P:829:TRP:CH2 | 2:Q:87:LYS:CE | 2.58 | 0.86 |
| 3:R:139:TYR:HA | 3:R:142:PHE:HB3 | 1.56 | 0.86 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:793:ARG:HH21 | 3:C:147:MET:CE | 1.89 | 0.85 |
| 1:D:813:ILE:CD1 | 2:E:128:PHE:CE1 | 2.57 | 0.85 |
| 1:J:732:ILE:HG23 | 1:J:747:LEU:HB2 | 1.57 | 0.85 |
| 1:M:549:SER:N | 4:2:47:MET:C | 2.15 | 0.85 |
| 1:P:819:ASN:OD1 | 2:Q:92:ASP:HB2 | 1.75 | 0.85 |
| 4:2:324:THR:OG1 | 4:4:244:ASP:HA | 1.76 | 0.85 |
| 1:D:636:LYS:H | 4:9:334:GLU:CD | 1.78 | 0.85 |
| 1:D:646:PHE:CE2 | 1:D:652:LEU:CD1 | 2.58 | 0.85 |
| 1:G:636:LYS:H | 4:V:334:GLU:CD | 1.78 | 0.85 |
| 1:J:538:GLU:N | 4:W:351:THR:N | 2.24 | 0.85 |
| 1:M:646:PHE:CE2 | 1:M:652:LEU:CD1 | 2.58 | 0.85 |
| 1:M:826:VAL:HG21 | 2:N:88:LEU:HD21 | 1.58 | 0.85 |
| 1:P:206:LYS:HD3 | 1:P:217:THR:CB | 2.06 | 0.85 |
| 1:P:538:GLU:N | 4:1:351:THR:N | 2.24 | 0.85 |
| 1:A:410:ASN:OD1 | 4:8:334:GLU:CA | 2.24 | 0.85 |
| 1:A:819:ASN:CB | 2:B:90:GLY:O | 2.24 | 0.85 |
| 1:G:410:ASN:OD1 | 4:V:334:GLU:CA | 2.24 | 0.85 |
| 1:G:553:MLY:HG3 | 4:X:45:VAL:C | 1.96 | 0.85 |
| 1:J:202:SER:HA | 1:J:207:LYS:HE2 | 0.85 | 0.85 |
| 1:J:599:ASN:OD1 | 1:J:649:VAL:CA | 2.25 | 0.85 |
| 1:J:736:GLN:HA | 1:J:743:ALA:HB2 | 1.50 | 0.85 |
| 1:J:754:ASP:HA | 1:J:780:ASP:OD2 | 1.76 | 0.85 |
| 1:M:821:ARG:HH22 | 2:N:127:ARG:HG2 | 1.39 | 0.85 |
| 1:P:93:MET:O | 1:P:713:SER:CA | 2.24 | 0.85 |
| 1:P:599:ASN:OD1 | 1:P:649:VAL:CA | 2.25 | 0.85 |
| 1:A:798:LEU:HD11 | 3:C:126:LEU:CG | 2.05 | 0.85 |
| 1:D:834:LEU:HG | 2:E:54:MET:CG | 2.02 | 0.85 |
| 2:E:162:ASP:O | 2:K:21:GLU:HB2 | 1.75 | 0.85 |
| 1:G:553:MLY:HH12 | 4:X:45:VAL:HG11 | 1.58 | 0.85 |
| 1:J:754:ASP:C | 1:J:780:ASP:OD2 | 2.14 | 0.85 |
| 1:A:502:GLU:CB | 1:A:761:GLY:HA3 | 2.07 | 0.85 |
| 1:A:505:MLY:HG3 | 1:A:741:LYS:HZ1 | 1.40 | 0.85 |
| 1:D:202:SER:HA | 1:D:207:LYS:HE2 | 0.85 | 0.85 |
| 1:J:215:GLN:H | 1:J:340:ILE:HG12 | 1.05 | 0.85 |
| 1:M:630:ALA:C | 4:Z:25:ASP:OD2 | 2.15 | 0.85 |
| 1:M:831:TRP:CZ2 | 2:N:47:LEU:HD22 | 2.11 | 0.85 |
| 1:D:215:GLN:H | 1:D:340:ILE:HG12 | 1.06 | 0.85 |
| 1:G:28:GLN:OE1 | 1:G:723:ARG:NH1 | 2.09 | 0.85 |
| 2:N:117:LEU:CG | 2:N:147:ASN:CG | 2.44 | 0.85 |
| 1:A:640:LYS:C | 4:8:23:GLY:O | 2.15 | 0.85 |
| 1:D:206:LYS:HD3 | 1:D:217:THR:CB | 2.06 | 0.85 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:727:LEU:HD11 | 1:D:782:MLY:CG | 2.06 | 0.85 |
| 1:J:567:LYS:HZ3 | 4:Y:92:ASN:HD22 | 1.23 | 0.85 |
| 1:P:202:SER:HA | 1:P:207:LYS:HE2 | 0.86 | 0.85 |
| 1:A:206:LYS:HD3 | 1:A:217:THR:CB | 2.06 | 0.85 |
| 1:D:599:ASN:OD1 | 1:D:649:VAL:CA | 2.25 | 0.85 |
| 1:D:646:PHE:CD2 | 1:D:652:LEU:HD11 | 2.09 | 0.85 |
| 1:M:202:SER:HA | 1:M:207:LYS:HE2 | 0.86 | 0.85 |
| 1:P:93:MET:HG2 | 1:P:714:ARG:C | 1.97 | 0.85 |
| 4:1:201:VAL:HG23 | 4:Y:287:ILE:CG1 | 2.07 | 0.85 |
| 1:A:204:GLU:H | 1:A:207:LYS:HE3 | 1.42 | 0.85 |
| 1:D:795:ARG:HH21 | 3:F:116:GLU:CG | 1.89 | 0.85 |
| 1:G:599:ASN:OD1 | 1:G:649:VAL:CA | 2.25 | 0.85 |
| 1:G:754:ASP:N | 1:G:776:GLU:OE1 | 2.09 | 0.85 |
| 1:M:797:PHE:CE1 | 3:O:146:ILE:HA | 2.12 | 0.85 |
| 1:P:530:MET:HG2 | 4:1:354:GLN:CG | 2.06 | 0.85 |
| 1:P:635:GLY:HA2 | 4:1:334:GLU:CG | 2.03 | 0.85 |
| 1:P:640:LYS:C | 4:1:23:GLY:O | 2.16 | 0.85 |
| 4:1:166:TYR:CE2 | 4:3:64:ILE:CG2 | 2.59 | 0.85 |
| 4:X:287:ILE:CB | 4:Z:205:GLU:CG | 1.90 | 0.85 |
| 3:F:139:TYR:HA | 3:F:142:PHE:HB3 | 1.56 | 0.85 |
| 1:G:204:GLU:H | 1:G:207:LYS:HE3 | 1.42 | 0.85 |
| 1:G:832:MET:SD | 2:H:84:PHE:CE2 | 2.65 | 0.85 |
| 1:M:538:GLU:OE2 | 4:Z:355:MET:HE3 | 1.76 | 0.85 |
| 1:M:821:ARG:NH2 | 2:N:127:ARG:CD | 2.38 | 0.85 |
| 4:1:112:PRO:CG | 4:2:195:GLU:O | 2.25 | 0.85 |
| 4:8:287:ILE:CG2 | 4:V:205:GLU:HG2 | 2.05 | 0.85 |
| 1:A:640:LYS:CB | 1:A:645:SER:OG | 2.25 | 0.84 |
| 1:D:640:LYS:CB | 1:D:645:SER:OG | 2.25 | 0.84 |
| 1:G:410:ASN:ND2 | 4:V:336:LYS:HG2 | 1.92 | 0.84 |
| 1:G:529:PRO:CB | 4:V:353:GLN:OE1 | 2.25 | 0.84 |
| 1:G:538:GLU:OE2 | 4:V:355:MET:HE3 | 1.76 | 0.84 |
| 1:J:310:TYR:CZ | 1:J:320:ILE:HD11 | 2.11 | 0.84 |
| 1:J:599:ASN:OD1 | 1:J:649:VAL:HB | 1.73 | 0.84 |
| 1:M:410:ASN:ND2 | 4:Z:336:LYS:HG2 | 1.92 | 0.84 |
| 1:M:640:LYS:CB | 1:M:645:SER:OG | 2.25 | 0.84 |
| 1:M:732:ILE:CG2 | 1:M:747:LEU:HD13 | 1.34 | 0.84 |
| 1:P:732:ILE:HG23 | 1:P:747:LEU:HB2 | 1.57 | 0.84 |
| 2:Q:144:VAL:HG13 | 2:Q:153:ILE:HG12 | 1.14 | 0.84 |
| 4:1:287:ILE:CG1 | 4:3:203:THR:H | 1.88 | 0.84 |
| 4:3:322:PRO:CB | 4:5:244:ASP:CB | 2.55 | 0.84 |
| 4:4:287:ILE:CD1 | 4:6:203:THR:HB | 2.06 | 0.84 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:797:PHE:CD1 | 3:C:146:ILE:HG23 | 2.10 | 0.84 |
| 1:D:310:TYR:CZ | 1:D:320:ILE:HD11 | 2.11 | 0.84 |
| 1:D:549:SER:O | 4:W:46:GLY:HA3 | 1.77 | 0.84 |
| 1:D:640:LYS:C | 4:9:23:GLY:O | 2.16 | 0.84 |
| 1:G:418:THR:HB | 1:G:421:GLU:HG3 | 1.60 | 0.84 |
| 1:G:567:LYS:HZ1 | 4:X:92:ASN:ND2 | 1.68 | 0.84 |
| 2:H:117:LEU:CG | 2:H:147:ASN:CG | 2.45 | 0.84 |
| 1:J:725:ARG:CD | 1:J:733:PRO:HB3 | 2.07 | 0.84 |
| 1:M:817:GLN:HB3 | 2:N:127:ARG:CD | 2.07 | 0.84 |
| 1:P:732:ILE:HG21 | 1:P:747:LEU:HD13 | 0.91 | 0.84 |
| 1:P:795:ARG:HG2 | 3:R:118:MET:HE3 | 0.85 | 0.84 |
| 4:2:202:THR:HG22 | 4:Z:290:ARG:HH22 | 1.33 | 0.84 |
| 4:7:287:ILE:CG2 | 4:9:205:GLU:HG2 | 2.05 | 0.84 |
| 1:A:149:GLN:HG2 | 1:A:719:ASP:OD1 | 1.77 | 0.84 |
| 1:A:418:THR:HB | 1:A:421:GLU:HG3 | 1.60 | 0.84 |
| 1:A:599:ASN:OD1 | 1:A:649:VAL:CA | 2.25 | 0.84 |
| 2:B:121:LEU:CA | 2:B:128:PHE:CB | 2.46 | 0.84 |
| 2:E:117:LEU:CG | 2:E:147:ASN:CG | 2.45 | 0.84 |
| 2:E:163:ALA:O | 2:K:21:GLU:N | 2.11 | 0.84 |
| 1:J:410:ASN:ND2 | 4:W:336:LYS:HG2 | 1.92 | 0.84 |
| 1:M:410:ASN:OD1 | 4:Z:334:GLU:CA | 2.24 | 0.84 |
| 1:M:534:SER:O | 4:Z:351:THR:HG23 | 1.13 | 0.84 |
| 1:M:538:GLU:N | 4:Z:351:THR:N | 2.24 | 0.84 |
| 1:M:599:ASN:OD1 | 1:M:649:VAL:CA | 2.25 | 0.84 |
| 1:P:410:ASN:OD1 | 4:1:334:GLU:CA | 2.24 | 0.84 |
| 1:P:410:ASN:ND2 | 4:1:336:LYS:HG2 | 1.92 | 0.84 |
| 2:Q:117:LEU:CG | 2:Q:147:ASN:CG | 2.44 | 0.84 |
| 1:A:795:ARG:CD | 3:C:35:ARG:NH1 | 2.34 | 0.84 |
| 1:D:538:GLU:N | 4:9:351:THR:N | 2.25 | 0.84 |
| 1:J:831:TRP:CZ2 | 2:K:47:LEU:HD21 | 2.12 | 0.84 |
| 1:P:599:ASN:OD1 | 1:P:649:VAL:HB | 1.73 | 0.84 |
| 1:A:202:SER:HA | 1:A:207:LYS:HE2 | 0.86 | 0.84 |
| 1:A:819:ASN:CG | 2:B:92:ASP:N | 2.30 | 0.84 |
| 1:D:557:GLU:N | 4:W:48:GLY:HA2 | 1.90 | 0.84 |
| 1:G:543:PRO:HG3 | 4:V:143:TYR:O | 1.78 | 0.84 |
| 1:G:817:GLN:HG2 | 2:H:127:ARG:CB | 2.07 | 0.84 |
| 1:M:529:PRO:CB | 4:Z:353:GLN:OE1 | 2.25 | 0.84 |
| 1:M:640:LYS:C | 4:Z:23:GLY:O | 2.15 | 0.84 |
| 1:P:821:ARG:HH22 | 2:Q:127:ARG:CG | 1.89 | 0.84 |
| 1:D:725:ARG:CD | 1:D:733:PRO:HB3 | 2.07 | 0.84 |
| 1:G:646:PHE:CE2 | 1:G:652:LEU:CD1 | 2.58 | 0.84 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:792:ALA:HB2 | 3:I:42:THR:HG23 | 1.54 | 0.84 |
| 1:J:204:GLU:H | 1:J:207:LYS:HE3 | 1.42 | 0.84 |
| 1:P:630:ALA:C | 4:1:25:ASP:OD2 | 2.15 | 0.84 |
| 1:P:725:ARG:CD | 1:P:733:PRO:HB3 | 2.07 | 0.84 |
| 1:P:732:ILE:CG2 | 1:P:747:LEU:HD13 | 1.34 | 0.84 |
| 4:2:322:PRO:HB2 | 4:4:244:ASP:HB3 | 1.57 | 0.84 |
| 4:W:291:LYS:HD2 | 4:Y:243:PRO:CB | 2.07 | 0.84 |
| 1:A:549:SER:O | 4:V:46:GLY:HA3 | 1.77 | 0.84 |
| 1:D:410:ASN:ND2 | 4:9:336:LYS:HG2 | 1.93 | 0.84 |
| 1:G:215:GLN:H | 1:G:340:ILE:CG1 | 1.73 | 0.84 |
| 1:G:553:MLY:CH1 | 4:X:45:VAL:CG1 | 2.49 | 0.84 |
| 1:G:831:TRP:CZ2 | 2:H:47:LEU:HD22 | 2.11 | 0.84 |
| 1:M:204:GLU:H | 1:M:207:LYS:HE3 | 1.42 | 0.84 |
| 1:M:829:TRP:CH2 | 2:N:87:LYS:CE | 2.59 | 0.84 |
| 1:A:505:MLY:CB | 1:A:762:HIS:N | 2.39 | 0.84 |
| 2:B:141:PRO:CB | 2:B:142:PRO:CD | 2.56 | 0.84 |
| 3:C:139:TYR:HA | 3:C:142:PHE:HB3 | 1.56 | 0.84 |
| 1:J:561:LYS:CE | 4:Y:48:GLY:HA3 | 2.07 | 0.84 |
| 1:J:640:LYS:C | 4:W:23:GLY:O | 2.16 | 0.84 |
| 1:J:648:THR:CG2 | 1:J:651:ALA:HB2 | 2.08 | 0.84 |
| 1:M:732:ILE:HG23 | 1:M:747:LEU:HB2 | 1.57 | 0.84 |
| 1:M:783:LEU:HA | 1:M:786:ILE:CD1 | 2.07 | 0.84 |
| 1:P:204:GLU:H | 1:P:207:LYS:HE3 | 1.42 | 0.84 |
| 4:X:237:GLU:HA | 4:X:251:GLY:HA2 | 1.60 | 0.84 |
| 4:Z:237:GLU:HA | 4:Z:251:GLY:HA2 | 1.60 | 0.84 |
| 1:D:410:ASN:OD1 | 4:9:334:GLU:CA | 2.24 | 0.84 |
| 1:G:725:ARG:CZ | 1:G:733:PRO:HB3 | 2.06 | 0.84 |
| 1:J:630:ALA:C | 4:W:25:ASP:OD2 | 2.15 | 0.84 |
| 1:J:795:ARG:NH2 | 3:L:116:GLU:CD | 2.31 | 0.84 |
| 1:M:542:PHE:CA | 4:Z:143:TYR:CE1 | 2.61 | 0.84 |
| 1:M:798:LEU:CG | 3:O:126:LEU:HD11 | 2.06 | 0.84 |
| 1:M:817:GLN:HB3 | 2:N:127:ARG:NH1 | 1.92 | 0.84 |
| 1:P:529:PRO:CB | 4:1:353:GLN:OE1 | 2.25 | 0.84 |
| 1:P:783:LEU:CD1 | 1:P:786:ILE:HD11 | 2.06 | 0.84 |
| 1:A:538:GLU:N | 4:8:351:THR:N | 2.24 | 0.84 |
| 1:D:529:PRO:CB | 4:9:353:GLN:OE1 | 2.25 | 0.84 |
| 1:D:557:GLU:H | 4:W:48:GLY:HA3 | 1.29 | 0.84 |
| 1:D:815:CYS:SG | 2:E:92:ASP:OD1 | 2.35 | 0.84 |
| 1:G:202:SER:HA | 1:G:207:LYS:HE2 | 0.86 | 0.84 |
| 1:J:817:GLN:HB3 | 2:K:127:ARG:HD2 | 1.39 | 0.84 |
| 1:J:836:PHE:CE1 | 2:K:159:HIS:CA | 2.56 | 0.84 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:P:648:THR:CG2 | 1:P:651:ALA:HB2 | 2.08 | 0.84 |
| 1:P:817:GLN:HB3 | 2:Q:127:ARG:HD2 | 1.55 | 0.84 |
| 4:2:287:ILE:HG21 | 4:4:204:ALA:H | 1.42 | 0.84 |
| 4:8:286:ASP:OD1 | 4:V:203:THR:CG2 | 2.26 | 0.84 |
| 1:A:641:LYS:HG2 | 1:A:647:GLN:HG3 | 1.60 | 0.83 |
| 1:D:732:ILE:HG21 | 1:D:747:LEU:HD13 | 0.91 | 0.83 |
| 1:G:792:ALA:CA | 3:I:42:THR:HG22 | 2.06 | 0.83 |
| 1:J:543:PRO:HG3 | 4:W:143:TYR:O | 1.77 | 0.83 |
| 1:M:725:ARG:CZ | 1:M:733:PRO:HB3 | 2.06 | 0.83 |
| 4:2:237:GLU:HA | 4:2:251:GLY:HA2 | 1.60 | 0.83 |
| 1:A:630:ALA:C | 4:8:25:ASP:OD2 | 2.15 | 0.83 |
| 1:D:648:THR:CG2 | 1:D:651:ALA:HB2 | 2.08 | 0.83 |
| 2:E:141:PRO:CB | 2:E:142:PRO:CD | 2.56 | 0.83 |
| 1:G:629:GLU:CG | 1:G:643:GLY:O | 2.26 | 0.83 |
| 1:M:629:GLU:CG | 1:M:643:GLY:O | 2.26 | 0.83 |
| 1:M:648:THR:CG2 | 1:M:651:ALA:HB2 | 2.08 | 0.83 |
| 2:N:141:PRO:CB | 2:N:142:PRO:CD | 2.56 | 0.83 |
| 1:P:806:MET:C | 1:P:807:VAL:CA | 2.45 | 0.83 |
| 1:A:629:GLU:CG | 1:A:643:GLY:O | 2.26 | 0.83 |
| 1:A:837:MLY:CH2 | 2:H:20:ASP:HA | 2.07 | 0.83 |
| 2:H:141:PRO:CB | 2:H:142:PRO:CD | 2.56 | 0.83 |
| 1:J:789:ALA:HB1 | 3:L:81:GLN:CD | 1.98 | 0.83 |
| 1:M:732:ILE:HG21 | 1:M:747:LEU:HD13 | 0.91 | 0.83 |
| 1:M:817:GLN:CG | 2:N:127:ARG:CD | 2.52 | 0.83 |
| 4:V:237:GLU:HA | 4:V:251:GLY:HA2 | 1.60 | 0.83 |
| 1:A:529:PRO:CB | 4:8:353:GLN:OE1 | 2.25 | 0.83 |
| 1:A:735:GLY:C | 1:A:743:ALA:HB2 | 1.82 | 0.83 |
| 1:A:795:ARG:HG2 | 3:C:118:MET:HE3 | 1.60 | 0.83 |
| 1:A:837:MLY:HH21 | 2:H:20:ASP:CB | 2.08 | 0.83 |
| 1:G:640:LYS:C | 4:V:23:GLY:O | 2.16 | 0.83 |
| 1:G:648:THR:CG2 | 1:G:651:ALA:HB2 | 2.08 | 0.83 |
| 1:G:725:ARG:CD | 1:G:733:PRO:HB3 | 2.07 | 0.83 |
| 1:J:542:PHE:CA | 4:W:143:TYR:CE1 | 2.61 | 0.83 |
| 2:K:141:PRO:CB | 2:K:142:PRO:CD | 2.56 | 0.83 |
| 1:M:635:GLY:HA2 | 4:Z:334:GLU:CG | 2.03 | 0.83 |
| 1:M:725:ARG:CD | 1:M:733:PRO:HB3 | 2.08 | 0.83 |
| 1:P:543:PRO:HG3 | 4:1:143:TYR:O | 1.77 | 0.83 |
| 1:P:546:THR:OG1 | 4:3:47:MET:N | 2.10 | 0.83 |
| 1:P:730:SER:O | 1:P:734:GLU:HG3 | 1.78 | 0.83 |
| 1:P:797:PHE:CD1 | 3:R:146:ILE:O | 2.31 | 0.83 |
| 4:5:237:GLU:HA | 4:5:251:GLY:HA2 | 1.60 | 0.83 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:8:237:GLU:HA | 4:8:251:GLY:HA2 | 1.60 | 0.83 |
| 1:D:818:TYR:CB | 2:E:90:GLY:N | 2.40 | 0.83 |
| 1:G:542:PHE:CA | 4:V:143:TYR:CE1 | 2.61 | 0.83 |
| 1:G:797:PHE:CD1 | 3:I:146:ILE:CG2 | 2.57 | 0.83 |
| 1:M:418:THR:HB | 1:M:421:GLU:HG3 | 1.60 | 0.83 |
| 1:M:735:GLY:C | 1:M:743:ALA:HB2 | 1.82 | 0.83 |
| 1:M:831:TRP:CH2 | 2:N:47:LEU:HD21 | 2.00 | 0.83 |
| 1:A:502:GLU:CG | 1:A:761:GLY:N | 2.41 | 0.83 |
| 1:A:725:ARG:CZ | 1:A:733:PRO:HB3 | 2.06 | 0.83 |
| 1:A:792:ALA:HB2 | 3:C:42:THR:HG22 | 0.86 | 0.83 |
| 1:D:725:ARG:CZ | 1:D:733:PRO:HB3 | 2.06 | 0.83 |
| 1:J:530:MET:CG | 4:W:354:GLN:CB | 2.30 | 0.83 |
| 1:J:732:ILE:CG2 | 1:J:747:LEU:HD13 | 1.34 | 0.83 |
| 1:J:797:PHE:CZ | 3:L:146:ILE:HD13 | 2.09 | 0.83 |
| 1:P:279:LEU:HB2 | 1:P:282:GLU:HG3 | 1.60 | 0.83 |
| 4:7:286:ASP:OD1 | 4:9:203:THR:CG2 | 2.26 | 0.83 |
| 1:A:542:PHE:CA | 4:8:143:TYR:CE1 | 2.61 | 0.83 |
| 1:D:204:GLU:H | 1:D:207:LYS:HE3 | 1.41 | 0.83 |
| 1:D:530:MET:CG | 4:9:354:GLN:CB | 2.30 | 0.83 |
| 1:D:542:PHE:CA | 4:9:143:TYR:CE1 | 2.61 | 0.83 |
| 1:D:543:PRO:HG3 | 4:9:143:TYR:O | 1.77 | 0.83 |
| 1:D:630:ALA:C | 4:9:25:ASP:OD2 | 2.15 | 0.83 |
| 1:D:795:ARG:HG2 | 3:F:118:MET:HE1 | 1.60 | 0.83 |
| 2:E:111:SER:OG | 2:E:148:VAL:C | 2.15 | 0.83 |
| 1:G:148:ARG:NE | 1:G:764:MLY:HH21 | 1.93 | 0.83 |
| 1:J:567:LYS:HZ1 | 4:Y:92:ASN:HD22 | 1.27 | 0.83 |
| 1:M:795:ARG:NE | 3:O:43:ASN:OD1 | 2.11 | 0.83 |
| 1:P:418:THR:HB | 1:P:421:GLU:HG3 | 1.60 | 0.83 |
| 1:P:542:PHE:CA | 4:1:143:TYR:CE1 | 2.61 | 0.83 |
| 1:P:769:ALA:CA | 1:P:770:GLY:N | 2.41 | 0.83 |
| 1:P:797:PHE:CE2 | 3:R:126:LEU:HD22 | 2.12 | 0.83 |
| 1:D:643:GLY:N | 4:9:24:ASP:HA | 1.93 | 0.83 |
| 1:D:730:SER:O | 1:D:734:GLU:HG3 | 1.79 | 0.83 |
| 1:G:730:SER:O | 1:G:734:GLU:HG3 | 1.79 | 0.83 |
| 1:G:795:ARG:NE | 3:I:116:GLU:CB | 2.12 | 0.83 |
| 1:M:279:LEU:HB2 | 1:M:282:GLU:HG3 | 1.60 | 0.83 |
| 4:1:287:ILE:HG21 | 4:3:203:THR:H | 1.43 | 0.83 |
| 4:2:43:VAL:O | 4:Z:167:GLU:CD | 2.15 | 0.83 |
| 4:X:287:ILE:HG21 | 4:Z:199:SER:O | 1.78 | 0.83 |
| 1:A:725:ARG:CD | 1:A:733:PRO:HB3 | 2.08 | 0.83 |
| 1:J:410:ASN:OD1 | 4:W:334:GLU:CA | 2.24 | 0.83 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:732:ILE:HG23 | 1:J:747:LEU:CB | 1.85 | 0.83 |
| 1:M:730:SER:O | 1:M:734:GLU:HG3 | 1.79 | 0.83 |
| 1:M:791:GLN:HE22 | 3:O:115:GLY:HA3 | 1.44 | 0.83 |
| 2:Q:141:PRO:CB | 2:Q:142:PRO:CD | 2.56 | 0.83 |
| 4:4:237:GLU:HA | 4:4:251:GLY:HA2 | 1.60 | 0.83 |
| 1:J:791:GLN:OE1 | 3:L:116:GLU:HG3 | 1.78 | 0.83 |
| 1:M:797:PHE:CD1 | 3:O:149:VAL:HG11 | 2.13 | 0.83 |
| 1:P:629:GLU:CG | 1:P:643:GLY:O | 2.26 | 0.83 |
| 1:P:641:LYS:HG2 | 1:P:647:GLN:HG3 | 1.61 | 0.83 |
| 1:A:543:PRO:HG3 | 4:8:143:TYR:O | 1.77 | 0.82 |
| 1:A:648:THR:CG2 | 1:A:651:ALA:HB2 | 2.08 | 0.82 |
| 1:D:506:GLU:CG | 1:D:764:MLY:HE2 | 2.07 | 0.82 |
| 1:D:727:LEU:H | 1:D:782:MLY:HH22 | 1.42 | 0.82 |
| 1:D:830:PRO:HG2 | 2:E:67:MET:HE1 | 1.60 | 0.82 |
| 1:M:218:LEU:HB3 | 1:M:221:GLN:HG3 | 1.61 | 0.82 |
| 1:M:530:MET:HE1 | 4:Z:355:MET:SD | 2.19 | 0.82 |
| 1:P:640:LYS:CB | 1:P:645:SER:OG | 2.25 | 0.82 |
| 1:P:796:GLY:CA | 3:R:35:ARG:HD3 | 2.07 | 0.82 |
| 4:2:203:THR:HB | 4:Z:287:ILE:HD13 | 1.61 | 0.82 |
| 1:A:730:SER:O | 1:A:734:GLU:HG3 | 1.78 | 0.82 |
| 2:E:117:LEU:CB | 2:E:147:ASN:ND2 | 2.35 | 0.82 |
| 1:G:93:MET:SD | 1:G:715:VAL:HA | 2.19 | 0.82 |
| 1:G:218:LEU:HB3 | 1:G:221:GLN:HG3 | 1.60 | 0.82 |
| 1:G:538:GLU:N | 4:V:351:THR:N | 2.24 | 0.82 |
| 1:J:529:PRO:CB | 4:W:353:GLN:OE1 | 2.25 | 0.82 |
| 1:J:798:LEU:HD11 | 3:L:126:LEU:HD13 | 1.59 | 0.82 |
| 1:P:149:GLN:HG2 | 1:P:716:LEU:HD11 | 1.61 | 0.82 |
| 1:P:795:ARG:CZ | 3:R:116:GLU:CD | 2.47 | 0.82 |
| 1:P:826:VAL:HG21 | 2:Q:88:LEU:HD21 | 1.58 | 0.82 |
| 4:3:237:GLU:HA | 4:3:251:GLY:HA2 | 1.60 | 0.82 |
| 4:V:325:MET:HE1 | 4:X:244:ASP:CG | 2.00 | 0.82 |
| 1:A:549:SER:O | 4:V:46:GLY:CA | 2.27 | 0.82 |
| 1:A:732:ILE:CG2 | 1:A:747:LEU:HD13 | 1.34 | 0.82 |
| 1:A:819:ASN:CG | 2:B:90:GLY:O | 2.16 | 0.82 |
| 1:D:727:LEU:CD1 | 1:D:782:MLY:CG | 2.57 | 0.82 |
| 1:G:795:ARG:HB2 | 3:I:35:ARG:NH1 | 1.94 | 0.82 |
| 1:J:418:THR:HB | 1:J:421:GLU:HG3 | 1.60 | 0.82 |
| 1:J:629:GLU:CG | 1:J:643:GLY:O | 2.26 | 0.82 |
| 1:J:639:GLY:CA | 4:W:344:SER:C | 2.48 | 0.82 |
| 2:K:111:SER:OG | 2:K:148:VAL:C | 2.15 | 0.82 |
| 1:M:107:MLY:HB3 | 1:M:686:MET:HE2 | 1.61 | 0.82 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:N:121:LEU:CG | 2:N:128:PHE:CA | 2.49 | 0.82 |
| 1:A:218:LEU:HD22 | 1:A:222:ILE:CG1 | 2.10 | 0.82 |
| 1:A:557:GLU:N | 4:V:48:GLY:HA2 | 1.90 | 0.82 |
| 1:A:795:ARG:HG2 | 3:C:118:MET:CE | 2.08 | 0.82 |
| 1:D:506:GLU:HG2 | 1:D:764:MLY:HE2 | 1.58 | 0.82 |
| 1:D:507:GLY:HA3 | 1:D:762:HIS:CB | 2.09 | 0.82 |
| 1:D:578:HIS:HB3 | 1:D:592:ILE:HD12 | 1.62 | 0.82 |
| 1:G:218:LEU:HD22 | 1:G:222:ILE:CG1 | 2.10 | 0.82 |
| 1:G:769:ALA:O | 1:G:773:GLY:HA3 | 1.77 | 0.82 |
| 1:J:640:LYS:CB | 1:J:645:SER:OG | 2.25 | 0.82 |
| 1:M:578:HIS:HD2 | 1:M:591:ASN:HA | 1.45 | 0.82 |
| 4:1:247:VAL:H | 4:Y:324:THR:CG2 | 1.92 | 0.82 |
| 4:9:286:ASP:OD1 | 4:W:203:THR:CG2 | 2.26 | 0.82 |
| 1:A:149:GLN:HG2 | 1:A:719:ASP:CB | 2.09 | 0.82 |
| 1:A:502:GLU:CG | 1:A:764:MLY:O | 2.26 | 0.82 |
| 1:A:542:PHE:CA | 4:8:143:TYR:HE1 | 1.92 | 0.82 |
| 1:D:813:ILE:CG2 | 2:E:128:PHE:CE1 | 2.62 | 0.82 |
| 1:G:755:HIS:H | 1:G:779:ARG:NE | 1.76 | 0.82 |
| 1:J:279:LEU:HB2 | 1:J:282:GLU:HG3 | 1.60 | 0.82 |
| 1:J:735:GLY:C | 1:J:743:ALA:HB1 | 1.84 | 0.82 |
| 1:A:218:LEU:HB3 | 1:A:221:GLN:HG3 | 1.60 | 0.82 |
| 1:A:410:ASN:ND2 | 4:8:336:LYS:HG2 | 1.93 | 0.82 |
| 1:D:279:LEU:HB2 | 1:D:282:GLU:HG3 | 1.60 | 0.82 |
| 1:D:629:GLU:CG | 1:D:643:GLY:O | 2.26 | 0.82 |
| 1:D:641:LYS:HG2 | 1:D:647:GLN:HG3 | 1.60 | 0.82 |
| 1:G:502:GLU:OE2 | 1:G:761:GLY:HA3 | 1.80 | 0.82 |
| 1:G:640:LYS:CB | 1:G:645:SER:OG | 2.25 | 0.82 |
| 2:H:111:SER:OG | 2:H:148:VAL:C | 2.15 | 0.82 |
| 1:M:215:GLN:H | 1:M:340:ILE:CG1 | 1.73 | 0.82 |
| 1:M:542:PHE:CA | 4:Z:143:TYR:HE1 | 1.92 | 0.82 |
| 1:P:93:MET:HG2 | 1:P:714:ARG:H | 1.45 | 0.82 |
| 1:P:641:LYS:HD2 | 4:1:348:SER:CA | 2.09 | 0.82 |
| 1:P:769:ALA:O | 1:P:771:LEU:HB3 | 1.79 | 0.82 |
| 1:A:643:GLY:N | 4:8:24:ASP:HA | 1.93 | 0.82 |
| 1:D:107:MLY:HB3 | 1:D:686:MET:HE2 | 1.61 | 0.82 |
| 1:D:418:THR:HB | 1:D:421:GLU:HG3 | 1.60 | 0.82 |
| 1:D:793:ARG:HH21 | 3:F:147:MET:CE | 1.93 | 0.82 |
| 1:J:798:LEU:CD1 | 3:L:126:LEU:CD1 | 2.28 | 0.82 |
| 1:J:817:GLN:HG2 | 2:K:127:ARG:HB3 | 1.57 | 0.82 |
| 1:P:599:ASN:CA | 1:P:649:VAL:CB | 2.53 | 0.82 |
| 4:6:237:GLU:HA | 4:6:251:GLY:HA2 | 1.60 | 0.82 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:8:290:ARG:NH1 | 4:V:202:THR:HG21 | 1.94 | 0.82 |
| 1:A:754:ASP:OD2 | 1:A:778:MET:HE1 | 1.79 | 0.82 |
| 1:D:736:GLN:HA | 1:D:743:ALA:HB2 | 1.51 | 0.82 |
| 1:G:578:HIS:HD2 | 1:G:591:ASN:HA | 1.45 | 0.82 |
| 1:J:721:LYS:CA | 1:J:736:GLN:NE2 | 2.43 | 0.82 |
| 1:M:543:PRO:HG3 | 4:Z:143:TYR:O | 1.77 | 0.82 |
| 1:M:800:ARG:HB3 | 3:O:149:VAL:HG22 | 1.61 | 0.82 |
| 4:1:244:ASP:N | 4:Y:291:LYS:CG | 2.43 | 0.82 |
| 1:D:530:MET:HE1 | 4:9:355:MET:SD | 2.20 | 0.82 |
| 1:G:734:GLU:O | 1:G:738:MET:CG | 2.28 | 0.82 |
| 1:J:480:ILE:HG22 | 1:J:481:ASN:HD22 | 1.45 | 0.82 |
| 1:M:641:LYS:HD2 | 4:Z:348:SER:CA | 2.09 | 0.82 |
| 1:P:818:TYR:CD1 | 2:Q:127:ARG:NH1 | 2.47 | 0.82 |
| 4:W:286:ASP:OD1 | 4:Y:203:THR:N | 2.11 | 0.82 |
| 1:A:93:MET:HG2 | 1:A:715:VAL:CG2 | 2.10 | 0.82 |
| 1:A:498:LEU:HD23 | 1:A:764:MLY:HH22 | 1.60 | 0.82 |
| 1:D:732:ILE:CG2 | 1:D:747:LEU:HD13 | 1.34 | 0.82 |
| 1:G:84:MLY:CH2 | 1:G:719:ASP:O | 2.28 | 0.82 |
| 1:G:732:ILE:HG21 | 1:G:747:LEU:HD13 | 0.91 | 0.82 |
| 1:G:755:HIS:HB2 | 1:G:779:ARG:HH22 | 1.44 | 0.82 |
| 1:M:95:THR:OG1 | 1:M:770:GLY:CA | 2.26 | 0.82 |
| 1:M:578:HIS:HB3 | 1:M:592:ILE:HD12 | 1.61 | 0.82 |
| 1:M:734:GLU:O | 1:M:738:MET:CG | 2.28 | 0.82 |
| 1:P:820:VAL:HG11 | 2:Q:136:MET:CE | 2.10 | 0.82 |
| 1:A:279:LEU:HB2 | 1:A:282:GLU:HG3 | 1.60 | 0.81 |
| 1:A:530:MET:HE3 | 4:8:354:GLN:HG2 | 1.60 | 0.81 |
| 1:D:732:ILE:CD1 | 1:D:782:MLY:HH11 | 2.10 | 0.81 |
| 1:J:505:MLY:CD | 1:J:762:HIS:HE1 | 1.88 | 0.81 |
| 1:M:480:ILE:HG22 | 1:M:481:ASN:HD22 | 1.45 | 0.81 |
| 1:M:639:GLY:CA | 4:Z:344:SER:C | 2.48 | 0.81 |
| 1:M:769:ALA:C | 1:M:770:GLY:N | 2.33 | 0.81 |
| 1:M:803:TYR:CD2 | 3:O:17:PHE:CZ | 2.68 | 0.81 |
| 1:M:821:ARG:HH22 | 2:N:127:ARG:CG | 1.88 | 0.81 |
| 1:P:218:LEU:HD22 | 1:P:222:ILE:CG1 | 2.10 | 0.81 |
| 1:P:734:GLU:O | 1:P:738:MET:CG | 2.28 | 0.81 |
| 1:A:480:ILE:HG22 | 1:A:481:ASN:HD22 | 1.46 | 0.81 |
| 1:D:553:MLY:HG2 | 4:W:47:MET:H | 1.44 | 0.81 |
| 1:D:639:GLY:CA | 4:9:344:SER:C | 2.48 | 0.81 |
| 1:G:107:MLY:HB3 | 1:G:686:MET:HE2 | 1.62 | 0.81 |
| 1:G:599:ASN:CA | 1:G:649:VAL:CB | 2.53 | 0.81 |
| 1:G:641:LYS:HG2 | 1:G:647:GLN:HG3 | 1.61 | 0.81 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:H:121:LEU:CA | 2:H:128:PHE:CB | 2.47 | 0.81 |
| 1:J:783:LEU:O | 1:J:787:ILE:HB | 1.79 | 0.81 |
| 1:J:831:TRP:CZ2 | 2:K:47:LEU:HD22 | 2.14 | 0.81 |
| 1:M:218:LEU:HD22 | 1:M:222:ILE:CG1 | 2.10 | 0.81 |
| 4:1:290:ARG:HH22 | 4:3:202:THR:HG22 | 1.42 | 0.81 |
| 4:7:237:GLU:HA | 4:7:251:GLY:HA2 | 1.60 | 0.81 |
| 4:V:325:MET:SD | 4:X:244:ASP:HB3 | 2.18 | 0.81 |
| 1:A:107:MLY:HB3 | 1:A:686:MET:HE2 | 1.63 | 0.81 |
| 1:A:553:MLY:HG2 | 4:V:47:MET:H | 1.44 | 0.81 |
| 1:A:571:ALA:O | 1:A:572:LYS:CG | 2.28 | 0.81 |
| 1:A:641:LYS:HD2 | 4:8:348:SER:CA | 2.10 | 0.81 |
| 1:D:549:SER:O | 4:W:46:GLY:CA | 2.27 | 0.81 |
| 1:D:641:LYS:HD2 | 4:9:348:SER:HB2 | 1.54 | 0.81 |
| 1:D:831:TRP:CE2 | 2:E:51:PHE:CZ | 2.68 | 0.81 |
| 1:G:93:MET:SD | 1:G:716:LEU:N | 2.53 | 0.81 |
| 1:G:797:PHE:CE2 | 3:I:126:LEU:HD13 | 2.15 | 0.81 |
| 1:G:797:PHE:CE1 | 3:I:146:ILE:CG2 | 2.61 | 0.81 |
| 1:J:215:GLN:N | 1:J:340:ILE:CD1 | 2.44 | 0.81 |
| 1:J:571:ALA:O | 1:J:572:LYS:CG | 2.28 | 0.81 |
| 1:J:641:LYS:HD2 | 4:W:348:SER:HB2 | 1.54 | 0.81 |
| 1:J:730:SER:O | 1:J:734:GLU:HG3 | 1.78 | 0.81 |
| 1:J:734:GLU:O | 1:J:738:MET:CG | 2.28 | 0.81 |
| 1:J:795:ARG:CZ | 3:L:116:GLU:CD | 2.48 | 0.81 |
| 1:P:544:LYS:HB3 | 4:3:45:VAL:HG22 | 1.62 | 0.81 |
| 1:P:544:LYS:HD3 | 4:3:45:VAL:HG21 | 1.63 | 0.81 |
| 1:P:571:ALA:O | 1:P:572:LYS:CG | 2.28 | 0.81 |
| 1:P:821:ARG:HH22 | 2:Q:127:ARG:HG2 | 1.36 | 0.81 |
| 4:1:237:GLU:HA | 4:1:251:GLY:HA2 | 1.60 | 0.81 |
| 4:7:290:ARG:NH1 | 4:9:202:THR:HG21 | 1.94 | 0.81 |
| 4:W:237:GLU:HA | 4:W:251:GLY:HA2 | 1.60 | 0.81 |
| 4:Y:237:GLU:HA | 4:Y:251:GLY:HA2 | 1.60 | 0.81 |
| 1:A:578:HIS:HD2 | 1:A:591:ASN:HA | 1.45 | 0.81 |
| 1:D:549:SER:O | 4:W:46:GLY:C | 2.18 | 0.81 |
| 1:D:830:PRO:HG2 | 2:E:67:MET:HE2 | 1.61 | 0.81 |
| 1:G:84:MLY:HB3 | 1:G:723:ARG:CZ | 2.10 | 0.81 |
| 1:J:819:ASN:ND2 | 2:K:92:ASP:CB | 2.39 | 0.81 |
| 1:M:641:LYS:HG2 | 1:M:647:GLN:HG3 | 1.61 | 0.81 |
| 1:P:218:LEU:HA | 1:P:221:GLN:HG2 | 1.62 | 0.81 |
| 1:P:639:GLY:CA | 4:1:344:SER:C | 2.48 | 0.81 |
| 1:P:646:PHE:CE2 | 1:P:652:LEU:HD21 | 2.15 | 0.81 |
| 4:4:322:PRO:HB3 | 4:6:244:ASP:OD2 | 1.79 | 0.81 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:232:PHE:CZ | 1:D:287:ILE:HD13 | 2.16 | 0.81 |
| 1:G:28:GLN:C | 1:G:723:ARG:HH22 | 1.82 | 0.81 |
| 1:G:215:GLN:N | 1:G:340:ILE:CD1 | 2.44 | 0.81 |
| 1:G:279:LEU:HB2 | 1:G:282:GLU:HG3 | 1.60 | 0.81 |
| 1:J:643:GLY:N | 4:W:24:ASP:HA | 1.94 | 0.81 |
| 1:M:218:LEU:CA | 1:M:221:GLN:HG2 | 2.10 | 0.81 |
| 1:M:571:ALA:O | 1:M:572:LYS:CG | 2.28 | 0.81 |
| 1:P:578:HIS:HB3 | 1:P:592:ILE:HD12 | 1.62 | 0.81 |
| 1:P:643:GLY:N | 4:1:24:ASP:HA | 1.94 | 0.81 |
| 2:Q:144:VAL:HG12 | 2:Q:153:ILE:CD1 | 2.10 | 0.81 |
| 1:A:502:GLU:HG3 | 1:A:761:GLY:HA3 | 1.58 | 0.81 |
| 1:D:538:GLU:CA | 4:9:351:THR:H | 1.93 | 0.81 |
| 1:D:641:LYS:HD2 | 4:9:348:SER:CA | 2.10 | 0.81 |
| 1:D:727:LEU:HG | 1:D:782:MLY:HG3 | 1.62 | 0.81 |
| 1:D:734:GLU:O | 1:D:738:MET:CG | 2.28 | 0.81 |
| 1:G:538:GLU:CA | 4:V:351:THR:H | 1.93 | 0.81 |
| 1:J:649:VAL:HG12 | 1:J:649:VAL:C | 1.98 | 0.81 |
| 1:P:218:LEU:HB3 | 1:P:221:GLN:HG3 | 1.61 | 0.81 |
| 1:A:218:LEU:CA | 1:A:221:GLN:HG2 | 2.10 | 0.81 |
| 1:A:734:GLU:O | 1:A:738:MET:CG | 2.28 | 0.81 |
| 1:A:798:LEU:HD21 | 3:C:126:LEU:HD11 | 1.62 | 0.81 |
| 1:A:836:PHE:CZ | 2:B:159:HIS:C | 2.54 | 0.81 |
| 1:D:215:GLN:N | 1:D:340:ILE:CD1 | 2.44 | 0.81 |
| 1:D:218:LEU:HA | 1:D:221:GLN:HG2 | 1.62 | 0.81 |
| 1:G:567:LYS:HZ3 | 4:X:92:ASN:ND2 | 1.75 | 0.81 |
| 1:G:721:LYS:CA | 1:G:736:GLN:NE2 | 2.43 | 0.81 |
| 1:M:643:GLY:N | 4:Z:24:ASP:HA | 1.93 | 0.81 |
| 1:M:646:PHE:CE2 | 1:M:652:LEU:HD21 | 2.15 | 0.81 |
| 1:P:107:MLY:HB3 | 1:P:686:MET:HE2 | 1.63 | 0.81 |
| 1:P:215:GLN:N | 1:P:340:ILE:CD1 | 2.44 | 0.81 |
| 1:P:783:LEU:CA | 1:P:786:ILE:CD1 | 2.58 | 0.81 |
| 4:6:223:PHE:HE1 | 4:6:255:PHE:HB2 | 1.46 | 0.81 |
| 4:9:290:ARG:NH1 | 4:W:202:THR:HG21 | 1.94 | 0.81 |
| 1:G:480:ILE:HG22 | 1:G:481:ASN:HD22 | 1.45 | 0.81 |
| 1:G:542:PHE:CA | 4:V:143:TYR:HE1 | 1.93 | 0.81 |
| 1:G:643:GLY:N | 4:V:24:ASP:HA | 1.94 | 0.81 |
| 1:G:757:GLN:OE1 | 1:G:772:LEU:C | 2.18 | 0.81 |
| 1:G:819:ASN:HA | 2:H:90:GLY:C | 1.98 | 0.81 |
| 1:J:578:HIS:HB3 | 1:J:592:ILE:HD12 | 1.62 | 0.81 |
| 1:J:797:PHE:HE1 | 3:L:146:ILE:HA | 1.44 | 0.81 |
| 2:K:117:LEU:CB | 2:K:147:ASN:ND2 | 2.35 | 0.81 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:N:144:VAL:HG12 | 2:N:153:ILE:CD1 | 2.09 | 0.81 |
| 1:P:783:LEU:CB | 1:P:786:ILE:CD1 | 2.58 | 0.81 |
| 1:A:538:GLU:CA | 4:8:351:THR:H | 1.93 | 0.81 |
| 1:A:639:GLY:CA | 4:8:344:SER:C | 2.48 | 0.81 |
| 1:G:127:ASN:HD22 | 1:G:128:PRO:HD2 | 1.45 | 0.81 |
| 2:H:141:PRO:HB2 | 2:H:142:PRO:CD | 2.11 | 0.81 |
| 1:J:641:LYS:HG2 | 1:J:647:GLN:HG3 | 1.61 | 0.81 |
| 1:P:578:HIS:HD2 | 1:P:591:ASN:HA | 1.45 | 0.81 |
| 4:3:290:ARG:HH21 | 4:5:202:THR:HG23 | 1.41 | 0.81 |
| 4:4:223:PHE:HE1 | 4:4:255:PHE:HB2 | 1.46 | 0.81 |
| 4:X:291:LYS:HB2 | 4:Z:245:GLY:H | 1.44 | 0.81 |
| 1:A:149:GLN:HE21 | 1:A:718:ALA:HB3 | 0.98 | 0.81 |
| 1:A:501:GLU:CG | 1:A:762:HIS:HD1 | 1.86 | 0.81 |
| 1:D:809:ARG:NH2 | 2:E:120:LEU:HD11 | 1.96 | 0.81 |
| 1:G:818:TYR:HB3 | 2:H:90:GLY:HA3 | 1.63 | 0.81 |
| 3:L:49:ILE:N | 3:L:52:ASN:ND2 | 2.29 | 0.81 |
| 1:M:218:LEU:HA | 1:M:221:GLN:HG2 | 1.62 | 0.81 |
| 1:P:538:GLU:CA | 4:1:351:THR:H | 1.93 | 0.81 |
| 4:1:201:VAL:HG23 | 4:Y:287:ILE:CG2 | 2.11 | 0.81 |
| 4:9:237:GLU:HA | 4:9:251:GLY:HA2 | 1.60 | 0.81 |
| 1:A:215:GLN:N | 1:A:340:ILE:CD1 | 2.44 | 0.80 |
| 1:A:549:SER:O | 4:V:46:GLY:C | 2.19 | 0.80 |
| 2:B:117:LEU:HB2 | 2:B:147:ASN:HD21 | 1.46 | 0.80 |
| 1:G:557:GLU:HB2 | 4:X:46:GLY:C | 2.00 | 0.80 |
| 1:G:641:LYS:HD2 | 4:V:348:SER:CA | 2.10 | 0.80 |
| 1:J:784:ALA:O | 1:J:788:THR:N | 2.14 | 0.80 |
| 1:M:127:ASN:HD22 | 1:M:128:PRO:HD2 | 1.45 | 0.80 |
| 1:M:232:PHE:CZ | 1:M:287:ILE:HD13 | 2.16 | 0.80 |
| 1:M:529:PRO:C | 4:Z:354:GLN:CB | 2.48 | 0.80 |
| 1:M:721:LYS:CA | 1:M:736:GLN:NE2 | 2.43 | 0.80 |
| 1:M:732:ILE:HG22 | 1:M:747:LEU:HD12 | 0.81 | 0.80 |
| 1:M:836:PHE:CE1 | 2:N:160:GLY:N | 2.45 | 0.80 |
| 1:P:232:PHE:CZ | 1:P:287:ILE:HD13 | 2.16 | 0.80 |
| 1:P:708:ARG:C | 1:P:710:GLY:N | 2.34 | 0.80 |
| 1:A:578:HIS:HB3 | 1:A:592:ILE:HD12 | 1.62 | 0.80 |
| 1:D:127:ASN:HD22 | 1:D:128:PRO:HD2 | 1.45 | 0.80 |
| 1:D:571:ALA:O | 1:D:572:LYS:CG | 2.28 | 0.80 |
| 1:J:107:MLY:HB3 | 1:J:686:MET:HE2 | 1.63 | 0.80 |
| 1:J:218:LEU:HD22 | 1:J:222:ILE:CG1 | 2.10 | 0.80 |
| 1:J:732:ILE:HG22 | 1:J:747:LEU:HD12 | 0.81 | 0.80 |
| 2:K:144:VAL:CA | 2:K:153:ILE:HD11 | 2.11 | 0.80 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:215:GLN:N | 1:M:340:ILE:CD1 | 2.44 | 0.80 |
| 1:M:538:GLU:CA | 4:Z:351:THR:H | 1.93 | 0.80 |
| 1:P:218:LEU:CA | 1:P:221:GLN:HG2 | 2.10 | 0.80 |
| 4:1:223:PHE:HE1 | 4:1:255:PHE:HB2 | 1.46 | 0.80 |
| 4:1:245:GLY:CA | 4:Y:324:THR:O | 2.29 | 0.80 |
| 4:5:223:PHE:HE1 | 4:5:255:PHE:HB2 | 1.46 | 0.80 |
| 4:X:223:PHE:HE1 | 4:X:255:PHE:HB2 | 1.46 | 0.80 |
| 1:A:218:LEU:HA | 1:A:221:GLN:HG2 | 1.62 | 0.80 |
| 1:A:530:MET:CG | 4:8:354:GLN:CB | 2.30 | 0.80 |
| 1:D:795:ARG:CD | 3:F:35:ARG:HH12 | 1.93 | 0.80 |
| 1:J:641:LYS:HD2 | 4:W:348:SER:CA | 2.09 | 0.80 |
| 4:1:112:PRO:HB3 | 4:2:195:GLU:O | 1.82 | 0.80 |
| 4:1:243:PRO:C | 4:Y:291:LYS:CD | 2.49 | 0.80 |
| 4:Z:223:PHE:HE1 | 4:Z:255:PHE:HB2 | 1.46 | 0.80 |
| 1:A:232:PHE:CZ | 1:A:287:ILE:HD13 | 2.16 | 0.80 |
| 1:A:732:ILE:HG22 | 1:A:747:LEU:HD12 | 0.81 | 0.80 |
| 1:D:218:LEU:HD22 | 1:D:222:ILE:CG1 | 2.10 | 0.80 |
| 1:G:578:HIS:HB3 | 1:G:592:ILE:HD12 | 1.62 | 0.80 |
| 1:G:735:GLY:C | 1:G:743:ALA:HB2 | 1.82 | 0.80 |
| 1:G:838:ILE:CD1 | 2:H:54:MET:HE1 | 2.07 | 0.80 |
| 2:H:144:VAL:CA | 2:H:153:ILE:HD11 | 2.11 | 0.80 |
| 1:J:218:LEU:HA | 1:J:221:GLN:HG2 | 1.62 | 0.80 |
| 1:J:232:PHE:CZ | 1:J:287:ILE:HD13 | 2.16 | 0.80 |
| 1:J:542:PHE:CA | 4:W:143:TYR:HE1 | 1.92 | 0.80 |
| 2:N:141:PRO:CB | 2:N:142:PRO:HD2 | 2.11 | 0.80 |
| 1:P:795:ARG:NE | 3:R:43:ASN:OD1 | 2.13 | 0.80 |
| 2:Q:141:PRO:HB2 | 2:Q:142:PRO:CD | 2.12 | 0.80 |
| 4:W:223:PHE:HE1 | 4:W:255:PHE:HB2 | 1.46 | 0.80 |
| 1:D:374:GLN:HG3 | 1:D:375:ALA:N | 1.96 | 0.80 |
| 1:D:480:ILE:HG22 | 1:D:481:ASN:HD22 | 1.45 | 0.80 |
| 1:D:578:HIS:HD2 | 1:D:591:ASN:HA | 1.45 | 0.80 |
| 1:D:649:VAL:HG12 | 1:D:649:VAL:C | 1.98 | 0.80 |
| 2:E:144:VAL:CA | 2:E:153:ILE:HD11 | 2.11 | 0.80 |
| 1:G:639:GLY:CA | 4:V:344:SER:C | 2.48 | 0.80 |
| 1:G:795:ARG:CZ | 3:I:116:GLU:HB3 | 2.11 | 0.80 |
| 1:G:820:VAL:HG11 | 2:H:136:MET:CE | 2.12 | 0.80 |
| 1:J:127:ASN:HD22 | 1:J:128:PRO:HD2 | 1.45 | 0.80 |
| 1:P:127:ASN:HD22 | 1:P:128:PRO:HD2 | 1.45 | 0.80 |
| 1:P:732:ILE:HG22 | 1:P:747:LEU:HD12 | 0.81 | 0.80 |
| 4:2:64:ILE:HG21 | 4:Z:166:TYR:HE2 | 1.44 | 0.80 |
| 4:3:223:PHE:HE1 | 4:3:255:PHE:HB2 | 1.46 | 0.80 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:144:VAL:CA | 2:B:153:ILE:HD11 | 2.11 | 0.80 |
| 1:D:732:ILE:HG22 | 1:D:747:LEU:HD12 | 0.81 | 0.80 |
| 3:F:49:ILE:N | 3:F:52:ASN:ND2 | 2.29 | 0.80 |
| 1:G:218:LEU:HA | 1:G:221:GLN:HG2 | 1.62 | 0.80 |
| 1:J:534:SER:O | 4:W:351:THR:HG23 | 1.13 | 0.80 |
| 2:K:141:PRO:HB2 | 2:K:142:PRO:CD | 2.12 | 0.80 |
| 1:P:793:ARG:HD3 | 3:R:40:ASN:ND2 | 1.96 | 0.80 |
| 1:A:127:ASN:HD22 | 1:A:128:PRO:HD2 | 1.45 | 0.80 |
| 1:A:149:GLN:CB | 1:A:718:ALA:CB | 2.52 | 0.80 |
| 1:A:409:GLY:N | 1:A:636:LYS:CG | 2.44 | 0.80 |
| 3:C:49:ILE:N | 3:C:52:ASN:ND2 | 2.29 | 0.80 |
| 1:D:550:PHE:N | 4:W:46:GLY:HA3 | 1.97 | 0.80 |
| 1:D:819:ASN:HB2 | 2:E:90:GLY:O | 1.82 | 0.80 |
| 1:G:218:LEU:CA | 1:G:221:GLN:HG2 | 2.10 | 0.80 |
| 1:G:232:PHE:CZ | 1:G:287:ILE:HD13 | 2.16 | 0.80 |
| 1:G:795:ARG:NH2 | 3:I:116:GLU:CD | 2.30 | 0.80 |
| 1:J:510:TRP:CH2 | 1:J:772:LEU:HD11 | 2.16 | 0.80 |
| 1:P:831:TRP:HZ3 | 2:Q:34:ILE:HD13 | 1.44 | 0.80 |
| 2:Q:141:PRO:CB | 2:Q:142:PRO:HD2 | 2.12 | 0.80 |
| 3:R:49:ILE:N | 3:R:52:ASN:ND2 | 2.30 | 0.80 |
| 1:A:550:PHE:CA | 4:V:46:GLY:CA | 2.59 | 0.80 |
| 1:G:571:ALA:O | 1:G:572:LYS:CG | 2.28 | 0.80 |
| 1:G:641:LYS:HD2 | 1:G:647:GLN:OE1 | 1.81 | 0.80 |
| 1:G:732:ILE:CG2 | 1:G:747:LEU:HD13 | 1.34 | 0.80 |
| 1:G:732:ILE:HG22 | 1:G:747:LEU:HD12 | 0.81 | 0.80 |
| 2:H:141:PRO:CB | 2:H:142:PRO:HD2 | 2.12 | 0.80 |
| 1:J:28:GLN:OE1 | 1:J:723:ARG:CG | 2.29 | 0.80 |
| 1:J:374:GLN:HG3 | 1:J:375:ALA:N | 1.96 | 0.80 |
| 1:M:797:PHE:CE1 | 3:O:149:VAL:HG12 | 2.15 | 0.80 |
| 1:P:480:ILE:HG22 | 1:P:481:ASN:HD22 | 1.45 | 0.80 |
| 4:2:223:PHE:HE1 | 4:2:255:PHE:HB2 | 1.46 | 0.80 |
| 4:8:223:PHE:HE1 | 4:8:255:PHE:HB2 | 1.46 | 0.80 |
| 1:A:505:MLY:HG3 | 1:A:741:LYS:NZ | 1.96 | 0.80 |
| 1:A:837:MLY:HH22 | 2:H:21:GLU:H | 1.43 | 0.80 |
| 1:M:374:GLN:HG3 | 1:M:375:ALA:N | 1.96 | 0.80 |
| 1:P:725:ARG:CZ | 1:P:733:PRO:HB3 | 2.06 | 0.80 |
| 1:D:550:PHE:CA | 4:W:46:GLY:CA | 2.59 | 0.80 |
| 1:D:831:TRP:CD1 | 2:E:51:PHE:CZ | 2.68 | 0.80 |
| 1:G:834:LEU:CD1 | 2:H:51:PHE:CE1 | 2.64 | 0.80 |
| 2:H:117:LEU:HB2 | 2:H:147:ASN:HD21 | 1.47 | 0.80 |
| 1:M:599:ASN:CA | 1:M:649:VAL:CB | 2.53 | 0.80 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:818:TYR:CD1 | 2:N:127:ARG:NH1 | 2.50 | 0.80 |
| 1:P:93:MET:HG3 | 1:P:714:ARG:HG3 | 1.62 | 0.80 |
| 1:P:542:PHE:CA | 4:1:143:TYR:HE1 | 1.93 | 0.80 |
| 1:D:409:GLY:N | 1:D:636:LYS:CG | 2.45 | 0.79 |
| 3:I:49:ILE:N | 3:I:52:ASN:ND2 | 2.29 | 0.79 |
| 1:J:538:GLU:CA | 4:W:351:THR:H | 1.93 | 0.79 |
| 1:M:785:GLU:O | 1:M:786:ILE:N | 2.16 | 0.79 |
| 2:N:141:PRO:HB2 | 2:N:142:PRO:CD | 2.11 | 0.79 |
| 1:A:149:GLN:CG | 1:A:719:ASP:CG | 2.49 | 0.79 |
| 1:D:795:ARG:CG | 3:F:35:ARG:HH12 | 1.95 | 0.79 |
| 1:J:409:GLY:N | 1:J:636:LYS:CG | 2.44 | 0.79 |
| 1:J:817:GLN:HG3 | 2:K:128:PHE:CE1 | 2.17 | 0.79 |
| 2:K:141:PRO:CB | 2:K:142:PRO:HD2 | 2.12 | 0.79 |
| 1:M:291:ILE:HA | 1:M:331:LEU:HD11 | 1.64 | 0.79 |
| 3:O:49:ILE:N | 3:O:52:ASN:ND2 | 2.30 | 0.79 |
| 1:P:821:ARG:HH21 | 2:Q:127:ARG:HG2 | 0.98 | 0.79 |
| 1:D:550:PHE:HA | 4:W:46:GLY:HA2 | 1.64 | 0.79 |
| 1:D:641:LYS:HD2 | 1:D:647:GLN:OE1 | 1.81 | 0.79 |
| 2:E:121:LEU:CG | 2:E:128:PHE:CA | 2.48 | 0.79 |
| 1:G:409:GLY:N | 1:G:636:LYS:CG | 2.44 | 0.79 |
| 1:J:291:ILE:HA | 1:J:331:LEU:HD11 | 1.64 | 0.79 |
| 2:K:117:LEU:HB2 | 2:K:147:ASN:HD21 | 1.47 | 0.79 |
| 2:N:144:VAL:CA | 2:N:153:ILE:HD11 | 2.11 | 0.79 |
| 1:A:721:LYS:CA | 1:A:736:GLN:NE2 | 2.43 | 0.79 |
| 1:D:646:PHE:CE2 | 1:D:652:LEU:HD21 | 2.15 | 0.79 |
| 1:G:795:ARG:NE | 3:I:116:GLU:OE2 | 2.14 | 0.79 |
| 1:J:646:PHE:CE2 | 1:J:652:LEU:HD21 | 2.15 | 0.79 |
| 1:P:374:GLN:HG3 | 1:P:375:ALA:N | 1.96 | 0.79 |
| 2:Q:144:VAL:CA | 2:Q:153:ILE:HD11 | 2.11 | 0.79 |
| 4:2:203:THR:H | 4:Z:287:ILE:CG2 | 1.94 | 0.79 |
| 2:E:141:PRO:CB | 2:E:142:PRO:HD2 | 2.12 | 0.79 |
| 1:G:374:GLN:HG3 | 1:G:375:ALA:N | 1.96 | 0.79 |
| 1:J:818:TYR:CD1 | 2:K:127:ARG:NH1 | 2.50 | 0.79 |
| 1:M:795:ARG:HB3 | 3:O:35:ARG:NH1 | 1.92 | 0.79 |
| 1:P:407:GLY:HA2 | 1:P:412:ALA:HA | 1.65 | 0.79 |
| 1:P:529:PRO:C | 4:1:354:GLN:CB | 2.49 | 0.79 |
| 4:2:324:THR:CG2 | 4:4:244:ASP:CA | 2.59 | 0.79 |
| 1:A:819:ASN:CG | 2:B:92:ASP:H | 1.83 | 0.79 |
| 2:B:141:PRO:CB | 2:B:142:PRO:HD2 | 2.12 | 0.79 |
| 2:B:144:VAL:HG12 | 2:B:153:ILE:CD1 | 2.09 | 0.79 |
| 1:D:642:LYS:HG2 | 4:9:22:ALA:HA | 1.65 | 0.79 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:721:LYS:HG2 | 1:D:736:GLN:CD | 1.86 | 0.79 |
| 1:D:721:LYS:CA | 1:D:736:GLN:NE2 | 2.43 | 0.79 |
| 1:D:724:TYR:CD1 | 1:D:782:MLY:HD3 | 2.17 | 0.79 |
| 1:M:769:ALA:C | 1:M:770:GLY:CA | 2.51 | 0.79 |
| 1:M:806:MET:CA | 1:M:807:VAL:N | 2.46 | 0.79 |
| 4:9:223:PHE:HE1 | 4:9:255:PHE:HB2 | 1.46 | 0.79 |
| 1:G:641:LYS:CE | 1:G:647:GLN:HB2 | 2.13 | 0.79 |
| 3:L:50:LEU:C | 3:L:53:PRO:HD2 | 2.03 | 0.79 |
| 1:M:407:GLY:HA2 | 1:M:412:ALA:HA | 1.65 | 0.79 |
| 1:M:409:GLY:N | 1:M:636:LYS:CG | 2.44 | 0.79 |
| 4:1:166:TYR:HE2 | 4:3:64:ILE:HG21 | 1.42 | 0.79 |
| 4:Y:223:PHE:HE1 | 4:Y:255:PHE:HB2 | 1.46 | 0.79 |
| 2:B:141:PRO:HB2 | 2:B:142:PRO:CD | 2.12 | 0.79 |
| 3:C:50:LEU:C | 3:C:53:PRO:HD2 | 2.03 | 0.79 |
| 1:D:174:SER:CB | 1:D:667:THR:HG21 | 2.13 | 0.79 |
| 1:D:291:ILE:HA | 1:D:331:LEU:HD11 | 1.64 | 0.79 |
| 1:J:218:LEU:CA | 1:J:221:GLN:HG2 | 2.10 | 0.79 |
| 1:J:732:ILE:HG21 | 1:J:747:LEU:HD13 | 0.91 | 0.79 |
| 1:J:756:THR:O | 1:J:776:GLU:OE1 | 2.01 | 0.79 |
| 1:M:641:LYS:CE | 1:M:647:GLN:HB2 | 2.13 | 0.79 |
| 1:M:817:GLN:HG2 | 2:N:127:ARG:CD | 2.11 | 0.79 |
| 1:P:409:GLY:N | 1:P:636:LYS:CG | 2.44 | 0.79 |
| 1:P:642:LYS:HG2 | 4:1:22:ALA:HA | 1.65 | 0.79 |
| 4:1:287:ILE:CG2 | 4:3:203:THR:H | 1.96 | 0.79 |
| 4:7:223:PHE:HE1 | 4:7:255:PHE:HB2 | 1.46 | 0.79 |
| 4:V:223:PHE:HE1 | 4:V:255:PHE:HB2 | 1.46 | 0.79 |
| 1:D:537:GLU:O | 4:9:350:SER:N | 2.16 | 0.79 |
| 1:D:538:GLU:HG3 | 4:9:351:THR:C | 2.03 | 0.79 |
| 2:E:162:ASP:O | 2:K:21:GLU:CB | 2.31 | 0.79 |
| 1:G:817:GLN:CD | 2:H:127:ARG:CD | 2.49 | 0.79 |
| 3:I:50:LEU:C | 3:I:53:PRO:HD2 | 2.03 | 0.79 |
| 1:J:174:SER:CB | 1:J:667:THR:HG21 | 2.13 | 0.79 |
| 1:J:537:GLU:O | 4:W:350:SER:N | 2.16 | 0.79 |
| 1:J:538:GLU:HG3 | 4:W:351:THR:C | 2.03 | 0.79 |
| 1:J:820:VAL:CG1 | 2:K:136:MET:HE1 | 2.12 | 0.79 |
| 1:M:735:GLY:C | 1:M:743:ALA:HB1 | 1.84 | 0.79 |
| 1:M:797:PHE:CE2 | 3:O:126:LEU:CD2 | 2.62 | 0.79 |
| 1:P:291:ILE:HA | 1:P:331:LEU:HD11 | 1.64 | 0.79 |
| 1:P:751:GLY:HA2 | 1:P:779:ARG:NH2 | 1.98 | 0.79 |
| 4:2:288:ASP:N | 4:4:203:THR:CG2 | 2.45 | 0.79 |
| 1:A:641:LYS:CE | 1:A:647:GLN:HB2 | 2.13 | 0.79 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:641:LYS:HD2 | 1:A:647:GLN:OE1 | 1.81 | 0.79 |
| 1:G:538:GLU:HG3 | 4:V:351:THR:C | 2.02 | 0.79 |
| 1:G:754:ASP:O | 1:G:776:GLU:OE1 | 1.99 | 0.79 |
| 2:H:144:VAL:HG12 | 2:H:153:ILE:CD1 | 2.09 | 0.79 |
| 1:J:578:HIS:HD2 | 1:J:591:ASN:HA | 1.45 | 0.79 |
| 1:M:537:GLU:O | 4:Z:350:SER:N | 2.16 | 0.79 |
| 1:P:817:GLN:HG2 | 2:Q:127:ARG:CD | 2.11 | 0.79 |
| 4:1:201:VAL:H | 4:Y:287:ILE:HG12 | 1.42 | 0.79 |
| 1:A:149:GLN:NE2 | 1:A:718:ALA:HB2 | 1.94 | 0.78 |
| 1:A:556:ASP:HA | 4:V:49:GLN:O | 1.70 | 0.78 |
| 1:D:542:PHE:CA | 4:9:143:TYR:HE1 | 1.92 | 0.78 |
| 2:E:144:VAL:HG12 | 2:E:153:ILE:CD1 | 2.10 | 0.78 |
| 1:G:530:MET:HE2 | 4:V:354:GLN:HG3 | 1.65 | 0.78 |
| 1:G:769:ALA:HB2 | 1:G:770:GLY:N | 1.97 | 0.78 |
| 1:G:791:GLN:HE22 | 3:I:115:GLY:HA2 | 1.48 | 0.78 |
| 1:J:599:ASN:CA | 1:J:649:VAL:CB | 2.53 | 0.78 |
| 1:M:795:ARG:HH22 | 3:O:116:GLU:CG | 1.95 | 0.78 |
| 1:A:291:ILE:HA | 1:A:331:LEU:HD11 | 1.64 | 0.78 |
| 1:A:374:GLN:HG3 | 1:A:375:ALA:N | 1.96 | 0.78 |
| 1:G:503:TYR:HE1 | 1:G:711:PHE:CD2 | 2.00 | 0.78 |
| 1:M:481:ASN:HD22 | 1:M:481:ASN:N | 1.82 | 0.78 |
| 1:P:537:GLU:O | 4:1:350:SER:N | 2.16 | 0.78 |
| 1:A:174:SER:CB | 1:A:667:THR:HG21 | 2.13 | 0.78 |
| 1:D:725:ARG:C | 1:D:782:MLY:CH2 | 2.52 | 0.78 |
| 1:D:795:ARG:HD2 | 3:F:35:ARG:HH12 | 1.48 | 0.78 |
| 1:G:407:GLY:HA2 | 1:G:412:ALA:HA | 1.65 | 0.78 |
| 1:G:708:ARG:HA | 1:G:712:PRO:CG | 2.13 | 0.78 |
| 1:G:757:GLN:CB | 1:G:776:GLU:CG | 2.60 | 0.78 |
| 1:J:84:MLY:CH1 | 1:J:720:PHE:HD1 | 1.88 | 0.78 |
| 1:J:407:GLY:HA2 | 1:J:412:ALA:HA | 1.65 | 0.78 |
| 2:K:144:VAL:HG12 | 2:K:153:ILE:CD1 | 2.10 | 0.78 |
| 1:M:805:ALA:C | 1:M:807:VAL:N | 2.37 | 0.78 |
| 1:P:538:GLU:HG3 | 4:1:351:THR:C | 2.03 | 0.78 |
| 3:F:50:LEU:C | 3:F:53:PRO:HD2 | 2.03 | 0.78 |
| 1:G:481:ASN:HD22 | 1:G:481:ASN:N | 1.82 | 0.78 |
| 1:M:542:PHE:HA | 4:Z:143:TYR:HE1 | 1.34 | 0.78 |
| 1:M:639:GLY:CA | 4:Z:345:ILE:N | 2.47 | 0.78 |
| 3:O:50:LEU:C | 3:O:53:PRO:HD2 | 2.03 | 0.78 |
| 1:P:641:LYS:CE | 1:P:647:GLN:HB2 | 2.13 | 0.78 |
| 1:P:821:ARG:NH2 | 2:Q:127:ARG:CD | 2.46 | 0.78 |
| 4:2:287:ILE:CB | 4:4:203:THR:HG22 | 2.14 | 0.78 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:9:287:ILE:HB | 4:W:204:ALA:N | 1.97 | 0.78 |
| 1:A:149:GLN:HA | 1:A:719:ASP:OD1 | 1.84 | 0.78 |
| 1:A:537:GLU:O | 4:8:350:SER:N | 2.16 | 0.78 |
| 1:A:550:PHE:N | 4:V:46:GLY:HA3 | 1.97 | 0.78 |
| 1:D:599:ASN:CA | 1:D:649:VAL:CB | 2.53 | 0.78 |
| 1:D:727:LEU:HD11 | 1:D:782:MLY:HG2 | 1.63 | 0.78 |
| 1:G:830:PRO:CB | 2:H:67:MET:CE | 2.61 | 0.78 |
| 1:J:756:THR:HG22 | 1:J:776:GLU:OE1 | 1.82 | 0.78 |
| 1:M:709:LYS:C | 1:M:710:GLY:CA | 2.51 | 0.78 |
| 1:P:95:THR:OG1 | 1:P:769:ALA:HA | 1.84 | 0.78 |
| 1:P:800:ARG:HB3 | 3:R:149:VAL:HG22 | 1.66 | 0.78 |
| 4:2:202:THR:HG21 | 4:Z:290:ARG:NH2 | 1.75 | 0.78 |
| 1:D:219:GLU:O | 1:D:223:ILE:HG13 | 1.84 | 0.78 |
| 1:G:291:ILE:HA | 1:G:331:LEU:HD11 | 1.64 | 0.78 |
| 1:G:639:GLY:CA | 4:V:345:ILE:N | 2.47 | 0.78 |
| 1:G:757:GLN:CB | 1:G:776:GLU:HG2 | 2.11 | 0.78 |
| 1:G:797:PHE:HE2 | 3:I:126:LEU:HD22 | 1.46 | 0.78 |
| 1:J:51:THR:O | 1:J:62:VAL:HG13 | 1.84 | 0.78 |
| 1:M:51:THR:O | 1:M:62:VAL:HG13 | 1.84 | 0.78 |
| 4:V:287:ILE:HD11 | 4:X:201:VAL:O | 1.76 | 0.78 |
| 1:G:755:HIS:N | 1:G:779:ARG:NH1 | 2.32 | 0.78 |
| 1:M:410:ASN:CG | 4:Z:334:GLU:CA | 2.47 | 0.78 |
| 1:M:817:GLN:HB3 | 2:N:127:ARG:HD2 | 1.63 | 0.78 |
| 4:1:112:PRO:CB | 4:2:195:GLU:O | 2.32 | 0.78 |
| 1:A:505:MLY:HB3 | 1:A:762:HIS:N | 1.99 | 0.78 |
| 3:C:3:SER:O | 3:C:4:LYS:HB2 | 1.84 | 0.78 |
| 1:D:51:THR:O | 1:D:62:VAL:HG13 | 1.84 | 0.78 |
| 1:D:407:GLY:HA2 | 1:D:412:ALA:HA | 1.65 | 0.78 |
| 1:D:635:GLY:HA3 | 4:9:341:ILE:CD1 | 2.14 | 0.78 |
| 1:D:639:GLY:CA | 4:9:345:ILE:N | 2.47 | 0.78 |
| 1:D:727:LEU:N | 1:D:782:MLY:CE | 2.47 | 0.78 |
| 1:G:51:THR:O | 1:G:62:VAL:HG13 | 1.84 | 0.78 |
| 1:G:721:LYS:HG2 | 1:G:736:GLN:CD | 1.86 | 0.78 |
| 1:J:635:GLY:HA3 | 4:W:341:ILE:CD1 | 2.14 | 0.78 |
| 1:J:646:PHE:HE2 | 1:J:652:LEU:CD2 | 1.97 | 0.78 |
| 1:J:725:ARG:CZ | 1:J:733:PRO:HB3 | 2.06 | 0.78 |
| 1:P:51:THR:O | 1:P:62:VAL:HG13 | 1.84 | 0.78 |
| 1:P:174:SER:CB | 1:P:667:THR:HG21 | 2.13 | 0.78 |
| 1:P:721:LYS:CA | 1:P:736:GLN:NE2 | 2.43 | 0.78 |
| 1:A:51:THR:O | 1:A:62:VAL:HG13 | 1.84 | 0.78 |
| 1:D:537:GLU:HG3 | 4:9:350:SER:O | 1.79 | 0.78 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:496:PHE:CD2 | 1:G:514:ASP:HA | 2.19 | 0.78 |
| 1:M:95:THR:OG1 | 1:M:770:GLY:HA2 | 1.82 | 0.78 |
| 1:P:818:TYR:CE1 | 2:Q:127:ARG:HH22 | 1.36 | 0.78 |
| 1:P:819:ASN:OD1 | 2:Q:92:ASP:CA | 2.31 | 0.78 |
| 4:2:324:THR:CB | 4:4:244:ASP:HA | 2.14 | 0.78 |
| 1:G:410:ASN:CG | 4:V:334:GLU:CA | 2.47 | 0.78 |
| 1:J:733:PRO:C | 1:J:737:PHE:HD1 | 1.88 | 0.78 |
| 1:M:816:ILE:HD11 | 2:N:100:ALA:HB1 | 1.65 | 0.78 |
| 1:P:496:PHE:CD2 | 1:P:514:ASP:HA | 2.19 | 0.78 |
| 4:2:203:THR:H | 4:Z:287:ILE:HG21 | 1.47 | 0.78 |
| 1:A:97:LEU:HD22 | 1:A:712:PRO:CB | 2.13 | 0.77 |
| 1:A:641:LYS:CE | 1:A:647:GLN:CG | 2.60 | 0.77 |
| 1:D:496:PHE:CD2 | 1:D:514:ASP:HA | 2.19 | 0.77 |
| 1:D:800:ARG:O | 3:F:149:VAL:CG2 | 2.32 | 0.77 |
| 1:G:505:MLY:CD | 1:G:762:HIS:NE2 | 2.47 | 0.77 |
| 1:G:707:CYS:SG | 1:G:714:ARG:NH1 | 2.57 | 0.77 |
| 1:J:642:LYS:HG2 | 4:W:22:ALA:HA | 1.65 | 0.77 |
| 1:J:756:THR:CG2 | 1:J:776:GLU:HB3 | 2.11 | 0.77 |
| 1:M:538:GLU:HG3 | 4:Z:351:THR:C | 2.03 | 0.77 |
| 1:M:783:LEU:CD1 | 1:M:786:ILE:HD11 | 2.14 | 0.77 |
| 1:M:798:LEU:HD21 | 3:O:126:LEU:HD11 | 1.66 | 0.77 |
| 4:7:287:ILE:HB | 4:9:204:ALA:N | 1.98 | 0.77 |
| 1:A:496:PHE:CD2 | 1:A:514:ASP:HA | 2.19 | 0.77 |
| 1:D:218:LEU:CA | 1:D:221:GLN:HG2 | 2.10 | 0.77 |
| 1:D:724:TYR:HD1 | 1:D:782:MLY:HD3 | 1.47 | 0.77 |
| 1:G:219:GLU:O | 1:G:223:ILE:HG13 | 1.84 | 0.77 |
| 1:G:641:LYS:CE | 1:G:647:GLN:CG | 2.61 | 0.77 |
| 3:I:3:SER:O | 3:I:4:LYS:HB2 | 1.84 | 0.77 |
| 1:M:174:SER:CB | 1:M:667:THR:HG21 | 2.13 | 0.77 |
| 1:M:496:PHE:CD2 | 1:M:514:ASP:HA | 2.19 | 0.77 |
| 2:Q:111:SER:OG | 2:Q:148:VAL:C | 2.15 | 0.77 |
| 4:8:287:ILE:HB | 4:V:204:ALA:N | 1.97 | 0.77 |
| 1:A:646:PHE:HE2 | 1:A:652:LEU:CD2 | 1.97 | 0.77 |
| 1:A:732:ILE:HG21 | 1:A:747:LEU:HD13 | 0.91 | 0.77 |
| 1:A:800:ARG:C | 3:C:149:VAL:HG21 | 2.04 | 0.77 |
| 1:D:727:LEU:CG | 1:D:782:MLY:CG | 2.63 | 0.77 |
| 1:G:537:GLU:O | 4:V:350:SER:N | 2.16 | 0.77 |
| 1:J:219:GLU:O | 1:J:223:ILE:HG13 | 1.84 | 0.77 |
| 1:M:641:LYS:HD2 | 1:M:647:GLN:OE1 | 1.81 | 0.77 |
| 1:M:797:PHE:CZ | 3:O:146:ILE:CD1 | 2.66 | 0.77 |
| 1:P:817:GLN:CB | 2:Q:127:ARG:CD | 2.61 | 0.77 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:R:50:LEU:C | 3:R:53:PRO:HD2 | 2.03 | 0.77 |
| 4:4:322:PRO:HB3 | 4:6:244:ASP:CB | 2.10 | 0.77 |
| 2:B:111:SER:OG | 2:B:148:VAL:C | 2.15 | 0.77 |
| 1:D:410:ASN:CG | 4:9:334:GLU:CA | 2.48 | 0.77 |
| 1:J:496:PHE:CD2 | 1:J:514:ASP:HA | 2.19 | 0.77 |
| 1:J:557:GLU:CA | 4:Y:47:MET:CA | 1.90 | 0.77 |
| 1:J:792:ALA:CA | 3:L:42:THR:HA | 2.10 | 0.77 |
| 1:M:635:GLY:HA3 | 4:Z:341:ILE:CD1 | 2.14 | 0.77 |
| 1:M:803:TYR:CD2 | 3:O:17:PHE:HZ | 2.01 | 0.77 |
| 1:P:732:ILE:HG23 | 1:P:747:LEU:CB | 1.84 | 0.77 |
| 4:X:223:PHE:HD2 | 4:X:312:ARG:HH21 | 1.33 | 0.77 |
| 1:A:550:PHE:HA | 4:V:46:GLY:HA2 | 1.65 | 0.77 |
| 3:C:49:ILE:N | 3:C:52:ASN:HD22 | 1.82 | 0.77 |
| 1:D:795:ARG:HB3 | 3:F:35:ARG:HH12 | 1.15 | 0.77 |
| 2:E:141:PRO:HB2 | 2:E:142:PRO:CD | 2.12 | 0.77 |
| 1:J:116:TYR:O | 1:J:153:PRO:HB2 | 1.85 | 0.77 |
| 1:J:529:PRO:C | 4:W:354:GLN:CB | 2.49 | 0.77 |
| 1:M:725:ARG:HG3 | 1:M:733:PRO:HA | 1.67 | 0.77 |
| 3:O:3:SER:O | 3:O:4:LYS:HB2 | 1.85 | 0.77 |
| 1:P:836:PHE:CE1 | 2:Q:160:GLY:N | 2.44 | 0.77 |
| 4:7:223:PHE:HD2 | 4:7:312:ARG:HH21 | 1.32 | 0.77 |
| 1:A:797:PHE:CE2 | 3:C:126:LEU:HD22 | 2.12 | 0.77 |
| 1:D:529:PRO:C | 4:9:354:GLN:CB | 2.49 | 0.77 |
| 1:D:727:LEU:HG | 1:D:782:MLY:CG | 2.13 | 0.77 |
| 1:D:747:LEU:CD1 | 1:D:782:MLY:HH21 | 2.13 | 0.77 |
| 1:M:544:LYS:HB3 | 4:2:45:VAL:HG22 | 1.64 | 0.77 |
| 1:M:817:GLN:HG2 | 2:N:127:ARG:CB | 2.14 | 0.77 |
| 1:P:646:PHE:HE2 | 1:P:652:LEU:CD2 | 1.97 | 0.77 |
| 1:P:733:PRO:C | 1:P:737:PHE:HD1 | 1.88 | 0.77 |
| 1:P:817:GLN:HB3 | 2:Q:127:ARG:NH1 | 1.98 | 0.77 |
| 4:2:287:ILE:HG21 | 4:4:202:THR:C | 2.05 | 0.77 |
| 4:4:288:ASP:N | 4:6:203:THR:CG2 | 2.46 | 0.77 |
| 4:9:223:PHE:HD2 | 4:9:312:ARG:HH21 | 1.32 | 0.77 |
| 1:A:538:GLU:HG3 | 4:8:351:THR:C | 2.03 | 0.77 |
| 1:A:639:GLY:CA | 4:8:345:ILE:N | 2.47 | 0.77 |
| 1:A:818:TYR:CB | 2:B:90:GLY:CA | 2.55 | 0.77 |
| 1:D:218:LEU:HB3 | 1:D:221:GLN:HG3 | 1.60 | 0.77 |
| 2:E:121:LEU:CG | 2:E:128:PHE:HA | 2.14 | 0.77 |
| 3:F:3:SER:O | 3:F:4:LYS:HB2 | 1.84 | 0.77 |
| 1:J:84:MLY:O | 1:J:723:ARG:HD2 | 1.84 | 0.77 |
| 1:M:641:LYS:CE | 1:M:647:GLN:CG | 2.60 | 0.77 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:817:GLN:CB | 2:N:127:ARG:HH11 | 1.95 | 0.77 |
| 4:1:203:THR:N | 4:Y:286:ASP:OD1 | 2.17 | 0.77 |
| 4:1:244:ASP:OD2 | 4:Y:325:MET:CE | 2.32 | 0.77 |
| 1:A:219:GLU:O | 1:A:223:ILE:HG13 | 1.84 | 0.77 |
| 1:D:641:LYS:CE | 1:D:647:GLN:HB2 | 2.13 | 0.77 |
| 1:G:505:MLY:CE | 1:G:762:HIS:CE1 | 2.65 | 0.77 |
| 1:G:629:GLU:HA | 1:G:643:GLY:C | 2.05 | 0.77 |
| 3:R:49:ILE:N | 3:R:52:ASN:HD22 | 1.82 | 0.77 |
| 4:4:223:PHE:HD2 | 4:4:312:ARG:HH21 | 1.33 | 0.77 |
| 1:A:534:SER:O | 4:8:351:THR:N | 2.18 | 0.77 |
| 1:A:629:GLU:HA | 1:A:643:GLY:C | 2.05 | 0.77 |
| 1:G:93:MET:CE | 1:G:764:MLY:CD | 2.63 | 0.77 |
| 1:G:506:GLU:OE2 | 1:G:760:PHE:O | 2.03 | 0.77 |
| 1:J:83:PRO:O | 1:J:723:ARG:NH2 | 2.18 | 0.77 |
| 1:J:218:LEU:HD22 | 1:J:222:ILE:HG12 | 1.67 | 0.77 |
| 3:L:49:ILE:N | 3:L:52:ASN:HD22 | 1.82 | 0.77 |
| 1:M:95:THR:HG1 | 1:M:770:GLY:N | 1.76 | 0.77 |
| 1:M:642:LYS:HG2 | 4:Z:22:ALA:HA | 1.65 | 0.77 |
| 1:M:831:TRP:HZ3 | 2:N:34:ILE:HD13 | 1.50 | 0.77 |
| 4:4:288:ASP:H | 4:6:203:THR:CG2 | 1.98 | 0.77 |
| 4:5:223:PHE:HD2 | 4:5:312:ARG:HH21 | 1.33 | 0.77 |
| 4:6:223:PHE:HD2 | 4:6:312:ARG:HH21 | 1.33 | 0.77 |
| 4:V:223:PHE:HD2 | 4:V:312:ARG:HH21 | 1.33 | 0.77 |
| 4:Z:223:PHE:HD2 | 4:Z:312:ARG:HH21 | 1.33 | 0.77 |
| 1:A:795:ARG:HH22 | 3:C:116:GLU:CD | 1.88 | 0.77 |
| 1:D:94:MET:CE | 1:D:101:ALA:HB1 | 2.15 | 0.77 |
| 3:F:49:ILE:N | 3:F:52:ASN:HD22 | 1.82 | 0.77 |
| 1:G:116:TYR:O | 1:G:153:PRO:HB2 | 1.85 | 0.77 |
| 1:G:174:SER:CB | 1:G:667:THR:HG21 | 2.13 | 0.77 |
| 1:G:642:LYS:HG2 | 4:V:22:ALA:HA | 1.65 | 0.77 |
| 1:G:646:PHE:HE2 | 1:G:652:LEU:CD2 | 1.97 | 0.77 |
| 1:J:796:GLY:N | 3:L:35:ARG:CZ | 2.48 | 0.77 |
| 1:M:623:PHE:CG | 1:M:623:PHE:CA | 2.68 | 0.77 |
| 1:M:646:PHE:HE2 | 1:M:652:LEU:CD2 | 1.97 | 0.77 |
| 1:M:795:ARG:HD2 | 3:O:35:ARG:HH12 | 1.49 | 0.77 |
| 1:P:94:MET:CE | 1:P:101:ALA:HB1 | 2.15 | 0.77 |
| 1:P:795:ARG:CB | 3:R:35:ARG:HH12 | 1.95 | 0.77 |
| 4:2:287:ILE:HG13 | 4:4:202:THR:HA | 1.64 | 0.77 |
| 4:8:223:PHE:HD2 | 4:8:312:ARG:HH21 | 1.33 | 0.77 |
| 4:W:223:PHE:HD2 | 4:W:312:ARG:HH21 | 1.32 | 0.77 |
| 1:D:556:ASP:HA | 4:W:49:GLN:O | 1.70 | 0.76 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:642:LYS:CG | 4:9:23:GLY:H | 1.77 | 0.76 |
| 1:D:725:ARG:HG3 | 1:D:733:PRO:HA | 1.68 | 0.76 |
| 1:G:817:GLN:CD | 2:H:127:ARG:HB2 | 2.06 | 0.76 |
| 1:J:795:ARG:NE | 3:L:116:GLU:CD | 2.38 | 0.76 |
| 1:M:629:GLU:HA | 1:M:643:GLY:C | 2.05 | 0.76 |
| 1:P:664:LEU:O | 1:P:667:THR:HB | 1.86 | 0.76 |
| 4:2:288:ASP:OD1 | 4:4:203:THR:HG23 | 1.84 | 0.76 |
| 4:2:324:THR:HG23 | 4:4:244:ASP:CA | 2.14 | 0.76 |
| 4:X:287:ILE:CD1 | 4:Z:205:GLU:HG3 | 2.15 | 0.76 |
| 1:D:646:PHE:HE2 | 1:D:652:LEU:CD2 | 1.97 | 0.76 |
| 1:G:797:PHE:HE2 | 3:I:126:LEU:HD13 | 1.49 | 0.76 |
| 1:J:94:MET:CE | 1:J:101:ALA:HB1 | 2.15 | 0.76 |
| 1:J:639:GLY:CA | 4:W:345:ILE:N | 2.46 | 0.76 |
| 3:L:3:SER:O | 3:L:4:LYS:HB2 | 1.85 | 0.76 |
| 1:M:732:ILE:N | 1:M:733:PRO:HD2 | 2.00 | 0.76 |
| 1:M:793:ARG:HH11 | 3:O:40:ASN:HD22 | 0.80 | 0.76 |
| 2:N:117:LEU:HB2 | 2:N:147:ASN:HD21 | 1.47 | 0.76 |
| 2:N:121:LEU:CG | 2:N:128:PHE:HA | 2.14 | 0.76 |
| 1:P:639:GLY:CA | 4:1:345:ILE:N | 2.47 | 0.76 |
| 4:2:223:PHE:HD2 | 4:2:312:ARG:HH21 | 1.33 | 0.76 |
| 1:A:407:GLY:HA2 | 1:A:412:ALA:HA | 1.65 | 0.76 |
| 1:A:721:LYS:CA | 1:A:736:GLN:OE1 | 2.33 | 0.76 |
| 1:A:818:TYR:CB | 2:B:90:GLY:N | 2.48 | 0.76 |
| 1:D:732:ILE:N | 1:D:733:PRO:HD2 | 2.00 | 0.76 |
| 1:G:94:MET:CE | 1:G:101:ALA:HB1 | 2.15 | 0.76 |
| 1:J:829:TRP:CE3 | 2:K:87:LYS:NZ | 2.54 | 0.76 |
| 1:J:836:PHE:CE2 | 2:K:160:GLY:N | 2.49 | 0.76 |
| 1:P:641:LYS:HD2 | 4:1:348:SER:HB2 | 1.54 | 0.76 |
| 1:P:769:ALA:O | 1:P:771:LEU:CA | 2.33 | 0.76 |
| 4:Y:223:PHE:HD2 | 4:Y:312:ARG:HH21 | 1.33 | 0.76 |
| 1:A:529:PRO:C | 4:8:354:GLN:CB | 2.49 | 0.76 |
| 1:A:623:PHE:CG | 1:A:623:PHE:CA | 2.68 | 0.76 |
| 1:A:800:ARG:O | 3:C:149:VAL:CG2 | 2.33 | 0.76 |
| 1:G:755:HIS:CG | 1:G:779:ARG:HH12 | 2.02 | 0.76 |
| 1:J:732:ILE:N | 1:J:733:PRO:HD2 | 2.01 | 0.76 |
| 1:J:834:LEU:HD12 | 2:K:51:PHE:HE1 | 1.49 | 0.76 |
| 1:M:642:LYS:CG | 4:Z:23:GLY:H | 1.77 | 0.76 |
| 1:M:797:PHE:CE1 | 3:O:149:VAL:HG11 | 2.20 | 0.76 |
| 3:O:49:ILE:N | 3:O:52:ASN:HD22 | 1.83 | 0.76 |
| 1:P:732:ILE:N | 1:P:733:PRO:HD2 | 2.00 | 0.76 |
| 1:A:732:ILE:N | 1:A:733:PRO:HD2 | 2.00 | 0.76 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:553:MLY:NZ | 4:W:45:VAL:HA | 1.84 | 0.76 |
| 2:E:117:LEU:HB2 | 2:E:147:ASN:HD21 | 1.47 | 0.76 |
| 1:J:789:ALA:CB | 3:L:81:GLN:CD | 2.53 | 0.76 |
| 1:J:798:LEU:HD11 | 3:L:126:LEU:HD11 | 0.78 | 0.76 |
| 1:J:821:ARG:HH21 | 2:K:127:ARG:HG2 | 1.51 | 0.76 |
| 1:M:94:MET:CE | 1:M:101:ALA:HB1 | 2.16 | 0.76 |
| 4:V:325:MET:CE | 4:X:244:ASP:OD2 | 2.34 | 0.76 |
| 1:A:97:LEU:HD22 | 1:A:712:PRO:HB3 | 1.66 | 0.76 |
| 1:A:116:TYR:O | 1:A:153:PRO:HB2 | 1.85 | 0.76 |
| 1:A:481:ASN:HD22 | 1:A:481:ASN:N | 1.82 | 0.76 |
| 1:A:664:LEU:O | 1:A:667:THR:HB | 1.86 | 0.76 |
| 1:D:623:PHE:CG | 1:D:623:PHE:CA | 2.68 | 0.76 |
| 1:D:831:TRP:CE2 | 2:E:47:LEU:CD2 | 2.55 | 0.76 |
| 1:G:635:GLY:HA3 | 4:V:341:ILE:CD1 | 2.14 | 0.76 |
| 1:G:732:ILE:N | 1:G:733:PRO:HD2 | 2.00 | 0.76 |
| 1:G:733:PRO:C | 1:G:737:PHE:HD1 | 1.88 | 0.76 |
| 1:G:831:TRP:HH2 | 2:H:47:LEU:HD21 | 0.94 | 0.76 |
| 1:J:530:MET:HE2 | 4:W:354:GLN:HG3 | 1.68 | 0.76 |
| 1:J:641:LYS:CE | 1:J:647:GLN:HB2 | 2.13 | 0.76 |
| 1:J:725:ARG:HG3 | 1:J:733:PRO:HA | 1.67 | 0.76 |
| 1:J:793:ARG:NH1 | 3:L:40:ASN:ND2 | 2.33 | 0.76 |
| 1:P:219:GLU:O | 1:P:223:ILE:HG13 | 1.84 | 0.76 |
| 1:P:623:PHE:CG | 1:P:623:PHE:CA | 2.68 | 0.76 |
| 1:P:641:LYS:CE | 1:P:647:GLN:CG | 2.60 | 0.76 |
| 1:P:783:LEU:HA | 1:P:786:ILE:HD11 | 1.61 | 0.76 |
| 4:3:223:PHE:HD2 | 4:3:312:ARG:HH21 | 1.33 | 0.76 |
| 4:3:288:ASP:H | 4:5:203:THR:CG2 | 1.98 | 0.76 |
| 1:A:642:LYS:HG2 | 4:8:22:ALA:HA | 1.66 | 0.76 |
| 1:A:646:PHE:CE2 | 1:A:652:LEU:HD21 | 2.15 | 0.76 |
| 1:D:735:GLY:C | 1:D:743:ALA:HB2 | 1.82 | 0.76 |
| 1:G:28:GLN:HB3 | 1:G:723:ARG:NH2 | 1.99 | 0.76 |
| 1:J:149:GLN:HG2 | 1:J:716:LEU:HD11 | 1.66 | 0.76 |
| 1:J:641:LYS:CE | 1:J:647:GLN:CG | 2.61 | 0.76 |
| 1:M:537:GLU:HG3 | 4:Z:350:SER:O | 1.78 | 0.76 |
| 1:M:709:LYS:CA | 1:M:710:GLY:N | 2.49 | 0.76 |
| 1:P:116:TYR:O | 1:P:153:PRO:HB2 | 1.85 | 0.76 |
| 1:P:629:GLU:HA | 1:P:643:GLY:C | 2.05 | 0.76 |
| 1:P:649:VAL:CG1 | 1:P:649:VAL:CB | 2.64 | 0.76 |
| 4:3:322:PRO:HB2 | 4:5:244:ASP:HB2 | 1.65 | 0.76 |
| 4:8:290:ARG:NH1 | 4:V:202:THR:CG2 | 2.49 | 0.76 |
| 1:A:218:LEU:HD22 | 1:A:222:ILE:HG12 | 1.67 | 0.76 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:635:GLY:HA3 | 4:8:341:ILE:CD1 | 2.14 | 0.76 |
| 1:A:733:PRO:C | 1:A:737:PHE:HD1 | 1.88 | 0.76 |
| 1:D:116:TYR:O | 1:D:153:PRO:HB2 | 1.85 | 0.76 |
| 1:D:534:SER:O | 4:9:351:THR:N | 2.19 | 0.76 |
| 1:D:727:LEU:N | 1:D:782:MLY:HE2 | 2.00 | 0.76 |
| 1:G:166:MET:HE1 | 1:G:254:PHE:HB2 | 1.67 | 0.76 |
| 1:G:817:GLN:CG | 2:H:127:ARG:HD2 | 2.16 | 0.76 |
| 1:J:534:SER:O | 4:W:351:THR:N | 2.19 | 0.76 |
| 1:P:218:LEU:HD22 | 1:P:222:ILE:HG12 | 1.67 | 0.76 |
| 1:P:549:SER:HA | 4:3:43:VAL:CG1 | 2.15 | 0.76 |
| 1:P:803:TYR:O | 1:P:807:VAL:N | 2.18 | 0.76 |
| 4:1:223:PHE:HD2 | 4:1:312:ARG:HH21 | 1.33 | 0.76 |
| 4:W:291:LYS:HB3 | 4:Y:244:ASP:HB3 | 1.66 | 0.76 |
| 1:A:94:MET:CE | 1:A:101:ALA:HB1 | 2.15 | 0.76 |
| 1:D:218:LEU:HD22 | 1:D:222:ILE:HG12 | 1.67 | 0.76 |
| 1:D:629:GLU:HA | 1:D:643:GLY:C | 2.05 | 0.76 |
| 1:D:831:TRP:CH2 | 2:E:34:ILE:CG2 | 2.65 | 0.76 |
| 1:G:218:LEU:HD22 | 1:G:222:ILE:HG12 | 1.66 | 0.76 |
| 3:I:49:ILE:N | 3:I:52:ASN:HD22 | 1.82 | 0.76 |
| 1:J:710:GLY:O | 1:J:772:LEU:HB2 | 1.86 | 0.76 |
| 1:J:756:THR:CG2 | 1:J:776:GLU:C | 2.46 | 0.76 |
| 1:J:769:ALA:CB | 1:J:770:GLY:CA | 2.64 | 0.76 |
| 1:M:116:TYR:O | 1:M:153:PRO:HB2 | 1.85 | 0.76 |
| 1:M:218:LEU:HD22 | 1:M:222:ILE:HG12 | 1.67 | 0.76 |
| 1:M:803:TYR:CE2 | 3:O:17:PHE:CZ | 2.73 | 0.76 |
| 2:N:111:SER:OG | 2:N:148:VAL:C | 2.14 | 0.76 |
| 4:2:203:THR:H | 4:Z:287:ILE:CB | 1.98 | 0.76 |
| 4:7:290:ARG:NH1 | 4:9:202:THR:CG2 | 2.49 | 0.76 |
| 1:D:649:VAL:CG1 | 1:D:649:VAL:CB | 2.64 | 0.76 |
| 1:G:623:PHE:CG | 1:G:623:PHE:CA | 2.68 | 0.76 |
| 1:J:410:ASN:CG | 4:W:334:GLU:CA | 2.47 | 0.76 |
| 1:J:629:GLU:HA | 1:J:643:GLY:C | 2.05 | 0.76 |
| 1:J:649:VAL:CG1 | 1:J:649:VAL:CB | 2.64 | 0.76 |
| 1:M:219:GLU:O | 1:M:223:ILE:HG13 | 1.84 | 0.76 |
| 1:M:530:MET:CG | 4:Z:354:GLN:CB | 2.30 | 0.76 |
| 1:P:93:MET:HG2 | 1:P:714:ARG:N | 2.01 | 0.76 |
| 1:P:636:LYS:O | 1:P:637:LYS:HB2 | 1.86 | 0.76 |
| 1:A:538:GLU:OE2 | 4:8:355:MET:HE3 | 1.85 | 0.75 |
| 1:A:649:VAL:CG1 | 1:A:649:VAL:CB | 2.64 | 0.75 |
| 1:A:800:ARG:HD2 | 3:C:149:VAL:C | 2.06 | 0.75 |
| 1:D:636:LYS:O | 1:D:637:LYS:HB2 | 1.86 | 0.75 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:664:LEU:O | 1:D:667:THR:HB | 1.86 | 0.75 |
| 1:D:727:LEU:HD12 | 1:D:782:MLY:HD3 | 1.27 | 0.75 |
| 1:D:767:PHE:O | 1:D:771:LEU:CD1 | 2.34 | 0.75 |
| 1:G:664:LEU:O | 1:G:667:THR:HB | 1.86 | 0.75 |
| 1:G:820:VAL:HG11 | 2:H:136:MET:HE3 | 1.67 | 0.75 |
| 2:K:121:LEU:CG | 2:K:128:PHE:HA | 2.14 | 0.75 |
| 2:E:163:ALA:C | 2:K:22:THR:N | 2.39 | 0.75 |
| 1:J:795:ARG:O | 3:L:35:ARG:NH2 | 2.18 | 0.75 |
| 1:J:817:GLN:HG2 | 2:K:127:ARG:CG | 2.15 | 0.75 |
| 1:M:664:LEU:O | 1:M:667:THR:HB | 1.86 | 0.75 |
| 1:M:721:LYS:CA | 1:M:736:GLN:OE1 | 2.33 | 0.75 |
| 4:1:167:GLU:CD | 4:3:43:VAL:O | 2.25 | 0.75 |
| 1:A:28:GLN:NE2 | 1:A:723:ARG:HH21 | 1.81 | 0.75 |
| 1:A:752:ASP:CG | 1:A:782:MLY:HD3 | 2.06 | 0.75 |
| 1:A:769:ALA:O | 1:A:772:LEU:N | 2.14 | 0.75 |
| 1:G:84:MLY:CB | 1:G:723:ARG:CZ | 2.64 | 0.75 |
| 1:G:503:TYR:CE1 | 1:G:711:PHE:HE2 | 2.04 | 0.75 |
| 1:J:623:PHE:CG | 1:J:623:PHE:CA | 2.68 | 0.75 |
| 1:P:218:LEU:HB2 | 1:P:221:GLN:CG | 2.10 | 0.75 |
| 1:P:831:TRP:HE1 | 2:Q:67:MET:HB3 | 1.52 | 0.75 |
| 4:X:288:ASP:HB3 | 4:Z:243:PRO:HG2 | 1.67 | 0.75 |
| 2:B:150:TYR:C | 2:B:151:LYS:CG | 2.49 | 0.75 |
| 1:G:649:VAL:CG1 | 1:G:649:VAL:CB | 2.64 | 0.75 |
| 1:J:826:VAL:HG21 | 2:K:88:LEU:CD2 | 2.16 | 0.75 |
| 1:P:410:ASN:CG | 4:1:334:GLU:CA | 2.47 | 0.75 |
| 3:R:3:SER:O | 3:R:4:LYS:HB2 | 1.85 | 0.75 |
| 2:B:121:LEU:CG | 2:B:128:PHE:HA | 2.14 | 0.75 |
| 1:D:721:LYS:CA | 1:D:736:GLN:OE1 | 2.33 | 0.75 |
| 1:D:799:MET:CE | 3:F:32:ASP:CB | 2.50 | 0.75 |
| 1:G:817:GLN:NE2 | 2:H:128:PHE:CE1 | 2.54 | 0.75 |
| 1:J:350:ALA:O | 1:J:354:LEU:HB2 | 1.87 | 0.75 |
| 1:J:710:GLY:CA | 1:J:772:LEU:CD2 | 2.35 | 0.75 |
| 2:N:114:LYS:HA | 2:N:146:GLY:C | 2.03 | 0.75 |
| 4:3:322:PRO:CB | 4:5:244:ASP:OD2 | 2.26 | 0.75 |
| 4:4:322:PRO:CB | 4:6:244:ASP:HB2 | 2.14 | 0.75 |
| 1:A:557:GLU:N | 4:V:48:GLY:HA3 | 1.90 | 0.75 |
| 2:E:163:ALA:C | 2:K:22:THR:H | 1.90 | 0.75 |
| 1:G:818:TYR:CZ | 2:H:127:ARG:NH1 | 2.53 | 0.75 |
| 1:P:534:SER:O | 4:1:351:THR:N | 2.19 | 0.75 |
| 1:P:725:ARG:HG3 | 1:P:733:PRO:HA | 1.67 | 0.75 |
| 4:1:244:ASP:H | 4:Y:291:LYS:HD2 | 1.51 | 0.75 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:1:287:ILE:HB | 4:3:203:THR:HG21 | 1.64 | 0.75 |
| 4:2:203:THR:CB | 4:Z:287:ILE:HB | 2.14 | 0.75 |
| 4:4:287:ILE:HB | 4:6:203:THR:HG22 | 1.69 | 0.75 |
| 1:A:149:GLN:CG | 1:A:719:ASP:N | 2.45 | 0.75 |
| 1:A:753:VAL:CG1 | 1:A:775:LEU:CG | 2.18 | 0.75 |
| 1:A:809:ARG:NH1 | 2:B:124:GLY:HA2 | 2.01 | 0.75 |
| 1:D:838:ILE:HD12 | 2:E:54:MET:HE3 | 1.59 | 0.75 |
| 1:A:537:GLU:HG3 | 4:8:350:SER:O | 1.79 | 0.75 |
| 1:D:350:ALA:O | 1:D:354:LEU:HB2 | 1.87 | 0.75 |
| 1:D:799:MET:SD | 3:F:32:ASP:CG | 2.64 | 0.75 |
| 1:G:148:ARG:HH21 | 1:G:764:MLY:HH21 | 1.51 | 0.75 |
| 1:G:538:GLU:O | 4:V:349:LEU:HG | 1.87 | 0.75 |
| 1:G:721:LYS:CA | 1:G:736:GLN:OE1 | 2.33 | 0.75 |
| 1:J:636:LYS:O | 1:J:637:LYS:HB2 | 1.86 | 0.75 |
| 1:M:350:ALA:O | 1:M:354:LEU:HB2 | 1.87 | 0.75 |
| 1:M:534:SER:O | 4:Z:351:THR:N | 2.19 | 0.75 |
| 1:M:649:VAL:CG1 | 1:M:649:VAL:CB | 2.64 | 0.75 |
| 1:M:795:ARG:CB | 3:O:35:ARG:HH12 | 2.00 | 0.75 |
| 4:1:205:GLU:CD | 4:Y:287:ILE:C | 2.43 | 0.75 |
| 4:5:253:GLU:HA | 4:5:256:ARG:HG3 | 1.69 | 0.75 |
| 1:G:92:ALA:O | 1:G:714:ARG:HG2 | 1.86 | 0.75 |
| 1:G:541:MET:O | 4:V:143:TYR:CZ | 2.40 | 0.75 |
| 1:G:817:GLN:HG2 | 2:H:127:ARG:HB2 | 1.66 | 0.75 |
| 1:J:310:TYR:CE2 | 1:J:320:ILE:HD11 | 2.22 | 0.75 |
| 1:J:541:MET:O | 4:W:143:TYR:CZ | 2.40 | 0.75 |
| 1:P:538:GLU:CD | 4:1:355:MET:HE3 | 2.08 | 0.75 |
| 4:8:253:GLU:HA | 4:8:256:ARG:HG3 | 1.69 | 0.75 |
| 4:9:288:ASP:H | 4:W:203:THR:HG22 | 1.52 | 0.75 |
| 1:A:85:TYR:HH | 1:A:772:LEU:HD23 | 0.93 | 0.74 |
| 1:A:797:PHE:HE2 | 3:C:126:LEU:CD2 | 2.00 | 0.74 |
| 1:D:541:MET:O | 4:9:143:TYR:CZ | 2.40 | 0.74 |
| 1:G:646:PHE:CE2 | 1:G:652:LEU:HD21 | 2.15 | 0.74 |
| 1:G:725:ARG:HG3 | 1:G:733:PRO:HA | 1.67 | 0.74 |
| 1:G:795:ARG:NE | 3:I:116:GLU:CD | 2.39 | 0.74 |
| 1:G:795:ARG:HH21 | 3:I:116:GLU:CB | 2.00 | 0.74 |
| 1:G:829:TRP:CZ2 | 2:H:83:MET:HE1 | 2.22 | 0.74 |
| 1:J:218:LEU:HB3 | 1:J:221:GLN:HG3 | 1.61 | 0.74 |
| 1:J:481:ASN:HD22 | 1:J:481:ASN:N | 1.82 | 0.74 |
| 1:J:721:LYS:CA | 1:J:736:GLN:OE1 | 2.33 | 0.74 |
| 1:J:829:TRP:HZ3 | 2:K:84:PHE:CZ | 2.03 | 0.74 |
| 1:J:831:TRP:HE1 | 2:K:67:MET:CB | 1.99 | 0.74 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:831:TRP:NE1 | 2:K:67:MET:HB3 | 1.99 | 0.74 |
| 1:M:707:CYS:O | 1:M:710:GLY:N | 2.20 | 0.74 |
| 1:M:795:ARG:CZ | 3:O:43:ASN:OD1 | 2.19 | 0.74 |
| 4:3:253:GLU:HA | 4:3:256:ARG:HG3 | 1.69 | 0.74 |
| 1:A:505:MLY:HB2 | 1:A:761:GLY:CA | 2.17 | 0.74 |
| 1:A:538:GLU:O | 4:8:349:LEU:HG | 1.86 | 0.74 |
| 1:A:725:ARG:HG3 | 1:A:733:PRO:HA | 1.67 | 0.74 |
| 1:A:800:ARG:C | 3:C:149:VAL:CG2 | 2.56 | 0.74 |
| 1:A:831:TRP:CZ2 | 2:B:50:THR:HB | 2.18 | 0.74 |
| 3:C:4:LYS:N | 3:C:5:ALA:O | 2.17 | 0.74 |
| 1:D:215:GLN:NE2 | 1:D:336:SER:O | 2.21 | 0.74 |
| 1:G:736:GLN:HA | 1:G:743:ALA:HB2 | 1.51 | 0.74 |
| 1:J:538:GLU:HA | 4:W:349:LEU:HD12 | 0.75 | 0.74 |
| 1:J:664:LEU:O | 1:J:667:THR:HB | 1.86 | 0.74 |
| 1:M:35:MLY:HG3 | 1:M:777:GLU:OE2 | 1.87 | 0.74 |
| 1:M:791:GLN:OE1 | 3:O:116:GLU:HG3 | 1.87 | 0.74 |
| 1:P:791:GLN:HE22 | 3:R:115:GLY:CA | 1.99 | 0.74 |
| 4:1:253:GLU:HA | 4:1:256:ARG:HG3 | 1.69 | 0.74 |
| 1:D:641:LYS:CE | 1:D:647:GLN:CG | 2.60 | 0.74 |
| 1:G:215:GLN:NE2 | 1:G:336:SER:O | 2.20 | 0.74 |
| 1:G:350:ALA:O | 1:G:354:LEU:HB2 | 1.87 | 0.74 |
| 1:G:757:GLN:OE1 | 1:G:772:LEU:CA | 2.35 | 0.74 |
| 1:M:541:MET:O | 4:Z:143:TYR:CZ | 2.40 | 0.74 |
| 1:P:538:GLU:HA | 4:1:349:LEU:HD12 | 0.74 | 0.74 |
| 1:P:817:GLN:HG3 | 2:Q:128:PHE:CE1 | 2.22 | 0.74 |
| 4:9:290:ARG:NH1 | 4:W:202:THR:CG2 | 2.49 | 0.74 |
| 4:V:253:GLU:HA | 4:V:256:ARG:HG3 | 1.69 | 0.74 |
| 4:W:324:THR:CG2 | 4:Y:247:VAL:HG22 | 2.17 | 0.74 |
| 1:D:733:PRO:C | 1:D:737:PHE:HD1 | 1.88 | 0.74 |
| 1:G:148:ARG:NH2 | 1:G:764:MLY:HH11 | 2.02 | 0.74 |
| 1:M:538:GLU:O | 4:Z:349:LEU:HG | 1.86 | 0.74 |
| 1:M:733:PRO:C | 1:M:737:PHE:HD1 | 1.88 | 0.74 |
| 1:M:800:ARG:HB3 | 3:O:149:VAL:CG2 | 2.17 | 0.74 |
| 1:P:537:GLU:HG3 | 4:1:350:SER:O | 1.78 | 0.74 |
| 1:P:541:MET:O | 4:1:143:TYR:CZ | 2.40 | 0.74 |
| 4:Z:253:GLU:HA | 4:Z:256:ARG:HG3 | 1.69 | 0.74 |
| 1:A:215:GLN:NE2 | 1:A:336:SER:O | 2.20 | 0.74 |
| 1:D:310:TYR:CE2 | 1:D:320:ILE:HD11 | 2.23 | 0.74 |
| 1:D:538:GLU:HA | 4:9:349:LEU:HD12 | 0.74 | 0.74 |
| 1:G:534:SER:O | 4:V:351:THR:N | 2.19 | 0.74 |
| 1:J:735:GLY:C | 1:J:743:ALA:HB2 | 1.82 | 0.74 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:486:MLY:HH13 | 1:M:527:GLU:OE1 | 1.88 | 0.74 |
| 1:P:481:ASN:HD22 | 1:P:481:ASN:N | 1.82 | 0.74 |
| 1:P:721:LYS:CA | 1:P:736:GLN:OE1 | 2.33 | 0.74 |
| 4:1:290:ARG:NH2 | 4:3:202:THR:HG21 | 1.87 | 0.74 |
| 1:A:350:ALA:O | 1:A:354:LEU:HB2 | 1.87 | 0.74 |
| 1:A:793:ARG:HH21 | 3:C:147:MET:HE3 | 1.50 | 0.74 |
| 1:A:823:PHE:CD1 | 2:B:160:GLY:HA2 | 2.21 | 0.74 |
| 1:D:732:ILE:N | 1:D:733:PRO:CD | 2.51 | 0.74 |
| 1:D:735:GLY:CA | 1:D:743:ALA:HA | 2.18 | 0.74 |
| 1:G:732:ILE:N | 1:G:733:PRO:CD | 2.51 | 0.74 |
| 1:M:218:LEU:HB2 | 1:M:221:GLN:CG | 2.09 | 0.74 |
| 1:M:436:MLY:HE3 | 1:M:626:TYR:CE1 | 2.23 | 0.74 |
| 1:M:640:LYS:O | 4:Z:23:GLY:O | 2.06 | 0.74 |
| 1:M:797:PHE:CE2 | 3:O:146:ILE:HD12 | 2.21 | 0.74 |
| 1:M:805:ALA:O | 1:M:809:ARG:CB | 2.35 | 0.74 |
| 4:1:243:PRO:C | 4:Y:291:LYS:HD2 | 2.07 | 0.74 |
| 1:A:541:MET:O | 4:8:143:TYR:CZ | 2.40 | 0.74 |
| 1:G:817:GLN:CG | 2:H:127:ARG:HB2 | 2.17 | 0.74 |
| 1:M:215:GLN:NE2 | 1:M:336:SER:O | 2.20 | 0.74 |
| 1:M:735:GLY:CA | 1:M:743:ALA:HA | 2.18 | 0.74 |
| 1:M:805:ALA:O | 1:M:809:ARG:N | 2.21 | 0.74 |
| 4:2:324:THR:OG1 | 4:4:244:ASP:N | 2.17 | 0.74 |
| 4:W:253:GLU:HA | 4:W:256:ARG:HG3 | 1.69 | 0.74 |
| 4:Y:253:GLU:HA | 4:Y:256:ARG:HG3 | 1.69 | 0.74 |
| 1:D:481:ASN:HD22 | 1:D:481:ASN:N | 1.82 | 0.74 |
| 1:G:84:MLY:HB3 | 1:G:723:ARG:CD | 2.13 | 0.74 |
| 1:G:84:MLY:CA | 1:G:723:ARG:CZ | 2.65 | 0.74 |
| 1:G:836:PHE:CZ | 2:H:159:HIS:HA | 2.23 | 0.74 |
| 1:J:537:GLU:HG3 | 4:W:350:SER:O | 1.78 | 0.74 |
| 1:M:640:LYS:O | 1:M:645:SER:OG | 2.06 | 0.74 |
| 1:M:836:PHE:CD2 | 2:N:160:GLY:N | 2.56 | 0.74 |
| 1:P:310:TYR:CE2 | 1:P:320:ILE:HD11 | 2.22 | 0.74 |
| 1:P:530:MET:HE2 | 4:1:354:GLN:HG3 | 1.66 | 0.74 |
| 4:X:253:GLU:HA | 4:X:256:ARG:HG3 | 1.70 | 0.74 |
| 1:A:310:TYR:CE2 | 1:A:320:ILE:HD11 | 2.22 | 0.74 |
| 1:A:797:PHE:CE1 | 3:C:146:ILE:C | 2.60 | 0.74 |
| 1:D:409:GLY:HA3 | 4:9:333:PRO:N | 2.03 | 0.74 |
| 1:D:834:LEU:HD11 | 2:E:54:MET:CB | 2.11 | 0.74 |
| 1:D:834:LEU:HD12 | 2:E:54:MET:HB2 | 1.67 | 0.74 |
| 2:E:130:PRO:O | 2:E:132:GLU:N | 2.21 | 0.74 |
| 1:G:310:TYR:CE2 | 1:G:320:ILE:HD11 | 2.22 | 0.74 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:538:GLU:O | 4:W:349:LEU:HG | 1.86 | 0.74 |
| 1:J:826:VAL:HG21 | 2:K:88:LEU:HD21 | 1.70 | 0.74 |
| 1:M:272:MLY:HH13 | 1:M:435:GLU:OE1 | 1.88 | 0.74 |
| 1:P:410:ASN:OD1 | 4:1:335:ARG:N | 2.21 | 0.74 |
| 1:P:641:LYS:HD2 | 1:P:647:GLN:OE1 | 1.81 | 0.74 |
| 1:P:829:TRP:HZ3 | 2:Q:84:PHE:CZ | 2.04 | 0.74 |
| 1:D:721:LYS:CB | 1:D:736:GLN:CD | 2.56 | 0.74 |
| 1:G:84:MLY:HH22 | 1:G:723:ARG:HB2 | 1.68 | 0.74 |
| 1:G:783:LEU:O | 1:G:787:ILE:CB | 2.35 | 0.74 |
| 1:J:215:GLN:NE2 | 1:J:336:SER:O | 2.21 | 0.74 |
| 1:J:410:ASN:OD1 | 4:W:335:ARG:N | 2.21 | 0.74 |
| 1:M:310:TYR:CE2 | 1:M:320:ILE:HD11 | 2.22 | 0.74 |
| 1:P:732:ILE:N | 1:P:733:PRO:CD | 2.51 | 0.74 |
| 1:P:735:GLY:CA | 1:P:743:ALA:HA | 2.18 | 0.74 |
| 4:3:322:PRO:HB2 | 4:5:244:ASP:HB3 | 1.70 | 0.74 |
| 1:A:272:MLY:HH13 | 1:A:435:GLU:OE1 | 1.88 | 0.73 |
| 1:A:640:LYS:O | 4:8:23:GLY:O | 2.06 | 0.73 |
| 1:D:272:MLY:HH13 | 1:D:435:GLU:OE1 | 1.87 | 0.73 |
| 1:G:640:LYS:O | 4:V:23:GLY:O | 2.06 | 0.73 |
| 1:J:292:MET:HE3 | 1:J:309:PRO:HA | 1.70 | 0.73 |
| 1:J:436:MLY:HE3 | 1:J:626:TYR:CE1 | 2.23 | 0.73 |
| 1:J:735:GLY:CA | 1:J:743:ALA:HA | 2.18 | 0.73 |
| 1:J:757:GLN:NE2 | 1:J:777:GLU:H | 1.84 | 0.73 |
| 2:K:130:PRO:O | 2:K:132:GLU:N | 2.21 | 0.73 |
| 1:M:732:ILE:N | 1:M:733:PRO:CD | 2.51 | 0.73 |
| 1:P:93:MET:HG2 | 1:P:714:ARG:CA | 2.18 | 0.73 |
| 1:P:350:ALA:O | 1:P:354:LEU:HB2 | 1.87 | 0.73 |
| 1:P:486:MLY:HH13 | 1:P:527:GLU:OE1 | 1.88 | 0.73 |
| 1:P:546:THR:HG21 | 4:3:47:MET:CA | 2.18 | 0.73 |
| 1:P:795:ARG:CG | 3:R:118:MET:HE1 | 2.18 | 0.73 |
| 1:P:820:VAL:CG1 | 2:Q:136:MET:CE | 2.66 | 0.73 |
| 4:2:287:ILE:HG13 | 4:4:202:THR:CA | 2.16 | 0.73 |
| 1:A:409:GLY:HA3 | 4:8:333:PRO:N | 2.03 | 0.73 |
| 1:A:436:MLY:HE3 | 1:A:626:TYR:CE1 | 2.23 | 0.73 |
| 1:A:721:LYS:CB | 1:A:736:GLN:CD | 2.56 | 0.73 |
| 1:A:732:ILE:N | 1:A:733:PRO:CD | 2.51 | 0.73 |
| 1:A:813:ILE:CG1 | 2:B:128:PHE:HE1 | 2.01 | 0.73 |
| 1:A:837:MLY:CH2 | 2:H:20:ASP:HB2 | 2.18 | 0.73 |
| 1:D:769:ALA:O | 1:D:774:LEU:HB2 | 1.88 | 0.73 |
| 1:G:769:ALA:HB1 | 1:G:770:GLY:CA | 2.10 | 0.73 |
| 1:G:829:TRP:CH2 | 2:H:83:MET:HE3 | 2.23 | 0.73 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:409:GLY:HA3 | 4:W:333:PRO:N | 2.03 | 0.73 |
| 1:J:721:LYS:CB | 1:J:736:GLN:CD | 2.56 | 0.73 |
| 1:P:733:PRO:C | 1:P:737:PHE:CD1 | 2.62 | 0.73 |
| 1:P:797:PHE:HE2 | 3:R:126:LEU:CD2 | 1.99 | 0.73 |
| 4:2:253:GLU:HA | 4:2:256:ARG:HG3 | 1.70 | 0.73 |
| 1:A:831:TRP:CH2 | 2:B:34:ILE:HG23 | 2.23 | 0.73 |
| 1:D:410:ASN:OD1 | 4:9:335:ARG:N | 2.22 | 0.73 |
| 1:G:436:MLY:HE3 | 1:G:626:TYR:CE1 | 2.23 | 0.73 |
| 1:G:486:MLY:HH13 | 1:G:527:GLU:OE1 | 1.88 | 0.73 |
| 1:G:636:LYS:O | 1:G:637:LYS:HB2 | 1.86 | 0.73 |
| 1:M:237:THR:HG22 | 1:M:239:ARG:H | 1.54 | 0.73 |
| 1:M:721:LYS:CB | 1:M:736:GLN:CD | 2.56 | 0.73 |
| 1:P:149:GLN:CD | 1:P:763:THR:HG21 | 2.08 | 0.73 |
| 1:P:214:MET:HA | 1:P:340:ILE:HD11 | 1.70 | 0.73 |
| 1:P:783:LEU:CG | 1:P:786:ILE:HD12 | 1.98 | 0.73 |
| 4:1:287:ILE:CG2 | 4:3:202:THR:HB | 2.19 | 0.73 |
| 4:W:324:THR:HG23 | 4:Y:247:VAL:HG22 | 1.70 | 0.73 |
| 1:A:536:LEU:HD13 | 1:A:550:PHE:CZ | 2.24 | 0.73 |
| 1:A:538:GLU:HA | 4:8:349:LEU:HD12 | 0.74 | 0.73 |
| 1:A:707:CYS:CA | 1:A:714:ARG:CZ | 2.64 | 0.73 |
| 1:A:735:GLY:CA | 1:A:743:ALA:HA | 2.18 | 0.73 |
| 1:A:798:LEU:CD1 | 3:C:126:LEU:CD1 | 2.58 | 0.73 |
| 1:G:149:GLN:HB3 | 1:G:716:LEU:HD21 | 1.70 | 0.73 |
| 1:G:538:GLU:HA | 4:V:349:LEU:HD12 | 0.74 | 0.73 |
| 1:G:640:LYS:O | 1:G:645:SER:OG | 2.06 | 0.73 |
| 1:G:755:HIS:H | 1:G:779:ARG:NH1 | 1.83 | 0.73 |
| 1:G:813:ILE:HG23 | 2:H:128:PHE:HZ | 1.50 | 0.73 |
| 1:J:272:MLY:HH13 | 1:J:435:GLU:OE1 | 1.87 | 0.73 |
| 1:J:641:LYS:HD2 | 1:J:647:GLN:OE1 | 1.81 | 0.73 |
| 1:J:754:ASP:CG | 1:J:780:ASP:OD2 | 2.13 | 0.73 |
| 1:M:21:GLU:O | 1:M:25:ILE:HG13 | 1.89 | 0.73 |
| 1:P:436:MLY:HE3 | 1:P:626:TYR:CE1 | 2.23 | 0.73 |
| 1:P:538:GLU:O | 4:1:349:LEU:HG | 1.86 | 0.73 |
| 1:P:635:GLY:HA3 | 4:1:341:ILE:CD1 | 2.14 | 0.73 |
| 1:P:802:GLU:O | 1:P:806:MET:HG3 | 1.89 | 0.73 |
| 4:1:243:PRO:HB2 | 4:Y:291:LYS:HD2 | 1.68 | 0.73 |
| 1:D:530:MET:CE | 4:9:355:MET:SD | 2.77 | 0.73 |
| 1:D:640:LYS:O | 4:9:23:GLY:O | 2.06 | 0.73 |
| 1:D:708:ARG:CA | 1:D:710:GLY:N | 2.51 | 0.73 |
| 1:G:536:LEU:HD13 | 1:G:550:PHE:CZ | 2.24 | 0.73 |
| 1:G:754:ASP:CA | 1:G:776:GLU:CD | 2.56 | 0.73 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:505:MLY:CG | 1:J:762:HIS:HE1 | 1.97 | 0.73 |
| 1:M:409:GLY:HA3 | 4:Z:333:PRO:N | 2.03 | 0.73 |
| 1:M:538:GLU:HA | 4:Z:349:LEU:HD12 | 0.75 | 0.73 |
| 1:M:798:LEU:HD13 | 3:O:126:LEU:HD11 | 1.67 | 0.73 |
| 1:P:536:LEU:HD13 | 1:P:550:PHE:CZ | 2.24 | 0.73 |
| 4:8:288:ASP:H | 4:V:203:THR:HG22 | 1.52 | 0.73 |
| 1:A:636:LYS:O | 1:A:637:LYS:HB2 | 1.87 | 0.73 |
| 1:A:813:ILE:HG12 | 2:B:128:PHE:HE1 | 1.53 | 0.73 |
| 1:D:131:TRP:C | 1:D:132:LEU:HD12 | 2.09 | 0.73 |
| 1:D:190:MLY:HE3 | 1:D:230:GLU:OE2 | 1.89 | 0.73 |
| 1:D:838:ILE:HD11 | 2:E:54:MET:SD | 2.27 | 0.73 |
| 1:G:84:MLY:HH21 | 1:G:720:PHE:HA | 1.69 | 0.73 |
| 1:G:190:MLY:HE3 | 1:G:230:GLU:OE2 | 1.89 | 0.73 |
| 1:G:237:THR:HG22 | 1:G:239:ARG:H | 1.54 | 0.73 |
| 1:G:272:MLY:HH13 | 1:G:435:GLU:OE1 | 1.88 | 0.73 |
| 1:G:441:MET:O | 1:G:445:ILE:HG13 | 1.88 | 0.73 |
| 1:G:487:LEU:O | 1:G:490:PHE:HB3 | 1.88 | 0.73 |
| 1:G:537:GLU:HG3 | 4:V:350:SER:O | 1.79 | 0.73 |
| 1:G:735:GLY:CA | 1:G:743:ALA:HA | 2.17 | 0.73 |
| 1:J:732:ILE:N | 1:J:733:PRO:CD | 2.51 | 0.73 |
| 1:P:272:MLY:HH13 | 1:P:435:GLU:OE1 | 1.87 | 0.73 |
| 1:P:487:LEU:O | 1:P:490:PHE:HB3 | 1.89 | 0.73 |
| 1:A:502:GLU:OE2 | 1:A:764:MLY:O | 2.07 | 0.73 |
| 1:D:507:GLY:O | 1:D:761:GLY:HA2 | 1.86 | 0.73 |
| 1:G:503:TYR:HE1 | 1:G:711:PHE:CE2 | 2.07 | 0.73 |
| 1:G:721:LYS:CB | 1:G:736:GLN:CD | 2.56 | 0.73 |
| 1:J:796:GLY:HA2 | 3:L:35:ARG:NE | 2.03 | 0.73 |
| 1:J:802:GLU:O | 1:J:806:MET:HG3 | 1.89 | 0.73 |
| 1:J:834:LEU:HD12 | 2:K:51:PHE:CE1 | 2.23 | 0.73 |
| 1:M:753:VAL:HG12 | 1:M:771:LEU:HD11 | 1.71 | 0.73 |
| 1:P:534:SER:CA | 4:1:351:THR:HA | 2.19 | 0.73 |
| 2:Q:117:LEU:HD12 | 2:Q:147:ASN:CA | 2.19 | 0.73 |
| 4:9:253:GLU:HA | 4:9:256:ARG:HG3 | 1.70 | 0.73 |
| 1:A:499:GLU:CD | 1:A:766:PHE:CE2 | 2.62 | 0.73 |
| 1:A:733:PRO:C | 1:A:737:PHE:CD1 | 2.62 | 0.73 |
| 1:A:830:PRO:HB2 | 2:B:51:PHE:CE1 | 2.23 | 0.73 |
| 1:A:831:TRP:HZ3 | 2:B:50:THR:CG2 | 1.54 | 0.73 |
| 1:D:436:MLY:HE3 | 1:D:626:TYR:CE1 | 2.23 | 0.73 |
| 1:G:817:GLN:OE1 | 2:H:127:ARG:CD | 2.28 | 0.73 |
| 1:M:190:MLY:HE3 | 1:M:230:GLU:OE2 | 1.89 | 0.73 |
| 1:P:215:GLN:NE2 | 1:P:336:SER:O | 2.21 | 0.73 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:P:783:LEU:O | 1:P:786:ILE:HG13 | 1.87 | 0.73 |
| 2:Q:130:PRO:O | 2:Q:132:GLU:N | 2.21 | 0.73 |
| 4:7:253:GLU:HA | 4:7:256:ARG:HG3 | 1.70 | 0.73 |
| 1:A:93:MET:CE | 1:A:715:VAL:CA | 2.43 | 0.73 |
| 1:A:530:MET:CE | 4:8:355:MET:SD | 2.76 | 0.73 |
| 1:A:542:PHE:CD2 | 4:8:143:TYR:CE1 | 2.77 | 0.73 |
| 1:D:530:MET:HE3 | 4:9:354:GLN:HG2 | 1.69 | 0.73 |
| 1:D:538:GLU:O | 4:9:349:LEU:HG | 1.86 | 0.73 |
| 1:J:190:MLY:HE3 | 1:J:230:GLU:OE2 | 1.89 | 0.73 |
| 1:P:721:LYS:CB | 1:P:736:GLN:CD | 2.56 | 0.73 |
| 4:4:288:ASP:CB | 4:6:203:THR:CG2 | 2.66 | 0.73 |
| 4:7:288:ASP:H | 4:9:203:THR:HG22 | 1.52 | 0.73 |
| 1:A:21:GLU:O | 1:A:25:ILE:HG13 | 1.89 | 0.73 |
| 1:A:487:LEU:O | 1:A:490:PHE:HB3 | 1.88 | 0.73 |
| 1:D:486:MLY:HH13 | 1:D:527:GLU:OE1 | 1.88 | 0.73 |
| 1:D:802:GLU:O | 1:D:806:MET:HG3 | 1.89 | 0.73 |
| 1:D:815:CYS:O | 2:E:90:GLY:O | 2.07 | 0.73 |
| 1:G:21:GLU:O | 1:G:25:ILE:HG13 | 1.89 | 0.73 |
| 1:G:834:LEU:HD12 | 2:H:51:PHE:CE1 | 2.23 | 0.73 |
| 1:J:214:MET:HA | 1:J:340:ILE:HD11 | 1.70 | 0.73 |
| 1:J:536:LEU:HD13 | 1:J:550:PHE:CZ | 2.24 | 0.73 |
| 1:J:542:PHE:CD2 | 4:W:143:TYR:CE1 | 2.77 | 0.73 |
| 1:J:640:LYS:O | 4:W:23:GLY:O | 2.06 | 0.73 |
| 1:J:801:VAL:HG21 | 3:L:126:LEU:CD2 | 2.19 | 0.73 |
| 1:M:487:LEU:O | 1:M:490:PHE:HB3 | 1.88 | 0.73 |
| 1:M:542:PHE:CD2 | 4:Z:143:TYR:CE1 | 2.77 | 0.73 |
| 1:M:636:LYS:O | 1:M:637:LYS:HB2 | 1.86 | 0.73 |
| 1:P:21:GLU:O | 1:P:25:ILE:HG13 | 1.88 | 0.73 |
| 1:P:782:MLY:O | 1:P:786:ILE:HG12 | 1.87 | 0.73 |
| 4:1:201:VAL:HG23 | 4:Y:287:ILE:HG23 | 1.70 | 0.73 |
| 4:4:253:GLU:HA | 4:4:256:ARG:HG3 | 1.70 | 0.73 |
| 1:A:640:LYS:O | 1:A:645:SER:OG | 2.06 | 0.72 |
| 1:A:813:ILE:CD1 | 2:B:128:PHE:HE1 | 2.02 | 0.72 |
| 3:C:24:LYS:CA | 3:C:63:ILE:O | 2.37 | 0.72 |
| 1:D:542:PHE:CD2 | 4:9:143:TYR:CE1 | 2.77 | 0.72 |
| 1:G:84:MLY:HG2 | 1:G:723:ARG:HD2 | 0.73 | 0.72 |
| 1:G:149:GLN:HG2 | 1:G:716:LEU:HD11 | 1.71 | 0.72 |
| 1:G:735:GLY:C | 1:G:743:ALA:HB1 | 1.84 | 0.72 |
| 1:G:819:ASN:N | 2:H:90:GLY:O | 2.21 | 0.72 |
| 2:H:130:PRO:O | 2:H:132:GLU:N | 2.21 | 0.72 |
| 1:J:21:GLU:O | 1:J:25:ILE:HG13 | 1.89 | 0.72 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:792:ALA:HB1 | 3:L:42:THR:N | 2.03 | 0.72 |
| 1:J:818:TYR:CZ | 2:K:127:ARG:CZ | 2.63 | 0.72 |
| 2:K:117:LEU:HD12 | 2:K:147:ASN:CA | 2.19 | 0.72 |
| 1:M:618:THR:O | 1:M:622:LEU:HD13 | 1.89 | 0.72 |
| 1:M:829:TRP:HZ3 | 2:N:84:PHE:CZ | 2.07 | 0.72 |
| 2:N:144:VAL:CB | 2:N:153:ILE:HD11 | 2.19 | 0.72 |
| 1:A:190:MLY:HE3 | 1:A:230:GLU:OE2 | 1.89 | 0.72 |
| 1:A:217:THR:C | 1:A:221:GLN:HE21 | 1.93 | 0.72 |
| 1:A:802:GLU:O | 1:A:806:MET:HG3 | 1.89 | 0.72 |
| 1:G:131:TRP:C | 1:G:132:LEU:HD12 | 2.09 | 0.72 |
| 1:G:290:GLN:C | 1:G:331:LEU:HD12 | 2.10 | 0.72 |
| 1:G:409:GLY:HA3 | 4:V:333:PRO:N | 2.03 | 0.72 |
| 1:G:410:ASN:OD1 | 4:V:335:ARG:N | 2.21 | 0.72 |
| 1:G:733:PRO:C | 1:G:737:PHE:CD1 | 2.62 | 0.72 |
| 1:J:36:SER:O | 1:J:52:ILE:HG12 | 1.90 | 0.72 |
| 1:J:487:LEU:O | 1:J:490:PHE:HB3 | 1.89 | 0.72 |
| 1:J:519:LEU:HD12 | 1:J:519:LEU:N | 2.04 | 0.72 |
| 1:M:131:TRP:C | 1:M:132:LEU:HD12 | 2.10 | 0.72 |
| 1:M:727:LEU:HD22 | 1:M:775:LEU:HG | 1.70 | 0.72 |
| 1:M:791:GLN:NE2 | 3:O:114:LEU:O | 2.22 | 0.72 |
| 2:N:130:PRO:O | 2:N:132:GLU:N | 2.21 | 0.72 |
| 3:O:24:LYS:CA | 3:O:63:ILE:O | 2.36 | 0.72 |
| 1:P:36:SER:O | 1:P:52:ILE:HG12 | 1.89 | 0.72 |
| 1:P:292:MET:HE3 | 1:P:309:PRO:HA | 1.71 | 0.72 |
| 1:P:409:GLY:HA3 | 4:1:333:PRO:N | 2.03 | 0.72 |
| 1:P:519:LEU:N | 1:P:519:LEU:HD12 | 2.05 | 0.72 |
| 1:P:640:LYS:O | 4:1:23:GLY:O | 2.06 | 0.72 |
| 1:A:441:MET:O | 1:A:445:ILE:HG13 | 1.88 | 0.72 |
| 2:B:130:PRO:O | 2:B:132:GLU:N | 2.21 | 0.72 |
| 1:D:618:THR:O | 1:D:622:LEU:HD13 | 1.89 | 0.72 |
| 1:J:486:MLY:HH13 | 1:J:527:GLU:OE1 | 1.87 | 0.72 |
| 1:J:530:MET:CE | 4:W:355:MET:SD | 2.77 | 0.72 |
| 1:J:791:GLN:HE21 | 3:L:115:GLY:HA3 | 1.54 | 0.72 |
| 1:M:290:GLN:C | 1:M:331:LEU:HD12 | 2.10 | 0.72 |
| 1:M:536:LEU:HD13 | 1:M:550:PHE:CZ | 2.24 | 0.72 |
| 2:N:150:TYR:C | 2:N:151:LYS:CG | 2.48 | 0.72 |
| 1:P:530:MET:CE | 4:1:355:MET:SD | 2.77 | 0.72 |
| 1:P:643:GLY:N | 4:1:24:ASP:CA | 2.46 | 0.72 |
| 3:R:24:LYS:CA | 3:R:63:ILE:O | 2.37 | 0.72 |
| 1:A:486:MLY:HH13 | 1:A:527:GLU:OE1 | 1.88 | 0.72 |
| 1:A:534:SER:CA | 4:8:351:THR:HA | 2.18 | 0.72 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:534:SER:CA | 4:9:351:THR:HA | 2.19 | 0.72 |
| 1:D:536:LEU:HD13 | 1:D:550:PHE:CZ | 2.23 | 0.72 |
| 1:D:798:LEU:HD21 | 3:F:122:GLU:HB3 | 1.69 | 0.72 |
| 3:F:24:LYS:CA | 3:F:63:ILE:O | 2.37 | 0.72 |
| 1:G:530:MET:CG | 4:V:354:GLN:CB | 2.30 | 0.72 |
| 2:H:121:LEU:CG | 2:H:128:PHE:HA | 2.14 | 0.72 |
| 1:J:166:MET:HE1 | 1:J:254:PHE:HB2 | 1.71 | 0.72 |
| 1:J:217:THR:C | 1:J:221:GLN:HE21 | 1.92 | 0.72 |
| 1:J:295:MLY:HG3 | 1:J:332:MET:CE | 2.19 | 0.72 |
| 3:L:24:LYS:CA | 3:L:63:ILE:O | 2.37 | 0.72 |
| 1:M:214:MET:HA | 1:M:340:ILE:HD11 | 1.70 | 0.72 |
| 1:M:534:SER:CA | 4:Z:351:THR:HA | 2.19 | 0.72 |
| 1:P:190:MLY:HE3 | 1:P:230:GLU:OE2 | 1.89 | 0.72 |
| 1:P:217:THR:C | 1:P:221:GLN:HE21 | 1.93 | 0.72 |
| 2:Q:117:LEU:HB2 | 2:Q:147:ASN:HD21 | 1.47 | 0.72 |
| 4:1:287:ILE:CG2 | 4:3:203:THR:CG2 | 2.61 | 0.72 |
| 1:A:36:SER:O | 1:A:52:ILE:HG12 | 1.90 | 0.72 |
| 1:A:214:MET:HA | 1:A:340:ILE:HD11 | 1.71 | 0.72 |
| 1:A:237:THR:HG22 | 1:A:239:ARG:H | 1.54 | 0.72 |
| 1:D:290:GLN:C | 1:D:331:LEU:HD12 | 2.09 | 0.72 |
| 1:G:214:MET:HA | 1:G:340:ILE:HD11 | 1.70 | 0.72 |
| 1:J:486:MLY:HH22 | 1:J:527:GLU:OE2 | 1.90 | 0.72 |
| 1:M:530:MET:HE3 | 4:Z:354:GLN:HG2 | 1.67 | 0.72 |
| 1:M:727:LEU:HD13 | 1:M:775:LEU:HD23 | 1.71 | 0.72 |
| 1:P:486:MLY:HH22 | 1:P:527:GLU:OE2 | 1.90 | 0.72 |
| 2:Q:144:VAL:CB | 2:Q:153:ILE:HD11 | 2.19 | 0.72 |
| 1:A:131:TRP:C | 1:A:132:LEU:HD12 | 2.10 | 0.72 |
| 1:A:176:LEU:N | 1:A:176:LEU:HD12 | 2.05 | 0.72 |
| 1:A:290:GLN:C | 1:A:331:LEU:HD12 | 2.09 | 0.72 |
| 1:A:553:MLY:NZ | 4:V:45:VAL:HA | 1.84 | 0.72 |
| 1:D:486:MLY:HH22 | 1:D:527:GLU:OE2 | 1.90 | 0.72 |
| 1:G:831:TRP:HH2 | 2:H:47:LEU:CD2 | 1.68 | 0.72 |
| 1:J:530:MET:HE1 | 4:W:355:MET:SD | 2.30 | 0.72 |
| 1:P:542:PHE:CD2 | 4:1:143:TYR:CE1 | 2.77 | 0.72 |
| 4:2:288:ASP:H | 4:4:203:THR:HG22 | 1.54 | 0.72 |
| 4:3:3:ASP:HA | 4:3:6:THR:CB | 2.18 | 0.72 |
| 4:6:253:GLU:HA | 4:6:256:ARG:HG3 | 1.70 | 0.72 |
| 1:A:486:MLY:HH22 | 1:A:527:GLU:OE2 | 1.90 | 0.72 |
| 1:A:519:LEU:HD12 | 1:A:519:LEU:N | 2.05 | 0.72 |
| 1:D:217:THR:C | 1:D:221:GLN:HE21 | 1.93 | 0.72 |
| 1:D:727:LEU:CG | 1:D:782:MLY:CD | 2.60 | 0.72 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:176:LEU:HD12 | 1:G:176:LEU:N | 2.05 | 0.72 |
| 1:G:534:SER:CA | 4:V:351:THR:HA | 2.20 | 0.72 |
| 1:G:556:ASP:OD2 | 4:X:47:MET:HE2 | 1.89 | 0.72 |
| 1:G:791:GLN:OE1 | 3:I:116:GLU:HG3 | 1.90 | 0.72 |
| 3:I:24:LYS:CA | 3:I:63:ILE:O | 2.37 | 0.72 |
| 1:J:131:TRP:C | 1:J:132:LEU:HD12 | 2.09 | 0.72 |
| 1:J:534:SER:CA | 4:W:351:THR:HA | 2.19 | 0.72 |
| 1:J:818:TYR:CG | 2:K:127:ARG:NH1 | 2.58 | 0.72 |
| 4:X:287:ILE:N | 4:Z:202:THR:CB | 2.52 | 0.72 |
| 1:A:149:GLN:HB2 | 1:A:718:ALA:HB1 | 1.68 | 0.72 |
| 1:A:295:MLY:HG3 | 1:A:332:MET:CE | 2.19 | 0.72 |
| 1:A:410:ASN:OD1 | 4:8:335:ARG:N | 2.22 | 0.72 |
| 1:A:791:GLN:OE1 | 3:C:116:GLU:CG | 2.29 | 0.72 |
| 1:D:237:THR:HG22 | 1:D:239:ARG:H | 1.54 | 0.72 |
| 1:D:487:LEU:O | 1:D:490:PHE:HB3 | 1.89 | 0.72 |
| 1:G:542:PHE:CD2 | 4:V:143:TYR:CE1 | 2.78 | 0.72 |
| 1:G:730:SER:HG | 3:I:113:THR:HG21 | 1.51 | 0.72 |
| 1:G:802:GLU:O | 1:G:806:MET:HG3 | 1.88 | 0.72 |
| 1:J:237:THR:HG22 | 1:J:239:ARG:H | 1.54 | 0.72 |
| 1:J:829:TRP:CZ3 | 2:K:84:PHE:CZ | 2.77 | 0.72 |
| 1:M:72:VAL:HG13 | 1:M:76:GLN:CB | 2.19 | 0.72 |
| 1:M:530:MET:CE | 4:Z:355:MET:SD | 2.77 | 0.72 |
| 1:M:838:ILE:HD11 | 2:N:54:MET:SD | 2.30 | 0.72 |
| 1:P:131:TRP:C | 1:P:132:LEU:HD12 | 2.10 | 0.72 |
| 1:P:618:THR:O | 1:P:622:LEU:HD13 | 1.89 | 0.72 |
| 4:2:3:ASP:HA | 4:2:6:THR:CB | 2.17 | 0.72 |
| 4:V:286:ASP:OD1 | 4:X:203:THR:N | 2.23 | 0.72 |
| 1:A:754:ASP:HB3 | 1:A:757:GLN:HG2 | 1.72 | 0.72 |
| 1:D:36:SER:O | 1:D:52:ILE:HG12 | 1.90 | 0.72 |
| 1:G:217:THR:C | 1:G:221:GLN:HE21 | 1.92 | 0.72 |
| 1:G:530:MET:CE | 4:V:355:MET:SD | 2.78 | 0.72 |
| 1:J:797:PHE:CE1 | 3:L:146:ILE:CB | 2.73 | 0.72 |
| 1:M:176:LEU:HD12 | 1:M:176:LEU:N | 2.05 | 0.72 |
| 1:M:519:LEU:N | 1:M:519:LEU:HD12 | 2.04 | 0.72 |
| 1:M:546:THR:HG22 | 1:M:548:THR:N | 2.05 | 0.72 |
| 1:M:733:PRO:C | 1:M:737:PHE:CD1 | 2.62 | 0.72 |
| 1:P:640:LYS:O | 1:P:645:SER:OG | 2.06 | 0.72 |
| 4:5:3:ASP:HA | 4:5:6:THR:CB | 2.18 | 0.72 |
| 1:A:97:LEU:CD2 | 1:A:712:PRO:HB2 | 2.20 | 0.72 |
| 1:A:546:THR:HG22 | 1:A:548:THR:N | 2.05 | 0.72 |
| 1:A:732:ILE:HG23 | 1:A:747:LEU:CB | 1.85 | 0.72 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:176:LEU:HD12 | 1:D:176:LEU:N | 2.05 | 0.72 |
| 1:D:507:GLY:O | 1:D:762:HIS:N | 2.23 | 0.72 |
| 2:E:114:LYS:HA | 2:E:146:GLY:C | 2.03 | 0.72 |
| 1:G:28:GLN:CA | 1:G:723:ARG:HH22 | 2.03 | 0.72 |
| 1:G:505:MLY:CH2 | 1:G:762:HIS:HE1 | 0.66 | 0.72 |
| 1:G:529:PRO:C | 4:V:354:GLN:CB | 2.50 | 0.72 |
| 1:G:557:GLU:HA | 4:X:48:GLY:CA | 2.18 | 0.72 |
| 2:H:117:LEU:HD12 | 2:H:147:ASN:CA | 2.20 | 0.72 |
| 2:H:136:MET:O | 2:H:140:PHE:HB2 | 1.90 | 0.72 |
| 1:J:97:LEU:HD22 | 1:J:712:PRO:HB2 | 1.72 | 0.72 |
| 1:M:441:MET:O | 1:M:445:ILE:HG13 | 1.88 | 0.72 |
| 1:M:802:GLU:O | 1:M:806:MET:HG3 | 1.89 | 0.72 |
| 2:Q:121:LEU:CG | 2:Q:128:PHE:HA | 2.14 | 0.72 |
| 1:A:499:GLU:OE2 | 1:A:766:PHE:CE2 | 2.43 | 0.71 |
| 1:D:14:ALA:HB3 | 1:D:15:PRO:HD3 | 1.72 | 0.71 |
| 1:D:21:GLU:O | 1:D:25:ILE:HG13 | 1.88 | 0.71 |
| 1:D:214:MET:HA | 1:D:340:ILE:HD11 | 1.71 | 0.71 |
| 1:D:295:MLY:HG3 | 1:D:332:MET:CE | 2.20 | 0.71 |
| 1:D:815:CYS:HG | 2:E:92:ASP:CG | 1.90 | 0.71 |
| 1:G:486:MLY:HH22 | 1:G:527:GLU:OE2 | 1.90 | 0.71 |
| 1:G:754:ASP:HB3 | 1:G:757:GLN:HG2 | 1.72 | 0.71 |
| 1:J:218:LEU:HB2 | 1:J:221:GLN:CG | 2.09 | 0.71 |
| 1:J:618:THR:O | 1:J:622:LEU:HD13 | 1.89 | 0.71 |
| 1:P:290:GLN:C | 1:P:331:LEU:HD12 | 2.09 | 0.71 |
| 1:P:817:GLN:CB | 2:Q:127:ARG:HH11 | 1.99 | 0.71 |
| 4:1:3:ASP:HA | 4:1:6:THR:CB | 2.18 | 0.71 |
| 1:A:768:MLY:HB3 | 1:A:771:LEU:HB2 | 0.82 | 0.71 |
| 1:D:754:ASP:HB3 | 1:D:757:GLN:HG2 | 1.72 | 0.71 |
| 2:E:136:MET:O | 2:E:140:PHE:HB2 | 1.90 | 0.71 |
| 1:J:14:ALA:HB3 | 1:J:15:PRO:HD3 | 1.73 | 0.71 |
| 1:M:217:THR:C | 1:M:221:GLN:HE21 | 1.92 | 0.71 |
| 1:M:410:ASN:OD1 | 4:Z:335:ARG:N | 2.21 | 0.71 |
| 1:P:14:ALA:HB3 | 1:P:15:PRO:HD3 | 1.73 | 0.71 |
| 1:P:707:CYS:O | 1:P:710:GLY:HA3 | 1.88 | 0.71 |
| 1:P:769:ALA:HA | 1:P:770:GLY:N | 2.03 | 0.71 |
| 4:Y:3:ASP:HA | 4:Y:6:THR:CB | 2.18 | 0.71 |
| 1:A:819:ASN:HB2 | 2:B:90:GLY:O | 1.89 | 0.71 |
| 2:B:144:VAL:CG1 | 2:B:153:ILE:HD13 | 2.19 | 0.71 |
| 1:D:519:LEU:HD12 | 1:D:519:LEU:N | 2.05 | 0.71 |
| 1:D:831:TRP:NE1 | 2:E:51:PHE:CZ | 2.58 | 0.71 |
| 1:G:643:GLY:N | 4:V:24:ASP:CA | 2.47 | 0.71 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:792:ALA:HA | 3:L:42:THR:CA | 2.13 | 0.71 |
| 1:J:817:GLN:OE1 | 2:K:127:ARG:CD | 2.36 | 0.71 |
| 1:M:166:MET:HE1 | 1:M:254:PHE:HB2 | 1.72 | 0.71 |
| 1:M:798:LEU:HD21 | 3:O:126:LEU:CD1 | 2.20 | 0.71 |
| 1:M:821:ARG:HH21 | 2:N:127:ARG:HG2 | 0.90 | 0.71 |
| 1:A:505:MLY:CB | 1:A:761:GLY:HA2 | 2.19 | 0.71 |
| 1:A:599:ASN:CA | 1:A:649:VAL:CB | 2.54 | 0.71 |
| 1:D:441:MET:O | 1:D:445:ILE:HG13 | 1.88 | 0.71 |
| 1:D:538:GLU:OE2 | 4:9:355:MET:HE3 | 1.87 | 0.71 |
| 1:G:217:THR:O | 1:G:220:ASP:HB2 | 1.91 | 0.71 |
| 1:J:441:MET:O | 1:J:445:ILE:HG13 | 1.88 | 0.71 |
| 1:J:538:GLU:OE2 | 4:W:355:MET:HE3 | 1.87 | 0.71 |
| 1:J:797:PHE:HE1 | 3:L:146:ILE:CA | 2.03 | 0.71 |
| 2:K:114:LYS:HA | 2:K:146:GLY:C | 2.03 | 0.71 |
| 2:K:136:MET:O | 2:K:140:PHE:HB2 | 1.90 | 0.71 |
| 1:M:783:LEU:HD12 | 1:M:786:ILE:HD11 | 1.72 | 0.71 |
| 1:P:86:ASP:OD2 | 1:P:87:MLY:HH13 | 1.91 | 0.71 |
| 1:P:441:MET:O | 1:P:445:ILE:HG13 | 1.88 | 0.71 |
| 1:P:754:ASP:HB3 | 1:P:757:GLN:HG2 | 1.72 | 0.71 |
| 2:Q:136:MET:O | 2:Q:140:PHE:HB2 | 1.90 | 0.71 |
| 4:W:325:MET:HE1 | 4:Y:244:ASP:CG | 2.11 | 0.71 |
| 1:A:643:GLY:N | 4:8:24:ASP:CA | 2.46 | 0.71 |
| 2:B:136:MET:O | 2:B:140:PHE:HB2 | 1.90 | 0.71 |
| 2:B:144:VAL:CB | 2:B:153:ILE:HD11 | 2.19 | 0.71 |
| 2:H:150:TYR:C | 2:H:151:LYS:CG | 2.48 | 0.71 |
| 1:M:36:SER:O | 1:M:52:ILE:HG12 | 1.90 | 0.71 |
| 1:M:486:MLY:HH22 | 1:M:527:GLU:OE2 | 1.90 | 0.71 |
| 1:P:786:ILE:CA | 1:P:787:ILE:N | 2.53 | 0.71 |
| 4:X:3:ASP:HA | 4:X:6:THR:CB | 2.17 | 0.71 |
| 1:A:206:LYS:HD3 | 1:A:217:THR:HG23 | 0.71 | 0.71 |
| 1:A:245:ARG:HD3 | 1:A:271:GLU:OE1 | 1.90 | 0.71 |
| 1:G:36:SER:O | 1:G:52:ILE:HG12 | 1.90 | 0.71 |
| 1:G:274:ARG:NH2 | 1:G:282:GLU:OE1 | 2.24 | 0.71 |
| 1:G:769:ALA:O | 1:G:773:GLY:HA2 | 1.89 | 0.71 |
| 1:J:290:GLN:C | 1:J:331:LEU:HD12 | 2.09 | 0.71 |
| 1:J:640:LYS:O | 1:J:645:SER:OG | 2.06 | 0.71 |
| 1:M:295:MLY:HG3 | 1:M:332:MET:CE | 2.20 | 0.71 |
| 1:P:534:SER:C | 4:1:351:THR:CA | 2.47 | 0.71 |
| 1:A:56:GLU:CB | 1:A:59:MLY:HB3 | 2.20 | 0.71 |
| 1:A:166:MET:HE1 | 1:A:254:PHE:HB2 | 1.72 | 0.71 |
| 1:A:217:THR:O | 1:A:220:ASP:HB2 | 1.91 | 0.71 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:813:ILE:HG12 | 2:B:128:PHE:CE1 | 2.25 | 0.71 |
| 1:D:217:THR:O | 1:D:220:ASP:HB2 | 1.91 | 0.71 |
| 1:G:86:ASP:OD2 | 1:G:87:MLY:HH13 | 1.91 | 0.71 |
| 1:G:295:MLY:HG3 | 1:G:332:MET:CE | 2.20 | 0.71 |
| 1:J:754:ASP:HB3 | 1:J:757:GLN:HG2 | 1.72 | 0.71 |
| 1:J:831:TRP:HZ3 | 2:K:34:ILE:HD13 | 1.56 | 0.71 |
| 2:K:144:VAL:CB | 2:K:153:ILE:HD11 | 2.19 | 0.71 |
| 1:M:217:THR:O | 1:M:220:ASP:HB2 | 1.91 | 0.71 |
| 1:M:641:LYS:HD2 | 4:Z:348:SER:HA | 1.73 | 0.71 |
| 1:P:829:TRP:CZ3 | 2:Q:84:PHE:CZ | 2.78 | 0.71 |
| 4:8:290:ARG:HH22 | 4:V:202:THR:HG23 | 1.50 | 0.71 |
| 4:X:287:ILE:CD1 | 4:Z:205:GLU:CG | 2.68 | 0.71 |
| 4:Z:3:ASP:HA | 4:Z:6:THR:CB | 2.18 | 0.71 |
| 1:A:72:VAL:HG13 | 1:A:76:GLN:CB | 2.19 | 0.71 |
| 1:A:618:THR:O | 1:A:622:LEU:HD13 | 1.89 | 0.71 |
| 1:A:739:ASP:CB | 1:A:742:LYS:HB3 | 2.13 | 0.71 |
| 1:D:218:LEU:HB2 | 1:D:221:GLN:CG | 2.09 | 0.71 |
| 1:D:245:ARG:HD3 | 1:D:271:GLU:OE1 | 1.90 | 0.71 |
| 1:D:274:ARG:NH2 | 1:D:282:GLU:OE1 | 2.24 | 0.71 |
| 1:G:72:VAL:HG13 | 1:G:76:GLN:CB | 2.19 | 0.71 |
| 2:H:144:VAL:CB | 2:H:153:ILE:HD11 | 2.19 | 0.71 |
| 1:J:733:PRO:C | 1:J:737:PHE:CD1 | 2.62 | 0.71 |
| 1:M:838:ILE:CD1 | 2:N:54:MET:HE3 | 2.11 | 0.71 |
| 4:W:3:ASP:HA | 4:W:6:THR:CB | 2.18 | 0.71 |
| 1:A:274:ARG:NH2 | 1:A:282:GLU:OE1 | 2.24 | 0.71 |
| 1:D:166:MET:HE1 | 1:D:254:PHE:HB2 | 1.72 | 0.71 |
| 2:E:144:VAL:CB | 2:E:153:ILE:HD11 | 2.19 | 0.71 |
| 1:G:618:THR:O | 1:G:622:LEU:HD13 | 1.89 | 0.71 |
| 1:G:732:ILE:HG23 | 1:G:747:LEU:CB | 1.85 | 0.71 |
| 1:M:14:ALA:HB3 | 1:M:15:PRO:HD3 | 1.72 | 0.71 |
| 2:N:136:MET:O | 2:N:140:PHE:HB2 | 1.90 | 0.71 |
| 1:P:791:GLN:CD | 3:R:116:GLU:H | 1.93 | 0.71 |
| 1:A:502:GLU:CD | 1:A:761:GLY:N | 2.44 | 0.71 |
| 1:D:86:ASP:OD2 | 1:D:87:MLY:HH13 | 1.91 | 0.71 |
| 1:D:550:PHE:HA | 4:W:46:GLY:HA3 | 1.66 | 0.71 |
| 1:D:640:LYS:O | 1:D:645:SER:OG | 2.06 | 0.71 |
| 1:G:14:ALA:HB3 | 1:G:15:PRO:HD3 | 1.72 | 0.71 |
| 1:G:519:LEU:HD12 | 1:G:519:LEU:N | 2.05 | 0.71 |
| 1:J:245:ARG:HD3 | 1:J:271:GLU:OE1 | 1.90 | 0.71 |
| 1:J:791:GLN:NE2 | 3:L:115:GLY:HA3 | 2.06 | 0.71 |
| 1:M:245:ARG:HD3 | 1:M:271:GLU:OE1 | 1.90 | 0.71 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:805:ALA:HA | 1:M:808:GLU:HB2 | 1.73 | 0.71 |
| 1:M:820:VAL:HG11 | 2:N:136:MET:CE | 2.20 | 0.71 |
| 1:P:295:MLY:HG3 | 1:P:332:MET:CE | 2.20 | 0.71 |
| 4:1:287:ILE:HB | 4:3:203:THR:CB | 2.19 | 0.71 |
| 4:8:3:ASP:HA | 4:8:6:THR:CB | 2.17 | 0.71 |
| 4:X:286:ASP:C | 4:Z:202:THR:OG1 | 2.22 | 0.71 |
| 1:D:795:ARG:HH21 | 3:F:116:GLU:CB | 2.02 | 0.70 |
| 1:J:86:ASP:OD2 | 1:J:87:MLY:HH13 | 1.91 | 0.70 |
| 1:J:176:LEU:HD12 | 1:J:176:LEU:N | 2.05 | 0.70 |
| 1:J:217:THR:O | 1:J:220:ASP:HB2 | 1.91 | 0.70 |
| 1:M:754:ASP:HB3 | 1:M:757:GLN:HG2 | 1.71 | 0.70 |
| 1:P:237:THR:HG22 | 1:P:239:ARG:H | 1.54 | 0.70 |
| 1:P:795:ARG:HB3 | 3:R:35:ARG:NH1 | 1.98 | 0.70 |
| 4:1:243:PRO:HB3 | 4:Y:291:LYS:CE | 2.02 | 0.70 |
| 1:A:123:CYS:HB2 | 1:A:158:ILE:HD11 | 1.73 | 0.70 |
| 1:G:829:TRP:HH2 | 2:H:83:MET:HE3 | 1.55 | 0.70 |
| 1:J:97:LEU:CD2 | 1:J:712:PRO:HB2 | 2.21 | 0.70 |
| 1:M:579:PHE:HD2 | 1:M:592:ILE:HD11 | 1.57 | 0.70 |
| 3:O:4:LYS:N | 3:O:5:ALA:O | 2.17 | 0.70 |
| 1:P:245:ARG:HD3 | 1:P:271:GLU:OE1 | 1.90 | 0.70 |
| 1:P:795:ARG:HH21 | 3:R:116:GLU:HB3 | 0.54 | 0.70 |
| 3:R:4:LYS:N | 3:R:5:ALA:O | 2.16 | 0.70 |
| 4:1:287:ILE:CB | 4:3:203:THR:CG2 | 2.34 | 0.70 |
| 4:2:64:ILE:CG2 | 4:Z:166:TYR:CE2 | 2.69 | 0.70 |
| 1:D:712:PRO:HG2 | 1:D:771:LEU:CB | 2.18 | 0.70 |
| 1:D:791:GLN:CD | 3:F:116:GLU:HG3 | 2.10 | 0.70 |
| 1:G:93:MET:HE2 | 1:G:764:MLY:HD3 | 1.71 | 0.70 |
| 1:G:97:LEU:HD23 | 1:G:712:PRO:HB3 | 0.78 | 0.70 |
| 1:G:795:ARG:CZ | 3:I:116:GLU:CB | 2.69 | 0.70 |
| 1:J:93:MET:HA | 1:J:714:ARG:H | 1.54 | 0.70 |
| 1:J:274:ARG:NH2 | 1:J:282:GLU:OE1 | 2.24 | 0.70 |
| 1:M:577:ALA:O | 1:M:578:HIS:CG | 2.44 | 0.70 |
| 1:M:797:PHE:CE2 | 3:O:146:ILE:CD1 | 2.75 | 0.70 |
| 1:M:821:ARG:HH22 | 2:N:127:ARG:NE | 1.90 | 0.70 |
| 1:P:641:LYS:HD2 | 4:1:348:SER:HA | 1.72 | 0.70 |
| 4:4:3:ASP:HA | 4:4:6:THR:CB | 2.17 | 0.70 |
| 4:7:290:ARG:HH22 | 4:9:202:THR:HG23 | 1.51 | 0.70 |
| 4:9:3:ASP:HA | 4:9:6:THR:CB | 2.18 | 0.70 |
| 1:G:56:GLU:CB | 1:G:59:MLY:HB3 | 2.19 | 0.70 |
| 1:G:97:LEU:HD22 | 1:G:712:PRO:HB2 | 1.73 | 0.70 |
| 1:G:810:ARG:HG2 | 1:G:810:ARG:HH11 | 1.56 | 0.70 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:817:GLN:HG3 | 2:H:128:PHE:CE1 | 2.27 | 0.70 |
| 1:M:56:GLU:CB | 1:M:59:MLY:HB3 | 2.19 | 0.70 |
| 1:M:86:ASP:OD2 | 1:M:87:MLY:HH13 | 1.91 | 0.70 |
| 1:P:579:PHE:HD2 | 1:P:592:ILE:HD11 | 1.57 | 0.70 |
| 1:P:791:GLN:NE2 | 3:R:116:GLU:H | 1.88 | 0.70 |
| 1:D:206:LYS:HD3 | 1:D:217:THR:HG23 | 0.70 | 0.70 |
| 1:G:84:MLY:HH22 | 1:G:719:ASP:O | 1.91 | 0.70 |
| 1:G:245:ARG:HD3 | 1:G:271:GLU:OE1 | 1.90 | 0.70 |
| 1:J:56:GLU:CB | 1:J:59:MLY:HB3 | 2.20 | 0.70 |
| 1:J:93:MET:SD | 1:J:716:LEU:N | 2.64 | 0.70 |
| 1:J:817:GLN:HB3 | 2:K:127:ARG:HH11 | 1.56 | 0.70 |
| 3:L:48:LYS:HB3 | 3:L:52:ASN:HD21 | 1.57 | 0.70 |
| 1:P:176:LEU:HD12 | 1:P:176:LEU:N | 2.05 | 0.70 |
| 1:A:14:ALA:HB3 | 1:A:15:PRO:HD3 | 1.72 | 0.70 |
| 1:A:550:PHE:HA | 4:V:46:GLY:HA3 | 1.66 | 0.70 |
| 1:A:579:PHE:HD2 | 1:A:592:ILE:HD11 | 1.57 | 0.70 |
| 1:D:819:ASN:CG | 2:E:90:GLY:O | 2.29 | 0.70 |
| 1:M:274:ARG:NH2 | 1:M:282:GLU:OE1 | 2.24 | 0.70 |
| 1:M:630:ALA:O | 4:Z:25:ASP:HB2 | 1.92 | 0.70 |
| 1:M:709:LYS:H | 1:M:710:GLY:N | 1.86 | 0.70 |
| 1:P:751:GLY:HA2 | 1:P:779:ARG:HH21 | 1.56 | 0.70 |
| 4:3:1:ASP:HA | 4:3:4:GLU:HB3 | 1.74 | 0.70 |
| 4:9:290:ARG:HH22 | 4:W:202:THR:HG23 | 1.51 | 0.70 |
| 1:D:123:CYS:HB2 | 1:D:158:ILE:HD11 | 1.73 | 0.70 |
| 1:D:782:MLY:C | 1:D:783:LEU:HD12 | 2.22 | 0.70 |
| 1:G:579:PHE:HD2 | 1:G:592:ILE:HD11 | 1.57 | 0.70 |
| 1:J:769:ALA:CB | 1:J:770:GLY:HA2 | 2.20 | 0.70 |
| 1:P:217:THR:O | 1:P:220:ASP:HB2 | 1.91 | 0.70 |
| 1:P:577:ALA:O | 1:P:578:HIS:CG | 2.45 | 0.70 |
| 1:P:831:TRP:CZ2 | 2:Q:47:LEU:CD2 | 2.70 | 0.70 |
| 3:R:25:ILE:O | 3:R:63:ILE:HB | 1.92 | 0.70 |
| 4:2:287:ILE:HG21 | 4:4:202:THR:OG1 | 1.89 | 0.70 |
| 4:Y:1:ASP:HA | 4:Y:4:GLU:HB3 | 1.74 | 0.70 |
| 1:A:577:ALA:O | 1:A:578:HIS:CG | 2.44 | 0.70 |
| 1:D:56:GLU:CB | 1:D:59:MLY:HB3 | 2.20 | 0.70 |
| 3:F:4:LYS:N | 3:F:5:ALA:O | 2.16 | 0.70 |
| 1:G:28:GLN:CB | 1:G:723:ARG:HH22 | 2.04 | 0.70 |
| 1:G:213:LYS:HA | 1:G:220:ASP:OD1 | 1.92 | 0.70 |
| 1:G:732:ILE:CG2 | 1:G:747:LEU:HD11 | 1.26 | 0.70 |
| 1:G:795:ARG:CB | 3:I:35:ARG:NH1 | 2.52 | 0.70 |
| 1:J:123:CYS:HB2 | 1:J:158:ILE:HD11 | 1.73 | 0.70 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:215:GLN:CA | 1:J:340:ILE:CG2 | 2.62 | 0.70 |
| 1:J:577:ALA:O | 1:J:578:HIS:CG | 2.45 | 0.70 |
| 1:J:782:MLY:C | 1:J:783:LEU:HD12 | 2.22 | 0.70 |
| 1:J:818:TYR:CE1 | 2:K:127:ARG:NH1 | 2.60 | 0.70 |
| 1:M:721:LYS:HG2 | 1:M:736:GLN:CD | 1.86 | 0.70 |
| 1:M:831:TRP:HE1 | 2:N:67:MET:HB3 | 1.56 | 0.70 |
| 1:P:274:ARG:NH2 | 1:P:282:GLU:OE1 | 2.24 | 0.70 |
| 1:P:792:ALA:CB | 3:R:42:THR:CG2 | 2.53 | 0.70 |
| 4:V:325:MET:CE | 4:X:244:ASP:CB | 2.70 | 0.70 |
| 1:D:577:ALA:O | 1:D:578:HIS:CG | 2.45 | 0.70 |
| 1:D:641:LYS:HD2 | 4:9:348:SER:HA | 1.73 | 0.70 |
| 3:F:48:LYS:HB3 | 3:F:52:ASN:HD21 | 1.57 | 0.70 |
| 1:G:206:LYS:HD3 | 1:G:217:THR:HG23 | 0.71 | 0.70 |
| 1:G:829:TRP:CE3 | 2:H:87:LYS:NZ | 2.59 | 0.70 |
| 1:J:732:ILE:CG2 | 1:J:747:LEU:HD11 | 1.26 | 0.70 |
| 1:J:818:TYR:CD1 | 2:K:127:ARG:CZ | 2.75 | 0.70 |
| 1:M:206:LYS:HD3 | 1:M:217:THR:HG23 | 0.71 | 0.70 |
| 2:N:117:LEU:HD12 | 2:N:147:ASN:CA | 2.20 | 0.70 |
| 4:W:1:ASP:HA | 4:W:4:GLU:HB3 | 1.74 | 0.70 |
| 4:W:324:THR:HG23 | 4:Y:247:VAL:H | 1.45 | 0.70 |
| 1:A:410:ASN:CG | 4:8:334:GLU:CA | 2.48 | 0.70 |
| 1:A:499:GLU:OE2 | 1:A:766:PHE:HE2 | 1.74 | 0.70 |
| 1:A:502:GLU:CA | 1:A:761:GLY:CA | 2.58 | 0.70 |
| 1:D:72:VAL:HG13 | 1:D:76:GLN:CB | 2.20 | 0.70 |
| 1:D:579:PHE:HD2 | 1:D:592:ILE:HD11 | 1.57 | 0.70 |
| 1:D:709:LYS:C | 1:D:710:GLY:HA2 | 2.12 | 0.70 |
| 1:D:834:LEU:CD2 | 2:E:54:MET:CE | 2.69 | 0.70 |
| 2:E:111:SER:OG | 2:E:148:VAL:HG12 | 1.92 | 0.70 |
| 1:G:577:ALA:O | 1:G:578:HIS:CG | 2.44 | 0.70 |
| 1:G:798:LEU:HG | 3:I:122:GLU:HB3 | 1.74 | 0.70 |
| 1:M:739:ASP:CB | 1:M:742:LYS:HB3 | 2.12 | 0.70 |
| 1:M:787:ILE:HG22 | 1:M:788:THR:N | 2.07 | 0.70 |
| 1:M:798:LEU:CD2 | 3:O:126:LEU:CD1 | 2.65 | 0.70 |
| 1:M:836:PHE:CD1 | 2:N:159:HIS:HA | 2.20 | 0.70 |
| 1:P:530:MET:CG | 4:1:354:GLN:CB | 2.30 | 0.70 |
| 1:P:791:GLN:NE2 | 3:R:115:GLY:HA3 | 2.06 | 0.70 |
| 2:Q:111:SER:OG | 2:Q:148:VAL:HG12 | 1.92 | 0.70 |
| 4:3:287:ILE:HB | 4:5:204:ALA:H | 1.55 | 0.70 |
| 4:8:1:ASP:HA | 4:8:4:GLU:HB3 | 1.74 | 0.70 |
| 4:Z:1:ASP:HA | 4:Z:4:GLU:HB3 | 1.74 | 0.70 |
| 1:A:86:ASP:OD2 | 1:A:87:MLY:HH13 | 1.91 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:C:25:ILE:O | 3:C:63:ILE:HB | 1.92 | 0.69 |
| 1:G:834:LEU:HD13 | 2:H:51:PHE:CE1 | 2.27 | 0.69 |
| 1:G:834:LEU:HD21 | 2:H:34:ILE:HG12 | 1.72 | 0.69 |
| 1:J:641:LYS:HD2 | 4:W:348:SER:HA | 1.73 | 0.69 |
| 1:M:797:PHE:CD1 | 3:O:146:ILE:O | 2.45 | 0.69 |
| 1:M:799:MET:SD | 3:O:32:ASP:OD2 | 2.50 | 0.69 |
| 1:P:206:LYS:HD3 | 1:P:217:THR:HG23 | 0.70 | 0.69 |
| 1:P:530:MET:HE1 | 4:1:355:MET:SD | 2.32 | 0.69 |
| 4:5:1:ASP:HA | 4:5:4:GLU:HB3 | 1.74 | 0.69 |
| 4:X:1:ASP:HA | 4:X:4:GLU:HB3 | 1.74 | 0.69 |
| 4:X:287:ILE:CG1 | 4:Z:201:VAL:N | 2.12 | 0.69 |
| 1:A:213:LYS:HA | 1:A:220:ASP:OD1 | 1.92 | 0.69 |
| 1:A:541:MET:CG | 4:8:345:ILE:O | 2.40 | 0.69 |
| 1:A:787:ILE:HG22 | 1:A:788:THR:N | 2.07 | 0.69 |
| 1:D:810:ARG:HG2 | 1:D:810:ARG:HH11 | 1.57 | 0.69 |
| 1:G:215:GLN:CA | 1:G:340:ILE:CG2 | 2.63 | 0.69 |
| 1:G:218:LEU:HB2 | 1:G:221:GLN:CG | 2.09 | 0.69 |
| 1:G:553:MLY:HH12 | 4:X:45:VAL:CG2 | 2.21 | 0.69 |
| 1:G:829:TRP:CZ2 | 2:H:83:MET:CE | 2.75 | 0.69 |
| 3:I:48:LYS:HB3 | 3:I:52:ASN:HD21 | 1.56 | 0.69 |
| 1:J:762:HIS:H | 1:J:762:HIS:CD2 | 2.08 | 0.69 |
| 2:K:150:TYR:C | 2:K:151:LYS:CG | 2.49 | 0.69 |
| 2:N:111:SER:OG | 2:N:148:VAL:HG12 | 1.92 | 0.69 |
| 1:P:787:ILE:HG22 | 1:P:788:THR:N | 2.07 | 0.69 |
| 1:P:795:ARG:CZ | 3:R:43:ASN:OD1 | 2.20 | 0.69 |
| 1:P:797:PHE:CE1 | 3:R:146:ILE:O | 2.45 | 0.69 |
| 3:R:48:LYS:HB3 | 3:R:52:ASN:HD21 | 1.57 | 0.69 |
| 4:4:324:THR:CG2 | 4:6:244:ASP:C | 2.55 | 0.69 |
| 4:V:1:ASP:HA | 4:V:4:GLU:HB3 | 1.74 | 0.69 |
| 1:A:630:ALA:O | 4:8:25:ASP:HB2 | 1.92 | 0.69 |
| 1:A:797:PHE:CD1 | 3:C:146:ILE:CG2 | 2.75 | 0.69 |
| 1:D:787:ILE:HG22 | 1:D:788:THR:N | 2.07 | 0.69 |
| 1:D:797:PHE:CE1 | 3:F:146:ILE:CG2 | 2.70 | 0.69 |
| 1:M:541:MET:CG | 4:Z:345:ILE:O | 2.40 | 0.69 |
| 3:O:25:ILE:O | 3:O:63:ILE:HB | 1.92 | 0.69 |
| 1:P:800:ARG:HB3 | 3:R:149:VAL:CG2 | 2.23 | 0.69 |
| 4:3:287:ILE:CG2 | 4:5:204:ALA:H | 2.04 | 0.69 |
| 4:V:3:ASP:HA | 4:V:6:THR:CB | 2.18 | 0.69 |
| 1:A:795:ARG:CB | 3:C:35:ARG:NH2 | 2.52 | 0.69 |
| 1:A:795:ARG:CD | 3:C:43:ASN:CG | 2.60 | 0.69 |
| 1:D:546:THR:HG22 | 1:D:548:THR:N | 2.05 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:831:TRP:CE3 | 2:E:34:ILE:HD13 | 2.27 | 0.69 |
| 1:G:553:MLY:CD | 4:X:45:VAL:HG12 | 2.23 | 0.69 |
| 1:G:782:MLY:C | 1:G:783:LEU:HD12 | 2.22 | 0.69 |
| 1:J:739:ASP:CB | 1:J:742:LYS:HB3 | 2.12 | 0.69 |
| 1:M:549:SER:HA | 4:2:43:VAL:HG11 | 1.74 | 0.69 |
| 1:M:797:PHE:HD1 | 3:O:149:VAL:CG1 | 2.02 | 0.69 |
| 1:M:807:VAL:O | 1:M:810:ARG:HB2 | 1.93 | 0.69 |
| 1:M:810:ARG:HG2 | 1:M:810:ARG:HH11 | 1.57 | 0.69 |
| 1:P:782:MLY:C | 1:P:783:LEU:HD12 | 2.22 | 0.69 |
| 1:P:819:ASN:OD1 | 2:Q:91:ALA:C | 2.29 | 0.69 |
| 4:1:247:VAL:H | 4:Y:324:THR:HB | 1.55 | 0.69 |
| 4:7:3:ASP:HA | 4:7:6:THR:CB | 2.18 | 0.69 |
| 4:9:1:ASP:HA | 4:9:4:GLU:HB3 | 1.74 | 0.69 |
| 1:A:149:GLN:CG | 1:A:718:ALA:HB3 | 2.23 | 0.69 |
| 1:D:733:PRO:C | 1:D:737:PHE:CD1 | 2.62 | 0.69 |
| 1:J:72:VAL:HG13 | 1:J:76:GLN:CB | 2.20 | 0.69 |
| 1:J:642:LYS:HB3 | 4:W:21:PHE:O | 1.92 | 0.69 |
| 1:J:769:ALA:HB2 | 1:J:770:GLY:CA | 2.21 | 0.69 |
| 1:J:807:VAL:O | 1:J:810:ARG:HB2 | 1.93 | 0.69 |
| 1:P:123:CYS:HB2 | 1:P:158:ILE:HD11 | 1.73 | 0.69 |
| 1:P:815:CYS:O | 1:P:819:ASN:HB2 | 1.93 | 0.69 |
| 4:3:290:ARG:NH2 | 4:5:202:THR:HG22 | 1.98 | 0.69 |
| 1:A:149:GLN:HG2 | 1:A:719:ASP:HB2 | 1.75 | 0.69 |
| 1:A:502:GLU:HG3 | 1:A:760:PHE:C | 2.11 | 0.69 |
| 1:A:800:ARG:HH22 | 3:C:40:ASN:CG | 1.83 | 0.69 |
| 1:A:810:ARG:HG2 | 1:A:810:ARG:HH11 | 1.57 | 0.69 |
| 1:G:541:MET:CG | 4:V:345:ILE:O | 2.41 | 0.69 |
| 1:G:829:TRP:CH2 | 2:H:87:LYS:HE2 | 2.27 | 0.69 |
| 2:H:111:SER:OG | 2:H:148:VAL:HG12 | 1.92 | 0.69 |
| 1:M:642:LYS:HB3 | 4:Z:21:PHE:O | 1.92 | 0.69 |
| 1:M:762:HIS:H | 1:M:762:HIS:CD2 | 2.07 | 0.69 |
| 1:M:782:MLY:C | 1:M:783:LEU:HD12 | 2.22 | 0.69 |
| 3:O:48:LYS:HB3 | 3:O:52:ASN:HD21 | 1.57 | 0.69 |
| 1:P:546:THR:HG22 | 1:P:548:THR:N | 2.05 | 0.69 |
| 1:P:630:ALA:O | 4:1:25:ASP:CB | 2.41 | 0.69 |
| 4:X:287:ILE:HG12 | 4:Z:201:VAL:H | 0.87 | 0.69 |
| 1:A:641:LYS:HD2 | 4:8:348:SER:HA | 1.73 | 0.69 |
| 1:A:782:MLY:C | 1:A:783:LEU:HD12 | 2.23 | 0.69 |
| 1:A:795:ARG:NH2 | 3:C:116:GLU:OE1 | 2.25 | 0.69 |
| 1:A:834:LEU:HD22 | 2:B:54:MET:HE2 | 1.75 | 0.69 |
| 1:D:762:HIS:H | 1:D:762:HIS:CD2 | 2.08 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:795:ARG:HB3 | 3:F:35:ARG:HH22 | 1.58 | 0.69 |
| 1:D:795:ARG:HH21 | 3:F:116:GLU:HB3 | 1.58 | 0.69 |
| 1:G:796:GLY:HA2 | 3:I:35:ARG:NE | 2.08 | 0.69 |
| 1:J:579:PHE:HD2 | 1:J:592:ILE:HD11 | 1.57 | 0.69 |
| 3:L:4:LYS:N | 3:L:5:ALA:O | 2.16 | 0.69 |
| 3:L:25:ILE:O | 3:L:63:ILE:HB | 1.92 | 0.69 |
| 1:M:213:LYS:HA | 1:M:220:ASP:OD1 | 1.92 | 0.69 |
| 1:P:149:GLN:CG | 1:P:716:LEU:HD11 | 2.22 | 0.69 |
| 1:A:642:LYS:HB3 | 4:8:21:PHE:O | 1.93 | 0.69 |
| 1:A:762:HIS:CD2 | 1:A:762:HIS:H | 2.08 | 0.69 |
| 1:A:800:ARG:HH22 | 3:C:40:ASN:HD21 | 0.72 | 0.69 |
| 1:A:802:GLU:OE1 | 1:A:802:GLU:HA | 1.93 | 0.69 |
| 2:B:117:LEU:HD12 | 2:B:147:ASN:CA | 2.20 | 0.69 |
| 1:D:533:PHE:O | 1:D:537:GLU:HG2 | 1.93 | 0.69 |
| 1:D:643:GLY:N | 4:9:24:ASP:CA | 2.46 | 0.69 |
| 1:D:725:ARG:O | 1:D:782:MLY:HH22 | 1.92 | 0.69 |
| 1:D:732:ILE:HG21 | 1:D:747:LEU:HD11 | 0.73 | 0.69 |
| 1:D:797:PHE:CZ | 3:F:126:LEU:HD22 | 2.20 | 0.69 |
| 1:D:802:GLU:OE1 | 1:D:802:GLU:HA | 1.93 | 0.69 |
| 1:D:807:VAL:O | 1:D:810:ARG:HB2 | 1.93 | 0.69 |
| 1:D:831:TRP:CZ3 | 2:E:34:ILE:HG21 | 2.27 | 0.69 |
| 1:G:123:CYS:HB2 | 1:G:158:ILE:HD11 | 1.73 | 0.69 |
| 1:G:641:LYS:HD2 | 4:V:348:SER:HA | 1.73 | 0.69 |
| 1:G:754:ASP:CG | 1:G:776:GLU:HA | 2.12 | 0.69 |
| 2:H:144:VAL:CG1 | 2:H:153:ILE:HD13 | 2.20 | 0.69 |
| 3:I:3:SER:O | 3:I:4:LYS:CB | 2.41 | 0.69 |
| 3:I:25:ILE:O | 3:I:63:ILE:HB | 1.92 | 0.69 |
| 1:J:123:CYS:HB2 | 1:J:158:ILE:CD1 | 2.23 | 0.69 |
| 1:J:546:THR:HG22 | 1:J:548:THR:N | 2.05 | 0.69 |
| 1:J:795:ARG:CZ | 3:L:116:GLU:OE1 | 2.41 | 0.69 |
| 2:K:117:LEU:CB | 2:K:147:ASN:OD1 | 2.39 | 0.69 |
| 1:M:783:LEU:CG | 1:M:786:ILE:HD11 | 2.23 | 0.69 |
| 1:M:791:GLN:CD | 3:O:116:GLU:H | 1.96 | 0.69 |
| 1:P:56:GLU:CB | 1:P:59:MLY:HB3 | 2.20 | 0.69 |
| 1:P:630:ALA:O | 4:1:25:ASP:HB2 | 1.91 | 0.69 |
| 1:P:642:LYS:HB3 | 4:1:21:PHE:O | 1.92 | 0.69 |
| 4:2:287:ILE:CG2 | 4:4:203:THR:N | 2.55 | 0.69 |
| 1:A:795:ARG:CG | 3:C:35:ARG:NH1 | 2.46 | 0.69 |
| 2:B:111:SER:OG | 2:B:148:VAL:HG12 | 1.92 | 0.69 |
| 1:D:123:CYS:HB2 | 1:D:158:ILE:CD1 | 2.23 | 0.69 |
| 1:G:530:MET:HE1 | 4:V:355:MET:SD | 2.33 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:I:48:LYS:C | 3:I:52:ASN:HD21 | 1.96 | 0.69 |
| 1:J:206:LYS:HD3 | 1:J:217:THR:HG23 | 0.71 | 0.69 |
| 2:K:111:SER:OG | 2:K:148:VAL:HG12 | 1.92 | 0.69 |
| 1:M:797:PHE:CD1 | 3:O:149:VAL:HG12 | 2.24 | 0.69 |
| 1:P:72:VAL:HG13 | 1:P:76:GLN:CB | 2.19 | 0.69 |
| 1:P:166:MET:HE3 | 1:P:254:PHE:CD2 | 2.28 | 0.69 |
| 1:P:541:MET:CG | 4:1:345:ILE:O | 2.40 | 0.69 |
| 1:P:728:ASN:OD1 | 3:R:93:VAL:CG1 | 2.41 | 0.69 |
| 1:P:739:ASP:CB | 1:P:742:LYS:HB3 | 2.12 | 0.69 |
| 4:6:3:ASP:HA | 4:6:6:THR:CB | 2.18 | 0.69 |
| 4:7:1:ASP:HA | 4:7:4:GLU:HB3 | 1.74 | 0.69 |
| 1:A:52:ILE:HD13 | 1:A:52:ILE:N | 2.08 | 0.69 |
| 2:B:117:LEU:CB | 2:B:147:ASN:OD1 | 2.39 | 0.69 |
| 1:G:533:PHE:O | 1:G:537:GLU:HG2 | 1.93 | 0.69 |
| 1:G:815:CYS:O | 1:G:819:ASN:HB2 | 1.93 | 0.69 |
| 1:J:630:ALA:O | 4:W:25:ASP:HB2 | 1.92 | 0.69 |
| 1:J:796:GLY:HA2 | 3:L:35:ARG:CG | 2.23 | 0.69 |
| 1:J:815:CYS:O | 1:J:819:ASN:HB2 | 1.93 | 0.69 |
| 1:J:817:GLN:CD | 2:K:127:ARG:CG | 2.61 | 0.69 |
| 1:M:538:GLU:CD | 4:Z:355:MET:CE | 2.62 | 0.69 |
| 1:M:785:GLU:O | 1:M:789:ALA:HB3 | 1.92 | 0.69 |
| 1:M:800:ARG:HH22 | 3:O:40:ASN:CG | 1.95 | 0.69 |
| 2:N:117:LEU:CB | 2:N:147:ASN:OD1 | 2.40 | 0.69 |
| 4:1:1:ASP:HA | 4:1:4:GLU:HB3 | 1.74 | 0.69 |
| 4:1:287:ILE:HD13 | 4:3:203:THR:HB | 1.75 | 0.69 |
| 1:A:218:LEU:HB2 | 1:A:221:GLN:CG | 2.10 | 0.68 |
| 1:A:836:PHE:CE1 | 2:B:159:HIS:CA | 2.75 | 0.68 |
| 1:D:727:LEU:H | 1:D:782:MLY:CH2 | 2.06 | 0.68 |
| 1:D:800:ARG:HB3 | 3:F:149:VAL:HG22 | 1.73 | 0.68 |
| 1:J:149:GLN:HB3 | 1:J:716:LEU:HD21 | 1.74 | 0.68 |
| 1:J:652:LEU:O | 1:J:655:GLU:N | 2.27 | 0.68 |
| 1:J:797:PHE:HE2 | 3:L:126:LEU:HD22 | 1.54 | 0.68 |
| 1:M:123:CYS:HB2 | 1:M:158:ILE:HD11 | 1.73 | 0.68 |
| 1:P:123:CYS:HB2 | 1:P:158:ILE:CD1 | 2.23 | 0.68 |
| 1:P:652:LEU:O | 1:P:655:GLU:N | 2.26 | 0.68 |
| 1:P:762:HIS:H | 1:P:762:HIS:CD2 | 2.08 | 0.68 |
| 2:Q:117:LEU:CB | 2:Q:147:ASN:OD1 | 2.39 | 0.68 |
| 4:1:243:PRO:C | 4:Y:291:LYS:CE | 2.62 | 0.68 |
| 4:3:324:THR:HG21 | 4:5:243:PRO:C | 2.11 | 0.68 |
| 1:A:553:MLY:HG2 | 4:V:47:MET:N | 2.07 | 0.68 |
| 1:A:753:VAL:HG11 | 1:A:775:LEU:CD2 | 2.23 | 0.68 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:F:25:ILE:O | 3:F:63:ILE:HB | 1.92 | 0.68 |
| 1:G:762:HIS:CD2 | 1:G:762:HIS:H | 2.08 | 0.68 |
| 1:G:795:ARG:N | 3:I:118:MET:CE | 2.55 | 0.68 |
| 1:G:797:PHE:CE2 | 3:I:126:LEU:CD1 | 2.76 | 0.68 |
| 3:I:4:LYS:N | 3:I:5:ALA:O | 2.16 | 0.68 |
| 1:M:643:GLY:N | 4:Z:24:ASP:CA | 2.46 | 0.68 |
| 1:M:783:LEU:HG | 1:M:786:ILE:HD11 | 1.73 | 0.68 |
| 1:M:795:ARG:HH22 | 3:O:116:GLU:CD | 1.97 | 0.68 |
| 1:P:797:PHE:CE1 | 3:R:149:VAL:HG11 | 2.27 | 0.68 |
| 4:4:322:PRO:CB | 4:6:244:ASP:CG | 2.54 | 0.68 |
| 1:A:215:GLN:CA | 1:A:340:ILE:CG2 | 2.63 | 0.68 |
| 1:A:630:ALA:O | 4:8:25:ASP:CB | 2.41 | 0.68 |
| 1:A:795:ARG:NH2 | 3:C:116:GLU:HB3 | 2.03 | 0.68 |
| 1:A:818:TYR:HB3 | 2:B:90:GLY:N | 2.07 | 0.68 |
| 3:C:3:SER:O | 3:C:4:LYS:CB | 2.41 | 0.68 |
| 2:E:117:LEU:HD12 | 2:E:147:ASN:CA | 2.20 | 0.68 |
| 2:E:144:VAL:CG1 | 2:E:153:ILE:HD13 | 2.19 | 0.68 |
| 1:G:807:VAL:O | 1:G:810:ARG:HB2 | 1.93 | 0.68 |
| 1:J:533:PHE:O | 1:J:537:GLU:HG2 | 1.93 | 0.68 |
| 1:M:538:GLU:CD | 4:Z:355:MET:HE3 | 2.13 | 0.68 |
| 1:M:817:GLN:HG3 | 2:N:128:PHE:CE1 | 2.27 | 0.68 |
| 1:P:91:MET:HE3 | 1:P:119:SER:HB2 | 1.75 | 0.68 |
| 1:P:213:LYS:HA | 1:P:220:ASP:OD1 | 1.92 | 0.68 |
| 1:P:803:TYR:CE2 | 3:R:17:PHE:CZ | 2.81 | 0.68 |
| 1:P:807:VAL:O | 1:P:810:ARG:HB2 | 1.93 | 0.68 |
| 1:P:810:ARG:HH11 | 1:P:810:ARG:HG2 | 1.57 | 0.68 |
| 3:R:3:SER:O | 3:R:4:LYS:CB | 2.41 | 0.68 |
| 4:3:160:THR:HG21 | 4:3:274:ILE:HD11 | 1.76 | 0.68 |
| 4:4:1:ASP:HA | 4:4:4:GLU:HB3 | 1.74 | 0.68 |
| 4:V:160:THR:HG21 | 4:V:274:ILE:HD11 | 1.76 | 0.68 |
| 1:D:652:LEU:O | 1:D:655:GLU:N | 2.27 | 0.68 |
| 1:D:727:LEU:H | 1:D:782:MLY:CE | 2.06 | 0.68 |
| 1:G:829:TRP:HZ2 | 2:H:83:MET:HE1 | 1.56 | 0.68 |
| 1:J:52:ILE:HD13 | 1:J:52:ILE:N | 2.09 | 0.68 |
| 1:J:769:ALA:HB3 | 1:J:770:GLY:CA | 2.23 | 0.68 |
| 1:M:62:VAL:HG12 | 1:M:63:MLY:O | 1.94 | 0.68 |
| 1:M:732:ILE:CG2 | 1:M:747:LEU:HD11 | 1.26 | 0.68 |
| 1:M:796:GLY:CA | 3:O:35:ARG:HD3 | 2.21 | 0.68 |
| 3:R:48:LYS:C | 3:R:52:ASN:HD21 | 1.96 | 0.68 |
| 4:6:1:ASP:HA | 4:6:4:GLU:HB3 | 1.74 | 0.68 |
| 4:8:160:THR:HG21 | 4:8:274:ILE:HD11 | 1.76 | 0.68 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:213:LYS:HA | 1:D:220:ASP:OD1 | 1.92 | 0.68 |
| 1:D:557:GLU:N | 4:W:48:GLY:HA3 | 1.90 | 0.68 |
| 1:G:538:GLU:CD | 4:V:355:MET:CE | 2.62 | 0.68 |
| 1:G:787:ILE:HG22 | 1:G:788:THR:N | 2.07 | 0.68 |
| 1:J:213:LYS:HA | 1:J:220:ASP:OD1 | 1.92 | 0.68 |
| 1:J:408:VAL:HG12 | 4:W:332:PRO:HB3 | 1.76 | 0.68 |
| 1:J:538:GLU:CD | 4:W:355:MET:CE | 2.62 | 0.68 |
| 1:J:796:GLY:CA | 3:L:35:ARG:HD3 | 2.23 | 0.68 |
| 1:M:802:GLU:OE1 | 1:M:802:GLU:HA | 1.93 | 0.68 |
| 1:M:829:TRP:CZ3 | 2:N:84:PHE:CZ | 2.82 | 0.68 |
| 1:P:802:GLU:OE1 | 1:P:802:GLU:HA | 1.92 | 0.68 |
| 1:A:62:VAL:HG12 | 1:A:63:MLY:O | 1.94 | 0.68 |
| 1:D:553:MLY:HG2 | 4:W:47:MET:N | 2.07 | 0.68 |
| 1:D:712:PRO:HB2 | 1:D:771:LEU:HD22 | 1.75 | 0.68 |
| 3:F:3:SER:O | 3:F:4:LYS:CB | 2.41 | 0.68 |
| 1:G:292:MET:HE3 | 1:G:309:PRO:HA | 1.74 | 0.68 |
| 1:G:754:ASP:OD2 | 1:G:776:GLU:HA | 1.93 | 0.68 |
| 1:J:541:MET:CG | 4:W:345:ILE:O | 2.41 | 0.68 |
| 1:J:630:ALA:O | 4:W:25:ASP:CB | 2.41 | 0.68 |
| 1:J:810:ARG:HG2 | 1:J:810:ARG:HH11 | 1.57 | 0.68 |
| 1:J:821:ARG:HH22 | 2:K:127:ARG:CG | 2.01 | 0.68 |
| 1:M:123:CYS:HB2 | 1:M:158:ILE:CD1 | 2.23 | 0.68 |
| 1:P:533:PHE:O | 1:P:537:GLU:HG2 | 1.93 | 0.68 |
| 1:A:538:GLU:CD | 4:8:355:MET:CE | 2.62 | 0.68 |
| 1:A:813:ILE:HG22 | 2:B:127:ARG:HD3 | 1.75 | 0.68 |
| 3:C:48:LYS:HB3 | 3:C:52:ASN:HD21 | 1.57 | 0.68 |
| 1:D:52:ILE:HD13 | 1:D:52:ILE:N | 2.09 | 0.68 |
| 1:D:91:MET:HE3 | 1:D:119:SER:HB2 | 1.76 | 0.68 |
| 1:D:815:CYS:O | 1:D:819:ASN:HB2 | 1.93 | 0.68 |
| 1:G:802:GLU:OE1 | 1:G:802:GLU:HA | 1.93 | 0.68 |
| 2:H:117:LEU:CB | 2:H:147:ASN:ND2 | 2.35 | 0.68 |
| 1:J:546:THR:H | 1:J:549:SER:HB3 | 1.59 | 0.68 |
| 1:P:166:MET:HE1 | 1:P:254:PHE:HB2 | 1.73 | 0.68 |
| 1:P:797:PHE:CZ | 3:R:146:ILE:HA | 2.29 | 0.68 |
| 1:P:836:PHE:CD2 | 2:Q:160:GLY:N | 2.61 | 0.68 |
| 4:2:153:LEU:HD11 | 4:2:274:ILE:HG13 | 1.76 | 0.68 |
| 1:A:815:CYS:O | 1:A:819:ASN:HB2 | 1.93 | 0.68 |
| 1:D:541:MET:CG | 4:9:345:ILE:O | 2.41 | 0.68 |
| 1:D:798:LEU:HD12 | 3:F:126:LEU:HD21 | 1.76 | 0.68 |
| 1:G:123:CYS:HB2 | 1:G:158:ILE:CD1 | 2.23 | 0.68 |
| 2:H:114:LYS:HA | 2:H:146:GLY:C | 2.03 | 0.68 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:630:ALA:O | 4:Z:25:ASP:CB | 2.41 | 0.68 |
| 1:P:546:THR:H | 1:P:549:SER:HB3 | 1.59 | 0.68 |
| 4:2:1:ASP:HA | 4:2:4:GLU:HB3 | 1.74 | 0.68 |
| 4:4:153:LEU:HD11 | 4:4:274:ILE:HG13 | 1.76 | 0.68 |
| 4:6:153:LEU:HD11 | 4:6:274:ILE:HG13 | 1.76 | 0.68 |
| 1:D:800:ARG:C | 3:F:149:VAL:HG21 | 2.14 | 0.68 |
| 1:G:52:ILE:HD13 | 1:G:52:ILE:N | 2.09 | 0.68 |
| 1:J:802:GLU:OE1 | 1:J:802:GLU:HA | 1.92 | 0.68 |
| 1:P:508:ILE:HD11 | 1:P:759:ALA:HB2 | 1.74 | 0.68 |
| 4:7:153:LEU:HD11 | 4:7:274:ILE:HG13 | 1.76 | 0.68 |
| 4:X:288:ASP:CB | 4:Z:204:ALA:HB1 | 2.24 | 0.68 |
| 4:Y:160:THR:HG21 | 4:Y:274:ILE:HD11 | 1.76 | 0.68 |
| 1:A:166:MET:HE3 | 1:A:254:PHE:CD2 | 2.29 | 0.68 |
| 1:D:408:VAL:HG12 | 4:9:332:PRO:HB3 | 1.76 | 0.68 |
| 1:D:538:GLU:CD | 4:9:355:MET:CE | 2.62 | 0.68 |
| 1:D:546:THR:H | 1:D:549:SER:HB3 | 1.59 | 0.68 |
| 1:D:798:LEU:CD1 | 3:F:126:LEU:HD21 | 2.24 | 0.68 |
| 1:M:52:ILE:HD13 | 1:M:52:ILE:N | 2.09 | 0.68 |
| 1:P:795:ARG:HH22 | 3:R:116:GLU:CG | 2.04 | 0.68 |
| 1:P:819:ASN:CG | 2:Q:90:GLY:O | 2.32 | 0.68 |
| 4:X:160:THR:HG21 | 4:X:274:ILE:HD11 | 1.76 | 0.68 |
| 2:B:117:LEU:CG | 2:B:147:ASN:HB3 | 2.24 | 0.67 |
| 1:D:630:ALA:O | 4:9:25:ASP:HB2 | 1.92 | 0.67 |
| 1:D:642:LYS:HB3 | 4:9:21:PHE:O | 1.93 | 0.67 |
| 1:G:550:PHE:HE2 | 1:G:592:ILE:HG23 | 1.59 | 0.67 |
| 3:L:102:VAL:HG23 | 3:L:139:TYR:HD1 | 1.60 | 0.67 |
| 1:M:795:ARG:HH21 | 3:O:116:GLU:HB3 | 0.51 | 0.67 |
| 1:M:819:ASN:CG | 2:N:90:GLY:O | 2.32 | 0.67 |
| 1:P:408:VAL:HG12 | 4:1:332:PRO:HB3 | 1.76 | 0.67 |
| 1:A:290:GLN:O | 1:A:331:LEU:HD12 | 1.95 | 0.67 |
| 1:A:505:MLY:CD | 1:A:762:HIS:CD2 | 2.77 | 0.67 |
| 1:D:800:ARG:HB3 | 3:F:149:VAL:CG2 | 2.24 | 0.67 |
| 1:G:612:GLN:NE2 | 1:G:627:GLY:N | 2.43 | 0.67 |
| 1:G:732:ILE:HG21 | 1:G:747:LEU:HD11 | 0.72 | 0.67 |
| 1:G:797:PHE:HE2 | 3:I:126:LEU:CD1 | 2.07 | 0.67 |
| 1:G:834:LEU:HD22 | 2:H:34:ILE:CD1 | 2.24 | 0.67 |
| 1:J:710:GLY:C | 1:J:772:LEU:HD22 | 2.14 | 0.67 |
| 1:J:817:GLN:CG | 2:K:127:ARG:CG | 2.70 | 0.67 |
| 1:M:533:PHE:O | 1:M:537:GLU:HG2 | 1.93 | 0.67 |
| 1:M:652:LEU:O | 1:M:655:GLU:N | 2.27 | 0.67 |
| 1:M:795:ARG:CG | 3:O:118:MET:HE1 | 2.24 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:O:3:SER:O | 3:O:4:LYS:CB | 2.41 | 0.67 |
| 1:P:93:MET:CA | 1:P:713:SER:HA | 2.24 | 0.67 |
| 4:1:247:VAL:N | 4:Y:324:THR:CG2 | 2.58 | 0.67 |
| 4:W:160:THR:HG21 | 4:W:274:ILE:HD11 | 1.76 | 0.67 |
| 4:X:287:ILE:N | 4:Z:202:THR:HG23 | 1.86 | 0.67 |
| 1:A:550:PHE:HE2 | 1:A:592:ILE:HG23 | 1.59 | 0.67 |
| 1:A:807:VAL:O | 1:A:810:ARG:HB2 | 1.93 | 0.67 |
| 2:B:141:PRO:O | 2:B:145:ALA:CB | 2.43 | 0.67 |
| 3:I:102:VAL:HG23 | 3:I:139:TYR:HD1 | 1.60 | 0.67 |
| 1:J:732:ILE:HG21 | 1:J:747:LEU:HD11 | 0.73 | 0.67 |
| 1:J:787:ILE:HG22 | 1:J:788:THR:N | 2.07 | 0.67 |
| 2:K:117:LEU:CG | 2:K:147:ASN:HB3 | 2.24 | 0.67 |
| 1:M:290:GLN:O | 1:M:331:LEU:HD12 | 1.95 | 0.67 |
| 1:M:550:PHE:HE2 | 1:M:592:ILE:HG23 | 1.59 | 0.67 |
| 4:1:166:TYR:CZ | 4:3:64:ILE:HG21 | 2.29 | 0.67 |
| 4:X:153:LEU:HD11 | 4:X:274:ILE:HG13 | 1.76 | 0.67 |
| 4:Z:160:THR:HG21 | 4:Z:274:ILE:HD11 | 1.76 | 0.67 |
| 1:A:58:GLY:HA2 | 1:A:74:GLU:OE1 | 1.94 | 0.67 |
| 1:D:290:GLN:O | 1:D:331:LEU:HD12 | 1.95 | 0.67 |
| 1:D:630:ALA:O | 4:9:25:ASP:CB | 2.41 | 0.67 |
| 1:G:62:VAL:HG12 | 1:G:63:MLY:O | 1.94 | 0.67 |
| 1:G:642:LYS:HB3 | 4:V:21:PHE:O | 1.92 | 0.67 |
| 1:J:215:GLN:HA | 1:J:340:ILE:CB | 2.23 | 0.67 |
| 1:J:792:ALA:CA | 3:L:42:THR:CA | 2.72 | 0.67 |
| 3:R:102:VAL:HG23 | 3:R:139:TYR:HD1 | 1.60 | 0.67 |
| 4:Z:153:LEU:HD11 | 4:Z:274:ILE:HG13 | 1.76 | 0.67 |
| 1:A:123:CYS:HB2 | 1:A:158:ILE:CD1 | 2.23 | 0.67 |
| 1:D:58:GLY:HA2 | 1:D:74:GLU:OE1 | 1.95 | 0.67 |
| 1:D:166:MET:HE3 | 1:D:254:PHE:CD2 | 2.29 | 0.67 |
| 2:E:117:LEU:CB | 2:E:147:ASN:OD1 | 2.39 | 0.67 |
| 1:G:752:ASP:O | 1:G:780:ASP:CG | 2.33 | 0.67 |
| 1:J:643:GLY:N | 4:W:24:ASP:CA | 2.46 | 0.67 |
| 1:M:826:VAL:HG21 | 2:N:88:LEU:HD23 | 1.76 | 0.67 |
| 1:P:202:SER:HA | 1:P:207:LYS:HE3 | 1.72 | 0.67 |
| 1:P:217:THR:O | 1:P:221:GLN:HG2 | 1.95 | 0.67 |
| 1:P:480:ILE:HG22 | 1:P:481:ASN:ND2 | 2.09 | 0.67 |
| 1:P:797:PHE:CD1 | 3:R:149:VAL:HG11 | 2.29 | 0.67 |
| 1:P:838:ILE:HD11 | 2:Q:54:MET:SD | 2.35 | 0.67 |
| 1:A:28:GLN:HE22 | 1:A:723:ARG:NH2 | 1.88 | 0.67 |
| 1:A:652:LEU:O | 1:A:655:GLU:N | 2.27 | 0.67 |
| 1:D:62:VAL:HG12 | 1:D:63:MLY:O | 1.94 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:E:141:PRO:O | 2:E:145:ALA:CB | 2.43 | 0.67 |
| 3:F:49:ILE:HA | 3:F:52:ASN:ND2 | 2.05 | 0.67 |
| 1:G:290:GLN:O | 1:G:331:LEU:HD12 | 1.95 | 0.67 |
| 1:J:62:VAL:HG12 | 1:J:63:MLY:O | 1.94 | 0.67 |
| 1:J:480:ILE:HG22 | 1:J:481:ASN:ND2 | 2.09 | 0.67 |
| 1:M:544:LYS:HD3 | 4:2:45:VAL:HG21 | 1.76 | 0.67 |
| 1:M:546:THR:H | 1:M:549:SER:HB3 | 1.60 | 0.67 |
| 1:M:815:CYS:O | 1:M:819:ASN:HB2 | 1.93 | 0.67 |
| 2:N:117:LEU:CG | 2:N:147:ASN:HB3 | 2.25 | 0.67 |
| 1:P:58:GLY:HA2 | 1:P:74:GLU:OE1 | 1.95 | 0.67 |
| 4:9:160:THR:HG21 | 4:9:274:ILE:HD11 | 1.76 | 0.67 |
| 4:V:153:LEU:HD11 | 4:V:274:ILE:HG13 | 1.76 | 0.67 |
| 1:D:217:THR:O | 1:D:221:GLN:HG2 | 1.95 | 0.67 |
| 1:D:480:ILE:HG22 | 1:D:481:ASN:ND2 | 2.09 | 0.67 |
| 1:D:538:GLU:CD | 4:9:355:MET:HE1 | 2.12 | 0.67 |
| 1:G:813:ILE:CG2 | 2:H:128:PHE:HE1 | 2.05 | 0.67 |
| 1:J:58:GLY:HA2 | 1:J:74:GLU:OE1 | 1.95 | 0.67 |
| 1:M:131:TRP:O | 1:M:132:LEU:HD12 | 1.95 | 0.67 |
| 2:N:141:PRO:O | 2:N:145:ALA:CB | 2.43 | 0.67 |
| 3:O:102:VAL:HG23 | 3:O:139:TYR:HD1 | 1.60 | 0.67 |
| 1:P:52:ILE:HD13 | 1:P:52:ILE:N | 2.09 | 0.67 |
| 1:D:374:GLN:HG3 | 1:D:375:ALA:H | 1.60 | 0.67 |
| 1:D:648:THR:CB | 4:9:350:SER:OG | 2.43 | 0.67 |
| 3:F:102:VAL:HG23 | 3:F:139:TYR:HD1 | 1.60 | 0.67 |
| 1:G:58:GLY:HA2 | 1:G:74:GLU:OE1 | 1.95 | 0.67 |
| 1:G:538:GLU:CD | 4:V:355:MET:HE3 | 2.14 | 0.67 |
| 1:J:537:GLU:C | 4:W:351:THR:H | 1.98 | 0.67 |
| 1:M:58:GLY:HA2 | 1:M:74:GLU:OE1 | 1.95 | 0.67 |
| 1:M:408:VAL:HG12 | 4:Z:332:PRO:HB3 | 1.76 | 0.67 |
| 1:M:783:LEU:C | 1:M:786:ILE:HG13 | 2.14 | 0.67 |
| 1:P:648:THR:CB | 4:1:350:SER:OG | 2.43 | 0.67 |
| 1:P:707:CYS:O | 1:P:710:GLY:CA | 2.42 | 0.67 |
| 4:3:287:ILE:HG22 | 4:5:204:ALA:HB3 | 1.76 | 0.67 |
| 4:9:153:LEU:HD11 | 4:9:274:ILE:HG13 | 1.76 | 0.67 |
| 1:A:642:LYS:CD | 4:8:24:ASP:O | 2.42 | 0.67 |
| 1:D:732:ILE:HG22 | 1:D:747:LEU:CD1 | 1.55 | 0.67 |
| 1:G:97:LEU:HD21 | 1:G:712:PRO:CB | 2.24 | 0.67 |
| 1:G:215:GLN:HA | 1:G:340:ILE:CB | 2.23 | 0.67 |
| 1:G:652:LEU:O | 1:G:655:GLU:N | 2.27 | 0.67 |
| 1:J:538:GLU:CD | 4:W:355:MET:HE1 | 2.12 | 0.67 |
| 2:K:141:PRO:O | 2:K:145:ALA:CB | 2.43 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:480:ILE:HG22 | 1:M:481:ASN:ND2 | 2.10 | 0.67 |
| 1:M:537:GLU:C | 4:Z:351:THR:H | 1.98 | 0.67 |
| 1:M:791:GLN:HE22 | 3:O:115:GLY:CA | 2.08 | 0.67 |
| 1:P:550:PHE:HE2 | 1:P:592:ILE:HG23 | 1.59 | 0.67 |
| 4:5:160:THR:HG21 | 4:5:274:ILE:HD11 | 1.76 | 0.67 |
| 1:A:501:GLU:HG2 | 1:A:762:HIS:CE1 | 2.25 | 0.67 |
| 1:A:533:PHE:O | 1:A:537:GLU:HG2 | 1.93 | 0.67 |
| 1:A:546:THR:H | 1:A:549:SER:HB3 | 1.60 | 0.67 |
| 1:A:553:MLY:CG | 4:V:47:MET:N | 2.54 | 0.67 |
| 1:D:831:TRP:CZ2 | 2:E:47:LEU:HB3 | 2.24 | 0.67 |
| 1:G:339:ASP:OD1 | 1:G:348:MLY:HH13 | 1.95 | 0.67 |
| 1:G:546:THR:H | 1:G:549:SER:HB3 | 1.60 | 0.67 |
| 3:I:24:LYS:HA | 3:I:63:ILE:O | 1.95 | 0.67 |
| 3:L:24:LYS:HA | 3:L:63:ILE:O | 1.95 | 0.67 |
| 1:M:215:GLN:HA | 1:M:340:ILE:CB | 2.23 | 0.67 |
| 1:P:62:VAL:HG12 | 1:P:63:MLY:O | 1.94 | 0.67 |
| 1:P:818:TYR:CE1 | 2:Q:127:ARG:NH1 | 2.62 | 0.67 |
| 2:Q:141:PRO:O | 2:Q:145:ALA:CB | 2.43 | 0.67 |
| 4:3:287:ILE:CD1 | 4:5:203:THR:HB | 2.19 | 0.67 |
| 1:A:131:TRP:O | 1:A:132:LEU:HD12 | 1.95 | 0.66 |
| 1:A:817:GLN:HG3 | 2:B:127:ARG:HB3 | 1.77 | 0.66 |
| 1:D:418:THR:HG22 | 1:D:419:VAL:N | 2.11 | 0.66 |
| 1:G:505:MLY:HH22 | 1:G:762:HIS:HE1 | 0.50 | 0.66 |
| 1:G:753:VAL:C | 1:G:779:ARG:HH11 | 1.89 | 0.66 |
| 1:G:831:TRP:HZ3 | 2:H:34:ILE:HG21 | 1.60 | 0.66 |
| 1:J:131:TRP:O | 1:J:132:LEU:HD12 | 1.95 | 0.66 |
| 1:J:217:THR:O | 1:J:221:GLN:HG2 | 1.95 | 0.66 |
| 1:J:550:PHE:HE2 | 1:J:592:ILE:HG23 | 1.59 | 0.66 |
| 1:J:648:THR:CB | 4:W:350:SER:OG | 2.43 | 0.66 |
| 3:L:3:SER:O | 3:L:4:LYS:CB | 2.41 | 0.66 |
| 1:M:174:SER:O | 1:M:670:HIS:HB2 | 1.95 | 0.66 |
| 1:M:612:GLN:NE2 | 1:M:627:GLY:N | 2.43 | 0.66 |
| 1:M:635:GLY:O | 4:Z:341:ILE:HG21 | 1.95 | 0.66 |
| 1:M:648:THR:CB | 4:Z:350:SER:OG | 2.43 | 0.66 |
| 1:P:166:MET:HE3 | 1:P:254:PHE:HD2 | 1.61 | 0.66 |
| 4:2:160:THR:HG21 | 4:2:274:ILE:HD11 | 1.76 | 0.66 |
| 1:A:339:ASP:OD1 | 1:A:348:MLY:HH13 | 1.95 | 0.66 |
| 1:A:612:GLN:NE2 | 1:A:627:GLY:N | 2.43 | 0.66 |
| 3:C:24:LYS:HA | 3:C:63:ILE:O | 1.95 | 0.66 |
| 1:D:61:THR:HG23 | 1:D:71:THR:OG1 | 1.95 | 0.66 |
| 1:D:530:MET:HE2 | 4:9:354:GLN:HG3 | 1.76 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:537:GLU:C | 4:9:351:THR:H | 1.98 | 0.66 |
| 1:D:550:PHE:HE2 | 1:D:592:ILE:HG23 | 1.59 | 0.66 |
| 1:G:541:MET:O | 4:V:143:TYR:OH | 2.14 | 0.66 |
| 1:G:829:TRP:CH2 | 2:H:84:PHE:CE1 | 2.83 | 0.66 |
| 1:P:541:MET:HG2 | 4:1:345:ILE:C | 2.16 | 0.66 |
| 2:Q:117:LEU:CG | 2:Q:147:ASN:HB3 | 2.24 | 0.66 |
| 4:1:160:THR:HG21 | 4:1:274:ILE:HD11 | 1.76 | 0.66 |
| 4:7:160:THR:HG21 | 4:7:274:ILE:HD11 | 1.76 | 0.66 |
| 4:W:153:LEU:HD11 | 4:W:274:ILE:HG13 | 1.76 | 0.66 |
| 1:A:78:PHE:HB3 | 1:A:98:HIS:CD2 | 2.30 | 0.66 |
| 1:A:505:MLY:N | 1:A:762:HIS:NE2 | 2.43 | 0.66 |
| 1:A:537:GLU:C | 4:8:351:THR:H | 1.99 | 0.66 |
| 1:A:599:ASN:OD1 | 1:A:649:VAL:N | 2.29 | 0.66 |
| 1:A:732:ILE:HG22 | 1:A:747:LEU:CD1 | 1.55 | 0.66 |
| 1:D:131:TRP:O | 1:D:132:LEU:HD12 | 1.95 | 0.66 |
| 1:G:78:PHE:HB3 | 1:G:98:HIS:CD2 | 2.30 | 0.66 |
| 1:G:732:ILE:HG22 | 1:G:747:LEU:CD1 | 1.55 | 0.66 |
| 1:G:783:LEU:O | 1:G:787:ILE:CA | 2.43 | 0.66 |
| 1:J:226:ASN:HB2 | 1:J:227:PRO:HD3 | 1.77 | 0.66 |
| 4:6:160:THR:HG21 | 4:6:274:ILE:HD11 | 1.76 | 0.66 |
| 1:A:408:VAL:HG12 | 4:8:332:PRO:HB3 | 1.76 | 0.66 |
| 1:A:498:LEU:HD21 | 1:A:764:MLY:CH2 | 2.18 | 0.66 |
| 1:A:502:GLU:C | 1:A:761:GLY:HA3 | 2.15 | 0.66 |
| 1:A:648:THR:CB | 4:8:350:SER:OG | 2.43 | 0.66 |
| 2:E:117:LEU:CG | 2:E:147:ASN:HB3 | 2.25 | 0.66 |
| 1:G:131:TRP:O | 1:G:132:LEU:HD12 | 1.95 | 0.66 |
| 1:G:174:SER:O | 1:G:670:HIS:HB2 | 1.96 | 0.66 |
| 1:G:830:PRO:HB3 | 2:H:67:MET:CE | 2.15 | 0.66 |
| 1:G:830:PRO:CG | 2:H:67:MET:HE2 | 2.26 | 0.66 |
| 1:J:174:SER:O | 1:J:670:HIS:HB2 | 1.96 | 0.66 |
| 1:M:166:MET:HE3 | 1:M:254:PHE:CD2 | 2.31 | 0.66 |
| 3:O:48:LYS:C | 3:O:52:ASN:HD21 | 1.96 | 0.66 |
| 1:P:290:GLN:O | 1:P:331:LEU:HD12 | 1.95 | 0.66 |
| 1:P:732:ILE:HG21 | 1:P:747:LEU:HD11 | 0.73 | 0.66 |
| 4:Y:153:LEU:HD11 | 4:Y:274:ILE:HG13 | 1.76 | 0.66 |
| 1:A:93:MET:HE2 | 1:A:715:VAL:HA | 0.78 | 0.66 |
| 1:D:78:PHE:HB3 | 1:D:98:HIS:CD2 | 2.30 | 0.66 |
| 2:E:141:PRO:O | 2:E:145:ALA:HB2 | 1.96 | 0.66 |
| 1:J:599:ASN:OD1 | 1:J:649:VAL:N | 2.29 | 0.66 |
| 1:J:797:PHE:CZ | 3:L:126:LEU:HD22 | 2.29 | 0.66 |
| 1:P:728:ASN:OD1 | 3:R:93:VAL:HG13 | 1.94 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:174:SER:O | 1:A:670:HIS:HB2 | 1.96 | 0.66 |
| 1:A:798:LEU:CD1 | 3:C:126:LEU:CD2 | 2.53 | 0.66 |
| 1:G:84:MLY:HG2 | 1:G:723:ARG:CG | 2.24 | 0.66 |
| 1:G:93:MET:SD | 1:G:715:VAL:CA | 2.83 | 0.66 |
| 1:G:754:ASP:CB | 1:G:776:GLU:OE1 | 2.36 | 0.66 |
| 1:G:754:ASP:C | 1:G:776:GLU:OE1 | 2.33 | 0.66 |
| 1:G:784:ALA:O | 1:G:788:THR:HB | 1.94 | 0.66 |
| 1:G:795:ARG:HB3 | 3:I:35:ARG:HH12 | 1.60 | 0.66 |
| 1:G:823:PHE:CE1 | 2:H:156:VAL:O | 2.49 | 0.66 |
| 1:J:541:MET:HG2 | 4:W:345:ILE:C | 2.16 | 0.66 |
| 1:J:612:GLN:NE2 | 1:J:627:GLY:N | 2.43 | 0.66 |
| 1:M:339:ASP:OD1 | 1:M:348:MLY:HH13 | 1.95 | 0.66 |
| 1:M:599:ASN:OD1 | 1:M:649:VAL:N | 2.29 | 0.66 |
| 1:P:131:TRP:O | 1:P:132:LEU:HD12 | 1.95 | 0.66 |
| 1:P:418:THR:HG22 | 1:P:419:VAL:N | 2.11 | 0.66 |
| 3:R:49:ILE:HA | 3:R:52:ASN:ND2 | 2.06 | 0.66 |
| 4:1:244:ASP:N | 4:Y:291:LYS:HG3 | 2.05 | 0.66 |
| 4:2:203:THR:HB | 4:Z:287:ILE:CD1 | 2.25 | 0.66 |
| 4:4:160:THR:HG21 | 4:4:274:ILE:HD11 | 1.76 | 0.66 |
| 1:D:166:MET:HE3 | 1:D:254:PHE:HD2 | 1.61 | 0.66 |
| 1:D:174:SER:O | 1:D:670:HIS:HB2 | 1.96 | 0.66 |
| 1:D:599:ASN:OD1 | 1:D:649:VAL:N | 2.29 | 0.66 |
| 1:G:322:VAL:HB | 1:G:325:ILE:CD1 | 2.26 | 0.66 |
| 1:G:635:GLY:O | 4:V:341:ILE:HG21 | 1.95 | 0.66 |
| 1:G:819:ASN:CG | 2:H:90:GLY:O | 2.32 | 0.66 |
| 2:H:141:PRO:O | 2:H:145:ALA:CB | 2.43 | 0.66 |
| 1:J:166:MET:HE3 | 1:J:254:PHE:CD2 | 2.30 | 0.66 |
| 1:J:418:THR:HG22 | 1:J:419:VAL:N | 2.11 | 0.66 |
| 1:J:567:LYS:NZ | 4:Y:92:ASN:HA | 2.10 | 0.66 |
| 1:M:61:THR:HG23 | 1:M:71:THR:OG1 | 1.95 | 0.66 |
| 1:M:530:MET:HE2 | 4:Z:354:GLN:HG3 | 1.77 | 0.66 |
| 1:M:786:ILE:HB | 1:M:787:ILE:N | 2.11 | 0.66 |
| 1:M:831:TRP:CZ2 | 2:N:47:LEU:CD2 | 2.74 | 0.66 |
| 1:P:226:ASN:HB2 | 1:P:227:PRO:HD3 | 1.77 | 0.66 |
| 1:P:537:GLU:C | 4:1:351:THR:H | 1.98 | 0.66 |
| 1:P:635:GLY:O | 4:1:341:ILE:HG21 | 1.95 | 0.66 |
| 4:1:153:LEU:HD11 | 4:1:274:ILE:HG13 | 1.76 | 0.66 |
| 4:8:153:LEU:HD11 | 4:8:274:ILE:HG13 | 1.76 | 0.66 |
| 4:V:324:THR:HG23 | 4:X:247:VAL:H | 1.61 | 0.66 |
| 1:A:149:GLN:CB | 1:A:718:ALA:C | 2.58 | 0.66 |
| 2:B:141:PRO:O | 2:B:145:ALA:HB2 | 1.96 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:612:GLN:NE2 | 1:D:627:GLY:N | 2.43 | 0.66 |
| 1:G:61:THR:HG23 | 1:G:71:THR:OG1 | 1.94 | 0.66 |
| 1:G:408:VAL:HG12 | 4:V:332:PRO:HB3 | 1.76 | 0.66 |
| 1:G:466:GLY:HA2 | 1:G:484:ASN:HD21 | 1.61 | 0.66 |
| 1:G:502:GLU:OE2 | 1:G:761:GLY:CA | 2.44 | 0.66 |
| 1:G:537:GLU:C | 4:V:351:THR:H | 1.99 | 0.66 |
| 1:G:546:THR:HG22 | 1:G:548:THR:N | 2.05 | 0.66 |
| 1:J:78:PHE:HB3 | 1:J:98:HIS:CD2 | 2.30 | 0.66 |
| 1:J:93:MET:HG2 | 1:J:715:VAL:HA | 1.77 | 0.66 |
| 1:J:530:MET:CA | 4:W:354:GLN:CB | 2.74 | 0.66 |
| 1:J:635:GLY:O | 4:W:341:ILE:HG21 | 1.95 | 0.66 |
| 1:M:217:THR:O | 1:M:221:GLN:HG2 | 1.95 | 0.66 |
| 1:M:322:VAL:HB | 1:M:325:ILE:CD1 | 2.26 | 0.66 |
| 1:M:530:MET:CA | 4:Z:354:GLN:CB | 2.74 | 0.66 |
| 1:M:541:MET:HG2 | 4:Z:345:ILE:C | 2.16 | 0.66 |
| 1:M:804:ARG:O | 1:M:808:GLU:N | 2.27 | 0.66 |
| 1:P:61:THR:HG23 | 1:P:71:THR:OG1 | 1.95 | 0.66 |
| 1:P:174:SER:O | 1:P:670:HIS:HB2 | 1.96 | 0.66 |
| 1:P:839:MLY:HH21 | 2:Q:158:THR:HG22 | 1.78 | 0.66 |
| 3:R:24:LYS:HA | 3:R:63:ILE:O | 1.95 | 0.66 |
| 4:1:247:VAL:H | 4:Y:324:THR:CB | 2.08 | 0.66 |
| 1:A:792:ALA:CB | 3:C:42:THR:CG2 | 2.53 | 0.66 |
| 3:C:102:VAL:HG23 | 3:C:139:TYR:HD1 | 1.60 | 0.66 |
| 1:G:161:ASN:O | 1:G:165:PHE:HB2 | 1.96 | 0.66 |
| 1:G:418:THR:HG22 | 1:G:419:VAL:N | 2.11 | 0.66 |
| 1:G:817:GLN:HG3 | 2:H:128:PHE:CZ | 2.31 | 0.66 |
| 1:G:838:ILE:CG1 | 2:H:54:MET:HE1 | 2.25 | 0.66 |
| 1:J:94:MET:O | 1:J:713:SER:CA | 2.43 | 0.66 |
| 1:J:290:GLN:O | 1:J:331:LEU:HD12 | 1.95 | 0.66 |
| 1:J:538:GLU:HA | 4:W:349:LEU:HB3 | 1.78 | 0.66 |
| 1:M:226:ASN:HB2 | 1:M:227:PRO:HD3 | 1.78 | 0.66 |
| 1:M:466:GLY:HA2 | 1:M:484:ASN:HD21 | 1.61 | 0.66 |
| 1:M:642:LYS:CD | 4:Z:24:ASP:O | 2.43 | 0.66 |
| 1:P:612:GLN:NE2 | 1:P:627:GLY:N | 2.43 | 0.66 |
| 4:1:202:THR:OG1 | 4:Y:286:ASP:OD1 | 2.14 | 0.66 |
| 4:4:288:ASP:CB | 4:6:203:THR:HG21 | 2.25 | 0.66 |
| 1:A:635:GLY:O | 4:8:341:ILE:HG21 | 1.95 | 0.66 |
| 1:D:507:GLY:HA2 | 1:D:762:HIS:CG | 2.31 | 0.66 |
| 1:G:557:GLU:HB2 | 4:X:47:MET:N | 2.11 | 0.66 |
| 1:G:818:TYR:CD1 | 2:H:127:ARG:NH1 | 2.63 | 0.66 |
| 1:G:831:TRP:HE1 | 2:H:67:MET:CB | 1.97 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:831:TRP:CZ3 | 2:H:34:ILE:HG21 | 2.31 | 0.66 |
| 2:H:117:LEU:CG | 2:H:147:ASN:HB3 | 2.25 | 0.66 |
| 1:J:374:GLN:HG3 | 1:J:375:ALA:H | 1.59 | 0.66 |
| 1:J:642:LYS:CD | 4:W:24:ASP:O | 2.43 | 0.66 |
| 1:M:374:GLN:HG3 | 1:M:375:ALA:H | 1.59 | 0.66 |
| 1:M:418:THR:HG22 | 1:M:419:VAL:N | 2.11 | 0.66 |
| 1:P:480:ILE:HG22 | 1:P:481:ASN:N | 2.12 | 0.66 |
| 1:A:144:ARG:NH1 | 1:A:160:ASP:OD1 | 2.29 | 0.65 |
| 1:A:541:MET:O | 4:8:143:TYR:OH | 2.14 | 0.65 |
| 1:A:612:GLN:HE22 | 1:A:627:GLY:N | 1.94 | 0.65 |
| 1:A:793:ARG:HH21 | 3:C:147:MET:HE1 | 1.59 | 0.65 |
| 2:B:146:GLY:O | 2:B:147:ASN:HB2 | 1.96 | 0.65 |
| 1:D:161:ASN:O | 1:D:165:PHE:HB2 | 1.96 | 0.65 |
| 1:D:480:ILE:HG22 | 1:D:481:ASN:N | 2.11 | 0.65 |
| 1:G:226:ASN:HB2 | 1:G:227:PRO:HD3 | 1.78 | 0.65 |
| 1:G:374:GLN:HG3 | 1:G:375:ALA:H | 1.60 | 0.65 |
| 1:G:795:ARG:NH2 | 3:I:116:GLU:CB | 2.56 | 0.65 |
| 1:G:831:TRP:CH2 | 2:H:47:LEU:HD22 | 2.20 | 0.65 |
| 1:M:791:GLN:NE2 | 3:O:116:GLU:H | 1.93 | 0.65 |
| 1:P:296:MLY:HH11 | 1:P:348:MLY:HH21 | 1.79 | 0.65 |
| 1:A:322:VAL:HB | 1:A:325:ILE:CD1 | 2.26 | 0.65 |
| 1:A:418:THR:HG22 | 1:A:419:VAL:N | 2.11 | 0.65 |
| 1:A:480:ILE:HG22 | 1:A:481:ASN:ND2 | 2.10 | 0.65 |
| 1:A:754:ASP:OD2 | 1:A:774:LEU:CD2 | 2.43 | 0.65 |
| 1:D:507:GLY:HA2 | 1:D:762:HIS:ND1 | 2.11 | 0.65 |
| 1:D:530:MET:CA | 4:9:354:GLN:CB | 2.74 | 0.65 |
| 3:F:24:LYS:HA | 3:F:63:ILE:O | 1.95 | 0.65 |
| 1:G:217:THR:O | 1:G:221:GLN:HG2 | 1.95 | 0.65 |
| 1:G:739:ASP:CB | 1:G:742:LYS:HB3 | 2.12 | 0.65 |
| 1:G:823:PHE:HE1 | 2:H:160:GLY:HA2 | 1.61 | 0.65 |
| 3:I:48:LYS:O | 3:I:52:ASN:CG | 2.34 | 0.65 |
| 1:J:61:THR:HG23 | 1:J:71:THR:OG1 | 1.95 | 0.65 |
| 1:J:161:ASN:O | 1:J:165:PHE:HB2 | 1.96 | 0.65 |
| 1:M:78:PHE:HB3 | 1:M:98:HIS:CD2 | 2.30 | 0.65 |
| 2:N:117:LEU:HD11 | 2:N:147:ASN:HB3 | 1.76 | 0.65 |
| 1:P:78:PHE:HB3 | 1:P:98:HIS:CD2 | 2.30 | 0.65 |
| 1:P:530:MET:CA | 4:1:354:GLN:CB | 2.74 | 0.65 |
| 1:P:642:LYS:CD | 4:1:24:ASP:O | 2.43 | 0.65 |
| 4:2:288:ASP:H | 4:4:203:THR:CG2 | 2.08 | 0.65 |
| 1:A:149:GLN:HG2 | 1:A:719:ASP:CG | 2.13 | 0.65 |
| 1:A:161:ASN:O | 1:A:165:PHE:HB2 | 1.96 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:501:GLU:CG | 1:A:762:HIS:ND1 | 2.42 | 0.65 |
| 1:A:541:MET:HG2 | 4:8:345:ILE:C | 2.16 | 0.65 |
| 1:A:818:TYR:HB2 | 2:B:90:GLY:N | 2.11 | 0.65 |
| 3:C:3:SER:HG | 3:C:5:ALA:N | 1.95 | 0.65 |
| 1:D:541:MET:HG2 | 4:9:345:ILE:C | 2.16 | 0.65 |
| 1:D:797:PHE:CE1 | 3:F:146:ILE:CB | 2.79 | 0.65 |
| 1:D:798:LEU:CG | 3:F:126:LEU:HD11 | 2.21 | 0.65 |
| 1:J:295:MLY:HG3 | 1:J:332:MET:HE1 | 1.78 | 0.65 |
| 1:J:480:ILE:HG22 | 1:J:481:ASN:N | 2.11 | 0.65 |
| 1:J:691:VAL:O | 1:J:695:LEU:HD13 | 1.97 | 0.65 |
| 1:M:466:GLY:HA2 | 1:M:484:ASN:ND2 | 2.12 | 0.65 |
| 1:M:691:VAL:O | 1:M:695:LEU:HD13 | 1.97 | 0.65 |
| 1:M:820:VAL:CG1 | 2:N:136:MET:CE | 2.74 | 0.65 |
| 1:P:374:GLN:HG3 | 1:P:375:ALA:H | 1.59 | 0.65 |
| 1:A:691:VAL:O | 1:A:695:LEU:HD13 | 1.97 | 0.65 |
| 1:D:107:MLY:HB3 | 1:D:686:MET:CE | 2.26 | 0.65 |
| 1:D:724:TYR:CA | 1:D:782:MLY:CD | 2.73 | 0.65 |
| 3:F:45:GLU:O | 3:F:49:ILE:HG13 | 1.97 | 0.65 |
| 3:F:48:LYS:O | 3:F:52:ASN:CG | 2.34 | 0.65 |
| 1:G:480:ILE:HG22 | 1:G:481:ASN:ND2 | 2.10 | 0.65 |
| 1:G:599:ASN:OD1 | 1:G:649:VAL:N | 2.28 | 0.65 |
| 1:G:648:THR:CB | 4:V:350:SER:OG | 2.44 | 0.65 |
| 1:G:691:VAL:O | 1:G:695:LEU:HD13 | 1.97 | 0.65 |
| 1:M:292:MET:HE3 | 1:M:309:PRO:HA | 1.77 | 0.65 |
| 1:M:735:GLY:O | 1:M:743:ALA:HA | 1.94 | 0.65 |
| 1:M:798:LEU:HD23 | 3:O:122:GLU:HB3 | 1.79 | 0.65 |
| 1:M:822:SER:O | 1:M:825:ASN:HB2 | 1.97 | 0.65 |
| 1:P:691:VAL:O | 1:P:695:LEU:HD13 | 1.97 | 0.65 |
| 4:4:288:ASP:OD2 | 4:6:203:THR:CB | 2.42 | 0.65 |
| 1:D:144:ARG:NH1 | 1:D:160:ASP:OD1 | 2.29 | 0.65 |
| 1:D:339:ASP:OD1 | 1:D:348:MLY:HH13 | 1.95 | 0.65 |
| 1:G:725:ARG:NE | 1:G:737:PHE:HE1 | 1.95 | 0.65 |
| 3:I:45:GLU:O | 3:I:49:ILE:HG13 | 1.97 | 0.65 |
| 2:K:144:VAL:CG1 | 2:K:153:ILE:HD13 | 2.20 | 0.65 |
| 3:L:3:SER:HG | 3:L:5:ALA:N | 1.95 | 0.65 |
| 1:M:530:MET:CG | 4:Z:354:GLN:CG | 2.72 | 0.65 |
| 1:M:541:MET:O | 4:Z:143:TYR:OH | 2.14 | 0.65 |
| 4:1:287:ILE:CG1 | 4:3:203:THR:HB | 2.27 | 0.65 |
| 1:A:642:LYS:HA | 4:8:21:PHE:O | 1.96 | 0.65 |
| 1:A:797:PHE:CZ | 3:C:146:ILE:HD12 | 2.02 | 0.65 |
| 1:D:322:VAL:HB | 1:D:325:ILE:CD1 | 2.26 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:541:MET:O | 4:9:143:TYR:OH | 2.14 | 0.65 |
| 1:D:691:VAL:O | 1:D:695:LEU:HD13 | 1.97 | 0.65 |
| 3:F:3:SER:HG | 3:F:5:ALA:N | 1.95 | 0.65 |
| 3:F:48:LYS:C | 3:F:52:ASN:HD21 | 1.97 | 0.65 |
| 1:G:144:ARG:NH1 | 1:G:160:ASP:OD1 | 2.29 | 0.65 |
| 1:G:505:MLY:HH23 | 1:G:762:HIS:CE1 | 0.20 | 0.65 |
| 1:G:796:GLY:CA | 3:I:35:ARG:HD3 | 2.16 | 0.65 |
| 1:J:466:GLY:HA2 | 1:J:484:ASN:HD21 | 1.62 | 0.65 |
| 1:J:466:GLY:HA2 | 1:J:484:ASN:ND2 | 2.12 | 0.65 |
| 1:J:556:ASP:O | 4:Y:48:GLY:N | 2.29 | 0.65 |
| 1:M:732:ILE:HG21 | 1:M:747:LEU:HD11 | 0.73 | 0.65 |
| 1:M:836:PHE:CD2 | 2:N:160:GLY:CA | 2.80 | 0.65 |
| 3:O:24:LYS:HA | 3:O:63:ILE:O | 1.95 | 0.65 |
| 1:P:322:VAL:HB | 1:P:325:ILE:CD1 | 2.26 | 0.65 |
| 1:P:642:LYS:HA | 4:1:21:PHE:O | 1.96 | 0.65 |
| 1:P:735:GLY:C | 1:P:743:ALA:HB1 | 1.84 | 0.65 |
| 2:Q:114:LYS:HA | 2:Q:146:GLY:C | 2.03 | 0.65 |
| 2:Q:141:PRO:O | 2:Q:145:ALA:HB2 | 1.96 | 0.65 |
| 4:2:287:ILE:HG13 | 4:4:202:THR:CB | 2.26 | 0.65 |
| 4:5:153:LEU:HD11 | 4:5:274:ILE:HG13 | 1.76 | 0.65 |
| 4:W:324:THR:HG22 | 4:Y:247:VAL:HG13 | 1.77 | 0.65 |
| 1:A:217:THR:O | 1:A:221:GLN:HG2 | 1.95 | 0.65 |
| 1:A:374:GLN:HG3 | 1:A:375:ALA:H | 1.60 | 0.65 |
| 1:A:530:MET:CA | 4:8:354:GLN:CB | 2.73 | 0.65 |
| 1:A:815:CYS:O | 2:B:90:GLY:O | 2.14 | 0.65 |
| 1:D:530:MET:CG | 4:9:354:GLN:CG | 2.71 | 0.65 |
| 1:D:792:ALA:CB | 3:F:42:THR:CG2 | 2.25 | 0.65 |
| 1:G:612:GLN:HE22 | 1:G:627:GLY:N | 1.94 | 0.65 |
| 1:G:795:ARG:CZ | 3:I:116:GLU:OE2 | 2.44 | 0.65 |
| 3:I:3:SER:HG | 3:I:5:ALA:N | 1.95 | 0.65 |
| 1:J:819:ASN:OD1 | 2:K:92:ASP:CB | 2.45 | 0.65 |
| 2:K:141:PRO:O | 2:K:145:ALA:HB2 | 1.96 | 0.65 |
| 3:L:48:LYS:O | 3:L:52:ASN:CG | 2.34 | 0.65 |
| 1:M:144:ARG:NH1 | 1:M:160:ASP:OD1 | 2.29 | 0.65 |
| 1:M:161:ASN:O | 1:M:165:PHE:HB2 | 1.96 | 0.65 |
| 1:M:612:GLN:HE22 | 1:M:627:GLY:N | 1.95 | 0.65 |
| 1:M:642:LYS:HA | 4:Z:21:PHE:O | 1.96 | 0.65 |
| 1:P:93:MET:HA | 1:P:713:SER:HA | 1.79 | 0.65 |
| 1:P:339:ASP:OD1 | 1:P:348:MLY:HH13 | 1.96 | 0.65 |
| 1:P:538:GLU:CD | 4:1:355:MET:CE | 2.62 | 0.65 |
| 3:R:3:SER:HG | 3:R:5:ALA:N | 1.95 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:1:202:THR:C | 4:Y:286:ASP:OD1 | 2.35 | 0.65 |
| 3:C:48:LYS:O | 3:C:52:ASN:CG | 2.34 | 0.65 |
| 1:D:635:GLY:O | 4:9:341:ILE:HG21 | 1.96 | 0.65 |
| 1:G:642:LYS:HA | 4:V:21:PHE:O | 1.97 | 0.65 |
| 1:M:636:LYS:HG3 | 4:Z:334:GLU:CD | 2.17 | 0.65 |
| 1:M:803:TYR:O | 1:M:807:VAL:N | 2.30 | 0.65 |
| 1:P:144:ARG:NH1 | 1:P:160:ASP:OD1 | 2.29 | 0.65 |
| 1:P:161:ASN:O | 1:P:165:PHE:HB2 | 1.96 | 0.65 |
| 4:3:153:LEU:HD11 | 4:3:274:ILE:HG13 | 1.76 | 0.65 |
| 1:A:61:THR:HG23 | 1:A:71:THR:OG1 | 1.95 | 0.65 |
| 1:A:202:SER:CA | 1:A:207:LYS:HE3 | 2.27 | 0.65 |
| 1:A:530:MET:CG | 4:8:354:GLN:CG | 2.71 | 0.65 |
| 1:G:834:LEU:CD2 | 2:H:34:ILE:HD11 | 2.27 | 0.65 |
| 2:H:141:PRO:O | 2:H:145:ALA:HB2 | 1.96 | 0.65 |
| 2:H:146:GLY:O | 2:H:147:ASN:HB2 | 1.96 | 0.65 |
| 1:M:544:LYS:HB3 | 4:2:45:VAL:CG2 | 2.27 | 0.65 |
| 1:P:466:GLY:HA2 | 1:P:484:ASN:HD21 | 1.62 | 0.65 |
| 1:P:466:GLY:HA2 | 1:P:484:ASN:ND2 | 2.12 | 0.65 |
| 1:P:549:SER:HB2 | 4:3:43:VAL:CG2 | 2.18 | 0.65 |
| 1:P:599:ASN:OD1 | 1:P:649:VAL:N | 2.29 | 0.65 |
| 2:Q:140:PHE:O | 2:Q:141:PRO:C | 2.33 | 0.65 |
| 1:A:133:PRO:O | 1:A:136:ASN:HB2 | 1.97 | 0.65 |
| 1:A:813:ILE:CG2 | 2:B:127:ARG:HB2 | 2.27 | 0.65 |
| 1:D:636:LYS:O | 1:D:637:LYS:CB | 2.45 | 0.65 |
| 1:D:642:LYS:CD | 4:9:24:ASP:O | 2.42 | 0.65 |
| 2:E:140:PHE:HB3 | 2:E:144:VAL:CG1 | 2.27 | 0.65 |
| 1:G:530:MET:CA | 4:V:354:GLN:CB | 2.75 | 0.65 |
| 1:G:818:TYR:HB3 | 2:H:90:GLY:CA | 2.27 | 0.65 |
| 1:G:822:SER:O | 1:G:825:ASN:HB2 | 1.97 | 0.65 |
| 1:G:831:TRP:CH2 | 2:H:47:LEU:HD23 | 2.21 | 0.65 |
| 1:J:757:GLN:N | 1:J:776:GLU:HB3 | 2.12 | 0.65 |
| 1:J:822:SER:O | 1:J:825:ASN:HB2 | 1.97 | 0.65 |
| 1:M:831:TRP:HE1 | 2:N:67:MET:CB | 2.10 | 0.65 |
| 3:R:45:GLU:O | 3:R:49:ILE:HG13 | 1.96 | 0.65 |
| 4:2:203:THR:HG21 | 4:Z:287:ILE:HB | 1.70 | 0.65 |
| 4:2:322:PRO:CB | 4:4:244:ASP:HB2 | 2.23 | 0.65 |
| 4:3:287:ILE:HD13 | 4:5:203:THR:CB | 1.97 | 0.65 |
| 4:V:288:ASP:H | 4:X:204:ALA:H | 1.43 | 0.65 |
| 4:X:287:ILE:H | 4:Z:202:THR:HG23 | 1.62 | 0.65 |
| 1:D:466:GLY:HA2 | 1:D:484:ASN:ND2 | 2.12 | 0.64 |
| 1:D:814:PHE:CA | 2:E:127:ARG:HH11 | 1.94 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:557:GLU:HB2 | 4:X:47:MET:C | 2.16 | 0.64 |
| 1:J:322:VAL:HB | 1:J:325:ILE:CD1 | 2.26 | 0.64 |
| 1:J:636:LYS:HG3 | 4:W:334:GLU:CD | 2.17 | 0.64 |
| 3:L:45:GLU:O | 3:L:49:ILE:HG13 | 1.96 | 0.64 |
| 2:N:140:PHE:HB3 | 2:N:144:VAL:CG1 | 2.28 | 0.64 |
| 2:N:141:PRO:O | 2:N:145:ALA:HB2 | 1.96 | 0.64 |
| 1:P:217:THR:HB | 1:P:220:ASP:OD2 | 1.97 | 0.64 |
| 1:P:538:GLU:HA | 4:1:349:LEU:HB3 | 1.78 | 0.64 |
| 1:P:820:VAL:CG1 | 2:Q:136:MET:HE1 | 2.26 | 0.64 |
| 1:A:91:MET:HE3 | 1:A:119:SER:HB2 | 1.79 | 0.64 |
| 1:A:479:CYS:HB3 | 1:A:653:PHE:CE2 | 2.32 | 0.64 |
| 1:D:217:THR:HB | 1:D:220:ASP:OD2 | 1.98 | 0.64 |
| 1:D:226:ASN:HB2 | 1:D:227:PRO:HD3 | 1.78 | 0.64 |
| 1:D:411:GLU:N | 4:9:333:PRO:HB2 | 2.11 | 0.64 |
| 1:D:612:GLN:HE22 | 1:D:627:GLY:N | 1.94 | 0.64 |
| 1:G:479:CYS:HB3 | 1:G:653:PHE:CE2 | 2.33 | 0.64 |
| 1:G:541:MET:HG2 | 4:V:345:ILE:C | 2.16 | 0.64 |
| 1:G:636:LYS:HG3 | 4:V:334:GLU:CD | 2.18 | 0.64 |
| 1:G:724:TYR:HB3 | 1:G:727:LEU:HD12 | 1.80 | 0.64 |
| 3:I:49:ILE:HA | 3:I:52:ASN:ND2 | 2.06 | 0.64 |
| 1:J:144:ARG:NH1 | 1:J:160:ASP:OD1 | 2.29 | 0.64 |
| 1:J:339:ASP:OD1 | 1:J:348:MLY:HH13 | 1.95 | 0.64 |
| 1:M:538:GLU:HA | 4:Z:349:LEU:HB3 | 1.78 | 0.64 |
| 1:M:831:TRP:HE1 | 2:N:67:MET:CG | 2.10 | 0.64 |
| 3:O:45:GLU:O | 3:O:49:ILE:HG13 | 1.97 | 0.64 |
| 1:P:783:LEU:CB | 1:P:786:ILE:HD12 | 2.24 | 0.64 |
| 1:P:826:VAL:HG21 | 2:Q:88:LEU:HD23 | 1.76 | 0.64 |
| 4:1:247:VAL:HG22 | 4:Y:324:THR:HG22 | 0.67 | 0.64 |
| 4:1:247:VAL:N | 4:Y:324:THR:HG21 | 2.11 | 0.64 |
| 4:2:204:ALA:H | 4:Z:287:ILE:HG21 | 1.62 | 0.64 |
| 4:W:325:MET:SD | 4:Y:244:ASP:CG | 2.75 | 0.64 |
| 1:A:226:ASN:HB2 | 1:A:227:PRO:HD3 | 1.78 | 0.64 |
| 1:A:480:ILE:HG22 | 1:A:481:ASN:N | 2.11 | 0.64 |
| 1:A:636:LYS:HG3 | 4:8:334:GLU:CD | 2.17 | 0.64 |
| 2:B:140:PHE:HB3 | 2:B:144:VAL:CG1 | 2.28 | 0.64 |
| 3:C:45:GLU:O | 3:C:49:ILE:HG13 | 1.96 | 0.64 |
| 1:D:296:MLY:HH11 | 1:D:348:MLY:HH21 | 1.79 | 0.64 |
| 1:D:806:MET:O | 1:D:809:ARG:HB2 | 1.98 | 0.64 |
| 1:G:636:LYS:O | 1:G:637:LYS:CB | 2.45 | 0.64 |
| 1:J:218:LEU:CD2 | 1:J:222:ILE:HG12 | 2.28 | 0.64 |
| 1:J:725:ARG:NE | 1:J:737:PHE:HE1 | 1.95 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:479:CYS:HB3 | 1:M:653:PHE:CE2 | 2.33 | 0.64 |
| 1:M:725:ARG:NE | 1:M:737:PHE:HE1 | 1.95 | 0.64 |
| 1:P:636:LYS:HG3 | 4:1:334:GLU:CD | 2.17 | 0.64 |
| 1:P:636:LYS:O | 1:P:637:LYS:CB | 2.45 | 0.64 |
| 2:Q:140:PHE:HB3 | 2:Q:144:VAL:CG1 | 2.28 | 0.64 |
| 4:3:324:THR:CG2 | 4:5:243:PRO:C | 2.57 | 0.64 |
| 1:A:166:MET:HE3 | 1:A:254:PHE:HD2 | 1.62 | 0.64 |
| 1:A:466:GLY:HA2 | 1:A:484:ASN:ND2 | 2.12 | 0.64 |
| 1:A:725:ARG:NE | 1:A:737:PHE:HE1 | 1.95 | 0.64 |
| 1:A:753:VAL:CG1 | 1:A:775:LEU:HD23 | 2.28 | 0.64 |
| 1:A:822:SER:O | 1:A:825:ASN:HB2 | 1.97 | 0.64 |
| 1:D:538:GLU:HA | 4:9:349:LEU:HB3 | 1.78 | 0.64 |
| 1:D:636:LYS:HG3 | 4:9:334:GLU:CD | 2.18 | 0.64 |
| 1:D:642:LYS:HA | 4:9:21:PHE:O | 1.96 | 0.64 |
| 1:G:278:GLN:CG | 1:G:317:GLU:HB2 | 2.27 | 0.64 |
| 1:G:466:GLY:HA2 | 1:G:484:ASN:ND2 | 2.12 | 0.64 |
| 2:H:117:LEU:CB | 2:H:147:ASN:OD1 | 2.39 | 0.64 |
| 2:H:140:PHE:HB3 | 2:H:144:VAL:CG1 | 2.28 | 0.64 |
| 1:J:296:MLY:HH11 | 1:J:348:MLY:HH21 | 1.78 | 0.64 |
| 1:J:541:MET:HG2 | 4:W:345:ILE:O | 1.98 | 0.64 |
| 1:J:636:LYS:O | 1:J:637:LYS:CB | 2.45 | 0.64 |
| 2:K:140:PHE:O | 2:K:141:PRO:C | 2.33 | 0.64 |
| 1:M:724:TYR:HB3 | 1:M:727:LEU:HD12 | 1.80 | 0.64 |
| 1:P:218:LEU:CD2 | 1:P:222:ILE:HG12 | 2.28 | 0.64 |
| 1:P:612:GLN:HE22 | 1:P:627:GLY:N | 1.95 | 0.64 |
| 4:2:287:ILE:HG23 | 4:4:202:THR:HB | 0.88 | 0.64 |
| 1:D:822:SER:O | 1:D:825:ASN:HB2 | 1.97 | 0.64 |
| 1:G:217:THR:HB | 1:G:220:ASP:OD2 | 1.97 | 0.64 |
| 1:G:755:HIS:CB | 1:G:779:ARG:NH2 | 2.61 | 0.64 |
| 1:G:819:ASN:ND2 | 2:H:92:ASP:CA | 2.59 | 0.64 |
| 1:M:217:THR:HB | 1:M:220:ASP:OD2 | 1.97 | 0.64 |
| 1:M:541:MET:HG2 | 4:Z:345:ILE:O | 1.98 | 0.64 |
| 1:M:636:LYS:O | 1:M:637:LYS:CB | 2.45 | 0.64 |
| 1:P:107:MLY:HB3 | 1:P:686:MET:CE | 2.27 | 0.64 |
| 1:P:149:GLN:HG2 | 1:P:716:LEU:CD1 | 2.26 | 0.64 |
| 1:P:816:ILE:HD11 | 2:Q:100:ALA:HB1 | 1.78 | 0.64 |
| 3:R:48:LYS:O | 3:R:52:ASN:CG | 2.35 | 0.64 |
| 4:2:287:ILE:HG21 | 4:4:204:ALA:N | 2.11 | 0.64 |
| 1:A:732:ILE:HG21 | 1:A:747:LEU:HD11 | 0.73 | 0.64 |
| 1:D:466:GLY:HA2 | 1:D:484:ASN:HD21 | 1.61 | 0.64 |
| 1:D:795:ARG:NH2 | 3:F:116:GLU:OE1 | 2.31 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:838:ILE:HD13 | 2:E:54:MET:HE3 | 1.66 | 0.64 |
| 1:G:133:PRO:O | 1:G:136:ASN:HB2 | 1.98 | 0.64 |
| 1:G:817:GLN:HB3 | 2:H:127:ARG:HD3 | 1.78 | 0.64 |
| 2:H:144:VAL:HA | 2:H:153:ILE:HD11 | 1.80 | 0.64 |
| 1:J:411:GLU:N | 4:W:333:PRO:HB2 | 2.11 | 0.64 |
| 1:J:791:GLN:NE2 | 3:L:116:GLU:N | 2.46 | 0.64 |
| 1:J:806:MET:O | 1:J:809:ARG:HB2 | 1.98 | 0.64 |
| 2:K:149:ASP:OD2 | 2:K:150:TYR:C | 2.36 | 0.64 |
| 1:M:91:MET:HE3 | 1:M:119:SER:HB2 | 1.79 | 0.64 |
| 1:M:732:ILE:HG23 | 1:M:747:LEU:CB | 1.85 | 0.64 |
| 2:N:146:GLY:O | 2:N:147:ASN:HB2 | 1.96 | 0.64 |
| 1:P:530:MET:CG | 4:1:354:GLN:CG | 2.72 | 0.64 |
| 2:Q:117:LEU:CG | 2:Q:147:ASN:CB | 2.76 | 0.64 |
| 1:A:94:MET:HE1 | 1:A:101:ALA:HB1 | 1.79 | 0.64 |
| 1:A:530:MET:HE3 | 4:8:354:GLN:CG | 2.18 | 0.64 |
| 1:A:541:MET:HG2 | 4:8:345:ILE:O | 1.98 | 0.64 |
| 1:D:202:SER:HA | 1:D:207:LYS:HE3 | 1.72 | 0.64 |
| 1:D:783:LEU:HD12 | 1:D:783:LEU:N | 2.13 | 0.64 |
| 1:D:819:ASN:N | 2:E:90:GLY:O | 2.31 | 0.64 |
| 1:G:789:ALA:HB1 | 3:I:81:GLN:CD | 2.18 | 0.64 |
| 1:G:796:GLY:N | 3:I:35:ARG:CZ | 2.61 | 0.64 |
| 1:M:537:GLU:HB3 | 1:M:648:THR:HB | 1.80 | 0.64 |
| 1:M:546:THR:HB | 4:2:47:MET:O | 1.98 | 0.64 |
| 1:M:720:PHE:HE1 | 1:M:772:LEU:HD11 | 1.63 | 0.64 |
| 1:M:803:TYR:HD2 | 3:O:17:PHE:CZ | 2.14 | 0.64 |
| 2:N:144:VAL:HA | 2:N:153:ILE:HD11 | 1.80 | 0.64 |
| 1:P:642:LYS:CA | 4:1:21:PHE:O | 2.45 | 0.64 |
| 1:P:725:ARG:NE | 1:P:737:PHE:HE1 | 1.95 | 0.64 |
| 1:P:797:PHE:HE1 | 3:R:149:VAL:HG12 | 1.60 | 0.64 |
| 2:Q:146:GLY:O | 2:Q:147:ASN:HB2 | 1.96 | 0.64 |
| 1:A:753:VAL:HG11 | 1:A:775:LEU:HD23 | 1.78 | 0.64 |
| 1:A:837:MLY:CH2 | 2:H:20:ASP:CB | 2.75 | 0.64 |
| 2:B:149:ASP:OD2 | 2:B:150:TYR:C | 2.36 | 0.64 |
| 1:D:133:PRO:O | 1:D:136:ASN:HB2 | 1.98 | 0.64 |
| 1:D:479:CYS:HB3 | 1:D:653:PHE:CE2 | 2.32 | 0.64 |
| 1:D:642:LYS:CA | 4:9:21:PHE:O | 2.46 | 0.64 |
| 1:D:713:SER:CB | 1:D:775:LEU:HD22 | 2.28 | 0.64 |
| 1:D:725:ARG:NE | 1:D:737:PHE:HE1 | 1.95 | 0.64 |
| 2:E:144:VAL:HA | 2:E:153:ILE:HD11 | 1.80 | 0.64 |
| 1:G:218:LEU:CD2 | 1:G:222:ILE:HG12 | 2.27 | 0.64 |
| 1:G:553:MLY:O | 4:X:46:GLY:CA | 2.45 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:642:LYS:CG | 4:V:22:ALA:C | 2.67 | 0.64 |
| 1:G:795:ARG:N | 3:I:118:MET:HE3 | 2.13 | 0.64 |
| 1:G:813:ILE:HG21 | 2:H:128:PHE:CE1 | 2.33 | 0.64 |
| 1:G:817:GLN:HG2 | 2:H:127:ARG:HB3 | 1.80 | 0.64 |
| 1:G:819:ASN:CB | 2:H:90:GLY:O | 2.45 | 0.64 |
| 1:J:217:THR:HB | 1:J:220:ASP:OD2 | 1.97 | 0.64 |
| 1:J:537:GLU:C | 4:W:351:THR:N | 2.51 | 0.64 |
| 1:J:567:LYS:HZ2 | 4:Y:92:ASN:HA | 1.63 | 0.64 |
| 1:J:769:ALA:CB | 1:J:770:GLY:HA3 | 2.28 | 0.64 |
| 1:J:829:TRP:CZ3 | 2:K:84:PHE:CE1 | 2.86 | 0.64 |
| 1:J:832:MET:SD | 2:K:84:PHE:HE2 | 2.20 | 0.64 |
| 2:K:117:LEU:CG | 2:K:147:ASN:CB | 2.76 | 0.64 |
| 2:K:140:PHE:HB3 | 2:K:144:VAL:CG1 | 2.28 | 0.64 |
| 2:K:146:GLY:O | 2:K:147:ASN:HB2 | 1.96 | 0.64 |
| 1:M:296:MLY:HH11 | 1:M:348:MLY:HH21 | 1.78 | 0.64 |
| 2:N:149:ASP:OD2 | 2:N:150:TYR:C | 2.36 | 0.64 |
| 1:A:217:THR:HB | 1:A:220:ASP:OD2 | 1.97 | 0.64 |
| 1:A:721:LYS:HG2 | 1:A:736:GLN:CD | 1.86 | 0.64 |
| 1:D:218:LEU:CD2 | 1:D:222:ILE:HG12 | 2.28 | 0.64 |
| 1:D:406:VAL:HG12 | 1:D:407:GLY:N | 2.13 | 0.64 |
| 1:D:795:ARG:CB | 3:F:35:ARG:NH2 | 2.56 | 0.64 |
| 1:J:107:MLY:HB3 | 1:J:686:MET:CE | 2.27 | 0.64 |
| 1:J:612:GLN:HE22 | 1:J:627:GLY:N | 1.95 | 0.64 |
| 1:J:791:GLN:NE2 | 3:L:115:GLY:CA | 2.61 | 0.64 |
| 1:J:818:TYR:HE1 | 2:K:127:ARG:NH2 | 1.79 | 0.64 |
| 2:K:146:GLY:O | 2:K:147:ASN:CB | 2.46 | 0.64 |
| 1:M:406:VAL:HG12 | 1:M:407:GLY:N | 2.13 | 0.64 |
| 1:M:537:GLU:C | 4:Z:351:THR:N | 2.51 | 0.64 |
| 1:M:544:LYS:HB2 | 4:Z:147:ARG:HA | 1.80 | 0.64 |
| 1:P:127:ASN:HD22 | 1:P:128:PRO:CD | 2.11 | 0.64 |
| 1:P:133:PRO:O | 1:P:136:ASN:HB2 | 1.97 | 0.64 |
| 4:2:203:THR:HB | 4:Z:287:ILE:CG1 | 2.28 | 0.64 |
| 4:3:148:THR:HG21 | 4:5:45:VAL:CG2 | 2.27 | 0.64 |
| 4:3:287:ILE:CB | 4:5:204:ALA:H | 2.11 | 0.64 |
| 4:4:190:MET:SD | 4:4:209:VAL:HG11 | 2.38 | 0.64 |
| 1:A:278:GLN:CG | 1:A:317:GLU:HB2 | 2.27 | 0.64 |
| 1:D:577:ALA:O | 1:D:578:HIS:CD2 | 2.51 | 0.64 |
| 1:G:107:MLY:HB3 | 1:G:686:MET:CE | 2.27 | 0.64 |
| 1:G:537:GLU:C | 4:V:351:THR:N | 2.51 | 0.64 |
| 2:H:149:ASP:OD2 | 2:H:150:TYR:C | 2.37 | 0.64 |
| 1:J:537:GLU:HB3 | 1:J:648:THR:HB | 1.80 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:541:MET:O | 4:W:143:TYR:OH | 2.14 | 0.64 |
| 1:J:756:THR:HA | 1:J:776:GLU:OE1 | 1.97 | 0.64 |
| 1:J:797:PHE:CE2 | 3:L:126:LEU:CD2 | 2.78 | 0.64 |
| 2:N:146:GLY:O | 2:N:147:ASN:CB | 2.46 | 0.64 |
| 1:P:541:MET:HG2 | 4:1:345:ILE:O | 1.98 | 0.64 |
| 1:P:791:GLN:NE2 | 3:R:114:LEU:O | 2.31 | 0.64 |
| 1:P:797:PHE:CE1 | 3:R:146:ILE:CA | 2.80 | 0.64 |
| 2:Q:149:ASP:OD2 | 2:Q:150:TYR:C | 2.36 | 0.64 |
| 4:7:190:MET:SD | 4:7:209:VAL:HG11 | 2.38 | 0.64 |
| 1:A:538:GLU:HA | 4:8:349:LEU:HB3 | 1.78 | 0.63 |
| 2:B:117:LEU:CG | 2:B:147:ASN:CB | 2.76 | 0.63 |
| 1:G:480:ILE:HG22 | 1:G:481:ASN:N | 2.11 | 0.63 |
| 2:H:146:GLY:O | 2:H:147:ASN:CB | 2.46 | 0.63 |
| 1:J:133:PRO:O | 1:J:136:ASN:HB2 | 1.98 | 0.63 |
| 1:J:813:ILE:HG22 | 2:K:128:PHE:HE1 | 1.60 | 0.63 |
| 1:M:133:PRO:O | 1:M:136:ASN:HB2 | 1.98 | 0.63 |
| 1:P:724:TYR:HB3 | 1:P:727:LEU:HD12 | 1.80 | 0.63 |
| 1:P:798:LEU:HD22 | 3:R:126:LEU:HD11 | 1.73 | 0.63 |
| 1:P:822:SER:O | 1:P:825:ASN:HB2 | 1.97 | 0.63 |
| 4:6:190:MET:SD | 4:6:209:VAL:HG11 | 2.38 | 0.63 |
| 4:X:190:MET:SD | 4:X:209:VAL:HG11 | 2.38 | 0.63 |
| 1:A:93:MET:CE | 1:A:715:VAL:CG1 | 2.68 | 0.63 |
| 1:A:149:GLN:HG2 | 1:A:719:ASP:N | 2.09 | 0.63 |
| 1:A:218:LEU:CD2 | 1:A:222:ILE:HG12 | 2.28 | 0.63 |
| 1:A:577:ALA:O | 1:A:578:HIS:CD2 | 2.52 | 0.63 |
| 1:A:725:ARG:NE | 1:A:737:PHE:CE1 | 2.67 | 0.63 |
| 1:D:724:TYR:HD1 | 1:D:727:LEU:HD11 | 1.64 | 0.63 |
| 1:D:732:ILE:HG23 | 1:D:747:LEU:CB | 1.84 | 0.63 |
| 1:D:739:ASP:CB | 1:D:742:LYS:HB3 | 2.12 | 0.63 |
| 2:E:121:LEU:HA | 2:E:128:PHE:CG | 2.34 | 0.63 |
| 1:G:406:VAL:HG12 | 1:G:407:GLY:N | 2.13 | 0.63 |
| 1:G:505:MLY:NZ | 1:G:762:HIS:NE2 | 2.32 | 0.63 |
| 1:G:537:GLU:HB3 | 1:G:648:THR:HB | 1.81 | 0.63 |
| 1:J:541:MET:CA | 4:W:143:TYR:OH | 2.46 | 0.63 |
| 1:J:642:LYS:HA | 4:W:21:PHE:O | 1.96 | 0.63 |
| 1:J:724:TYR:HB3 | 1:J:727:LEU:HD12 | 1.80 | 0.63 |
| 1:J:836:PHE:CE2 | 2:K:160:GLY:HA3 | 2.32 | 0.63 |
| 2:K:144:VAL:HA | 2:K:153:ILE:HD11 | 1.80 | 0.63 |
| 1:M:543:PRO:HG2 | 4:Z:143:TYR:O | 1.98 | 0.63 |
| 1:M:549:SER:HB2 | 4:2:43:VAL:CG2 | 2.24 | 0.63 |
| 1:M:642:LYS:CG | 4:Z:22:ALA:C | 2.67 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:O:48:LYS:O | 3:O:52:ASN:CG | 2.34 | 0.63 |
| 1:P:530:MET:HA | 4:1:354:GLN:CB | 2.28 | 0.63 |
| 1:P:530:MET:HE3 | 4:1:355:MET:SD | 2.38 | 0.63 |
| 1:P:537:GLU:C | 4:1:351:THR:N | 2.51 | 0.63 |
| 1:P:541:MET:O | 4:1:143:TYR:OH | 2.14 | 0.63 |
| 2:Q:150:TYR:C | 2:Q:151:LYS:CG | 2.49 | 0.63 |
| 4:2:167:GLU:OE1 | 4:4:44:MET:HA | 1.97 | 0.63 |
| 4:2:257:CYS:HB3 | 4:2:258:PRO:HD3 | 1.81 | 0.63 |
| 4:8:190:MET:SD | 4:8:209:VAL:HG11 | 2.38 | 0.63 |
| 4:V:257:CYS:HB3 | 4:V:258:PRO:HD3 | 1.81 | 0.63 |
| 1:A:466:GLY:HA2 | 1:A:484:ASN:HD21 | 1.61 | 0.63 |
| 1:A:502:GLU:HG2 | 1:A:764:MLY:O | 1.97 | 0.63 |
| 1:A:783:LEU:HD12 | 1:A:783:LEU:N | 2.13 | 0.63 |
| 1:D:831:TRP:CG | 2:E:51:PHE:HZ | 2.15 | 0.63 |
| 1:G:94:MET:HE1 | 1:G:101:ALA:HB1 | 1.80 | 0.63 |
| 1:G:636:LYS:N | 4:V:334:GLU:OE1 | 2.31 | 0.63 |
| 1:G:784:ALA:O | 1:G:788:THR:CB | 2.45 | 0.63 |
| 1:G:795:ARG:HB3 | 3:I:35:ARG:HH22 | 1.63 | 0.63 |
| 1:J:530:MET:CG | 4:W:354:GLN:CG | 2.72 | 0.63 |
| 1:J:789:ALA:HB1 | 3:L:81:GLN:CG | 2.29 | 0.63 |
| 1:M:480:ILE:HG22 | 1:M:481:ASN:N | 2.11 | 0.63 |
| 1:P:541:MET:CA | 4:1:143:TYR:OH | 2.46 | 0.63 |
| 1:P:577:ALA:O | 1:P:578:HIS:CD2 | 2.51 | 0.63 |
| 1:P:642:LYS:CG | 4:1:22:ALA:C | 2.67 | 0.63 |
| 4:1:243:PRO:C | 4:Y:291:LYS:HE2 | 2.19 | 0.63 |
| 4:Z:190:MET:SD | 4:Z:209:VAL:HG11 | 2.38 | 0.63 |
| 1:A:636:LYS:O | 1:A:637:LYS:CB | 2.46 | 0.63 |
| 1:A:823:PHE:CD1 | 2:B:160:GLY:CA | 2.80 | 0.63 |
| 1:A:839:MLY:CH1 | 2:B:159:HIS:CD2 | 2.81 | 0.63 |
| 2:B:140:PHE:O | 2:B:141:PRO:C | 2.33 | 0.63 |
| 1:D:537:GLU:C | 4:9:351:THR:N | 2.51 | 0.63 |
| 1:G:577:ALA:O | 1:G:578:HIS:CD2 | 2.52 | 0.63 |
| 1:G:642:LYS:CA | 4:V:21:PHE:O | 2.46 | 0.63 |
| 2:H:117:LEU:CG | 2:H:147:ASN:CB | 2.76 | 0.63 |
| 2:H:132:GLU:O | 2:H:136:MET:HG2 | 1.98 | 0.63 |
| 1:J:530:MET:HA | 4:W:354:GLN:CB | 2.29 | 0.63 |
| 1:J:642:LYS:CA | 4:W:21:PHE:O | 2.46 | 0.63 |
| 1:J:735:GLY:O | 1:J:743:ALA:HA | 1.94 | 0.63 |
| 1:J:817:GLN:CD | 2:K:127:ARG:HB2 | 2.18 | 0.63 |
| 1:M:642:LYS:CA | 4:Z:21:PHE:O | 2.45 | 0.63 |
| 1:M:783:LEU:O | 1:M:786:ILE:N | 2.31 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:795:ARG:HE | 3:O:118:MET:HE1 | 1.63 | 0.63 |
| 1:M:821:ARG:HH12 | 2:N:127:ARG:CZ | 2.11 | 0.63 |
| 1:P:479:CYS:HB3 | 1:P:653:PHE:CE2 | 2.33 | 0.63 |
| 1:P:544:LYS:HB2 | 4:1:147:ARG:HA | 1.80 | 0.63 |
| 4:4:257:CYS:HB3 | 4:4:258:PRO:HD3 | 1.81 | 0.63 |
| 4:X:257:CYS:HB3 | 4:X:258:PRO:HD3 | 1.81 | 0.63 |
| 4:X:291:LYS:NZ | 4:Z:243:PRO:HB2 | 2.10 | 0.63 |
| 4:Z:257:CYS:HB3 | 4:Z:258:PRO:HD3 | 1.81 | 0.63 |
| 1:A:537:GLU:C | 4:8:351:THR:N | 2.52 | 0.63 |
| 1:A:543:PRO:HG2 | 4:8:143:TYR:O | 1.98 | 0.63 |
| 1:D:127:ASN:HD22 | 1:D:128:PRO:CD | 2.11 | 0.63 |
| 1:D:541:MET:CA | 4:9:143:TYR:OH | 2.47 | 0.63 |
| 1:D:831:TRP:CZ2 | 2:E:47:LEU:CG | 2.80 | 0.63 |
| 2:E:146:GLY:O | 2:E:147:ASN:HB2 | 1.96 | 0.63 |
| 1:G:127:ASN:HD22 | 1:G:128:PRO:CD | 2.11 | 0.63 |
| 1:G:771:LEU:O | 1:G:774:LEU:N | 2.32 | 0.63 |
| 1:G:792:ALA:HB1 | 3:I:42:THR:N | 2.13 | 0.63 |
| 1:J:166:MET:HE3 | 1:J:254:PHE:HD2 | 1.63 | 0.63 |
| 1:M:831:TRP:HH2 | 2:N:47:LEU:HD23 | 1.55 | 0.63 |
| 2:N:132:GLU:O | 2:N:136:MET:HG2 | 1.99 | 0.63 |
| 1:P:724:TYR:HD1 | 1:P:727:LEU:HD11 | 1.64 | 0.63 |
| 1:P:725:ARG:NE | 1:P:737:PHE:CE1 | 2.66 | 0.63 |
| 4:2:190:MET:SD | 4:2:209:VAL:HG11 | 2.38 | 0.63 |
| 4:9:190:MET:SD | 4:9:209:VAL:HG11 | 2.38 | 0.63 |
| 1:A:107:MLY:HB3 | 1:A:686:MET:CE | 2.27 | 0.63 |
| 1:A:296:MLY:HH11 | 1:A:348:MLY:HH21 | 1.78 | 0.63 |
| 1:A:406:VAL:HG12 | 1:A:407:GLY:N | 2.13 | 0.63 |
| 1:A:795:ARG:NH2 | 3:C:116:GLU:OE2 | 1.97 | 0.63 |
| 1:A:831:TRP:CG | 2:B:51:PHE:CE1 | 2.79 | 0.63 |
| 1:A:837:MLY:CH2 | 2:H:20:ASP:CA | 2.73 | 0.63 |
| 2:B:132:GLU:O | 2:B:136:MET:HG2 | 1.99 | 0.63 |
| 2:B:146:GLY:O | 2:B:147:ASN:CB | 2.46 | 0.63 |
| 1:D:215:GLN:CA | 1:D:340:ILE:CG2 | 2.63 | 0.63 |
| 1:D:724:TYR:HB3 | 1:D:727:LEU:HD12 | 1.80 | 0.63 |
| 2:E:117:LEU:HD11 | 2:E:147:ASN:HB3 | 1.76 | 0.63 |
| 1:G:28:GLN:CG | 1:G:723:ARG:HH12 | 2.10 | 0.63 |
| 1:G:534:SER:C | 4:V:351:THR:CA | 2.48 | 0.63 |
| 1:G:541:MET:HG2 | 4:V:345:ILE:O | 1.98 | 0.63 |
| 1:J:544:LYS:HB2 | 4:W:147:ARG:HA | 1.80 | 0.63 |
| 1:J:783:LEU:HD12 | 1:J:783:LEU:N | 2.13 | 0.63 |
| 3:L:48:LYS:C | 3:L:52:ASN:HD21 | 1.96 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:N:117:LEU:CG | 2:N:147:ASN:CB | 2.76 | 0.63 |
| 2:Q:132:GLU:O | 2:Q:136:MET:HG2 | 1.99 | 0.63 |
| 1:D:636:LYS:N | 4:9:334:GLU:OE1 | 2.31 | 0.63 |
| 1:D:831:TRP:CD2 | 2:E:51:PHE:CZ | 2.87 | 0.63 |
| 2:E:132:GLU:O | 2:E:136:MET:HG2 | 1.99 | 0.63 |
| 1:G:795:ARG:NE | 3:I:116:GLU:CG | 2.59 | 0.63 |
| 1:G:806:MET:O | 1:G:809:ARG:HB2 | 1.98 | 0.63 |
| 1:J:406:VAL:HG12 | 1:J:407:GLY:N | 2.13 | 0.63 |
| 1:J:642:LYS:CG | 4:W:22:ALA:C | 2.67 | 0.63 |
| 1:M:821:ARG:NH2 | 2:N:127:ARG:NE | 2.47 | 0.63 |
| 1:P:537:GLU:HB3 | 1:P:648:THR:HB | 1.80 | 0.63 |
| 1:P:643:GLY:H | 4:1:23:GLY:C | 2.01 | 0.63 |
| 4:6:257:CYS:HB3 | 4:6:258:PRO:HD3 | 1.81 | 0.63 |
| 1:D:251:ARG:HB2 | 1:D:264:ASP:CB | 2.29 | 0.63 |
| 1:D:541:MET:HG2 | 4:9:345:ILE:O | 1.98 | 0.63 |
| 1:D:542:PHE:CZ | 1:D:553:MLY:HH11 | 2.34 | 0.63 |
| 1:D:834:LEU:CD1 | 2:E:54:MET:HB2 | 2.25 | 0.63 |
| 1:G:510:TRP:CZ2 | 1:G:768:MLY:HH11 | 2.34 | 0.63 |
| 1:G:754:ASP:O | 1:G:776:GLU:CD | 2.37 | 0.63 |
| 1:J:141:LEU:H | 1:J:141:LEU:HD12 | 1.64 | 0.63 |
| 1:J:541:MET:C | 4:W:143:TYR:CZ | 2.73 | 0.63 |
| 1:J:577:ALA:O | 1:J:578:HIS:CD2 | 2.51 | 0.63 |
| 1:M:166:MET:HE3 | 1:M:254:PHE:HD2 | 1.63 | 0.63 |
| 1:M:210:GLN:O | 1:M:211:SER:OG | 2.15 | 0.63 |
| 1:M:218:LEU:CD2 | 1:M:222:ILE:HG12 | 2.28 | 0.63 |
| 1:M:783:LEU:HD12 | 1:M:783:LEU:N | 2.13 | 0.63 |
| 1:M:818:TYR:CE1 | 2:N:127:ARG:NH1 | 2.66 | 0.63 |
| 1:P:302:MET:HG2 | 1:P:303:LEU:CD1 | 2.29 | 0.63 |
| 2:Q:144:VAL:HA | 2:Q:153:ILE:HD11 | 1.80 | 0.63 |
| 4:8:257:CYS:HB3 | 4:8:258:PRO:HD3 | 1.81 | 0.63 |
| 4:V:190:MET:SD | 4:V:209:VAL:HG11 | 2.38 | 0.63 |
| 1:A:797:PHE:CD2 | 3:C:146:ILE:HG23 | 2.33 | 0.63 |
| 1:A:831:TRP:HZ3 | 2:B:50:THR:HG21 | 0.73 | 0.63 |
| 2:B:144:VAL:HA | 2:B:153:ILE:HD11 | 1.80 | 0.63 |
| 1:D:94:MET:HE1 | 1:D:101:ALA:HB1 | 1.80 | 0.63 |
| 1:D:538:GLU:HA | 4:9:349:LEU:CG | 2.28 | 0.63 |
| 1:G:783:LEU:HD12 | 1:G:783:LEU:N | 2.13 | 0.63 |
| 1:G:818:TYR:HH | 2:H:127:ARG:NH2 | 1.93 | 0.63 |
| 1:J:636:LYS:N | 4:W:334:GLU:OE1 | 2.31 | 0.63 |
| 1:J:725:ARG:NE | 1:J:737:PHE:CE1 | 2.67 | 0.63 |
| 1:M:127:ASN:HD22 | 1:M:128:PRO:CD | 2.11 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:577:ALA:O | 1:M:578:HIS:CD2 | 2.51 | 0.63 |
| 1:M:730:SER:C | 1:M:733:PRO:HD2 | 2.20 | 0.63 |
| 4:W:190:MET:SD | 4:W:209:VAL:HG11 | 2.38 | 0.63 |
| 1:A:141:LEU:H | 1:A:141:LEU:HD12 | 1.64 | 0.62 |
| 1:A:642:LYS:CG | 4:8:22:ALA:C | 2.67 | 0.62 |
| 1:D:642:LYS:CG | 4:9:22:ALA:C | 2.67 | 0.62 |
| 1:D:730:SER:C | 1:D:733:PRO:HD2 | 2.20 | 0.62 |
| 1:G:296:MLY:HH11 | 1:G:348:MLY:HH21 | 1.79 | 0.62 |
| 1:G:505:MLY:HH21 | 1:G:762:HIS:HD1 | 1.61 | 0.62 |
| 1:G:725:ARG:NE | 1:G:737:PHE:CE1 | 2.66 | 0.62 |
| 1:G:799:MET:SD | 3:I:32:ASP:CG | 2.77 | 0.62 |
| 1:J:127:ASN:HD22 | 1:J:128:PRO:CD | 2.11 | 0.62 |
| 1:J:302:MET:HG2 | 1:J:303:LEU:CD1 | 2.29 | 0.62 |
| 1:J:479:CYS:HB3 | 1:J:653:PHE:CE2 | 2.33 | 0.62 |
| 1:J:771:LEU:O | 1:J:774:LEU:N | 2.32 | 0.62 |
| 1:M:821:ARG:HH22 | 2:N:127:ARG:HE | 1.45 | 0.62 |
| 2:N:140:PHE:O | 2:N:141:PRO:C | 2.33 | 0.62 |
| 1:P:98:HIS:HB3 | 1:P:100:PRO:CD | 2.26 | 0.62 |
| 1:P:406:VAL:HG12 | 1:P:407:GLY:N | 2.13 | 0.62 |
| 2:Q:121:LEU:HA | 2:Q:128:PHE:CG | 2.34 | 0.62 |
| 1:A:642:LYS:CA | 4:8:21:PHE:O | 2.46 | 0.62 |
| 1:A:836:PHE:CE2 | 2:B:160:GLY:N | 2.67 | 0.62 |
| 1:D:541:MET:C | 4:9:143:TYR:CZ | 2.73 | 0.62 |
| 1:G:556:ASP:OD2 | 4:X:47:MET:CE | 2.40 | 0.62 |
| 2:K:132:GLU:O | 2:K:136:MET:HG2 | 1.99 | 0.62 |
| 1:M:411:GLU:N | 4:Z:333:PRO:HB2 | 2.11 | 0.62 |
| 1:M:725:ARG:NE | 1:M:737:PHE:CE1 | 2.66 | 0.62 |
| 1:P:541:MET:C | 4:1:143:TYR:CZ | 2.73 | 0.62 |
| 1:P:636:LYS:N | 4:1:334:GLU:OE1 | 2.31 | 0.62 |
| 1:P:730:SER:C | 1:P:733:PRO:HD2 | 2.20 | 0.62 |
| 2:Q:111:SER:OG | 2:Q:148:VAL:CG1 | 2.48 | 0.62 |
| 4:1:287:ILE:CB | 4:3:203:THR:H | 2.12 | 0.62 |
| 1:A:210:GLN:O | 1:A:211:SER:OG | 2.15 | 0.62 |
| 1:A:251:ARG:HB2 | 1:A:264:ASP:CB | 2.29 | 0.62 |
| 1:A:537:GLU:HB3 | 1:A:648:THR:HB | 1.80 | 0.62 |
| 1:A:538:GLU:CD | 4:8:355:MET:HE1 | 2.17 | 0.62 |
| 1:A:544:LYS:HB2 | 4:8:147:ARG:HA | 1.80 | 0.62 |
| 1:A:717:TYR:HD1 | 1:A:744:SER:HG | 1.47 | 0.62 |
| 1:A:724:TYR:HB3 | 1:A:727:LEU:HD12 | 1.80 | 0.62 |
| 1:D:202:SER:CA | 1:D:207:LYS:HE3 | 2.27 | 0.62 |
| 1:D:302:MET:HG2 | 1:D:303:LEU:CD1 | 2.30 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:507:GLY:O | 1:D:761:GLY:HA3 | 2.00 | 0.62 |
| 1:D:551:MLY:C | 4:W:46:GLY:O | 2.47 | 0.62 |
| 1:D:643:GLY:H | 4:9:23:GLY:C | 2.02 | 0.62 |
| 2:E:117:LEU:CG | 2:E:147:ASN:CB | 2.76 | 0.62 |
| 2:E:149:ASP:OD2 | 2:E:150:TYR:C | 2.37 | 0.62 |
| 1:G:538:GLU:HA | 4:V:349:LEU:HB3 | 1.79 | 0.62 |
| 1:G:557:GLU:CB | 4:X:47:MET:C | 2.50 | 0.62 |
| 1:M:251:ARG:HB2 | 1:M:264:ASP:CB | 2.29 | 0.62 |
| 1:M:546:THR:HG21 | 4:2:47:MET:HA | 1.80 | 0.62 |
| 1:M:636:LYS:N | 4:Z:334:GLU:OE1 | 2.31 | 0.62 |
| 3:O:24:LYS:HB3 | 3:O:63:ILE:H | 1.64 | 0.62 |
| 1:P:546:THR:HG21 | 4:3:47:MET:HA | 1.79 | 0.62 |
| 1:P:831:TRP:HE1 | 2:Q:67:MET:CB | 2.11 | 0.62 |
| 4:1:190:MET:SD | 4:1:209:VAL:HG11 | 2.38 | 0.62 |
| 4:7:257:CYS:HB3 | 4:7:258:PRO:HD3 | 1.81 | 0.62 |
| 1:A:127:ASN:HD22 | 1:A:128:PRO:CD | 2.11 | 0.62 |
| 1:A:411:GLU:N | 4:8:333:PRO:HB2 | 2.11 | 0.62 |
| 1:A:636:LYS:N | 4:8:334:GLU:OE1 | 2.31 | 0.62 |
| 1:A:724:TYR:HD1 | 1:A:727:LEU:HD11 | 1.64 | 0.62 |
| 3:C:48:LYS:C | 3:C:52:ASN:HD21 | 1.97 | 0.62 |
| 1:D:278:GLN:CG | 1:D:317:GLU:HB2 | 2.27 | 0.62 |
| 1:D:542:PHE:N | 4:9:143:TYR:OH | 2.33 | 0.62 |
| 1:D:838:ILE:HD11 | 2:E:54:MET:HE1 | 1.79 | 0.62 |
| 1:G:578:HIS:CB | 1:G:592:ILE:HD12 | 2.30 | 0.62 |
| 1:G:799:MET:SD | 3:I:32:ASP:OD2 | 2.56 | 0.62 |
| 1:G:829:TRP:CH2 | 2:H:87:LYS:CE | 2.83 | 0.62 |
| 1:G:834:LEU:CD2 | 2:H:34:ILE:CD1 | 2.77 | 0.62 |
| 1:J:84:MLY:HH12 | 1:J:720:PHE:HD1 | 1.63 | 0.62 |
| 2:K:121:LEU:HA | 2:K:128:PHE:CG | 2.34 | 0.62 |
| 3:L:24:LYS:HB3 | 3:L:63:ILE:H | 1.64 | 0.62 |
| 1:M:107:MLY:HB3 | 1:M:686:MET:CE | 2.27 | 0.62 |
| 1:M:724:TYR:HD1 | 1:M:727:LEU:HD11 | 1.64 | 0.62 |
| 1:M:771:LEU:O | 1:M:774:LEU:N | 2.32 | 0.62 |
| 1:P:735:GLY:O | 1:P:743:ALA:HA | 1.94 | 0.62 |
| 1:P:771:LEU:O | 1:P:774:LEU:N | 2.32 | 0.62 |
| 1:P:798:LEU:HD21 | 3:R:126:LEU:HD12 | 1.78 | 0.62 |
| 1:A:551:MLY:C | 4:V:46:GLY:O | 2.47 | 0.62 |
| 1:A:553:MLY:O | 4:V:48:GLY:HA2 | 2.00 | 0.62 |
| 1:A:580:SER:HA | 1:A:588:VAL:O | 2.00 | 0.62 |
| 2:B:121:LEU:HA | 2:B:128:PHE:CG | 2.34 | 0.62 |
| 1:D:274:ARG:HB2 | 1:D:285:TYR:CE2 | 2.34 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:543:PRO:HG2 | 4:9:143:TYR:O | 1.98 | 0.62 |
| 1:D:771:LEU:O | 1:D:774:LEU:N | 2.32 | 0.62 |
| 1:G:541:MET:CA | 4:V:143:TYR:OH | 2.47 | 0.62 |
| 1:G:542:PHE:CZ | 1:G:553:MLY:HH11 | 2.34 | 0.62 |
| 1:G:543:PRO:HG2 | 4:V:143:TYR:O | 1.98 | 0.62 |
| 1:G:757:GLN:OE1 | 1:G:772:LEU:HA | 1.97 | 0.62 |
| 2:H:121:LEU:HA | 2:H:128:PHE:CG | 2.34 | 0.62 |
| 1:J:542:PHE:N | 4:W:143:TYR:OH | 2.33 | 0.62 |
| 1:J:543:PRO:HG2 | 4:W:143:TYR:O | 1.98 | 0.62 |
| 1:M:578:HIS:CB | 1:M:592:ILE:HD12 | 2.30 | 0.62 |
| 1:M:643:GLY:H | 4:Z:23:GLY:C | 2.02 | 0.62 |
| 1:P:795:ARG:NH2 | 3:R:116:GLU:HG2 | 2.08 | 0.62 |
| 4:5:257:CYS:HB3 | 4:5:258:PRO:HD3 | 1.81 | 0.62 |
| 1:A:771:LEU:O | 1:A:774:LEU:N | 2.32 | 0.62 |
| 1:D:544:LYS:HB2 | 4:9:147:ARG:HA | 1.80 | 0.62 |
| 1:D:725:ARG:NE | 1:D:737:PHE:CE1 | 2.67 | 0.62 |
| 1:G:530:MET:HE3 | 4:V:355:MET:SD | 2.39 | 0.62 |
| 1:G:580:SER:HA | 1:G:588:VAL:O | 2.00 | 0.62 |
| 1:G:795:ARG:C | 3:I:35:ARG:NH2 | 2.53 | 0.62 |
| 1:J:154:HIS:CE1 | 1:J:156:PHE:CD2 | 2.88 | 0.62 |
| 1:J:506:GLU:CG | 1:J:760:PHE:O | 2.47 | 0.62 |
| 1:M:798:LEU:CD2 | 3:O:122:GLU:HB3 | 2.30 | 0.62 |
| 1:M:821:ARG:HH12 | 2:N:127:ARG:NE | 1.97 | 0.62 |
| 1:P:93:MET:CG | 1:P:714:ARG:H | 2.13 | 0.62 |
| 1:P:251:ARG:HB2 | 1:P:264:ASP:CB | 2.29 | 0.62 |
| 1:P:278:GLN:HG3 | 1:P:318:GLY:N | 2.15 | 0.62 |
| 1:P:542:PHE:N | 4:1:143:TYR:OH | 2.33 | 0.62 |
| 4:2:287:ILE:HD13 | 4:4:203:THR:N | 2.13 | 0.62 |
| 4:7:361:GLU:HB3 | 4:7:369:ILE:HG12 | 1.82 | 0.62 |
| 4:8:361:GLU:HB3 | 4:8:369:ILE:HG12 | 1.82 | 0.62 |
| 4:V:361:GLU:HB3 | 4:V:369:ILE:HG12 | 1.82 | 0.62 |
| 1:A:542:PHE:CZ | 1:A:553:MLY:HH11 | 2.34 | 0.62 |
| 1:A:813:ILE:O | 1:A:817:GLN:N | 2.30 | 0.62 |
| 2:B:111:SER:OG | 2:B:148:VAL:CG1 | 2.47 | 0.62 |
| 1:D:537:GLU:HB3 | 1:D:648:THR:HB | 1.80 | 0.62 |
| 1:D:831:TRP:NE1 | 2:E:47:LEU:HD22 | 2.13 | 0.62 |
| 1:J:721:LYS:HG2 | 1:J:736:GLN:CD | 1.86 | 0.62 |
| 1:J:724:TYR:HD1 | 1:J:727:LEU:HD11 | 1.64 | 0.62 |
| 1:J:730:SER:C | 1:J:733:PRO:HD2 | 2.20 | 0.62 |
| 3:L:49:ILE:HA | 3:L:52:ASN:ND2 | 2.06 | 0.62 |
| 2:Q:114:LYS:HG3 | 2:Q:146:GLY:HA2 | 1.82 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:1:201:VAL:HG23 | 4:Y:287:ILE:HG12 | 1.80 | 0.62 |
| 4:9:257:CYS:HB3 | 4:9:258:PRO:HD3 | 1.81 | 0.62 |
| 4:9:361:GLU:HB3 | 4:9:369:ILE:HG12 | 1.82 | 0.62 |
| 4:X:287:ILE:HD13 | 4:Z:205:GLU:CG | 2.30 | 0.62 |
| 1:A:274:ARG:HB2 | 1:A:285:TYR:CE2 | 2.34 | 0.62 |
| 1:A:292:MET:HE3 | 1:A:309:PRO:HA | 1.81 | 0.62 |
| 1:A:295:MLY:HG3 | 1:A:332:MET:HE1 | 1.80 | 0.62 |
| 1:A:806:MET:O | 1:A:809:ARG:HB2 | 1.98 | 0.62 |
| 1:D:506:GLU:CD | 1:D:764:MLY:HE3 | 2.09 | 0.62 |
| 1:D:798:LEU:HD11 | 3:F:126:LEU:CD2 | 2.30 | 0.62 |
| 1:G:641:LYS:CE | 1:G:647:GLN:CB | 2.75 | 0.62 |
| 1:G:817:GLN:HB3 | 2:H:127:ARG:CD | 2.30 | 0.62 |
| 3:I:49:ILE:CA | 3:I:52:ASN:ND2 | 2.53 | 0.62 |
| 1:J:84:MLY:HH21 | 1:J:720:PHE:C | 2.20 | 0.62 |
| 1:J:278:GLN:HG3 | 1:J:318:GLY:N | 2.15 | 0.62 |
| 1:M:141:LEU:H | 1:M:141:LEU:HD12 | 1.64 | 0.62 |
| 2:N:144:VAL:CG1 | 2:N:153:ILE:HD13 | 2.20 | 0.62 |
| 1:P:161:ASN:HA | 1:P:164:GLN:HE21 | 1.64 | 0.62 |
| 1:P:542:PHE:CZ | 1:P:553:MLY:HH11 | 2.34 | 0.62 |
| 4:1:287:ILE:HG22 | 4:3:203:THR:HG22 | 1.72 | 0.62 |
| 4:3:257:CYS:HB3 | 4:3:258:PRO:HD3 | 1.81 | 0.62 |
| 4:6:361:GLU:HB3 | 4:6:369:ILE:HG12 | 1.82 | 0.62 |
| 4:W:361:GLU:HB3 | 4:W:369:ILE:HG12 | 1.82 | 0.62 |
| 4:Y:361:GLU:HB3 | 4:Y:369:ILE:HG12 | 1.82 | 0.62 |
| 1:A:278:GLN:HG3 | 1:A:318:GLY:N | 2.15 | 0.62 |
| 1:A:541:MET:HE2 | 4:8:346:LEU:HD12 | 1.82 | 0.62 |
| 1:A:709:LYS:O | 1:A:710:GLY:N | 2.32 | 0.62 |
| 1:A:730:SER:C | 1:A:733:PRO:HD2 | 2.20 | 0.62 |
| 1:D:831:TRP:CG | 2:E:51:PHE:CZ | 2.87 | 0.62 |
| 2:E:114:LYS:HG3 | 2:E:146:GLY:HA2 | 1.82 | 0.62 |
| 2:E:146:GLY:O | 2:E:147:ASN:CB | 2.46 | 0.62 |
| 3:F:24:LYS:HB3 | 3:F:63:ILE:H | 1.64 | 0.62 |
| 1:G:295:MLY:HG3 | 1:G:332:MET:HE1 | 1.80 | 0.62 |
| 1:G:411:GLU:N | 4:V:333:PRO:HB2 | 2.11 | 0.62 |
| 1:G:730:SER:C | 1:G:733:PRO:HD2 | 2.20 | 0.62 |
| 1:J:274:ARG:HB2 | 1:J:285:TYR:CE2 | 2.34 | 0.62 |
| 1:J:542:PHE:CZ | 1:J:553:MLY:HH11 | 2.34 | 0.62 |
| 1:J:755:HIS:HA | 1:J:758:TYR:HE1 | 1.65 | 0.62 |
| 2:K:111:SER:OG | 2:K:148:VAL:CG1 | 2.48 | 0.62 |
| 1:M:541:MET:SD | 4:Z:346:LEU:O | 2.48 | 0.62 |
| 2:N:121:LEU:HA | 2:N:128:PHE:CG | 2.34 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:3:190:MET:SD | 4:3:209:VAL:HG11 | 2.39 | 0.62 |
| 4:Y:190:MET:SD | 4:Y:209:VAL:HG11 | 2.39 | 0.62 |
| 1:A:541:MET:CA | 4:8:143:TYR:OH | 2.47 | 0.62 |
| 1:A:542:PHE:CB | 4:8:143:TYR:HE1 | 2.12 | 0.62 |
| 1:A:578:HIS:CB | 1:A:592:ILE:HD12 | 2.29 | 0.62 |
| 1:A:792:ALA:HB2 | 3:C:42:THR:HG23 | 1.72 | 0.62 |
| 1:D:553:MLY:O | 4:W:48:GLY:HA2 | 1.99 | 0.62 |
| 1:D:580:SER:HA | 1:D:588:VAL:O | 2.00 | 0.62 |
| 1:D:724:TYR:HB3 | 1:D:782:MLY:NZ | 2.14 | 0.62 |
| 1:D:735:GLY:O | 1:D:743:ALA:HA | 1.94 | 0.62 |
| 1:G:278:GLN:HG3 | 1:G:318:GLY:N | 2.14 | 0.62 |
| 1:G:520:ALA:O | 1:G:524:GLU:HG2 | 2.00 | 0.62 |
| 1:G:797:PHE:HE1 | 3:I:146:ILE:HA | 1.65 | 0.62 |
| 1:J:202:SER:CA | 1:J:207:LYS:HE3 | 2.27 | 0.62 |
| 1:J:795:ARG:HG3 | 3:L:116:GLU:OE2 | 1.99 | 0.62 |
| 1:M:274:ARG:HB2 | 1:M:285:TYR:CE2 | 2.34 | 0.62 |
| 1:M:520:ALA:O | 1:M:524:GLU:HG2 | 2.00 | 0.62 |
| 1:M:541:MET:CA | 4:Z:143:TYR:OH | 2.46 | 0.62 |
| 1:P:578:HIS:CB | 1:P:592:ILE:HD12 | 2.30 | 0.62 |
| 1:P:821:ARG:HH22 | 2:Q:127:ARG:NE | 1.98 | 0.62 |
| 4:3:288:ASP:N | 4:5:203:THR:CG2 | 2.56 | 0.62 |
| 4:5:190:MET:SD | 4:5:209:VAL:HG11 | 2.38 | 0.62 |
| 4:X:361:GLU:HB3 | 4:X:369:ILE:HG12 | 1.82 | 0.62 |
| 4:Y:265:SER:CB | 4:Z:39:ARG:HH21 | 2.13 | 0.62 |
| 1:A:755:HIS:HA | 1:A:758:TYR:HE1 | 1.65 | 0.61 |
| 3:C:50:LEU:O | 3:C:53:PRO:HD2 | 2.00 | 0.61 |
| 1:D:278:GLN:HG3 | 1:D:318:GLY:N | 2.15 | 0.61 |
| 1:D:520:ALA:O | 1:D:524:GLU:HG2 | 2.00 | 0.61 |
| 1:D:579:PHE:CE1 | 1:D:581:LEU:HD13 | 2.35 | 0.61 |
| 2:E:111:SER:OG | 2:E:148:VAL:CG1 | 2.48 | 0.61 |
| 1:G:251:ARG:HB2 | 1:G:264:ASP:CB | 2.29 | 0.61 |
| 1:G:642:LYS:CD | 4:V:24:ASP:O | 2.43 | 0.61 |
| 1:G:829:TRP:CH2 | 2:H:83:MET:CE | 2.82 | 0.61 |
| 1:J:251:ARG:HB2 | 1:J:264:ASP:CB | 2.29 | 0.61 |
| 1:J:278:GLN:CG | 1:J:317:GLU:HB2 | 2.27 | 0.61 |
| 2:K:117:LEU:HD11 | 2:K:147:ASN:HB3 | 1.76 | 0.61 |
| 1:M:94:MET:HE1 | 1:M:101:ALA:HB1 | 1.80 | 0.61 |
| 1:M:161:ASN:HA | 1:M:164:GLN:HE21 | 1.64 | 0.61 |
| 1:M:530:MET:HA | 4:Z:354:GLN:CB | 2.28 | 0.61 |
| 1:P:639:GLY:N | 4:I:344:SER:C | 2.54 | 0.61 |
| 2:Q:146:GLY:O | 2:Q:147:ASN:CB | 2.47 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 4:2:203:THR:N | 4:Z:287:ILE:CG2 | 2.51 | 0.61 |
| 4:W:257:CYS:HB3 | 4:W:258:PRO:HD3 | 1.81 | 0.61 |
| 1:A:501:GLU:O | 1:A:762:HIS:NE2 | 2.33 | 0.61 |
| 1:A:623:PHE:CG | 1:A:623:PHE:HA | 2.35 | 0.61 |
| 1:A:799:MET:SD | 3:C:32:ASP:C | 2.78 | 0.61 |
| 1:A:819:ASN:OD1 | 2:B:91:ALA:CA | 2.34 | 0.61 |
| 1:D:530:MET:HA | 4:9:354:GLN:CB | 2.29 | 0.61 |
| 1:G:166:MET:HE3 | 1:G:254:PHE:CD2 | 2.36 | 0.61 |
| 1:G:274:ARG:HB2 | 1:G:285:TYR:CE2 | 2.34 | 0.61 |
| 1:G:541:MET:HE2 | 4:V:346:LEU:HD12 | 1.83 | 0.61 |
| 1:G:544:LYS:HB2 | 4:V:147:ARG:HA | 1.81 | 0.61 |
| 1:G:792:ALA:HB3 | 3:I:42:THR:CG2 | 1.91 | 0.61 |
| 1:G:795:ARG:HG2 | 3:I:118:MET:HE1 | 1.16 | 0.61 |
| 2:H:111:SER:OG | 2:H:148:VAL:CG1 | 2.47 | 0.61 |
| 3:I:50:LEU:O | 3:I:53:PRO:HD2 | 2.00 | 0.61 |
| 1:J:99:GLU:OE2 | 1:J:696:ARG:NH2 | 2.30 | 0.61 |
| 1:J:530:MET:HE3 | 4:W:355:MET:SD | 2.40 | 0.61 |
| 1:J:579:PHE:CE1 | 1:J:581:LEU:HD13 | 2.36 | 0.61 |
| 1:J:643:GLY:H | 4:W:23:GLY:C | 2.01 | 0.61 |
| 1:J:831:TRP:CZ3 | 2:K:34:ILE:HD13 | 2.36 | 0.61 |
| 1:M:81:ASN:OD1 | 1:M:96:HIS:HB2 | 2.00 | 0.61 |
| 1:M:530:MET:CG | 4:Z:354:GLN:HG3 | 2.30 | 0.61 |
| 1:M:542:PHE:CZ | 1:M:553:MLY:HH11 | 2.34 | 0.61 |
| 1:M:580:SER:HA | 1:M:588:VAL:O | 2.00 | 0.61 |
| 1:M:817:GLN:CB | 2:N:127:ARG:CD | 2.68 | 0.61 |
| 3:O:52:ASN:N | 3:O:53:PRO:HD2 | 2.16 | 0.61 |
| 1:P:81:ASN:OD1 | 1:P:96:HIS:HB2 | 2.00 | 0.61 |
| 1:P:541:MET:HE2 | 4:1:346:LEU:HD12 | 1.81 | 0.61 |
| 1:P:543:PRO:HG2 | 4:1:143:TYR:O | 1.98 | 0.61 |
| 1:P:795:ARG:HD2 | 3:R:35:ARG:HH12 | 1.65 | 0.61 |
| 4:1:361:GLU:HB3 | 4:1:369:ILE:HG12 | 1.82 | 0.61 |
| 4:3:361:GLU:HB3 | 4:3:369:ILE:HG12 | 1.82 | 0.61 |
| 4:Y:257:CYS:HB3 | 4:Y:258:PRO:HD3 | 1.81 | 0.61 |
| 1:A:578:HIS:CD2 | 1:A:591:ASN:HA | 2.31 | 0.61 |
| 1:A:634:GLY:N | 4:8:25:ASP:O | 2.31 | 0.61 |
| 1:A:643:GLY:H | 4:8:23:GLY:C | 2.02 | 0.61 |
| 1:A:799:MET:HE3 | 3:C:32:ASP:HB3 | 1.77 | 0.61 |
| 1:D:141:LEU:H | 1:D:141:LEU:HD12 | 1.64 | 0.61 |
| 1:D:541:MET:HE2 | 4:9:346:LEU:HD12 | 1.82 | 0.61 |
| 1:D:713:SER:HB2 | 1:D:775:LEU:HD21 | 1.81 | 0.61 |
| 1:G:530:MET:CG | 4:V:354:GLN:CG | 2.72 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:530:MET:CG | 4:V:354:GLN:HG3 | 2.30 | 0.61 |
| 1:G:542:PHE:CB | 4:V:143:TYR:HE1 | 2.13 | 0.61 |
| 1:G:686:MET:HG3 | 1:G:691:VAL:HG21 | 1.83 | 0.61 |
| 1:J:98:HIS:HB3 | 1:J:100:PRO:CD | 2.25 | 0.61 |
| 1:J:578:HIS:CB | 1:J:592:ILE:HD12 | 2.30 | 0.61 |
| 1:J:580:SER:HA | 1:J:588:VAL:O | 2.00 | 0.61 |
| 1:J:830:PRO:HB3 | 2:K:67:MET:HE1 | 1.82 | 0.61 |
| 1:M:541:MET:C | 4:Z:143:TYR:CZ | 2.72 | 0.61 |
| 1:P:520:ALA:O | 1:P:524:GLU:HG2 | 2.00 | 0.61 |
| 1:P:580:SER:HA | 1:P:588:VAL:O | 2.00 | 0.61 |
| 1:P:782:MLY:O | 1:P:786:ILE:CG1 | 2.47 | 0.61 |
| 2:Q:117:LEU:HD11 | 2:Q:147:ASN:HB3 | 1.76 | 0.61 |
| 4:1:257:CYS:HB3 | 4:1:258:PRO:HD3 | 1.81 | 0.61 |
| 2:B:117:LEU:HD11 | 2:B:147:ASN:HB3 | 1.76 | 0.61 |
| 1:D:98:HIS:HB3 | 1:D:100:PRO:CD | 2.25 | 0.61 |
| 1:D:161:ASN:HA | 1:D:164:GLN:HE21 | 1.64 | 0.61 |
| 1:D:210:GLN:O | 1:D:211:SER:OG | 2.15 | 0.61 |
| 3:F:50:LEU:O | 3:F:53:PRO:HD2 | 2.00 | 0.61 |
| 1:G:154:HIS:CE1 | 1:G:156:PHE:CD2 | 2.88 | 0.61 |
| 1:G:161:ASN:HA | 1:G:164:GLN:HE21 | 1.64 | 0.61 |
| 1:G:538:GLU:HA | 4:V:349:LEU:CG | 2.29 | 0.61 |
| 2:H:114:LYS:HG3 | 2:H:146:GLY:HA2 | 1.82 | 0.61 |
| 1:J:541:MET:HE2 | 4:W:346:LEU:HD12 | 1.82 | 0.61 |
| 1:M:541:MET:HE2 | 4:Z:346:LEU:HD12 | 1.82 | 0.61 |
| 2:N:111:SER:OG | 2:N:148:VAL:CG1 | 2.47 | 0.61 |
| 1:P:94:MET:HE1 | 1:P:101:ALA:HB1 | 1.81 | 0.61 |
| 1:P:141:LEU:HD12 | 1:P:141:LEU:H | 1.64 | 0.61 |
| 1:P:295:MLY:HG3 | 1:P:332:MET:HE1 | 1.80 | 0.61 |
| 1:P:623:PHE:CG | 1:P:623:PHE:HA | 2.35 | 0.61 |
| 1:P:795:ARG:HD2 | 3:R:43:ASN:CG | 2.17 | 0.61 |
| 4:Z:361:GLU:HB3 | 4:Z:369:ILE:HG12 | 1.82 | 0.61 |
| 3:C:63:ILE:HG22 | 3:C:64:THR:O | 2.01 | 0.61 |
| 1:D:578:HIS:CB | 1:D:592:ILE:HD12 | 2.30 | 0.61 |
| 1:D:800:ARG:CB | 3:F:149:VAL:HG22 | 2.30 | 0.61 |
| 1:G:643:GLY:H | 4:V:23:GLY:C | 2.02 | 0.61 |
| 1:G:717:TYR:HD1 | 1:G:744:SER:HG | 1.48 | 0.61 |
| 1:G:797:PHE:HE2 | 3:I:126:LEU:CG | 2.12 | 0.61 |
| 3:I:24:LYS:HB3 | 3:I:63:ILE:H | 1.64 | 0.61 |
| 1:P:154:HIS:CE1 | 1:P:156:PHE:CD2 | 2.88 | 0.61 |
| 1:P:274:ARG:HB2 | 1:P:285:TYR:CE2 | 2.34 | 0.61 |
| 2:Q:34:ILE:O | 2:Q:46:ASP:HB3 | 2.01 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:302:MET:HG2 | 1:A:303:LEU:CD1 | 2.30 | 0.61 |
| 1:A:686:MET:HG3 | 1:A:691:VAL:HG21 | 1.83 | 0.61 |
| 1:A:797:PHE:CD1 | 3:C:146:ILE:C | 2.71 | 0.61 |
| 3:C:24:LYS:HB3 | 3:C:63:ILE:H | 1.64 | 0.61 |
| 1:D:154:HIS:CE1 | 1:D:156:PHE:CD2 | 2.88 | 0.61 |
| 1:D:639:GLY:N | 4:9:344:SER:C | 2.54 | 0.61 |
| 1:D:713:SER:HB2 | 1:D:775:LEU:CD2 | 2.30 | 0.61 |
| 1:G:541:MET:C | 4:V:143:TYR:CZ | 2.73 | 0.61 |
| 1:M:278:GLN:HG3 | 1:M:318:GLY:N | 2.15 | 0.61 |
| 1:M:506:GLU:O | 1:M:762:HIS:NE2 | 2.34 | 0.61 |
| 1:M:542:PHE:CB | 4:Z:143:TYR:HE1 | 2.13 | 0.61 |
| 1:P:202:SER:CA | 1:P:207:LYS:HE3 | 2.27 | 0.61 |
| 1:P:578:HIS:CD2 | 1:P:591:ASN:HA | 2.31 | 0.61 |
| 1:P:821:ARG:HH12 | 2:Q:127:ARG:NE | 1.99 | 0.61 |
| 3:R:52:ASN:N | 3:R:53:PRO:HD2 | 2.15 | 0.61 |
| 4:2:203:THR:CG2 | 4:Z:287:ILE:CB | 2.34 | 0.61 |
| 4:X:291:LYS:CB | 4:Z:245:GLY:N | 2.64 | 0.61 |
| 1:A:530:MET:CG | 4:8:354:GLN:HG3 | 2.30 | 0.61 |
| 1:A:541:MET:C | 4:8:143:TYR:CZ | 2.73 | 0.61 |
| 1:A:798:LEU:CG | 3:C:126:LEU:HD11 | 2.31 | 0.61 |
| 1:A:800:ARG:HD2 | 3:C:149:VAL:O | 2.01 | 0.61 |
| 1:A:836:PHE:CZ | 2:B:159:HIS:CA | 2.83 | 0.61 |
| 2:B:114:LYS:HG3 | 2:B:146:GLY:HA2 | 1.82 | 0.61 |
| 1:D:643:GLY:O | 1:D:644:SER:CB | 2.48 | 0.61 |
| 1:G:81:ASN:OD1 | 1:G:96:HIS:HB2 | 2.00 | 0.61 |
| 1:G:302:MET:HG2 | 1:G:303:LEU:CD1 | 2.30 | 0.61 |
| 1:G:724:TYR:HD1 | 1:G:727:LEU:HD11 | 1.64 | 0.61 |
| 1:J:161:ASN:HA | 1:J:164:GLN:HE21 | 1.64 | 0.61 |
| 1:J:524:GLU:O | 1:J:528:MLY:HB3 | 2.01 | 0.61 |
| 1:J:578:HIS:CD2 | 1:J:591:ASN:HA | 2.31 | 0.61 |
| 2:K:34:ILE:O | 2:K:46:ASP:HB3 | 2.01 | 0.61 |
| 3:L:50:LEU:O | 3:L:53:PRO:HD2 | 2.00 | 0.61 |
| 1:M:542:PHE:N | 4:Z:143:TYR:OH | 2.33 | 0.61 |
| 1:M:686:MET:HG3 | 1:M:691:VAL:HG21 | 1.83 | 0.61 |
| 1:M:798:LEU:HD22 | 3:O:126:LEU:HD11 | 1.79 | 0.61 |
| 1:P:217:THR:C | 1:P:221:GLN:HG2 | 2.21 | 0.61 |
| 3:R:50:LEU:O | 3:R:53:PRO:HD2 | 2.00 | 0.61 |
| 1:A:542:PHE:N | 4:8:143:TYR:OH | 2.33 | 0.61 |
| 1:A:735:GLY:C | 1:A:743:ALA:HB1 | 1.84 | 0.61 |
| 2:B:34:ILE:O | 2:B:46:ASP:HB3 | 2.01 | 0.61 |
| 1:G:217:THR:C | 1:G:221:GLN:HG2 | 2.21 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:643:GLY:O | 1:G:644:SER:CB | 2.48 | 0.61 |
| 1:J:732:ILE:HG22 | 1:J:747:LEU:CD1 | 1.55 | 0.61 |
| 1:M:154:HIS:CE1 | 1:M:156:PHE:CD2 | 2.88 | 0.61 |
| 1:M:302:MET:HG2 | 1:M:303:LEU:CD1 | 2.30 | 0.61 |
| 1:M:634:GLY:N | 4:Z:25:ASP:O | 2.31 | 0.61 |
| 1:M:816:ILE:HD11 | 2:N:100:ALA:CB | 2.31 | 0.61 |
| 1:P:836:PHE:CD1 | 2:Q:159:HIS:HA | 2.23 | 0.61 |
| 3:R:63:ILE:HG22 | 3:R:64:THR:O | 2.01 | 0.61 |
| 1:A:81:ASN:OD1 | 1:A:96:HIS:HB2 | 2.00 | 0.61 |
| 1:A:149:GLN:OE1 | 1:A:716:LEU:CG | 2.46 | 0.61 |
| 1:A:520:ALA:O | 1:A:524:GLU:HG2 | 2.00 | 0.61 |
| 1:A:576:GLU:CG | 1:A:577:ALA:N | 2.44 | 0.61 |
| 1:D:800:ARG:CD | 3:F:149:VAL:C | 2.68 | 0.61 |
| 1:G:795:ARG:HA | 3:I:118:MET:SD | 2.41 | 0.61 |
| 1:G:819:ASN:CB | 2:H:92:ASP:HB2 | 2.27 | 0.61 |
| 1:J:81:ASN:OD1 | 1:J:96:HIS:HB2 | 2.00 | 0.61 |
| 1:J:557:GLU:HG3 | 1:J:557:GLU:O | 2.00 | 0.61 |
| 1:P:783:LEU:HD12 | 1:P:783:LEU:N | 2.13 | 0.61 |
| 4:X:287:ILE:H | 4:Z:202:THR:CB | 2.12 | 0.61 |
| 1:A:161:ASN:HA | 1:A:164:GLN:HE21 | 1.64 | 0.61 |
| 1:A:217:THR:C | 1:A:221:GLN:HG2 | 2.21 | 0.61 |
| 1:A:538:GLU:HA | 4:8:349:LEU:CG | 2.27 | 0.61 |
| 1:A:541:MET:SD | 4:8:346:LEU:O | 2.48 | 0.61 |
| 1:A:579:PHE:CE1 | 1:A:581:LEU:HD13 | 2.35 | 0.61 |
| 1:G:579:PHE:CE1 | 1:G:581:LEU:HD13 | 2.35 | 0.61 |
| 1:G:755:HIS:H | 1:G:779:ARG:NH2 | 1.92 | 0.61 |
| 1:J:623:PHE:CG | 1:J:623:PHE:HA | 2.36 | 0.61 |
| 1:J:643:GLY:O | 1:J:644:SER:CB | 2.49 | 0.61 |
| 1:J:817:GLN:CB | 2:K:127:ARG:HD3 | 2.12 | 0.61 |
| 3:L:63:ILE:HG22 | 3:L:64:THR:O | 2.01 | 0.61 |
| 1:M:217:THR:C | 1:M:221:GLN:HG2 | 2.22 | 0.61 |
| 1:M:278:GLN:CG | 1:M:317:GLU:HB2 | 2.27 | 0.61 |
| 1:M:549:SER:CB | 4:2:47:MET:O | 2.48 | 0.61 |
| 1:M:806:MET:C | 1:M:807:VAL:CA | 2.68 | 0.61 |
| 1:M:837:MLY:O | 1:M:840:PRO:HD2 | 2.01 | 0.61 |
| 1:P:40:VAL:HG22 | 1:P:41:VAL:N | 2.16 | 0.61 |
| 4:2:288:ASP:CB | 4:4:203:THR:HG21 | 2.29 | 0.61 |
| 4:2:361:GLU:HB3 | 4:2:369:ILE:HG12 | 1.82 | 0.61 |
| 1:A:124:VAL:CG1 | 1:A:675:ILE:HD13 | 2.31 | 0.60 |
| 1:A:557:GLU:HG3 | 1:A:557:GLU:O | 2.01 | 0.60 |
| 1:A:809:ARG:NH1 | 2:B:124:GLY:CA | 2.64 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:C:52:ASN:N | 3:C:53:PRO:HD2 | 2.16 | 0.60 |
| 1:D:81:ASN:OD1 | 1:D:96:HIS:HB2 | 2.00 | 0.60 |
| 1:G:99:GLU:OE2 | 1:G:696:ARG:NH2 | 2.30 | 0.60 |
| 1:G:141:LEU:H | 1:G:141:LEU:HD12 | 1.64 | 0.60 |
| 1:J:217:THR:C | 1:J:221:GLN:HG2 | 2.21 | 0.60 |
| 1:J:797:PHE:CE1 | 3:L:146:ILE:CA | 2.84 | 0.60 |
| 1:M:40:VAL:HG22 | 1:M:41:VAL:N | 2.16 | 0.60 |
| 1:M:557:GLU:HG3 | 1:M:557:GLU:O | 2.00 | 0.60 |
| 1:M:579:PHE:CE1 | 1:M:581:LEU:HD13 | 2.35 | 0.60 |
| 1:M:720:PHE:CE1 | 1:M:772:LEU:HD11 | 2.36 | 0.60 |
| 1:P:99:GLU:OE2 | 1:P:696:ARG:NH2 | 2.31 | 0.60 |
| 1:P:278:GLN:CG | 1:P:317:GLU:HB2 | 2.27 | 0.60 |
| 1:P:524:GLU:O | 1:P:528:MLY:HB3 | 2.01 | 0.60 |
| 4:4:361:GLU:HB3 | 4:4:369:ILE:HG12 | 1.82 | 0.60 |
| 4:6:223:PHE:HD2 | 4:6:312:ARG:NH2 | 1.99 | 0.60 |
| 4:W:223:PHE:HD2 | 4:W:312:ARG:NH2 | 1.99 | 0.60 |
| 1:A:154:HIS:CE1 | 1:A:156:PHE:CD2 | 2.88 | 0.60 |
| 1:A:524:GLU:O | 1:A:528:MLY:HB3 | 2.01 | 0.60 |
| 1:D:124:VAL:CG1 | 1:D:675:ILE:HD13 | 2.32 | 0.60 |
| 1:D:217:THR:C | 1:D:221:GLN:HG2 | 2.21 | 0.60 |
| 1:D:686:MET:HG3 | 1:D:691:VAL:HG21 | 1.83 | 0.60 |
| 1:G:797:PHE:CE2 | 3:I:126:LEU:CG | 2.84 | 0.60 |
| 1:J:124:VAL:CG1 | 1:J:675:ILE:HD13 | 2.31 | 0.60 |
| 1:M:643:GLY:O | 1:M:644:SER:CB | 2.49 | 0.60 |
| 2:N:130:PRO:HA | 2:N:133:ILE:HD12 | 1.83 | 0.60 |
| 1:P:838:ILE:CD1 | 2:Q:54:MET:HE3 | 2.13 | 0.60 |
| 1:A:38:VAL:HB | 1:A:52:ILE:HD11 | 1.84 | 0.60 |
| 1:A:95:THR:HG23 | 1:A:96:HIS:ND1 | 2.17 | 0.60 |
| 1:A:643:GLY:O | 1:A:644:SER:CB | 2.48 | 0.60 |
| 1:G:578:HIS:CD2 | 1:G:591:ASN:HA | 2.31 | 0.60 |
| 1:G:623:PHE:CG | 1:G:623:PHE:HA | 2.36 | 0.60 |
| 1:G:639:GLY:N | 4:V:344:SER:C | 2.54 | 0.60 |
| 1:G:834:LEU:HD12 | 2:H:51:PHE:HE1 | 1.66 | 0.60 |
| 1:G:834:LEU:CD2 | 2:H:34:ILE:HG12 | 2.30 | 0.60 |
| 1:J:38:VAL:HB | 1:J:52:ILE:HD11 | 1.83 | 0.60 |
| 1:J:756:THR:HG21 | 1:J:776:GLU:HA | 1.64 | 0.60 |
| 1:M:7:MET:HE3 | 1:M:14:ALA:HB1 | 1.83 | 0.60 |
| 1:M:38:VAL:HB | 1:M:52:ILE:HD11 | 1.84 | 0.60 |
| 1:M:95:THR:HG23 | 1:M:96:HIS:ND1 | 2.17 | 0.60 |
| 1:M:524:GLU:O | 1:M:528:MLY:HB3 | 2.01 | 0.60 |
| 1:M:642:LYS:CD | 4:Z:340:TRP:CZ3 | 2.79 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:O:50:LEU:O | 3:O:53:PRO:HD2 | 2.00 | 0.60 |
| 1:P:156:PHE:CD1 | 1:P:195:TYR:CD1 | 2.90 | 0.60 |
| 1:P:538:GLU:HA | 4:1:349:LEU:CG | 2.28 | 0.60 |
| 1:P:579:PHE:CE1 | 1:P:581:LEU:HD13 | 2.35 | 0.60 |
| 1:P:686:MET:HG3 | 1:P:691:VAL:HG21 | 1.83 | 0.60 |
| 4:2:243:PRO:O | 4:Z:324:THR:HG23 | 2.02 | 0.60 |
| 4:3:223:PHE:HD2 | 4:3:312:ARG:NH2 | 1.99 | 0.60 |
| 1:A:40:VAL:HG22 | 1:A:41:VAL:N | 2.16 | 0.60 |
| 1:A:93:MET:CE | 1:A:715:VAL:CB | 2.80 | 0.60 |
| 2:B:114:LYS:HA | 2:B:146:GLY:C | 2.03 | 0.60 |
| 1:D:156:PHE:CD1 | 1:D:195:TYR:CD1 | 2.90 | 0.60 |
| 1:D:524:GLU:O | 1:D:528:MLY:HB3 | 2.01 | 0.60 |
| 1:D:623:PHE:CG | 1:D:623:PHE:HA | 2.36 | 0.60 |
| 1:D:732:ILE:CG2 | 1:D:747:LEU:HD11 | 1.26 | 0.60 |
| 1:D:732:ILE:HD13 | 1:D:782:MLY:HH11 | 1.81 | 0.60 |
| 3:F:52:ASN:N | 3:F:53:PRO:HD2 | 2.16 | 0.60 |
| 1:G:40:VAL:HG22 | 1:G:41:VAL:N | 2.16 | 0.60 |
| 1:J:686:MET:HG3 | 1:J:691:VAL:HG21 | 1.83 | 0.60 |
| 1:J:795:ARG:HD2 | 3:L:43:ASN:N | 2.15 | 0.60 |
| 1:J:795:ARG:HH21 | 3:L:116:GLU:CD | 2.04 | 0.60 |
| 2:K:130:PRO:HA | 2:K:133:ILE:HD12 | 1.84 | 0.60 |
| 1:M:124:VAL:CG1 | 1:M:675:ILE:HD13 | 2.32 | 0.60 |
| 2:N:34:ILE:O | 2:N:46:ASP:HB3 | 2.01 | 0.60 |
| 1:P:97:LEU:HD21 | 1:P:712:PRO:CB | 2.22 | 0.60 |
| 1:P:795:ARG:HE | 3:R:118:MET:HE1 | 1.66 | 0.60 |
| 1:P:817:GLN:HB3 | 2:Q:127:ARG:HD3 | 1.83 | 0.60 |
| 4:1:243:PRO:C | 4:Y:291:LYS:HG3 | 2.21 | 0.60 |
| 4:3:324:THR:CG2 | 4:5:243:PRO:O | 2.49 | 0.60 |
| 4:9:223:PHE:HD2 | 4:9:312:ARG:NH2 | 1.99 | 0.60 |
| 1:A:124:VAL:HG13 | 1:A:675:ILE:HD13 | 1.84 | 0.60 |
| 1:A:639:GLY:N | 4:8:344:SER:C | 2.54 | 0.60 |
| 1:D:665:ARG:C | 1:D:667:THR:H | 2.05 | 0.60 |
| 1:D:798:LEU:CD2 | 3:F:122:GLU:HB3 | 2.31 | 0.60 |
| 1:G:124:VAL:CG1 | 1:G:675:ILE:HD13 | 2.31 | 0.60 |
| 1:G:524:GLU:O | 1:G:528:MLY:HB3 | 2.01 | 0.60 |
| 1:G:542:PHE:N | 4:V:143:TYR:OH | 2.33 | 0.60 |
| 1:G:557:GLU:HG3 | 1:G:557:GLU:O | 2.01 | 0.60 |
| 2:H:130:PRO:HA | 2:H:133:ILE:HD12 | 1.83 | 0.60 |
| 1:J:757:GLN:HA | 1:J:776:GLU:CG | 2.27 | 0.60 |
| 1:J:813:ILE:O | 1:J:817:GLN:N | 2.30 | 0.60 |
| 1:M:576:GLU:CG | 1:M:577:ALA:N | 2.44 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:P:717:TYR:HD1 | 1:P:744:SER:HG | 1.50 | 0.60 |
| 3:R:24:LYS:HB3 | 3:R:63:ILE:H | 1.64 | 0.60 |
| 4:1:223:PHE:HD2 | 4:1:312:ARG:NH2 | 1.99 | 0.60 |
| 4:1:287:ILE:HG21 | 4:3:203:THR:HG22 | 1.79 | 0.60 |
| 4:4:287:ILE:H | 4:4:287:ILE:HD12 | 1.67 | 0.60 |
| 4:6:287:ILE:H | 4:6:287:ILE:HD12 | 1.67 | 0.60 |
| 4:X:287:ILE:HB | 4:Z:205:GLU:HG3 | 0.62 | 0.60 |
| 1:A:831:TRP:CG | 2:B:51:PHE:HE1 | 2.17 | 0.60 |
| 1:G:84:MLY:CG | 1:G:723:ARG:NE | 2.50 | 0.60 |
| 1:G:612:GLN:HE22 | 1:G:627:GLY:HA2 | 1.66 | 0.60 |
| 1:G:817:GLN:CG | 2:H:127:ARG:CD | 2.80 | 0.60 |
| 1:G:834:LEU:CD1 | 2:H:51:PHE:HE1 | 2.15 | 0.60 |
| 1:J:710:GLY:C | 1:J:772:LEU:CD2 | 2.68 | 0.60 |
| 1:J:769:ALA:HB3 | 1:J:770:GLY:HA3 | 1.83 | 0.60 |
| 3:L:52:ASN:N | 3:L:53:PRO:CD | 2.65 | 0.60 |
| 1:M:530:MET:HE3 | 4:Z:354:GLN:CG | 2.26 | 0.60 |
| 1:M:546:THR:HG22 | 1:M:547:ASP:N | 2.17 | 0.60 |
| 3:O:3:SER:HG | 3:O:5:ALA:N | 1.98 | 0.60 |
| 1:P:38:VAL:HB | 1:P:52:ILE:HD11 | 1.83 | 0.60 |
| 1:P:643:GLY:O | 1:P:644:SER:CB | 2.49 | 0.60 |
| 1:P:665:ARG:C | 1:P:667:THR:H | 2.05 | 0.60 |
| 4:4:324:THR:HG21 | 4:6:244:ASP:N | 1.80 | 0.60 |
| 4:5:223:PHE:HD2 | 4:5:312:ARG:NH2 | 1.99 | 0.60 |
| 1:A:837:MLY:O | 1:A:840:PRO:HD2 | 2.01 | 0.60 |
| 1:D:38:VAL:HB | 1:D:52:ILE:HD11 | 1.84 | 0.60 |
| 1:D:127:ASN:ND2 | 1:D:128:PRO:HD2 | 2.16 | 0.60 |
| 1:D:553:MLY:NZ | 4:W:45:VAL:HG13 | 2.17 | 0.60 |
| 1:D:755:HIS:HA | 1:D:758:TYR:HE1 | 1.64 | 0.60 |
| 1:D:795:ARG:CG | 3:F:118:MET:CE | 2.74 | 0.60 |
| 1:G:28:GLN:CB | 1:G:723:ARG:NH1 | 2.27 | 0.60 |
| 1:G:38:VAL:HB | 1:G:52:ILE:HD11 | 1.84 | 0.60 |
| 1:G:60:VAL:O | 1:G:71:THR:HA | 2.02 | 0.60 |
| 1:G:95:THR:HG23 | 1:G:96:HIS:ND1 | 2.17 | 0.60 |
| 1:J:60:VAL:O | 1:J:71:THR:HA | 2.02 | 0.60 |
| 3:L:52:ASN:N | 3:L:53:PRO:HD2 | 2.15 | 0.60 |
| 1:M:538:GLU:HA | 4:Z:349:LEU:CG | 2.28 | 0.60 |
| 1:P:95:THR:HG23 | 1:P:96:HIS:ND1 | 2.17 | 0.60 |
| 4:5:361:GLU:HB3 | 4:5:369:ILE:HG12 | 1.82 | 0.60 |
| 1:A:546:THR:HG22 | 1:A:547:ASP:N | 2.17 | 0.60 |
| 1:D:530:MET:CG | 4:9:354:GLN:HG3 | 2.30 | 0.60 |
| 1:G:202:SER:CA | 1:G:207:LYS:HE3 | 2.28 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:530:MET:HA | 4:V:354:GLN:CB | 2.29 | 0.60 |
| 1:J:93:MET:CG | 1:J:715:VAL:HA | 2.32 | 0.60 |
| 1:J:520:ALA:O | 1:J:524:GLU:HG2 | 2.01 | 0.60 |
| 1:J:530:MET:CG | 4:W:354:GLN:HG3 | 2.30 | 0.60 |
| 1:J:553:MLY:HE3 | 4:Y:45:VAL:HG12 | 1.80 | 0.60 |
| 1:J:642:LYS:CD | 4:W:340:TRP:CZ3 | 2.79 | 0.60 |
| 1:J:755:HIS:N | 1:J:780:ASP:OD2 | 2.34 | 0.60 |
| 1:J:839:MLY:HH21 | 2:K:158:THR:HG22 | 1.84 | 0.60 |
| 2:N:114:LYS:HG3 | 2:N:146:GLY:HA2 | 1.82 | 0.60 |
| 3:O:63:ILE:HG22 | 3:O:64:THR:O | 2.01 | 0.60 |
| 1:P:542:PHE:CB | 4:1:143:TYR:HE1 | 2.13 | 0.60 |
| 1:P:836:PHE:CD2 | 2:Q:160:GLY:CA | 2.84 | 0.60 |
| 4:1:245:GLY:C | 4:Y:324:THR:O | 2.39 | 0.60 |
| 4:3:287:ILE:H | 4:3:287:ILE:HD12 | 1.67 | 0.60 |
| 4:5:287:ILE:H | 4:5:287:ILE:HD12 | 1.67 | 0.60 |
| 4:V:286:ASP:OD1 | 4:X:202:THR:HB | 2.02 | 0.60 |
| 1:A:60:VAL:O | 1:A:71:THR:HA | 2.02 | 0.60 |
| 1:D:546:THR:HG22 | 1:D:547:ASP:N | 2.17 | 0.60 |
| 1:D:823:PHE:CD1 | 2:E:160:GLY:CA | 2.84 | 0.60 |
| 2:E:34:ILE:O | 2:E:46:ASP:HB3 | 2.01 | 0.60 |
| 1:G:788:THR:O | 3:I:42:THR:CG2 | 2.47 | 0.60 |
| 3:I:52:ASN:N | 3:I:53:PRO:HD2 | 2.16 | 0.60 |
| 1:J:84:MLY:HH22 | 1:J:719:ASP:O | 2.02 | 0.60 |
| 1:J:94:MET:HE1 | 1:J:101:ALA:HB1 | 1.81 | 0.60 |
| 1:J:542:PHE:CB | 4:W:143:TYR:HE1 | 2.13 | 0.60 |
| 2:K:114:LYS:HG3 | 2:K:146:GLY:HA2 | 1.82 | 0.60 |
| 1:P:210:GLN:O | 1:P:211:SER:OG | 2.15 | 0.60 |
| 1:P:546:THR:HG22 | 1:P:547:ASP:N | 2.17 | 0.60 |
| 1:P:599:ASN:CB | 1:P:649:VAL:HB | 2.32 | 0.60 |
| 1:P:803:TYR:CD2 | 3:R:17:PHE:CZ | 2.89 | 0.60 |
| 4:1:167:GLU:OE2 | 4:3:43:VAL:O | 2.20 | 0.60 |
| 4:2:287:ILE:H | 4:2:287:ILE:HD12 | 1.67 | 0.60 |
| 4:Y:265:SER:CB | 4:Z:39:ARG:NH2 | 2.64 | 0.60 |
| 1:A:85:TYR:HH | 1:A:772:LEU:CD2 | 1.86 | 0.60 |
| 1:A:553:MLY:NZ | 4:V:45:VAL:HG13 | 2.16 | 0.60 |
| 3:C:52:ASN:N | 3:C:53:PRO:CD | 2.65 | 0.60 |
| 1:D:40:VAL:HG22 | 1:D:41:VAL:N | 2.16 | 0.60 |
| 1:G:92:ALA:O | 1:G:714:ARG:N | 2.35 | 0.60 |
| 1:G:124:VAL:HG13 | 1:G:675:ILE:HD13 | 1.84 | 0.60 |
| 1:G:553:MLY:HB2 | 4:X:46:GLY:HA3 | 1.83 | 0.60 |
| 1:G:795:ARG:HE | 3:I:116:GLU:HB3 | 0.52 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:127:ASN:ND2 | 1:J:128:PRO:HD2 | 2.16 | 0.60 |
| 1:J:156:PHE:CD1 | 1:J:195:TYR:CD1 | 2.90 | 0.60 |
| 1:M:49:MLY:HH13 | 1:M:108:GLU:OE2 | 2.02 | 0.60 |
| 1:P:550:PHE:CE2 | 1:P:592:ILE:HG23 | 2.37 | 0.60 |
| 1:P:769:ALA:O | 1:P:771:LEU:HB2 | 1.97 | 0.60 |
| 4:1:202:THR:CG2 | 4:Y:285:CYS:O | 2.46 | 0.60 |
| 4:2:287:ILE:CG2 | 4:4:202:THR:C | 2.69 | 0.60 |
| 4:V:223:PHE:HD2 | 4:V:312:ARG:NH2 | 2.00 | 0.60 |
| 1:A:542:PHE:CD1 | 4:8:143:TYR:CE1 | 2.90 | 0.59 |
| 1:A:550:PHE:CE2 | 1:A:592:ILE:HG23 | 2.37 | 0.59 |
| 1:D:60:VAL:O | 1:D:71:THR:HA | 2.02 | 0.59 |
| 1:D:507:GLY:HA2 | 1:D:762:HIS:CE1 | 2.37 | 0.59 |
| 1:D:542:PHE:CD1 | 4:9:143:TYR:CE1 | 2.90 | 0.59 |
| 1:D:578:HIS:CD2 | 1:D:591:ASN:HA | 2.31 | 0.59 |
| 1:D:787:ILE:O | 1:D:790:THR:N | 2.35 | 0.59 |
| 1:D:793:ARG:HH21 | 3:F:147:MET:HE1 | 1.66 | 0.59 |
| 2:H:34:ILE:O | 2:H:46:ASP:HB3 | 2.01 | 0.59 |
| 1:J:599:ASN:CB | 1:J:649:VAL:HB | 2.32 | 0.59 |
| 1:M:124:VAL:HG13 | 1:M:675:ILE:HD13 | 1.84 | 0.59 |
| 3:O:52:ASN:HB2 | 3:O:53:PRO:CD | 2.28 | 0.59 |
| 1:P:135:TYR:N | 1:P:135:TYR:CD1 | 2.70 | 0.59 |
| 2:Q:130:PRO:HA | 2:Q:133:ILE:HD12 | 1.84 | 0.59 |
| 2:Q:144:VAL:CG1 | 2:Q:153:ILE:HD13 | 2.20 | 0.59 |
| 4:7:223:PHE:HD2 | 4:7:312:ARG:NH2 | 1.99 | 0.59 |
| 4:X:287:ILE:H | 4:X:287:ILE:HD12 | 1.67 | 0.59 |
| 1:A:534:SER:C | 4:8:351:THR:CA | 2.47 | 0.59 |
| 1:D:230:GLU:O | 1:D:234:ASN:HB2 | 2.02 | 0.59 |
| 1:D:550:PHE:CE2 | 1:D:592:ILE:HG23 | 2.37 | 0.59 |
| 1:D:837:MLY:O | 1:D:840:PRO:HD2 | 2.02 | 0.59 |
| 1:G:148:ARG:HE | 1:G:764:MLY:HH21 | 1.67 | 0.59 |
| 1:G:530:MET:HE3 | 4:V:354:GLN:HG2 | 1.81 | 0.59 |
| 1:G:665:ARG:C | 1:G:667:THR:H | 2.05 | 0.59 |
| 1:G:792:ALA:HB1 | 3:I:42:THR:CA | 2.29 | 0.59 |
| 1:J:40:VAL:HG22 | 1:J:41:VAL:N | 2.16 | 0.59 |
| 1:J:776:GLU:O | 1:J:779:ARG:HB3 | 2.03 | 0.59 |
| 1:J:836:PHE:CE2 | 2:K:160:GLY:CA | 2.85 | 0.59 |
| 1:M:40:VAL:HG22 | 1:M:41:VAL:H | 1.67 | 0.59 |
| 1:M:623:PHE:CG | 1:M:623:PHE:HA | 2.36 | 0.59 |
| 1:M:795:ARG:NH2 | 3:O:116:GLU:HG2 | 2.09 | 0.59 |
| 1:P:93:MET:CE | 1:P:714:ARG:O | 2.50 | 0.59 |
| 1:P:549:SER:OG | 1:P:550:PHE:N | 2.35 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:P:787:ILE:O | 1:P:790:THR:N | 2.35 | 0.59 |
| 1:P:797:PHE:HZ | 3:R:146:ILE:HD13 | 1.60 | 0.59 |
| 4:1:287:ILE:H | 4:1:287:ILE:HD12 | 1.67 | 0.59 |
| 4:2:223:PHE:HD2 | 4:2:312:ARG:NH2 | 1.99 | 0.59 |
| 4:V:286:ASP:OD2 | 4:X:203:THR:CG2 | 2.47 | 0.59 |
| 1:A:530:MET:HE2 | 4:8:354:GLN:HG3 | 1.84 | 0.59 |
| 2:B:117:LEU:CB | 2:B:147:ASN:ND2 | 2.35 | 0.59 |
| 1:D:542:PHE:CB | 4:9:143:TYR:HE1 | 2.13 | 0.59 |
| 1:D:793:ARG:NH2 | 3:F:147:MET:CE | 2.65 | 0.59 |
| 1:D:795:ARG:CG | 3:F:118:MET:HE3 | 2.30 | 0.59 |
| 1:G:40:VAL:HG22 | 1:G:41:VAL:H | 1.67 | 0.59 |
| 1:G:91:MET:HE3 | 1:G:119:SER:HB2 | 1.84 | 0.59 |
| 1:G:156:PHE:CD1 | 1:G:195:TYR:CD1 | 2.90 | 0.59 |
| 1:G:508:ILE:CD1 | 1:G:759:ALA:CB | 2.65 | 0.59 |
| 1:G:536:LEU:HD13 | 1:G:550:PHE:CE1 | 2.37 | 0.59 |
| 1:G:801:VAL:HG23 | 3:I:126:LEU:HD21 | 1.83 | 0.59 |
| 1:J:40:VAL:HG22 | 1:J:41:VAL:H | 1.67 | 0.59 |
| 1:J:530:MET:HE3 | 4:W:354:GLN:HG2 | 1.80 | 0.59 |
| 1:J:550:PHE:CE2 | 1:J:592:ILE:HG23 | 2.37 | 0.59 |
| 1:J:665:ARG:C | 1:J:667:THR:H | 2.05 | 0.59 |
| 1:J:769:ALA:HB3 | 1:J:770:GLY:HA2 | 1.83 | 0.59 |
| 1:J:784:ALA:O | 1:J:788:THR:HB | 2.02 | 0.59 |
| 1:J:829:TRP:CE2 | 2:K:87:LYS:HE2 | 2.35 | 0.59 |
| 1:M:536:LEU:HD13 | 1:M:550:PHE:CE1 | 2.37 | 0.59 |
| 1:M:776:GLU:O | 1:M:779:ARG:HB3 | 2.02 | 0.59 |
| 1:P:709:LYS:CA | 1:P:710:GLY:N | 2.65 | 0.59 |
| 1:P:776:GLU:O | 1:P:779:ARG:HB3 | 2.03 | 0.59 |
| 1:P:831:TRP:HH2 | 2:Q:47:LEU:HD23 | 1.56 | 0.59 |
| 4:Z:287:ILE:HD12 | 4:Z:287:ILE:H | 1.67 | 0.59 |
| 1:D:95:THR:HG23 | 1:D:96:HIS:ND1 | 2.17 | 0.59 |
| 1:D:536:LEU:HD13 | 1:D:550:PHE:CE1 | 2.37 | 0.59 |
| 1:D:599:ASN:CB | 1:D:649:VAL:HB | 2.32 | 0.59 |
| 1:G:800:ARG:HH22 | 3:I:40:ASN:CG | 2.05 | 0.59 |
| 1:J:542:PHE:CD1 | 4:W:143:TYR:CE1 | 2.91 | 0.59 |
| 1:J:567:LYS:NZ | 4:Y:92:ASN:ND2 | 2.36 | 0.59 |
| 1:M:135:TYR:N | 1:M:135:TYR:CD1 | 2.70 | 0.59 |
| 1:P:124:VAL:CG1 | 1:P:675:ILE:HD13 | 2.32 | 0.59 |
| 1:P:839:MLY:HH21 | 2:Q:158:THR:CG2 | 2.33 | 0.59 |
| 3:R:46:ILE:O | 3:R:50:LEU:CG | 2.47 | 0.59 |
| 4:1:201:VAL:CG2 | 4:Y:287:ILE:CG1 | 2.79 | 0.59 |
| 4:1:201:VAL:CG2 | 4:Y:287:ILE:HG12 | 2.32 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:8:287:ILE:H | 4:8:287:ILE:HD12 | 1.67 | 0.59 |
| 1:A:536:LEU:HD13 | 1:A:550:PHE:CE1 | 2.38 | 0.59 |
| 1:A:549:SER:OG | 1:A:550:PHE:N | 2.36 | 0.59 |
| 1:A:787:ILE:O | 1:A:790:THR:N | 2.35 | 0.59 |
| 1:D:819:ASN:CA | 2:E:90:GLY:O | 2.51 | 0.59 |
| 1:G:265:ILE:HG22 | 1:G:266:GLU:N | 2.18 | 0.59 |
| 1:G:505:MLY:HE3 | 1:G:762:HIS:NE2 | 2.18 | 0.59 |
| 1:G:549:SER:OG | 1:G:550:PHE:N | 2.36 | 0.59 |
| 1:G:752:ASP:O | 1:G:780:ASP:CB | 2.50 | 0.59 |
| 1:M:542:PHE:CD1 | 4:Z:143:TYR:CE1 | 2.91 | 0.59 |
| 1:P:40:VAL:HG22 | 1:P:41:VAL:H | 1.67 | 0.59 |
| 1:P:124:VAL:HG13 | 1:P:675:ILE:HD13 | 1.84 | 0.59 |
| 1:P:530:MET:CG | 4:1:354:GLN:HG3 | 2.30 | 0.59 |
| 1:P:783:LEU:CA | 1:P:786:ILE:HD11 | 2.27 | 0.59 |
| 1:A:464:ILE:HG22 | 1:A:465:ALA:N | 2.18 | 0.59 |
| 3:C:49:ILE:HA | 3:C:52:ASN:ND2 | 2.05 | 0.59 |
| 1:D:7:MET:HE3 | 1:D:14:ALA:HB1 | 1.84 | 0.59 |
| 1:D:557:GLU:HG3 | 1:D:557:GLU:O | 2.00 | 0.59 |
| 1:G:166:MET:HE3 | 1:G:254:PHE:HD2 | 1.68 | 0.59 |
| 1:G:481:ASN:N | 1:G:481:ASN:ND2 | 2.51 | 0.59 |
| 1:G:546:THR:HG22 | 1:G:547:ASP:N | 2.17 | 0.59 |
| 1:G:776:GLU:O | 1:G:779:ARG:HB3 | 2.02 | 0.59 |
| 3:I:63:ILE:HG22 | 3:I:64:THR:O | 2.01 | 0.59 |
| 1:J:230:GLU:O | 1:J:234:ASN:HB2 | 2.03 | 0.59 |
| 1:J:541:MET:SD | 4:W:346:LEU:O | 2.48 | 0.59 |
| 1:J:796:GLY:CA | 3:L:35:ARG:NE | 2.65 | 0.59 |
| 1:M:578:HIS:CD2 | 1:M:591:ASN:HA | 2.31 | 0.59 |
| 1:M:599:ASN:CB | 1:M:649:VAL:HB | 2.32 | 0.59 |
| 1:M:612:GLN:HE22 | 1:M:627:GLY:HA2 | 1.67 | 0.59 |
| 1:M:639:GLY:N | 4:Z:344:SER:C | 2.54 | 0.59 |
| 1:P:230:GLU:O | 1:P:234:ASN:HB2 | 2.03 | 0.59 |
| 1:P:715:VAL:HG11 | 1:P:720:PHE:HD1 | 1.68 | 0.59 |
| 4:9:287:ILE:H | 4:9:287:ILE:HD12 | 1.67 | 0.59 |
| 1:A:156:PHE:CD1 | 1:A:195:TYR:CD1 | 2.89 | 0.59 |
| 1:A:481:ASN:N | 1:A:481:ASN:ND2 | 2.51 | 0.59 |
| 1:A:665:ARG:C | 1:A:667:THR:H | 2.05 | 0.59 |
| 2:B:130:PRO:HA | 2:B:133:ILE:HD12 | 1.84 | 0.59 |
| 1:D:642:LYS:CD | 4:9:340:TRP:CZ3 | 2.79 | 0.59 |
| 1:G:787:ILE:O | 1:G:790:THR:N | 2.35 | 0.59 |
| 3:I:52:ASN:N | 3:I:53:PRO:CD | 2.65 | 0.59 |
| 3:L:52:ASN:HB2 | 3:L:53:PRO:CD | 2.28 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:L:102:VAL:HG11 | 3:L:107:LEU:HB2 | 1.85 | 0.59 |
| 1:M:60:VAL:O | 1:M:71:THR:HA | 2.02 | 0.59 |
| 1:M:156:PHE:CD1 | 1:M:195:TYR:CD1 | 2.90 | 0.59 |
| 1:M:819:ASN:HA | 2:N:90:GLY:C | 2.05 | 0.59 |
| 1:P:795:ARG:NE | 3:R:116:GLU:HB3 | 2.17 | 0.59 |
| 1:P:797:PHE:CD1 | 3:R:149:VAL:HG12 | 2.30 | 0.59 |
| 4:Y:223:PHE:HD2 | 4:Y:312:ARG:NH2 | 1.99 | 0.59 |
| 1:D:195:TYR:O | 1:D:199:ILE:HG23 | 2.03 | 0.59 |
| 1:D:783:LEU:O | 1:D:787:ILE:N | 2.28 | 0.59 |
| 1:G:503:TYR:CZ | 1:G:711:PHE:HE2 | 2.18 | 0.59 |
| 1:J:95:THR:HG23 | 1:J:96:HIS:ND1 | 2.17 | 0.59 |
| 1:J:553:MLY:CH1 | 4:Y:45:VAL:HG11 | 2.32 | 0.59 |
| 1:J:757:GLN:CA | 1:J:776:GLU:HG3 | 2.30 | 0.59 |
| 1:M:481:ASN:N | 1:M:481:ASN:ND2 | 2.51 | 0.59 |
| 1:P:195:TYR:O | 1:P:199:ILE:HG23 | 2.03 | 0.59 |
| 1:P:542:PHE:CD1 | 4:1:143:TYR:CE1 | 2.91 | 0.59 |
| 1:P:786:ILE:CG2 | 1:P:787:ILE:N | 2.65 | 0.59 |
| 1:P:837:MLY:O | 1:P:840:PRO:HD2 | 2.02 | 0.59 |
| 1:A:49:MLY:HH13 | 1:A:108:GLU:OE2 | 2.02 | 0.59 |
| 1:A:776:GLU:O | 1:A:779:ARG:HB3 | 2.03 | 0.59 |
| 1:D:40:VAL:HG22 | 1:D:41:VAL:H | 1.67 | 0.59 |
| 1:D:646:PHE:CD2 | 1:D:652:LEU:CD1 | 2.85 | 0.59 |
| 2:E:130:PRO:HA | 2:E:133:ILE:HD12 | 1.84 | 0.59 |
| 1:G:48:VAL:HG22 | 1:G:49:MLY:N | 2.18 | 0.59 |
| 1:G:542:PHE:CD1 | 4:V:143:TYR:CE1 | 2.91 | 0.59 |
| 1:J:124:VAL:HG13 | 1:J:675:ILE:HD13 | 1.84 | 0.59 |
| 1:J:549:SER:OG | 1:J:550:PHE:N | 2.36 | 0.59 |
| 1:J:553:MLY:HG3 | 4:Y:45:VAL:O | 2.03 | 0.59 |
| 1:J:795:ARG:HG2 | 3:L:118:MET:HE1 | 1.84 | 0.59 |
| 1:M:195:TYR:O | 1:M:199:ILE:HG23 | 2.03 | 0.59 |
| 1:M:665:ARG:C | 1:M:667:THR:H | 2.05 | 0.59 |
| 1:M:786:ILE:N | 1:M:787:ILE:N | 2.51 | 0.59 |
| 1:M:813:ILE:O | 1:M:817:GLN:N | 2.30 | 0.59 |
| 3:O:52:ASN:N | 3:O:53:PRO:CD | 2.65 | 0.59 |
| 1:P:546:THR:CB | 4:3:46:GLY:CA | 2.75 | 0.59 |
| 1:P:634:GLY:N | 4:1:25:ASP:O | 2.31 | 0.59 |
| 4:3:322:PRO:CB | 4:5:244:ASP:HB2 | 2.26 | 0.59 |
| 1:A:48:VAL:HG22 | 1:A:49:MLY:N | 2.18 | 0.59 |
| 1:A:601:ASP:N | 1:A:602:PRO:HD3 | 2.18 | 0.59 |
| 1:D:732:ILE:CD1 | 1:D:782:MLY:CH1 | 2.79 | 0.59 |
| 1:G:28:GLN:HB3 | 1:G:723:ARG:HH22 | 1.61 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:601:ASP:N | 1:G:602:PRO:HD3 | 2.18 | 0.59 |
| 1:G:829:TRP:CE2 | 2:H:87:LYS:HE2 | 2.38 | 0.59 |
| 1:J:84:MLY:CH2 | 1:J:719:ASP:O | 2.51 | 0.59 |
| 1:J:195:TYR:O | 1:J:199:ILE:HG23 | 2.03 | 0.59 |
| 1:M:629:GLU:HB3 | 1:M:645:SER:N | 2.18 | 0.59 |
| 1:P:49:MLY:HH13 | 1:P:108:GLU:OE2 | 2.02 | 0.59 |
| 1:P:411:GLU:N | 4:1:333:PRO:HB2 | 2.11 | 0.59 |
| 1:P:813:ILE:O | 1:P:817:GLN:N | 2.30 | 0.59 |
| 1:A:7:MET:HE3 | 1:A:14:ALA:HB1 | 1.85 | 0.58 |
| 1:A:230:GLU:O | 1:A:234:ASN:HB2 | 2.03 | 0.58 |
| 1:A:813:ILE:HD13 | 2:B:128:PHE:HE1 | 1.66 | 0.58 |
| 1:G:210:GLN:O | 1:G:211:SER:OG | 2.15 | 0.58 |
| 1:G:646:PHE:CD2 | 1:G:652:LEU:CD1 | 2.85 | 0.58 |
| 1:J:48:VAL:HG22 | 1:J:49:MLY:N | 2.18 | 0.58 |
| 1:J:210:GLN:O | 1:J:211:SER:OG | 2.15 | 0.58 |
| 1:J:629:GLU:HB3 | 1:J:645:SER:N | 2.18 | 0.58 |
| 1:J:787:ILE:O | 1:J:790:THR:N | 2.35 | 0.58 |
| 1:J:837:MLY:O | 1:J:840:PRO:HD2 | 2.02 | 0.58 |
| 1:M:48:VAL:HG22 | 1:M:49:MLY:N | 2.18 | 0.58 |
| 1:M:464:ILE:HG22 | 1:M:465:ALA:N | 2.18 | 0.58 |
| 1:M:538:GLU:O | 1:M:541:MET:HB2 | 2.03 | 0.58 |
| 1:M:549:SER:CA | 4:2:43:VAL:HG11 | 2.32 | 0.58 |
| 1:P:48:VAL:HG22 | 1:P:49:MLY:N | 2.18 | 0.58 |
| 1:P:536:LEU:HD13 | 1:P:550:PHE:CE1 | 2.37 | 0.58 |
| 1:P:538:GLU:O | 1:P:541:MET:HB2 | 2.04 | 0.58 |
| 4:X:291:LYS:HB2 | 4:Z:245:GLY:N | 2.14 | 0.58 |
| 4:Z:223:PHE:HD2 | 4:Z:312:ARG:NH2 | 2.00 | 0.58 |
| 1:A:599:ASN:CB | 1:A:649:VAL:HB | 2.32 | 0.58 |
| 1:A:629:GLU:HB3 | 1:A:645:SER:N | 2.19 | 0.58 |
| 1:D:726:VAL:CG1 | 1:D:785:GLU:CG | 2.79 | 0.58 |
| 3:F:52:ASN:N | 3:F:53:PRO:CD | 2.65 | 0.58 |
| 1:G:116:TYR:HB2 | 1:G:153:PRO:O | 2.03 | 0.58 |
| 1:G:141:LEU:O | 1:G:144:ARG:HB3 | 2.03 | 0.58 |
| 1:G:629:GLU:HB3 | 1:G:645:SER:N | 2.18 | 0.58 |
| 1:G:789:ALA:CB | 3:I:81:GLN:CD | 2.71 | 0.58 |
| 1:J:49:MLY:HH13 | 1:J:108:GLU:OE2 | 2.02 | 0.58 |
| 1:J:634:GLY:N | 4:W:25:ASP:O | 2.31 | 0.58 |
| 1:M:116:TYR:HB2 | 1:M:153:PRO:O | 2.03 | 0.58 |
| 1:M:265:ILE:HG22 | 1:M:266:GLU:N | 2.18 | 0.58 |
| 1:M:787:ILE:O | 1:M:790:THR:N | 2.35 | 0.58 |
| 1:P:60:VAL:O | 1:P:71:THR:HA | 2.02 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:P:218:LEU:N | 1:P:221:GLN:HE21 | 2.01 | 0.58 |
| 1:P:529:PRO:HG3 | 4:1:353:GLN:OE1 | 2.04 | 0.58 |
| 1:P:646:PHE:CD2 | 1:P:652:LEU:CD1 | 2.85 | 0.58 |
| 1:P:799:MET:SD | 3:R:32:ASP:OD2 | 2.61 | 0.58 |
| 3:R:52:ASN:HB2 | 3:R:53:PRO:CD | 2.28 | 0.58 |
| 4:2:287:ILE:HG23 | 4:4:202:THR:HG1 | 1.66 | 0.58 |
| 4:X:223:PHE:HD2 | 4:X:312:ARG:NH2 | 2.00 | 0.58 |
| 1:A:141:LEU:O | 1:A:144:ARG:HB3 | 2.03 | 0.58 |
| 1:A:612:GLN:HE22 | 1:A:627:GLY:HA2 | 1.66 | 0.58 |
| 1:D:506:GLU:O | 1:D:763:THR:N | 2.36 | 0.58 |
| 1:D:529:PRO:HG3 | 4:9:353:GLN:OE1 | 2.03 | 0.58 |
| 3:F:63:ILE:HG22 | 3:F:64:THR:O | 2.01 | 0.58 |
| 1:G:599:ASN:CB | 1:G:649:VAL:HB | 2.32 | 0.58 |
| 1:J:135:TYR:N | 1:J:135:TYR:CD1 | 2.70 | 0.58 |
| 1:J:538:GLU:HA | 4:W:349:LEU:CG | 2.28 | 0.58 |
| 1:J:546:THR:HG22 | 1:J:547:ASP:N | 2.17 | 0.58 |
| 1:J:601:ASP:N | 1:J:602:PRO:HD3 | 2.18 | 0.58 |
| 1:M:141:LEU:O | 1:M:144:ARG:HB3 | 2.03 | 0.58 |
| 1:P:557:GLU:HG3 | 1:P:557:GLU:O | 2.00 | 0.58 |
| 1:P:629:GLU:HB3 | 1:P:645:SER:N | 2.18 | 0.58 |
| 1:P:818:TYR:CD1 | 2:Q:127:ARG:CZ | 2.83 | 0.58 |
| 4:8:223:PHE:HD2 | 4:8:312:ARG:NH2 | 1.99 | 0.58 |
| 1:A:40:VAL:HG22 | 1:A:41:VAL:H | 1.67 | 0.58 |
| 1:A:175:ILE:HA | 1:A:670:HIS:O | 2.04 | 0.58 |
| 1:A:642:LYS:CD | 4:8:340:TRP:CZ3 | 2.79 | 0.58 |
| 1:A:752:ASP:O | 1:A:778:MET:HB3 | 2.02 | 0.58 |
| 3:C:102:VAL:HG11 | 3:C:107:LEU:HB2 | 1.85 | 0.58 |
| 1:D:49:MLY:HH13 | 1:D:108:GLU:OE2 | 2.02 | 0.58 |
| 1:D:116:TYR:HB2 | 1:D:153:PRO:O | 2.03 | 0.58 |
| 1:D:124:VAL:HG13 | 1:D:675:ILE:HD13 | 1.84 | 0.58 |
| 1:D:265:ILE:HG22 | 1:D:266:GLU:N | 2.18 | 0.58 |
| 1:D:834:LEU:HD22 | 2:E:50:THR:HG22 | 1.86 | 0.58 |
| 3:F:52:ASN:HB2 | 3:F:53:PRO:CD | 2.28 | 0.58 |
| 1:G:195:TYR:O | 1:G:199:ILE:HG23 | 2.03 | 0.58 |
| 1:G:715:VAL:HG11 | 1:G:720:PHE:HD1 | 1.68 | 0.58 |
| 1:G:837:MLY:O | 1:G:840:PRO:HD2 | 2.02 | 0.58 |
| 2:H:117:LEU:HD11 | 2:H:147:ASN:HB3 | 1.76 | 0.58 |
| 1:J:91:MET:HE3 | 1:J:119:SER:HB2 | 1.85 | 0.58 |
| 1:J:124:VAL:HG13 | 1:J:675:ILE:CD1 | 2.33 | 0.58 |
| 1:M:124:VAL:HG13 | 1:M:675:ILE:CD1 | 2.33 | 0.58 |
| 1:M:175:ILE:HA | 1:M:670:HIS:O | 2.04 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:202:SER:CA | 1:M:207:LYS:HE3 | 2.27 | 0.58 |
| 1:M:550:PHE:CE2 | 1:M:592:ILE:HG23 | 2.37 | 0.58 |
| 1:P:265:ILE:HG22 | 1:P:266:GLU:N | 2.18 | 0.58 |
| 1:P:601:ASP:N | 1:P:602:PRO:HD3 | 2.18 | 0.58 |
| 1:P:612:GLN:HE22 | 1:P:627:GLY:HA2 | 1.66 | 0.58 |
| 3:R:102:VAL:HG11 | 3:R:107:LEU:HB2 | 1.85 | 0.58 |
| 1:A:794:CYS:O | 1:A:798:LEU:N | 2.37 | 0.58 |
| 2:B:144:VAL:HG12 | 2:B:153:ILE:HD11 | 1.75 | 0.58 |
| 1:D:464:ILE:HG22 | 1:D:465:ALA:N | 2.18 | 0.58 |
| 1:G:92:ALA:O | 1:G:714:ARG:CG | 2.51 | 0.58 |
| 1:J:116:TYR:HB2 | 1:J:153:PRO:O | 2.03 | 0.58 |
| 1:J:646:PHE:CD2 | 1:J:652:LEU:CD1 | 2.85 | 0.58 |
| 1:J:715:VAL:HG11 | 1:J:720:PHE:HD1 | 1.68 | 0.58 |
| 1:J:717:TYR:HD1 | 1:J:744:SER:HG | 1.50 | 0.58 |
| 1:M:230:GLU:O | 1:M:234:ASN:HB2 | 2.03 | 0.58 |
| 1:M:549:SER:OG | 1:M:550:PHE:N | 2.36 | 0.58 |
| 1:M:643:GLY:HA2 | 4:Z:24:ASP:OD1 | 2.04 | 0.58 |
| 1:M:791:GLN:NE2 | 3:O:115:GLY:HA3 | 2.17 | 0.58 |
| 1:P:220:ASP:O | 1:P:224:SER:N | 2.27 | 0.58 |
| 1:P:254:PHE:CE2 | 1:P:459:ILE:HD12 | 2.39 | 0.58 |
| 3:R:52:ASN:N | 3:R:53:PRO:CD | 2.65 | 0.58 |
| 4:4:287:ILE:HG21 | 4:6:204:ALA:H | 1.67 | 0.58 |
| 1:A:135:TYR:N | 1:A:135:TYR:CD1 | 2.70 | 0.58 |
| 1:A:643:GLY:HA2 | 4:8:24:ASP:OD1 | 2.04 | 0.58 |
| 1:A:768:MLY:CG | 1:A:771:LEU:HD13 | 2.27 | 0.58 |
| 1:A:836:PHE:HD2 | 2:B:161:GLU:OE1 | 1.86 | 0.58 |
| 1:D:64:THR:HG22 | 1:D:65:GLU:N | 2.19 | 0.58 |
| 1:D:715:VAL:HG11 | 1:D:720:PHE:HD1 | 1.68 | 0.58 |
| 1:D:776:GLU:O | 1:D:779:ARG:HB3 | 2.03 | 0.58 |
| 1:D:813:ILE:O | 1:D:817:GLN:N | 2.30 | 0.58 |
| 1:D:829:TRP:HE1 | 2:E:67:MET:HG2 | 1.69 | 0.58 |
| 1:G:175:ILE:HA | 1:G:670:HIS:O | 2.04 | 0.58 |
| 1:G:550:PHE:CE2 | 1:G:592:ILE:HG23 | 2.37 | 0.58 |
| 1:J:64:THR:HG22 | 1:J:65:GLU:N | 2.19 | 0.58 |
| 1:J:254:PHE:CE2 | 1:J:459:ILE:HD12 | 2.39 | 0.58 |
| 1:J:536:LEU:HD13 | 1:J:550:PHE:CE1 | 2.37 | 0.58 |
| 1:M:64:THR:HG22 | 1:M:65:GLU:N | 2.19 | 0.58 |
| 1:M:643:GLY:N | 4:Z:23:GLY:C | 2.55 | 0.58 |
| 1:P:796:GLY:HA2 | 3:R:35:ARG:CG | 2.33 | 0.58 |
| 4:7:287:ILE:HD12 | 4:7:287:ILE:H | 1.67 | 0.58 |
| 1:A:715:VAL:HG11 | 1:A:720:PHE:HD1 | 1.68 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:C:46:ILE:O | 3:C:50:LEU:CG | 2.47 | 0.58 |
| 1:D:135:TYR:N | 1:D:135:TYR:CD1 | 2.70 | 0.58 |
| 1:D:141:LEU:O | 1:D:144:ARG:HB3 | 2.04 | 0.58 |
| 1:D:175:ILE:HA | 1:D:670:HIS:O | 2.03 | 0.58 |
| 1:D:418:THR:HG22 | 1:D:419:VAL:H | 1.69 | 0.58 |
| 1:D:629:GLU:HB3 | 1:D:645:SER:N | 2.18 | 0.58 |
| 1:G:49:MLY:HH13 | 1:G:108:GLU:OE2 | 2.03 | 0.58 |
| 1:G:538:GLU:O | 1:G:541:MET:HB2 | 2.04 | 0.58 |
| 1:J:538:GLU:O | 1:J:541:MET:HB2 | 2.03 | 0.58 |
| 1:J:795:ARG:HH21 | 3:L:116:GLU:CG | 2.17 | 0.58 |
| 1:M:254:PHE:CE2 | 1:M:459:ILE:HD12 | 2.39 | 0.58 |
| 1:M:836:PHE:CZ | 2:N:159:HIS:HA | 2.23 | 0.58 |
| 1:P:116:TYR:HB2 | 1:P:153:PRO:O | 2.03 | 0.58 |
| 1:P:464:ILE:HG22 | 1:P:465:ALA:N | 2.19 | 0.58 |
| 4:X:287:ILE:H | 4:Z:202:THR:CG2 | 2.17 | 0.58 |
| 1:A:195:TYR:O | 1:A:199:ILE:HG23 | 2.03 | 0.58 |
| 1:D:254:PHE:CE2 | 1:D:459:ILE:HD12 | 2.39 | 0.58 |
| 1:G:643:GLY:HA2 | 4:V:24:ASP:OD1 | 2.04 | 0.58 |
| 1:G:815:CYS:SG | 2:H:92:ASP:OD1 | 2.61 | 0.58 |
| 1:J:791:GLN:NE2 | 3:L:116:GLU:H | 2.02 | 0.58 |
| 1:M:676:ILE:O | 1:M:676:ILE:HG23 | 2.03 | 0.58 |
| 1:M:839:MLY:HH21 | 2:N:158:THR:HG22 | 1.84 | 0.58 |
| 1:P:93:MET:HA | 1:P:714:ARG:H | 1.67 | 0.58 |
| 4:I:243:PRO:CB | 4:Y:291:LYS:CD | 2.69 | 0.58 |
| 1:A:279:LEU:HB3 | 1:A:280:PRO:HD2 | 1.86 | 0.58 |
| 3:C:52:ASN:HB2 | 3:C:53:PRO:CD | 2.28 | 0.58 |
| 1:D:549:SER:OG | 1:D:550:PHE:N | 2.36 | 0.58 |
| 1:D:642:LYS:CG | 4:9:22:ALA:CA | 2.80 | 0.58 |
| 1:G:813:ILE:O | 1:G:817:GLN:N | 2.30 | 0.58 |
| 1:J:7:MET:HE3 | 1:J:14:ALA:HB1 | 1.84 | 0.58 |
| 1:J:819:ASN:HD21 | 2:K:92:ASP:HB2 | 1.55 | 0.58 |
| 1:M:220:ASP:O | 1:M:224:SER:N | 2.27 | 0.58 |
| 1:M:279:LEU:HB3 | 1:M:280:PRO:HD2 | 1.86 | 0.58 |
| 1:M:322:VAL:HG11 | 1:M:325:ILE:HD11 | 1.86 | 0.58 |
| 1:M:534:SER:C | 4:Z:351:THR:CA | 2.47 | 0.58 |
| 1:M:755:HIS:HA | 1:M:758:TYR:HE1 | 1.65 | 0.58 |
| 1:M:821:ARG:NH1 | 2:N:127:ARG:NE | 2.52 | 0.58 |
| 1:P:124:VAL:HG13 | 1:P:675:ILE:CD1 | 2.33 | 0.58 |
| 1:A:116:TYR:HB2 | 1:A:153:PRO:O | 2.03 | 0.58 |
| 1:A:265:ILE:HG22 | 1:A:266:GLU:N | 2.18 | 0.58 |
| 1:A:707:CYS:C | 1:A:714:ARG:HH22 | 2.03 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:124:VAL:HG13 | 1:G:675:ILE:CD1 | 2.33 | 0.58 |
| 1:G:279:LEU:HB3 | 1:G:280:PRO:HD2 | 1.86 | 0.58 |
| 1:G:557:GLU:HB2 | 4:X:47:MET:O | 2.04 | 0.58 |
| 1:G:643:GLY:N | 4:V:23:GLY:C | 2.55 | 0.58 |
| 1:G:798:LEU:HD22 | 3:I:118:MET:HG3 | 1.86 | 0.58 |
| 1:J:265:ILE:HG22 | 1:J:266:GLU:N | 2.18 | 0.58 |
| 1:J:801:VAL:HG21 | 3:L:126:LEU:HD21 | 1.84 | 0.58 |
| 1:M:642:LYS:CG | 4:Z:22:ALA:CA | 2.80 | 0.58 |
| 1:P:64:THR:HG22 | 1:P:65:GLU:N | 2.19 | 0.58 |
| 1:P:279:LEU:HB3 | 1:P:280:PRO:HD2 | 1.86 | 0.58 |
| 1:P:642:LYS:CD | 4:1:340:TRP:CZ3 | 2.79 | 0.58 |
| 1:P:721:LYS:HG2 | 1:P:736:GLN:CD | 1.86 | 0.58 |
| 1:P:732:ILE:HG22 | 1:P:747:LEU:CD1 | 1.55 | 0.58 |
| 1:P:813:ILE:O | 1:P:816:ILE:N | 2.37 | 0.58 |
| 1:P:821:ARG:HH12 | 2:Q:127:ARG:CZ | 2.17 | 0.58 |
| 4:1:203:THR:HG22 | 4:Y:286:ASP:OD2 | 2.04 | 0.58 |
| 4:W:286:ASP:OD1 | 4:Y:203:THR:HG22 | 2.04 | 0.58 |
| 1:A:218:LEU:N | 1:A:221:GLN:HE21 | 2.01 | 0.57 |
| 3:C:49:ILE:CA | 3:C:52:ASN:ND2 | 2.53 | 0.57 |
| 1:D:124:VAL:HG13 | 1:D:675:ILE:CD1 | 2.33 | 0.57 |
| 1:D:831:TRP:CH2 | 2:E:47:LEU:CA | 2.56 | 0.57 |
| 1:G:135:TYR:N | 1:G:135:TYR:CD1 | 2.70 | 0.57 |
| 1:J:175:ILE:HA | 1:J:670:HIS:O | 2.03 | 0.57 |
| 1:J:464:ILE:HG22 | 1:J:465:ALA:N | 2.18 | 0.57 |
| 1:J:784:ALA:O | 1:J:788:THR:CB | 2.52 | 0.57 |
| 1:J:795:ARG:CA | 3:L:35:ARG:NH2 | 2.62 | 0.57 |
| 1:M:601:ASP:N | 1:M:602:PRO:HD3 | 2.18 | 0.57 |
| 2:N:117:LEU:CB | 2:N:147:ASN:ND2 | 2.35 | 0.57 |
| 1:P:642:LYS:CG | 4:1:22:ALA:CA | 2.80 | 0.57 |
| 4:1:247:VAL:N | 4:Y:324:THR:HB | 2.18 | 0.57 |
| 4:W:285:CYS:O | 4:Y:202:THR:CG2 | 2.52 | 0.57 |
| 4:X:287:ILE:HD13 | 4:Z:202:THR:O | 2.03 | 0.57 |
| 1:A:676:ILE:HG23 | 1:A:676:ILE:O | 2.03 | 0.57 |
| 1:D:48:VAL:HG22 | 1:D:49:MLY:N | 2.19 | 0.57 |
| 1:D:99:GLU:OE2 | 1:D:696:ARG:NH2 | 2.31 | 0.57 |
| 1:D:601:ASP:N | 1:D:602:PRO:HD3 | 2.18 | 0.57 |
| 1:D:717:TYR:HD1 | 1:D:744:SER:HG | 1.53 | 0.57 |
| 1:G:230:GLU:O | 1:G:234:ASN:HB2 | 2.03 | 0.57 |
| 1:G:464:ILE:HG22 | 1:G:465:ALA:N | 2.18 | 0.57 |
| 1:G:757:GLN:HG3 | 1:G:776:GLU:CB | 2.21 | 0.57 |
| 2:H:112:ILE:C | 2:H:147:ASN:O | 2.43 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:710:GLY:N | 1:J:772:LEU:HD22 | 2.15 | 0.57 |
| 3:R:102:VAL:HG23 | 3:R:139:TYR:CD1 | 2.39 | 0.57 |
| 4:2:287:ILE:HB | 4:4:203:THR:CA | 2.33 | 0.57 |
| 4:4:223:PHE:HD2 | 4:4:312:ARG:NH2 | 2.00 | 0.57 |
| 1:A:124:VAL:HG13 | 1:A:675:ILE:CD1 | 2.33 | 0.57 |
| 1:A:831:TRP:CD2 | 2:B:51:PHE:CE1 | 2.84 | 0.57 |
| 1:D:712:PRO:CB | 1:D:771:LEU:HD22 | 2.33 | 0.57 |
| 1:G:642:LYS:CD | 4:V:340:TRP:CZ3 | 2.80 | 0.57 |
| 1:J:279:LEU:HB3 | 1:J:280:PRO:HD2 | 1.86 | 0.57 |
| 1:J:568:PRO:HG3 | 1:J:578:HIS:H | 1.69 | 0.57 |
| 1:J:676:ILE:HG23 | 1:J:676:ILE:O | 2.03 | 0.57 |
| 3:L:102:VAL:HG23 | 3:L:139:TYR:CD1 | 2.39 | 0.57 |
| 1:M:709:LYS:C | 1:M:710:GLY:HA2 | 2.24 | 0.57 |
| 3:O:49:ILE:HA | 3:O:52:ASN:ND2 | 2.06 | 0.57 |
| 1:A:529:PRO:HG3 | 4:8:353:GLN:OE1 | 2.03 | 0.57 |
| 1:A:568:PRO:HG3 | 1:A:578:HIS:H | 1.69 | 0.57 |
| 1:A:813:ILE:O | 1:A:816:ILE:N | 2.37 | 0.57 |
| 1:D:220:ASP:O | 1:D:224:SER:N | 2.27 | 0.57 |
| 1:D:599:ASN:CG | 1:D:649:VAL:HB | 2.25 | 0.57 |
| 1:G:7:MET:HE3 | 1:G:14:ALA:HB1 | 1.86 | 0.57 |
| 1:G:529:PRO:HG3 | 4:V:353:GLN:OE1 | 2.04 | 0.57 |
| 1:G:747:LEU:HD23 | 1:G:747:LEU:O | 2.05 | 0.57 |
| 3:I:102:VAL:HG11 | 3:I:107:LEU:HB2 | 1.85 | 0.57 |
| 1:J:530:MET:CA | 4:W:354:GLN:HB3 | 2.35 | 0.57 |
| 1:J:794:CYS:O | 1:J:798:LEU:N | 2.37 | 0.57 |
| 1:M:646:PHE:CD2 | 1:M:652:LEU:CD1 | 2.85 | 0.57 |
| 1:M:715:VAL:HG11 | 1:M:720:PHE:HD1 | 1.68 | 0.57 |
| 1:M:747:LEU:O | 1:M:747:LEU:HD23 | 2.05 | 0.57 |
| 2:N:144:VAL:HG12 | 2:N:153:ILE:HD11 | 1.75 | 0.57 |
| 1:P:175:ILE:HA | 1:P:670:HIS:O | 2.04 | 0.57 |
| 1:P:409:GLY:HA3 | 4:1:333:PRO:CD | 2.35 | 0.57 |
| 1:P:676:ILE:O | 1:P:676:ILE:HG23 | 2.03 | 0.57 |
| 1:A:254:PHE:CE2 | 1:A:459:ILE:HD12 | 2.39 | 0.57 |
| 1:A:538:GLU:O | 1:A:541:MET:HB2 | 2.04 | 0.57 |
| 1:A:783:LEU:O | 1:A:787:ILE:N | 2.28 | 0.57 |
| 1:A:798:LEU:HD12 | 3:C:126:LEU:HD21 | 1.80 | 0.57 |
| 1:A:839:MLY:CH1 | 2:B:159:HIS:HD2 | 2.17 | 0.57 |
| 1:D:530:MET:CA | 4:9:354:GLN:HB3 | 2.35 | 0.57 |
| 1:D:538:GLU:O | 1:D:541:MET:HB2 | 2.04 | 0.57 |
| 1:D:676:ILE:HG23 | 1:D:676:ILE:O | 2.03 | 0.57 |
| 1:D:727:LEU:HG | 1:D:782:MLY:CD | 2.30 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:798:LEU:HD11 | 3:F:126:LEU:HD11 | 0.58 | 0.57 |
| 3:F:102:VAL:HG11 | 3:F:107:LEU:HB2 | 1.84 | 0.57 |
| 1:G:220:ASP:O | 1:G:224:SER:N | 2.28 | 0.57 |
| 1:G:813:ILE:O | 1:G:816:ILE:N | 2.37 | 0.57 |
| 1:J:409:GLY:HA3 | 4:W:333:PRO:CD | 2.35 | 0.57 |
| 1:J:599:ASN:CG | 1:J:649:VAL:HB | 2.25 | 0.57 |
| 1:M:568:PRO:HG3 | 1:M:578:HIS:H | 1.69 | 0.57 |
| 1:M:579:PHE:CD2 | 1:M:592:ILE:HD11 | 2.40 | 0.57 |
| 1:P:92:ALA:O | 1:P:712:PRO:O | 2.23 | 0.57 |
| 1:P:418:THR:HG22 | 1:P:419:VAL:H | 1.69 | 0.57 |
| 4:1:246:GLN:N | 4:Y:324:THR:HB | 2.19 | 0.57 |
| 1:A:322:VAL:HG11 | 1:A:325:ILE:HD11 | 1.86 | 0.57 |
| 1:D:279:LEU:HB3 | 1:D:280:PRO:HD2 | 1.86 | 0.57 |
| 1:D:295:MLY:HG3 | 1:D:332:MET:HE1 | 1.87 | 0.57 |
| 1:D:409:GLY:HA3 | 4:9:333:PRO:CD | 2.35 | 0.57 |
| 1:D:507:GLY:HA3 | 1:D:762:HIS:CA | 2.34 | 0.57 |
| 1:G:218:LEU:N | 1:G:221:GLN:HE21 | 2.01 | 0.57 |
| 1:G:510:TRP:CH2 | 1:G:768:MLY:HH11 | 2.39 | 0.57 |
| 1:G:677:PRO:HB2 | 1:G:678:ASN:ND2 | 2.20 | 0.57 |
| 1:G:754:ASP:O | 1:G:776:GLU:OE2 | 2.23 | 0.57 |
| 1:J:141:LEU:O | 1:J:144:ARG:HB3 | 2.04 | 0.57 |
| 1:J:567:LYS:HZ3 | 4:Y:92:ASN:ND2 | 1.98 | 0.57 |
| 1:J:642:LYS:CG | 4:W:22:ALA:CA | 2.80 | 0.57 |
| 1:M:218:LEU:N | 1:M:221:GLN:HE21 | 2.01 | 0.57 |
| 1:M:717:TYR:HD1 | 1:M:744:SER:HG | 1.50 | 0.57 |
| 1:P:530:MET:CA | 4:1:354:GLN:HB3 | 2.35 | 0.57 |
| 1:P:649:VAL:HA | 1:P:649:VAL:HG22 | 1.80 | 0.57 |
| 1:P:747:LEU:O | 1:P:747:LEU:HD23 | 2.05 | 0.57 |
| 1:P:836:PHE:CE1 | 2:Q:159:HIS:C | 2.78 | 0.57 |
| 4:1:243:PRO:CA | 4:Y:291:LYS:CE | 2.81 | 0.57 |
| 1:A:409:GLY:HA3 | 4:8:333:PRO:CD | 2.34 | 0.57 |
| 1:A:530:MET:CA | 4:8:354:GLN:HB3 | 2.34 | 0.57 |
| 1:A:541:MET:HG2 | 4:8:345:ILE:CG2 | 2.35 | 0.57 |
| 1:A:747:LEU:HD23 | 1:A:747:LEU:O | 2.05 | 0.57 |
| 1:A:800:ARG:CD | 3:C:149:VAL:C | 2.73 | 0.57 |
| 1:D:109:ARG:O | 1:D:114:MET:N | 2.37 | 0.57 |
| 1:D:541:MET:HG2 | 4:9:345:ILE:CG2 | 2.35 | 0.57 |
| 1:D:795:ARG:HD2 | 3:F:35:ARG:NH1 | 2.18 | 0.57 |
| 1:D:813:ILE:O | 1:D:816:ILE:N | 2.38 | 0.57 |
| 2:E:140:PHE:O | 2:E:141:PRO:C | 2.33 | 0.57 |
| 1:G:22:LYS:O | 1:G:26:GLU:N | 2.30 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:418:THR:HG22 | 1:J:419:VAL:H | 1.69 | 0.57 |
| 1:J:630:ALA:CA | 4:W:25:ASP:OD2 | 2.53 | 0.57 |
| 1:M:529:PRO:HG3 | 4:Z:353:GLN:OE1 | 2.04 | 0.57 |
| 1:P:173:GLN:C | 1:P:667:THR:HG23 | 2.25 | 0.57 |
| 1:P:630:ALA:CA | 4:1:25:ASP:OD2 | 2.53 | 0.57 |
| 4:1:287:ILE:CD1 | 4:3:203:THR:HB | 2.34 | 0.57 |
| 4:X:288:ASP:CB | 4:Z:204:ALA:HB3 | 2.05 | 0.57 |
| 1:A:530:MET:HE3 | 4:8:354:GLN:CB | 2.33 | 0.57 |
| 1:D:218:LEU:N | 1:D:221:GLN:HE21 | 2.01 | 0.57 |
| 1:D:798:LEU:CD1 | 3:F:126:LEU:CD2 | 2.83 | 0.57 |
| 1:G:638:GLY:CA | 4:V:345:ILE:H | 2.18 | 0.57 |
| 1:G:829:TRP:HZ2 | 2:H:83:MET:CE | 2.15 | 0.57 |
| 1:J:481:ASN:N | 1:J:481:ASN:ND2 | 2.51 | 0.57 |
| 1:J:561:LYS:HE3 | 4:Y:48:GLY:CA | 2.29 | 0.57 |
| 1:M:409:GLY:HA3 | 4:Z:333:PRO:CD | 2.35 | 0.57 |
| 1:M:638:GLY:CA | 4:Z:345:ILE:H | 2.18 | 0.57 |
| 1:M:836:PHE:CE1 | 2:N:159:HIS:C | 2.78 | 0.57 |
| 1:P:141:LEU:O | 1:P:144:ARG:HB3 | 2.04 | 0.57 |
| 1:P:568:PRO:HG3 | 1:P:578:HIS:H | 1.69 | 0.57 |
| 1:P:805:ALA:O | 1:P:809:ARG:HB2 | 2.04 | 0.57 |
| 4:1:202:THR:CA | 4:Y:286:ASP:OD1 | 2.52 | 0.57 |
| 4:4:287:ILE:HB | 4:6:203:THR:CG2 | 2.35 | 0.57 |
| 1:A:649:VAL:HA | 1:A:649:VAL:HG23 | 1.83 | 0.57 |
| 1:D:834:LEU:HG | 2:E:54:MET:SD | 2.44 | 0.57 |
| 1:G:568:PRO:HG3 | 1:G:578:HIS:H | 1.69 | 0.57 |
| 1:G:676:ILE:HG23 | 1:G:676:ILE:O | 2.03 | 0.57 |
| 1:J:529:PRO:HG3 | 4:W:353:GLN:OE1 | 2.04 | 0.57 |
| 1:J:643:GLY:N | 4:W:23:GLY:C | 2.55 | 0.57 |
| 1:J:813:ILE:O | 1:J:816:ILE:N | 2.38 | 0.57 |
| 1:M:82:PRO:HD2 | 1:M:85:TYR:CD2 | 2.40 | 0.57 |
| 2:N:112:ILE:C | 2:N:147:ASN:O | 2.43 | 0.57 |
| 1:P:82:PRO:HD2 | 1:P:85:TYR:CD2 | 2.40 | 0.57 |
| 1:P:127:ASN:ND2 | 1:P:128:PRO:HD2 | 2.16 | 0.57 |
| 1:P:579:PHE:CD2 | 1:P:592:ILE:HD11 | 2.40 | 0.57 |
| 1:P:643:GLY:N | 4:1:23:GLY:C | 2.55 | 0.57 |
| 1:A:173:GLN:C | 1:A:667:THR:HG23 | 2.25 | 0.57 |
| 1:A:677:PRO:HB2 | 1:A:678:ASN:ND2 | 2.20 | 0.57 |
| 2:B:112:ILE:C | 2:B:147:ASN:O | 2.42 | 0.57 |
| 3:F:102:VAL:HG23 | 3:F:139:TYR:CD1 | 2.39 | 0.57 |
| 1:G:64:THR:HG22 | 1:G:65:GLU:N | 2.19 | 0.57 |
| 1:G:173:GLN:C | 1:G:667:THR:HG23 | 2.25 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:635:GLY:HA3 | 4:V:334:GLU:CG | 2.30 | 0.57 |
| 1:J:534:SER:C | 4:W:351:THR:CA | 2.47 | 0.57 |
| 1:J:643:GLY:HA2 | 4:W:24:ASP:OD1 | 2.04 | 0.57 |
| 1:J:783:LEU:O | 1:J:787:ILE:CB | 2.52 | 0.57 |
| 1:M:173:GLN:C | 1:M:667:THR:HG23 | 2.25 | 0.57 |
| 1:M:530:MET:CA | 4:Z:354:GLN:HB3 | 2.34 | 0.57 |
| 1:M:818:TYR:CD1 | 2:N:127:ARG:CZ | 2.87 | 0.57 |
| 3:O:102:VAL:HG11 | 3:O:107:LEU:HB2 | 1.85 | 0.57 |
| 1:P:643:GLY:HA2 | 4:1:24:ASP:OD1 | 2.04 | 0.57 |
| 1:A:92:ALA:O | 1:A:713:SER:CA | 2.47 | 0.56 |
| 1:A:646:PHE:CD2 | 1:A:652:LEU:CD1 | 2.85 | 0.56 |
| 1:A:707:CYS:HA | 1:A:714:ARG:HH22 | 1.70 | 0.56 |
| 1:D:302:MET:HG2 | 1:D:303:LEU:HD13 | 1.87 | 0.56 |
| 1:D:529:PRO:CG | 4:9:353:GLN:OE1 | 2.53 | 0.56 |
| 1:D:541:MET:SD | 4:9:346:LEU:O | 2.48 | 0.56 |
| 1:D:568:PRO:HG3 | 1:D:578:HIS:H | 1.69 | 0.56 |
| 1:D:795:ARG:HE | 3:F:116:GLU:HB3 | 1.69 | 0.56 |
| 2:E:150:TYR:C | 2:E:151:LYS:CG | 2.48 | 0.56 |
| 1:G:794:CYS:O | 1:G:798:LEU:N | 2.37 | 0.56 |
| 1:J:97:LEU:HD22 | 1:J:712:PRO:CB | 2.29 | 0.56 |
| 1:J:639:GLY:N | 4:W:344:SER:C | 2.54 | 0.56 |
| 1:M:99:GLU:OE2 | 1:M:696:ARG:NH2 | 2.31 | 0.56 |
| 1:M:677:PRO:HB2 | 1:M:678:ASN:ND2 | 2.20 | 0.56 |
| 1:P:541:MET:HG2 | 4:1:345:ILE:CG2 | 2.35 | 0.56 |
| 1:P:798:LEU:HD13 | 3:R:126:LEU:CD1 | 2.30 | 0.56 |
| 4:1:201:VAL:HG23 | 4:Y:287:ILE:HG13 | 1.85 | 0.56 |
| 1:A:116:TYR:CE2 | 1:A:154:HIS:CD2 | 2.94 | 0.56 |
| 1:A:752:ASP:OD2 | 1:A:782:MLY:HD3 | 2.05 | 0.56 |
| 3:C:102:VAL:HG23 | 3:C:139:TYR:CD1 | 2.39 | 0.56 |
| 1:D:823:PHE:CD1 | 2:E:160:GLY:HA3 | 2.39 | 0.56 |
| 1:G:254:PHE:CE2 | 1:G:459:ILE:HD12 | 2.39 | 0.56 |
| 1:G:411:GLU:H | 4:V:333:PRO:HG2 | 1.70 | 0.56 |
| 1:G:707:CYS:HB3 | 1:G:712:PRO:HA | 1.86 | 0.56 |
| 1:J:541:MET:HG2 | 4:W:345:ILE:CG2 | 2.35 | 0.56 |
| 1:J:733:PRO:CA | 1:J:737:PHE:HE1 | 2.18 | 0.56 |
| 1:J:796:GLY:CA | 3:L:35:ARG:CD | 2.71 | 0.56 |
| 1:P:109:ARG:O | 1:P:114:MET:N | 2.37 | 0.56 |
| 1:A:64:THR:HG22 | 1:A:65:GLU:N | 2.19 | 0.56 |
| 1:A:82:PRO:HD2 | 1:A:85:TYR:CD2 | 2.40 | 0.56 |
| 1:A:109:ARG:O | 1:A:114:MET:N | 2.37 | 0.56 |
| 1:A:127:ASN:ND2 | 1:A:128:PRO:HD2 | 2.17 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:635:GLY:HA3 | 4:8:334:GLU:CG | 2.30 | 0.56 |
| 1:A:638:GLY:CA | 4:8:345:ILE:H | 2.19 | 0.56 |
| 1:D:135:TYR:N | 1:D:135:TYR:HD1 | 2.04 | 0.56 |
| 1:D:173:GLN:C | 1:D:667:THR:HG23 | 2.25 | 0.56 |
| 1:D:630:ALA:CA | 4:9:25:ASP:OD2 | 2.53 | 0.56 |
| 1:D:726:VAL:HG11 | 1:D:785:GLU:HB3 | 1.87 | 0.56 |
| 1:D:727:LEU:CA | 1:D:782:MLY:HE2 | 2.22 | 0.56 |
| 3:F:46:ILE:O | 3:F:50:LEU:CG | 2.47 | 0.56 |
| 1:G:22:LYS:HA | 1:G:25:ILE:HB | 1.87 | 0.56 |
| 1:G:82:PRO:HD2 | 1:G:85:TYR:CD2 | 2.40 | 0.56 |
| 1:G:322:VAL:HG11 | 1:G:325:ILE:HD11 | 1.86 | 0.56 |
| 1:J:218:LEU:N | 1:J:221:GLN:HE21 | 2.01 | 0.56 |
| 1:J:338:ILE:HG21 | 1:J:348:MLY:HB3 | 1.87 | 0.56 |
| 1:J:561:LYS:CE | 4:Y:48:GLY:CA | 2.82 | 0.56 |
| 1:J:642:LYS:CA | 4:W:22:ALA:C | 2.70 | 0.56 |
| 1:M:22:LYS:HA | 1:M:25:ILE:HB | 1.88 | 0.56 |
| 1:M:34:ALA:HB3 | 1:M:777:GLU:CD | 2.24 | 0.56 |
| 1:M:135:TYR:N | 1:M:135:TYR:HD1 | 2.04 | 0.56 |
| 1:M:217:THR:HG22 | 1:M:218:LEU:O | 2.06 | 0.56 |
| 1:M:813:ILE:O | 1:M:816:ILE:N | 2.38 | 0.56 |
| 1:P:338:ILE:HG21 | 1:P:348:MLY:HB3 | 1.87 | 0.56 |
| 1:P:411:GLU:H | 4:1:333:PRO:HG2 | 1.71 | 0.56 |
| 1:P:599:ASN:CG | 1:P:649:VAL:HB | 2.25 | 0.56 |
| 4:2:287:ILE:HG21 | 4:4:203:THR:N | 2.19 | 0.56 |
| 4:V:288:ASP:N | 4:X:204:ALA:H | 2.03 | 0.56 |
| 4:Z:365:ALA:HB3 | 4:Z:369:ILE:HB | 1.88 | 0.56 |
| 1:A:599:ASN:CG | 1:A:649:VAL:HB | 2.25 | 0.56 |
| 1:D:649:VAL:HA | 1:D:649:VAL:HG23 | 1.82 | 0.56 |
| 1:G:116:TYR:CE2 | 1:G:154:HIS:CD2 | 2.94 | 0.56 |
| 1:G:541:MET:HG2 | 4:V:345:ILE:CG2 | 2.35 | 0.56 |
| 1:G:792:ALA:CA | 3:I:42:THR:HA | 2.35 | 0.56 |
| 1:J:173:GLN:C | 1:J:667:THR:HG23 | 2.25 | 0.56 |
| 1:J:710:GLY:O | 1:J:772:LEU:CB | 2.52 | 0.56 |
| 1:P:7:MET:HE3 | 1:P:14:ALA:HB1 | 1.86 | 0.56 |
| 4:1:247:VAL:CG2 | 4:Y:324:THR:HG21 | 2.30 | 0.56 |
| 4:X:365:ALA:HB3 | 4:X:369:ILE:HB | 1.88 | 0.56 |
| 1:A:411:GLU:H | 4:8:333:PRO:HG2 | 1.71 | 0.56 |
| 1:A:795:ARG:HG2 | 3:C:118:MET:HE1 | 1.86 | 0.56 |
| 1:D:338:ILE:HG21 | 1:D:348:MLY:HB3 | 1.87 | 0.56 |
| 1:D:411:GLU:H | 4:9:333:PRO:HG2 | 1.70 | 0.56 |
| 1:D:546:THR:HG21 | 1:D:548:THR:HB | 1.88 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:D:643:GLY:HA2 | 4:9:24:ASP:OD1 | 2.04 | 0.56 |
| 1:D:677:PRO:HB2 | 1:D:678:ASN:ND2 | 2.20 | 0.56 |
| 1:G:506:GLU:OE2 | 1:G:760:PHE:CB | 2.46 | 0.56 |
| 1:G:541:MET:SD | 4:V:346:LEU:O | 2.49 | 0.56 |
| 1:J:411:GLU:H | 4:W:333:PRO:HG2 | 1.71 | 0.56 |
| 1:J:733:PRO:CB | 1:J:737:PHE:HE1 | 2.19 | 0.56 |
| 1:J:747:LEU:O | 1:J:747:LEU:HD23 | 2.05 | 0.56 |
| 1:J:817:GLN:CB | 2:K:127:ARG:HH11 | 2.18 | 0.56 |
| 1:M:649:VAL:HA | 1:M:649:VAL:HG23 | 1.83 | 0.56 |
| 1:M:836:PHE:CD2 | 2:N:160:GLY:HA3 | 2.39 | 0.56 |
| 1:P:529:PRO:CG | 4:1:353:GLN:OE1 | 2.54 | 0.56 |
| 1:P:649:VAL:CG1 | 1:P:649:VAL:HA | 2.35 | 0.56 |
| 1:P:677:PRO:HB2 | 1:P:678:ASN:ND2 | 2.20 | 0.56 |
| 4:3:287:ILE:HB | 4:5:204:ALA:N | 2.21 | 0.56 |
| 4:X:288:ASP:HB3 | 4:Z:204:ALA:HB1 | 1.86 | 0.56 |
| 1:A:579:PHE:CD2 | 1:A:592:ILE:HD11 | 2.40 | 0.56 |
| 1:A:733:PRO:CA | 1:A:737:PHE:HE1 | 2.19 | 0.56 |
| 1:D:82:PRO:HD2 | 1:D:85:TYR:CD2 | 2.40 | 0.56 |
| 1:D:508:ILE:CA | 1:D:761:GLY:HA3 | 2.26 | 0.56 |
| 1:G:135:TYR:N | 1:G:135:TYR:HD1 | 2.04 | 0.56 |
| 1:G:796:GLY:HA2 | 3:I:35:ARG:CZ | 2.35 | 0.56 |
| 1:G:817:GLN:CG | 2:H:127:ARG:CB | 2.79 | 0.56 |
| 1:M:435:GLU:O | 1:M:438:PHE:HB3 | 2.06 | 0.56 |
| 1:M:794:CYS:O | 1:M:798:LEU:N | 2.37 | 0.56 |
| 1:P:797:PHE:CE2 | 3:R:126:LEU:CD2 | 2.83 | 0.56 |
| 4:5:365:ALA:HB3 | 4:5:369:ILE:HB | 1.88 | 0.56 |
| 4:V:365:ALA:HB3 | 4:V:369:ILE:HB | 1.88 | 0.56 |
| 1:A:93:MET:C | 1:A:713:SER:HB3 | 2.26 | 0.56 |
| 1:A:499:GLU:CD | 1:A:766:PHE:HE2 | 2.09 | 0.56 |
| 1:A:823:PHE:CE1 | 2:B:160:GLY:HA3 | 2.39 | 0.56 |
| 1:G:127:ASN:ND2 | 1:G:128:PRO:HD2 | 2.17 | 0.56 |
| 1:G:409:GLY:HA3 | 4:V:333:PRO:CD | 2.35 | 0.56 |
| 1:G:506:GLU:OE2 | 1:G:760:PHE:C | 2.44 | 0.56 |
| 1:G:649:VAL:HA | 1:G:649:VAL:HG22 | 1.80 | 0.56 |
| 1:G:753:VAL:HA | 1:G:780:ASP:CG | 2.19 | 0.56 |
| 1:G:798:LEU:CD2 | 3:I:118:MET:CB | 2.82 | 0.56 |
| 3:I:52:ASN:HB2 | 3:I:53:PRO:CD | 2.28 | 0.56 |
| 1:J:206:LYS:HB3 | 1:J:217:THR:OG1 | 2.06 | 0.56 |
| 1:J:302:MET:HG2 | 1:J:303:LEU:HD13 | 1.87 | 0.56 |
| 1:M:116:TYR:CE2 | 1:M:154:HIS:CD2 | 2.94 | 0.56 |
| 1:P:7:MET:HE3 | 1:P:14:ALA:CB | 2.36 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:P:32:PHE:CG | 1:P:83:PRO:HD3 | 2.41 | 0.56 |
| 1:P:135:TYR:N | 1:P:135:TYR:HD1 | 2.04 | 0.56 |
| 1:P:206:LYS:HB3 | 1:P:217:THR:OG1 | 2.06 | 0.56 |
| 1:P:217:THR:HG22 | 1:P:218:LEU:O | 2.05 | 0.56 |
| 1:P:537:GLU:HB3 | 1:P:648:THR:CB | 2.36 | 0.56 |
| 4:8:288:ASP:CA | 4:V:204:ALA:HB2 | 2.32 | 0.56 |
| 4:V:291:LYS:HD2 | 4:X:243:PRO:HB2 | 1.87 | 0.56 |
| 1:A:22:LYS:HA | 1:A:25:ILE:HB | 1.88 | 0.56 |
| 1:A:649:VAL:HA | 1:A:649:VAL:HG22 | 1.81 | 0.56 |
| 1:D:747:LEU:HD23 | 1:D:747:LEU:O | 2.05 | 0.56 |
| 1:D:795:ARG:CG | 3:F:118:MET:HE1 | 2.34 | 0.56 |
| 1:G:406:VAL:HG12 | 1:G:407:GLY:H | 1.71 | 0.56 |
| 1:G:553:MLY:HH12 | 4:X:45:VAL:CG1 | 2.29 | 0.56 |
| 1:G:599:ASN:CG | 1:G:649:VAL:HB | 2.25 | 0.56 |
| 1:G:755:HIS:HA | 1:G:758:TYR:HE1 | 1.64 | 0.56 |
| 1:G:792:ALA:HA | 3:I:42:THR:HA | 1.88 | 0.56 |
| 3:I:46:ILE:O | 3:I:50:LEU:CG | 2.47 | 0.56 |
| 1:J:217:THR:HG22 | 1:J:218:LEU:O | 2.05 | 0.56 |
| 1:J:604:ASN:OD1 | 1:J:607:VAL:HG23 | 2.06 | 0.56 |
| 1:J:677:PRO:HB2 | 1:J:678:ASN:ND2 | 2.20 | 0.56 |
| 1:M:295:MLY:HG3 | 1:M:332:MET:HE1 | 1.86 | 0.56 |
| 1:M:506:GLU:O | 1:M:762:HIS:CD2 | 2.58 | 0.56 |
| 1:M:798:LEU:HD13 | 3:O:126:LEU:CD1 | 2.29 | 0.56 |
| 1:P:302:MET:HG2 | 1:P:303:LEU:HD13 | 1.87 | 0.56 |
| 1:P:322:VAL:HG11 | 1:P:325:ILE:HD11 | 1.86 | 0.56 |
| 1:P:755:HIS:HA | 1:P:758:TYR:HE1 | 1.64 | 0.56 |
| 1:P:798:LEU:HD23 | 3:R:122:GLU:HB3 | 1.86 | 0.56 |
| 1:A:22:LYS:O | 1:A:26:GLU:HG3 | 2.06 | 0.56 |
| 1:A:217:THR:HG22 | 1:A:218:LEU:O | 2.05 | 0.56 |
| 1:A:530:MET:CB | 4:8:354:GLN:HG3 | 2.36 | 0.56 |
| 1:A:630:ALA:CA | 4:8:25:ASP:OD2 | 2.53 | 0.56 |
| 1:D:116:TYR:CE2 | 1:D:154:HIS:CD2 | 2.94 | 0.56 |
| 1:D:322:VAL:HG11 | 1:D:325:ILE:HD11 | 1.86 | 0.56 |
| 1:G:22:LYS:O | 1:G:26:GLU:HG3 | 2.06 | 0.56 |
| 1:G:435:GLU:O | 1:G:438:PHE:HB3 | 2.06 | 0.56 |
| 1:G:579:PHE:CD2 | 1:G:592:ILE:HD11 | 2.40 | 0.56 |
| 1:G:649:VAL:CG1 | 1:G:649:VAL:HA | 2.35 | 0.56 |
| 1:G:783:LEU:HA | 1:G:786:ILE:HB | 1.87 | 0.56 |
| 1:J:82:PRO:HD2 | 1:J:85:TYR:CD2 | 2.40 | 0.56 |
| 1:J:109:ARG:O | 1:J:114:MET:N | 2.37 | 0.56 |
| 1:J:529:PRO:CB | 4:W:354:GLN:HA | 2.36 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:537:GLU:HB3 | 1:J:648:THR:CB | 2.36 | 0.56 |
| 1:M:541:MET:HG2 | 4:Z:345:ILE:CG2 | 2.35 | 0.56 |
| 1:M:630:ALA:CA | 4:Z:25:ASP:OD2 | 2.53 | 0.56 |
| 1:M:640:LYS:C | 1:M:645:SER:OG | 2.44 | 0.56 |
| 1:P:733:PRO:CA | 1:P:737:PHE:HE1 | 2.18 | 0.56 |
| 4:2:324:THR:OG1 | 4:4:244:ASP:CB | 2.53 | 0.56 |
| 4:8:365:ALA:HB3 | 4:8:369:ILE:HB | 1.88 | 0.56 |
| 1:A:97:LEU:HD22 | 1:A:712:PRO:HB2 | 1.81 | 0.56 |
| 1:A:290:GLN:HG2 | 1:A:331:LEU:HA | 1.87 | 0.56 |
| 1:A:435:GLU:O | 1:A:438:PHE:HB3 | 2.06 | 0.56 |
| 1:A:529:PRO:CB | 4:8:354:GLN:HA | 2.36 | 0.56 |
| 1:A:629:GLU:O | 1:A:643:GLY:HA3 | 2.06 | 0.56 |
| 1:A:640:LYS:C | 1:A:645:SER:OG | 2.44 | 0.56 |
| 1:D:435:GLU:O | 1:D:438:PHE:HB3 | 2.06 | 0.56 |
| 1:G:538:GLU:CG | 4:V:351:THR:C | 2.73 | 0.56 |
| 1:G:629:GLU:O | 1:G:643:GLY:HA3 | 2.06 | 0.56 |
| 1:G:754:ASP:HB2 | 1:G:776:GLU:CG | 2.34 | 0.56 |
| 1:J:322:VAL:HG11 | 1:J:325:ILE:HD11 | 1.86 | 0.56 |
| 1:J:529:PRO:CG | 4:W:353:GLN:OE1 | 2.54 | 0.56 |
| 1:J:819:ASN:OD1 | 2:K:91:ALA:C | 2.40 | 0.56 |
| 1:M:127:ASN:ND2 | 1:M:128:PRO:HD2 | 2.16 | 0.56 |
| 1:M:206:LYS:HB3 | 1:M:217:THR:OG1 | 2.06 | 0.56 |
| 1:M:410:ASN:CG | 4:Z:334:GLU:C | 2.65 | 0.56 |
| 1:M:733:PRO:CB | 1:M:737:PHE:HE1 | 2.19 | 0.56 |
| 1:P:604:ASN:OD1 | 1:P:607:VAL:HG23 | 2.06 | 0.56 |
| 1:P:733:PRO:CB | 1:P:737:PHE:HE1 | 2.19 | 0.56 |
| 4:3:365:ALA:HB3 | 4:3:369:ILE:HB | 1.88 | 0.56 |
| 4:Y:365:ALA:HB3 | 4:Y:369:ILE:HB | 1.88 | 0.56 |
| 3:C:123:VAL:O | 3:C:127:MET:HG2 | 2.07 | 0.55 |
| 1:D:206:LYS:HB3 | 1:D:217:THR:OG1 | 2.07 | 0.55 |
| 1:D:345:ALA:O | 1:D:349:THR:N | 2.40 | 0.55 |
| 1:D:406:VAL:HG12 | 1:D:407:GLY:H | 1.71 | 0.55 |
| 1:D:733:PRO:CB | 1:D:737:PHE:HE1 | 2.19 | 0.55 |
| 1:G:829:TRP:CH2 | 2:H:87:LYS:NZ | 2.73 | 0.55 |
| 1:J:612:GLN:HE22 | 1:J:627:GLY:HA2 | 1.66 | 0.55 |
| 1:J:756:THR:CG2 | 1:J:776:GLU:O | 2.32 | 0.55 |
| 1:M:338:ILE:HG21 | 1:M:348:MLY:HB3 | 1.87 | 0.55 |
| 1:M:599:ASN:CG | 1:M:649:VAL:HB | 2.25 | 0.55 |
| 1:M:629:GLU:O | 1:M:643:GLY:HA3 | 2.06 | 0.55 |
| 1:M:733:PRO:CA | 1:M:737:PHE:HE1 | 2.19 | 0.55 |
| 1:P:290:GLN:HG2 | 1:P:331:LEU:HA | 1.87 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:4:365:ALA:HB3 | 4:4:369:ILE:HB | 1.88 | 0.55 |
| 1:A:32:PHE:CG | 1:A:83:PRO:HD3 | 2.42 | 0.55 |
| 1:A:99:GLU:OE2 | 1:A:696:ARG:NH2 | 2.31 | 0.55 |
| 1:A:529:PRO:CG | 4:8:353:GLN:OE1 | 2.53 | 0.55 |
| 1:A:530:MET:HA | 4:8:354:GLN:CD | 2.11 | 0.55 |
| 1:A:796:GLY:HA3 | 3:C:40:ASN:OD1 | 2.07 | 0.55 |
| 1:D:537:GLU:HB3 | 1:D:648:THR:CB | 2.36 | 0.55 |
| 1:D:604:ASN:OD1 | 1:D:607:VAL:HG23 | 2.06 | 0.55 |
| 1:D:643:GLY:N | 4:9:23:GLY:C | 2.55 | 0.55 |
| 1:D:735:GLY:C | 1:D:743:ALA:HB1 | 1.84 | 0.55 |
| 1:D:813:ILE:HG21 | 2:E:128:PHE:CE1 | 2.41 | 0.55 |
| 1:J:435:GLU:O | 1:J:438:PHE:HB3 | 2.07 | 0.55 |
| 1:J:649:VAL:CG1 | 1:J:649:VAL:HA | 2.35 | 0.55 |
| 3:L:123:VAL:O | 3:L:127:MET:HG2 | 2.07 | 0.55 |
| 1:M:548:THR:CG2 | 4:2:47:MET:HG3 | 2.31 | 0.55 |
| 1:P:406:VAL:HG12 | 1:P:407:GLY:H | 1.71 | 0.55 |
| 4:2:287:ILE:HB | 4:4:203:THR:CB | 2.35 | 0.55 |
| 1:A:94:MET:O | 1:A:713:SER:HB3 | 2.05 | 0.55 |
| 1:A:732:ILE:CG2 | 1:A:747:LEU:HD11 | 1.26 | 0.55 |
| 3:C:35:ARG:HA | 3:C:39:GLN:O | 2.07 | 0.55 |
| 1:D:529:PRO:CB | 4:9:354:GLN:HA | 2.36 | 0.55 |
| 1:D:530:MET:HE3 | 4:9:354:GLN:CG | 2.28 | 0.55 |
| 1:D:546:THR:HB | 1:D:549:SER:H | 1.71 | 0.55 |
| 1:D:629:GLU:O | 1:D:643:GLY:HA3 | 2.06 | 0.55 |
| 1:D:794:CYS:O | 1:D:798:LEU:N | 2.37 | 0.55 |
| 1:G:735:GLY:O | 1:G:743:ALA:HA | 1.95 | 0.55 |
| 1:J:116:TYR:CE2 | 1:J:154:HIS:CD2 | 2.94 | 0.55 |
| 1:J:629:GLU:O | 1:J:643:GLY:HA3 | 2.06 | 0.55 |
| 1:M:32:PHE:CG | 1:M:83:PRO:HD3 | 2.42 | 0.55 |
| 1:M:604:ASN:OD1 | 1:M:607:VAL:HG23 | 2.06 | 0.55 |
| 1:P:116:TYR:CE2 | 1:P:154:HIS:CD2 | 2.94 | 0.55 |
| 1:P:794:CYS:O | 1:P:798:LEU:N | 2.37 | 0.55 |
| 1:A:135:TYR:N | 1:A:135:TYR:HD1 | 2.04 | 0.55 |
| 1:A:795:ARG:NH2 | 3:C:116:GLU:CB | 2.52 | 0.55 |
| 1:A:797:PHE:CE1 | 3:C:146:ILE:HG23 | 2.41 | 0.55 |
| 1:A:837:MLY:HH22 | 2:H:21:GLU:N | 2.19 | 0.55 |
| 1:D:725:ARG:HG3 | 1:D:733:PRO:CA | 2.36 | 0.55 |
| 1:D:813:ILE:CG2 | 2:E:128:PHE:HE1 | 2.14 | 0.55 |
| 3:I:35:ARG:HA | 3:I:39:GLN:O | 2.07 | 0.55 |
| 1:J:32:PHE:CG | 1:J:83:PRO:HD3 | 2.41 | 0.55 |
| 1:J:725:ARG:HG3 | 1:J:733:PRO:CA | 2.36 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:345:ALA:O | 1:M:349:THR:N | 2.40 | 0.55 |
| 1:M:529:PRO:CB | 4:Z:354:GLN:HA | 2.36 | 0.55 |
| 1:M:725:ARG:HG3 | 1:M:733:PRO:CA | 2.36 | 0.55 |
| 1:P:82:PRO:HD2 | 1:P:85:TYR:HD2 | 1.71 | 0.55 |
| 1:P:149:GLN:HB3 | 1:P:716:LEU:HD11 | 1.87 | 0.55 |
| 1:P:546:THR:HG21 | 4:3:47:MET:N | 2.21 | 0.55 |
| 1:P:546:THR:HG21 | 1:P:548:THR:HB | 1.88 | 0.55 |
| 1:P:546:THR:HB | 1:P:549:SER:H | 1.71 | 0.55 |
| 1:P:630:ALA:HA | 4:1:25:ASP:OD2 | 2.07 | 0.55 |
| 1:P:839:MLY:HH13 | 2:Q:159:HIS:HD2 | 1.71 | 0.55 |
| 3:R:35:ARG:HA | 3:R:39:GLN:O | 2.07 | 0.55 |
| 1:A:345:ALA:O | 1:A:349:THR:N | 2.40 | 0.55 |
| 1:A:418:THR:HG22 | 1:A:419:VAL:H | 1.70 | 0.55 |
| 1:D:733:PRO:CA | 1:D:737:PHE:HE1 | 2.19 | 0.55 |
| 1:D:769:ALA:C | 1:D:774:LEU:CB | 2.64 | 0.55 |
| 3:F:123:VAL:O | 3:F:127:MET:HG2 | 2.07 | 0.55 |
| 1:G:82:PRO:HD2 | 1:G:85:TYR:HD2 | 1.72 | 0.55 |
| 1:G:217:THR:HG22 | 1:G:218:LEU:O | 2.06 | 0.55 |
| 1:G:290:GLN:HG2 | 1:G:331:LEU:HA | 1.88 | 0.55 |
| 1:G:646:PHE:CE2 | 1:G:652:LEU:CG | 2.90 | 0.55 |
| 1:G:796:GLY:CA | 3:I:35:ARG:CZ | 2.84 | 0.55 |
| 1:J:22:LYS:HA | 1:J:25:ILE:HB | 1.87 | 0.55 |
| 1:J:82:PRO:HD2 | 1:J:85:TYR:HD2 | 1.72 | 0.55 |
| 1:J:290:GLN:HG2 | 1:J:331:LEU:HA | 1.87 | 0.55 |
| 1:J:406:VAL:HG12 | 1:J:407:GLY:H | 1.71 | 0.55 |
| 1:J:630:ALA:HA | 4:W:25:ASP:OD2 | 2.07 | 0.55 |
| 1:J:640:LYS:C | 1:J:645:SER:OG | 2.44 | 0.55 |
| 2:K:121:LEU:CA | 2:K:128:PHE:CG | 2.89 | 0.55 |
| 1:M:290:GLN:NE2 | 1:M:334:THR:OG1 | 2.40 | 0.55 |
| 1:M:820:VAL:CG1 | 2:N:136:MET:HE1 | 2.36 | 0.55 |
| 1:P:435:GLU:O | 1:P:438:PHE:HB3 | 2.06 | 0.55 |
| 3:R:123:VAL:O | 3:R:127:MET:HG2 | 2.07 | 0.55 |
| 4:W:365:ALA:HB3 | 4:W:369:ILE:HB | 1.88 | 0.55 |
| 1:A:302:MET:HG2 | 1:A:303:LEU:HD13 | 1.87 | 0.55 |
| 1:A:338:ILE:HG21 | 1:A:348:MLY:HB3 | 1.87 | 0.55 |
| 1:A:406:VAL:HG12 | 1:A:407:GLY:H | 1.71 | 0.55 |
| 1:A:537:GLU:HB3 | 1:A:648:THR:CB | 2.36 | 0.55 |
| 1:A:546:THR:HG21 | 1:A:548:THR:HB | 1.88 | 0.55 |
| 1:A:646:PHE:CE2 | 1:A:652:LEU:CG | 2.90 | 0.55 |
| 1:D:22:LYS:HA | 1:D:25:ILE:HB | 1.87 | 0.55 |
| 1:D:32:PHE:CG | 1:D:83:PRO:HD3 | 2.41 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:292:MET:HE3 | 1:D:309:PRO:HA | 1.88 | 0.55 |
| 1:D:649:VAL:CG1 | 1:D:649:VAL:HA | 2.35 | 0.55 |
| 2:E:112:ILE:C | 2:E:147:ASN:O | 2.42 | 0.55 |
| 1:G:733:PRO:CB | 1:G:737:PHE:HE1 | 2.19 | 0.55 |
| 1:J:22:LYS:O | 1:J:26:GLU:HG3 | 2.07 | 0.55 |
| 1:J:84:MLY:O | 1:J:723:ARG:CD | 2.52 | 0.55 |
| 1:J:649:VAL:HA | 1:J:649:VAL:HG23 | 1.83 | 0.55 |
| 1:J:756:THR:HG23 | 1:J:776:GLU:OE1 | 2.05 | 0.55 |
| 1:J:791:GLN:OE1 | 3:L:116:GLU:CG | 2.52 | 0.55 |
| 1:M:292:MET:HE1 | 1:M:309:PRO:CD | 2.37 | 0.55 |
| 1:M:418:THR:HG22 | 1:M:419:VAL:H | 1.69 | 0.55 |
| 1:M:546:THR:HG21 | 1:M:548:THR:HB | 1.88 | 0.55 |
| 3:O:35:ARG:HA | 3:O:39:GLN:O | 2.06 | 0.55 |
| 1:P:22:LYS:HA | 1:P:25:ILE:HB | 1.87 | 0.55 |
| 1:P:22:LYS:O | 1:P:26:GLU:HG3 | 2.07 | 0.55 |
| 1:P:640:LYS:C | 1:P:645:SER:OG | 2.45 | 0.55 |
| 1:P:646:PHE:CE2 | 1:P:652:LEU:CG | 2.90 | 0.55 |
| 1:P:805:ALA:O | 1:P:808:GLU:N | 2.39 | 0.55 |
| 1:P:817:GLN:CG | 2:Q:127:ARG:HB2 | 2.29 | 0.55 |
| 4:1:365:ALA:HB3 | 4:1:369:ILE:HB | 1.88 | 0.55 |
| 1:A:725:ARG:HG3 | 1:A:733:PRO:CA | 2.35 | 0.55 |
| 1:A:799:MET:SD | 3:C:32:ASP:O | 2.65 | 0.55 |
| 1:D:217:THR:HG22 | 1:D:218:LEU:O | 2.05 | 0.55 |
| 1:D:481:ASN:N | 1:D:481:ASN:ND2 | 2.51 | 0.55 |
| 2:E:144:VAL:HG12 | 2:E:153:ILE:HD11 | 1.75 | 0.55 |
| 1:G:7:MET:HE3 | 1:G:14:ALA:CB | 2.36 | 0.55 |
| 1:G:345:ALA:O | 1:G:349:THR:N | 2.40 | 0.55 |
| 1:G:634:GLY:N | 4:V:25:ASP:O | 2.31 | 0.55 |
| 1:G:640:LYS:C | 1:G:645:SER:OG | 2.44 | 0.55 |
| 1:G:765:VAL:HG12 | 1:G:766:PHE:N | 2.22 | 0.55 |
| 1:J:7:MET:HE3 | 1:J:14:ALA:CB | 2.36 | 0.55 |
| 1:J:135:TYR:N | 1:J:135:TYR:HD1 | 2.04 | 0.55 |
| 1:J:546:THR:HB | 1:J:549:SER:H | 1.71 | 0.55 |
| 1:J:546:THR:HG21 | 1:J:548:THR:HB | 1.88 | 0.55 |
| 2:K:156:VAL:HA | 2:K:159:HIS:O | 2.07 | 0.55 |
| 1:M:22:LYS:O | 1:M:26:GLU:HG3 | 2.07 | 0.55 |
| 1:M:529:PRO:CG | 4:Z:353:GLN:OE1 | 2.54 | 0.55 |
| 1:M:821:ARG:CZ | 2:N:127:ARG:CD | 2.85 | 0.55 |
| 3:O:102:VAL:HG23 | 3:O:139:TYR:CD1 | 2.39 | 0.55 |
| 1:P:290:GLN:NE2 | 1:P:334:THR:OG1 | 2.40 | 0.55 |
| 1:P:723:ARG:HH11 | 1:P:723:ARG:CG | 2.20 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:7:MET:HE3 | 1:A:14:ALA:CB | 2.36 | 0.55 |
| 1:A:82:PRO:HD2 | 1:A:85:TYR:HD2 | 1.72 | 0.55 |
| 1:A:206:LYS:HB3 | 1:A:217:THR:OG1 | 2.06 | 0.55 |
| 1:A:538:GLU:CD | 4:8:355:MET:HE3 | 2.26 | 0.55 |
| 1:A:579:PHE:HE1 | 1:A:581:LEU:HD13 | 1.72 | 0.55 |
| 1:A:604:ASN:OD1 | 1:A:607:VAL:HG23 | 2.06 | 0.55 |
| 1:A:733:PRO:CB | 1:A:737:PHE:HE1 | 2.19 | 0.55 |
| 1:D:630:ALA:HA | 4:9:25:ASP:OD2 | 2.07 | 0.55 |
| 1:G:206:LYS:HB3 | 1:G:217:THR:OG1 | 2.06 | 0.55 |
| 1:G:302:MET:HG2 | 1:G:303:LEU:HD13 | 1.88 | 0.55 |
| 1:G:338:ILE:HG21 | 1:G:348:MLY:HB3 | 1.87 | 0.55 |
| 1:G:537:GLU:HB3 | 1:G:648:THR:CB | 2.37 | 0.55 |
| 1:G:546:THR:HG21 | 1:G:548:THR:HB | 1.88 | 0.55 |
| 1:G:638:GLY:HA2 | 4:V:345:ILE:H | 1.72 | 0.55 |
| 1:J:530:MET:CB | 4:W:354:GLN:HG3 | 2.36 | 0.55 |
| 1:J:579:PHE:HE1 | 1:J:581:LEU:HD13 | 1.72 | 0.55 |
| 1:J:638:GLY:CA | 4:W:345:ILE:H | 2.18 | 0.55 |
| 1:J:646:PHE:CE2 | 1:J:652:LEU:CG | 2.90 | 0.55 |
| 3:O:46:ILE:O | 3:O:50:LEU:CG | 2.47 | 0.55 |
| 1:P:805:ALA:O | 1:P:809:ARG:CB | 2.55 | 0.55 |
| 1:P:829:TRP:HZ3 | 2:Q:84:PHE:CE2 | 2.25 | 0.55 |
| 4:7:288:ASP:CA | 4:9:204:ALA:HB2 | 2.32 | 0.55 |
| 4:7:365:ALA:HB3 | 4:7:369:ILE:HB | 1.88 | 0.55 |
| 4:9:365:ALA:HB3 | 4:9:369:ILE:HB | 1.88 | 0.55 |
| 1:D:22:LYS:O | 1:D:26:GLU:HG3 | 2.07 | 0.55 |
| 1:D:305:ILE:HG22 | 1:D:312:TYR:CE2 | 2.42 | 0.55 |
| 1:D:534:SER:C | 4:9:351:THR:CA | 2.47 | 0.55 |
| 1:D:759:ALA:O | 1:D:766:PHE:N | 2.32 | 0.55 |
| 1:G:292:MET:HE1 | 1:G:309:PRO:CD | 2.37 | 0.55 |
| 1:G:305:ILE:HG22 | 1:G:312:TYR:CZ | 2.42 | 0.55 |
| 1:G:529:PRO:CG | 4:V:353:GLN:OE1 | 2.54 | 0.55 |
| 1:G:649:VAL:HA | 1:G:649:VAL:HG23 | 1.83 | 0.55 |
| 3:I:102:VAL:HG23 | 3:I:139:TYR:CD1 | 2.39 | 0.55 |
| 1:J:78:PHE:HB3 | 1:J:98:HIS:NE2 | 2.22 | 0.55 |
| 1:J:345:ALA:O | 1:J:349:THR:N | 2.40 | 0.55 |
| 1:M:10:PHE:O | 1:M:12:GLU:N | 2.40 | 0.55 |
| 1:M:302:MET:HG2 | 1:M:303:LEU:HD13 | 1.87 | 0.55 |
| 1:M:537:GLU:HB3 | 1:M:648:THR:CB | 2.37 | 0.55 |
| 3:O:123:VAL:O | 3:O:127:MET:HG2 | 2.07 | 0.55 |
| 1:P:629:GLU:O | 1:P:643:GLY:HA3 | 2.06 | 0.55 |
| 4:2:243:PRO:O | 4:Z:324:THR:CG2 | 2.55 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:2:365:ALA:HB3 | 4:2:369:ILE:HB | 1.88 | 0.55 |
| 1:A:202:SER:HA | 1:A:207:LYS:HE3 | 1.72 | 0.55 |
| 1:A:649:VAL:CG1 | 1:A:649:VAL:HA | 2.35 | 0.55 |
| 1:A:765:VAL:HG12 | 1:A:766:PHE:N | 2.22 | 0.55 |
| 1:D:135:TYR:HD2 | 1:D:191:ARG:HG2 | 1.72 | 0.55 |
| 1:D:290:GLN:NE2 | 1:D:334:THR:OG1 | 2.40 | 0.55 |
| 1:D:612:GLN:HE22 | 1:D:627:GLY:HA2 | 1.67 | 0.55 |
| 1:D:642:LYS:CA | 4:9:22:ALA:C | 2.71 | 0.55 |
| 1:G:135:TYR:HD2 | 1:G:191:ARG:HG2 | 1.72 | 0.55 |
| 1:G:733:PRO:CA | 1:G:737:PHE:HE1 | 2.19 | 0.55 |
| 3:I:123:VAL:O | 3:I:127:MET:HG2 | 2.07 | 0.55 |
| 1:J:834:LEU:CD1 | 2:K:51:PHE:CD1 | 2.89 | 0.55 |
| 1:M:290:GLN:HG2 | 1:M:331:LEU:HA | 1.88 | 0.55 |
| 1:M:765:VAL:HG12 | 1:M:766:PHE:N | 2.22 | 0.55 |
| 2:N:156:VAL:HA | 2:N:159:HIS:O | 2.07 | 0.55 |
| 1:P:642:LYS:CA | 4:1:22:ALA:C | 2.70 | 0.55 |
| 1:P:831:TRP:HE1 | 2:Q:67:MET:CG | 2.20 | 0.55 |
| 4:9:288:ASP:CA | 4:W:204:ALA:HB2 | 2.32 | 0.55 |
| 1:A:305:ILE:HG22 | 1:A:312:TYR:CZ | 2.42 | 0.54 |
| 1:A:546:THR:HB | 1:A:549:SER:H | 1.71 | 0.54 |
| 1:A:638:GLY:HA2 | 4:8:345:ILE:H | 1.72 | 0.54 |
| 1:A:642:LYS:HG2 | 4:8:22:ALA:C | 2.28 | 0.54 |
| 1:A:707:CYS:CA | 1:A:714:ARG:HH22 | 2.20 | 0.54 |
| 1:D:78:PHE:HB3 | 1:D:98:HIS:NE2 | 2.23 | 0.54 |
| 1:D:538:GLU:CG | 4:9:351:THR:C | 2.74 | 0.54 |
| 1:D:553:MLY:HG3 | 4:W:44:MET:O | 2.07 | 0.54 |
| 1:D:579:PHE:HE1 | 1:D:581:LEU:HD13 | 1.72 | 0.54 |
| 1:D:646:PHE:CE2 | 1:D:652:LEU:CG | 2.90 | 0.54 |
| 1:D:765:VAL:HG12 | 1:D:766:PHE:N | 2.22 | 0.54 |
| 1:G:10:PHE:O | 1:G:12:GLU:N | 2.40 | 0.54 |
| 1:G:305:ILE:HG22 | 1:G:312:TYR:CE2 | 2.42 | 0.54 |
| 1:G:552:ASN:C | 4:X:47:MET:HE1 | 2.26 | 0.54 |
| 1:G:830:PRO:CG | 2:H:67:MET:CE | 2.85 | 0.54 |
| 1:M:638:GLY:HA2 | 4:Z:345:ILE:H | 1.72 | 0.54 |
| 1:M:732:ILE:HG22 | 1:M:747:LEU:CD1 | 1.55 | 0.54 |
| 1:M:795:ARG:CD | 3:O:35:ARG:HH12 | 2.17 | 0.54 |
| 1:P:721:LYS:C | 1:P:736:GLN:OE1 | 2.46 | 0.54 |
| 1:P:765:VAL:HG12 | 1:P:766:PHE:N | 2.22 | 0.54 |
| 4:X:325:MET:HE2 | 4:Z:246:GLN:HG2 | 1.89 | 0.54 |
| 1:A:290:GLN:NE2 | 1:A:334:THR:OG1 | 2.39 | 0.54 |
| 1:A:723:ARG:CG | 1:A:723:ARG:HH11 | 2.20 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:156:VAL:HA | 2:B:159:HIS:O | 2.07 | 0.54 |
| 1:D:290:GLN:HG2 | 1:D:331:LEU:HA | 1.87 | 0.54 |
| 1:D:642:LYS:HG2 | 4:9:22:ALA:C | 2.27 | 0.54 |
| 1:G:290:GLN:NE2 | 1:G:334:THR:OG1 | 2.40 | 0.54 |
| 1:J:290:GLN:NE2 | 1:J:334:THR:OG1 | 2.40 | 0.54 |
| 1:J:721:LYS:C | 1:J:736:GLN:OE1 | 2.46 | 0.54 |
| 1:P:529:PRO:CB | 4:1:354:GLN:HA | 2.36 | 0.54 |
| 1:P:579:PHE:HE1 | 1:P:581:LEU:HD13 | 1.72 | 0.54 |
| 1:P:817:GLN:CD | 2:Q:127:ARG:CD | 2.70 | 0.54 |
| 2:Q:156:VAL:HA | 2:Q:159:HIS:O | 2.07 | 0.54 |
| 1:A:292:MET:HE1 | 1:A:309:PRO:CD | 2.37 | 0.54 |
| 1:A:813:ILE:HD13 | 2:B:128:PHE:CE1 | 2.41 | 0.54 |
| 1:D:10:PHE:O | 1:D:12:GLU:N | 2.41 | 0.54 |
| 1:D:723:ARG:CG | 1:D:723:ARG:HH11 | 2.20 | 0.54 |
| 1:G:28:GLN:CD | 1:G:723:ARG:HH12 | 2.10 | 0.54 |
| 1:G:530:MET:CB | 4:V:354:GLN:HG3 | 2.37 | 0.54 |
| 1:J:797:PHE:CE1 | 3:L:146:ILE:HA | 2.34 | 0.54 |
| 1:M:305:ILE:HG22 | 1:M:312:TYR:CZ | 2.42 | 0.54 |
| 1:M:411:GLU:H | 4:Z:333:PRO:HG2 | 1.70 | 0.54 |
| 1:M:530:MET:CB | 4:Z:354:GLN:HG3 | 2.37 | 0.54 |
| 1:P:345:ALA:O | 1:P:349:THR:N | 2.40 | 0.54 |
| 1:P:638:GLY:HA2 | 4:1:345:ILE:H | 1.72 | 0.54 |
| 1:P:797:PHE:HD1 | 3:R:149:VAL:CG1 | 2.18 | 0.54 |
| 2:Q:146:GLY:O | 2:Q:147:ASN:ND2 | 2.41 | 0.54 |
| 1:A:10:PHE:O | 1:A:12:GLU:N | 2.41 | 0.54 |
| 1:A:135:TYR:HD2 | 1:A:191:ARG:HG2 | 1.72 | 0.54 |
| 1:A:149:GLN:HA | 1:A:719:ASP:CG | 2.27 | 0.54 |
| 1:D:82:PRO:HD2 | 1:D:85:TYR:HD2 | 1.72 | 0.54 |
| 1:D:576:GLU:CG | 1:D:577:ALA:N | 2.44 | 0.54 |
| 1:D:638:GLY:CA | 4:9:345:ILE:H | 2.19 | 0.54 |
| 1:G:32:PHE:CG | 1:G:83:PRO:HD3 | 2.41 | 0.54 |
| 1:J:292:MET:HE1 | 1:J:309:PRO:CD | 2.37 | 0.54 |
| 1:J:629:GLU:CB | 1:J:643:GLY:C | 2.76 | 0.54 |
| 1:M:78:PHE:HB3 | 1:M:98:HIS:NE2 | 2.23 | 0.54 |
| 1:M:629:GLU:CB | 1:M:643:GLY:C | 2.76 | 0.54 |
| 1:M:646:PHE:CE2 | 1:M:652:LEU:CG | 2.90 | 0.54 |
| 1:M:721:LYS:C | 1:M:736:GLN:OE1 | 2.46 | 0.54 |
| 1:P:305:ILE:HG22 | 1:P:312:TYR:CE2 | 2.42 | 0.54 |
| 4:6:365:ALA:HB3 | 4:6:369:ILE:HB | 1.88 | 0.54 |
| 1:A:410:ASN:CG | 4:8:334:GLU:C | 2.65 | 0.54 |
| 1:A:791:GLN:O | 1:A:794:CYS:HB2 | 2.08 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:292:MET:HE1 | 1:D:309:PRO:CD | 2.38 | 0.54 |
| 1:D:629:GLU:CB | 1:D:643:GLY:C | 2.76 | 0.54 |
| 1:G:148:ARG:NH2 | 1:G:764:MLY:CH2 | 2.62 | 0.54 |
| 1:G:553:MLY:HH13 | 4:X:45:VAL:CG1 | 2.25 | 0.54 |
| 1:J:305:ILE:HG22 | 1:J:312:TYR:CE2 | 2.43 | 0.54 |
| 1:M:538:GLU:CG | 4:Z:351:THR:C | 2.73 | 0.54 |
| 1:M:723:ARG:HH11 | 1:M:723:ARG:CG | 2.20 | 0.54 |
| 1:P:292:MET:HE1 | 1:P:309:PRO:CD | 2.37 | 0.54 |
| 1:P:538:GLU:CG | 4:1:351:THR:C | 2.73 | 0.54 |
| 1:P:831:TRP:CZ3 | 2:Q:34:ILE:HD13 | 2.34 | 0.54 |
| 4:V:291:LYS:HD2 | 4:X:243:PRO:CB | 2.38 | 0.54 |
| 1:D:7:MET:HE3 | 1:D:14:ALA:CB | 2.37 | 0.54 |
| 1:D:640:LYS:C | 1:D:645:SER:OG | 2.45 | 0.54 |
| 1:G:126:VAL:HG13 | 1:G:675:ILE:HG22 | 1.90 | 0.54 |
| 1:G:604:ASN:OD1 | 1:G:607:VAL:HG23 | 2.06 | 0.54 |
| 1:G:629:GLU:CB | 1:G:643:GLY:C | 2.76 | 0.54 |
| 1:J:10:PHE:O | 1:J:12:GLU:N | 2.40 | 0.54 |
| 1:J:538:GLU:CG | 4:W:351:THR:C | 2.73 | 0.54 |
| 3:L:35:ARG:HA | 3:L:39:GLN:O | 2.07 | 0.54 |
| 1:M:126:VAL:HG13 | 1:M:675:ILE:HG22 | 1.90 | 0.54 |
| 1:P:10:PHE:O | 1:P:12:GLU:N | 2.41 | 0.54 |
| 1:P:410:ASN:CG | 4:1:334:GLU:C | 2.65 | 0.54 |
| 1:P:530:MET:CB | 4:1:354:GLN:HG3 | 2.36 | 0.54 |
| 1:P:541:MET:SD | 4:1:346:LEU:O | 2.48 | 0.54 |
| 1:P:791:GLN:O | 1:P:794:CYS:HB2 | 2.08 | 0.54 |
| 1:P:821:ARG:NH1 | 2:Q:127:ARG:NE | 2.56 | 0.54 |
| 4:3:148:THR:HG21 | 4:5:45:VAL:HG21 | 1.89 | 0.54 |
| 1:A:640:LYS:C | 4:8:23:GLY:CA | 2.64 | 0.54 |
| 2:E:146:GLY:O | 2:E:147:ASN:ND2 | 2.41 | 0.54 |
| 1:G:78:PHE:HB3 | 1:G:98:HIS:NE2 | 2.23 | 0.54 |
| 1:G:410:ASN:CG | 4:V:334:GLU:C | 2.64 | 0.54 |
| 1:G:642:LYS:CG | 4:V:22:ALA:CA | 2.80 | 0.54 |
| 1:G:791:GLN:O | 1:G:794:CYS:HB2 | 2.08 | 0.54 |
| 2:H:146:GLY:O | 2:H:147:ASN:ND2 | 2.41 | 0.54 |
| 1:J:305:ILE:HG22 | 1:J:312:TYR:CZ | 2.42 | 0.54 |
| 1:J:410:ASN:CG | 4:W:334:GLU:C | 2.65 | 0.54 |
| 1:J:759:ALA:O | 1:J:766:PHE:N | 2.32 | 0.54 |
| 1:M:630:ALA:HA | 4:Z:25:ASP:OD2 | 2.07 | 0.54 |
| 1:P:642:LYS:HG2 | 4:1:22:ALA:C | 2.27 | 0.54 |
| 2:Q:121:LEU:CA | 2:Q:128:PHE:CG | 2.89 | 0.54 |
| 1:A:305:ILE:HG22 | 1:A:312:TYR:CE2 | 2.43 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:A:470:PHE:O | 1:A:473:ASN:ND2 | 2.40 | 0.54 |
| 1:A:571:ALA:O | 1:A:572:LYS:CB | 2.56 | 0.54 |
| 1:A:642:LYS:CA | 4:8:22:ALA:C | 2.71 | 0.54 |
| 1:D:38:VAL:CB | 1:D:52:ILE:HD11 | 2.38 | 0.54 |
| 1:D:135:TYR:HD2 | 1:D:191:ARG:HD3 | 1.73 | 0.54 |
| 1:D:800:ARG:HD3 | 3:F:149:VAL:C | 2.28 | 0.54 |
| 3:F:35:ARG:HA | 3:F:39:GLN:O | 2.07 | 0.54 |
| 1:G:529:PRO:CB | 4:V:354:GLN:HA | 2.37 | 0.54 |
| 1:G:556:ASP:OD2 | 4:X:44:MET:HG3 | 2.08 | 0.54 |
| 1:G:721:LYS:C | 1:G:736:GLN:OE1 | 2.46 | 0.54 |
| 1:J:538:GLU:HG3 | 4:W:352:PHE:CA | 2.38 | 0.54 |
| 1:J:795:ARG:HE | 3:L:116:GLU:CD | 2.09 | 0.54 |
| 1:J:826:VAL:HG21 | 2:K:88:LEU:HD23 | 1.90 | 0.54 |
| 1:M:406:VAL:HG12 | 1:M:407:GLY:H | 1.71 | 0.54 |
| 1:M:571:ALA:O | 1:M:572:LYS:CB | 2.56 | 0.54 |
| 1:P:493:HIS:ND1 | 1:P:514:ASP:OD2 | 2.41 | 0.54 |
| 1:P:546:THR:CB | 4:3:47:MET:N | 2.68 | 0.54 |
| 4:W:325:MET:SD | 4:Y:244:ASP:HB3 | 2.43 | 0.54 |
| 1:D:305:ILE:HG22 | 1:D:312:TYR:CZ | 2.43 | 0.54 |
| 1:D:404:PRO:CG | 1:D:417:GLU:HG3 | 2.38 | 0.54 |
| 1:G:470:PHE:O | 1:G:473:ASN:ND2 | 2.40 | 0.54 |
| 1:G:546:THR:HB | 1:G:549:SER:H | 1.71 | 0.54 |
| 1:J:505:MLY:HG3 | 1:J:762:HIS:HE1 | 1.56 | 0.54 |
| 2:K:112:ILE:C | 2:K:147:ASN:O | 2.42 | 0.54 |
| 1:P:404:PRO:CG | 1:P:417:GLU:HG3 | 2.38 | 0.54 |
| 3:R:92:ARG:HA | 3:R:139:TYR:OH | 2.08 | 0.54 |
| 1:A:38:VAL:CB | 1:A:52:ILE:HD11 | 2.38 | 0.54 |
| 1:A:553:MLY:HG3 | 4:V:44:MET:O | 2.07 | 0.54 |
| 1:A:630:ALA:HA | 4:8:25:ASP:OD2 | 2.07 | 0.54 |
| 1:A:732:ILE:HG23 | 1:A:747:LEU:CD1 | 1.04 | 0.54 |
| 1:A:839:MLY:HH11 | 2:B:159:HIS:HD2 | 1.72 | 0.54 |
| 1:D:530:MET:CB | 4:9:354:GLN:HG3 | 2.36 | 0.54 |
| 1:D:638:GLY:HA2 | 4:9:345:ILE:H | 1.72 | 0.54 |
| 1:G:404:PRO:CG | 1:G:417:GLU:HG3 | 2.38 | 0.54 |
| 1:G:505:MLY:HE3 | 1:G:762:HIS:CE1 | 2.42 | 0.54 |
| 1:G:530:MET:CA | 4:V:354:GLN:HB3 | 2.35 | 0.54 |
| 1:J:32:PHE:CD1 | 1:J:83:PRO:HD3 | 2.43 | 0.54 |
| 1:M:7:MET:HE3 | 1:M:14:ALA:CB | 2.37 | 0.54 |
| 1:M:82:PRO:HD2 | 1:M:85:TYR:HD2 | 1.72 | 0.54 |
| 1:M:548:THR:HG21 | 4:2:47:MET:HB3 | 1.87 | 0.54 |
| 1:P:638:GLY:CA | 4:1:345:ILE:H | 2.18 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:P:707:CYS:O | 1:P:710:GLY:N | 2.41 | 0.54 |
| 1:P:821:ARG:HH22 | 2:Q:127:ARG:HE | 1.54 | 0.54 |
| 1:P:836:PHE:CD2 | 2:Q:160:GLY:HA3 | 2.42 | 0.54 |
| 4:2:287:ILE:HG22 | 4:4:204:ALA:H | 1.69 | 0.54 |
| 1:A:93:MET:CE | 1:A:715:VAL:HG22 | 2.38 | 0.53 |
| 1:A:98:HIS:HB3 | 1:A:100:PRO:CD | 2.25 | 0.53 |
| 1:D:126:VAL:HG13 | 1:D:675:ILE:HG22 | 1.90 | 0.53 |
| 1:D:507:GLY:C | 1:D:762:HIS:H | 2.11 | 0.53 |
| 1:D:538:GLU:HG3 | 4:9:352:PHE:CA | 2.39 | 0.53 |
| 1:D:571:ALA:O | 1:D:572:LYS:CB | 2.56 | 0.53 |
| 1:D:834:LEU:CD2 | 2:E:50:THR:HG22 | 2.38 | 0.53 |
| 1:G:84:MLY:HA | 1:G:723:ARG:NH2 | 2.23 | 0.53 |
| 1:G:418:THR:HG22 | 1:G:419:VAL:H | 1.69 | 0.53 |
| 1:J:571:ALA:O | 1:J:572:LYS:CB | 2.56 | 0.53 |
| 1:J:791:GLN:O | 1:J:794:CYS:HB2 | 2.08 | 0.53 |
| 2:K:146:GLY:O | 2:K:147:ASN:ND2 | 2.41 | 0.53 |
| 1:M:32:PHE:CD1 | 1:M:83:PRO:HD3 | 2.44 | 0.53 |
| 1:M:305:ILE:HG22 | 1:M:312:TYR:CE2 | 2.43 | 0.53 |
| 1:M:803:TYR:HE2 | 3:O:17:PHE:CZ | 2.26 | 0.53 |
| 1:P:305:ILE:HG22 | 1:P:312:TYR:CZ | 2.42 | 0.53 |
| 1:P:757:GLN:HG3 | 1:P:772:LEU:HD11 | 1.91 | 0.53 |
| 1:P:803:TYR:CD2 | 3:R:17:PHE:HZ | 2.27 | 0.53 |
| 4:X:325:MET:CE | 4:Z:246:GLN:HG2 | 2.39 | 0.53 |
| 1:A:126:VAL:HG13 | 1:A:675:ILE:HG22 | 1.90 | 0.53 |
| 1:A:154:HIS:CE1 | 1:A:156:PHE:HD2 | 2.26 | 0.53 |
| 1:A:530:MET:CE | 4:8:354:GLN:HG3 | 2.35 | 0.53 |
| 1:A:553:MLY:O | 4:V:48:GLY:CA | 2.57 | 0.53 |
| 1:A:629:GLU:CB | 1:A:643:GLY:C | 2.75 | 0.53 |
| 2:B:146:GLY:O | 2:B:147:ASN:ND2 | 2.41 | 0.53 |
| 1:D:32:PHE:CD1 | 1:D:83:PRO:HD3 | 2.43 | 0.53 |
| 1:D:553:MLY:O | 4:W:48:GLY:CA | 2.56 | 0.53 |
| 1:D:713:SER:HB3 | 1:D:775:LEU:HD22 | 1.91 | 0.53 |
| 1:D:721:LYS:C | 1:D:736:GLN:OE1 | 2.46 | 0.53 |
| 1:G:38:VAL:CB | 1:G:52:ILE:HD11 | 2.38 | 0.53 |
| 1:G:154:HIS:CE1 | 1:G:156:PHE:HD2 | 2.26 | 0.53 |
| 1:G:579:PHE:HE1 | 1:G:581:LEU:HD13 | 1.72 | 0.53 |
| 1:G:723:ARG:CG | 1:G:723:ARG:HH11 | 2.20 | 0.53 |
| 1:G:789:ALA:HB1 | 3:I:81:GLN:NE2 | 2.23 | 0.53 |
| 1:G:795:ARG:CD | 3:I:116:GLU:OE2 | 2.56 | 0.53 |
| 1:J:493:HIS:ND1 | 1:J:514:ASP:OD2 | 2.41 | 0.53 |
| 1:J:819:ASN:CB | 2:K:90:GLY:O | 2.56 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:831:TRP:CH2 | 2:K:47:LEU:HD23 | 2.34 | 0.53 |
| 2:K:149:ASP:CG | 2:K:150:TYR:N | 2.49 | 0.53 |
| 3:L:92:ARG:HA | 3:L:139:TYR:OH | 2.08 | 0.53 |
| 1:M:135:TYR:HD2 | 1:M:191:ARG:HG2 | 1.72 | 0.53 |
| 1:M:277:PHE:CG | 1:M:278:GLN:N | 2.76 | 0.53 |
| 1:M:759:ALA:O | 1:M:766:PHE:N | 2.32 | 0.53 |
| 1:M:795:ARG:HD2 | 3:O:43:ASN:CG | 2.26 | 0.53 |
| 1:P:126:VAL:HG13 | 1:P:675:ILE:HG22 | 1.90 | 0.53 |
| 1:P:538:GLU:HG3 | 4:1:352:PHE:CA | 2.38 | 0.53 |
| 1:P:629:GLU:CB | 1:P:643:GLY:C | 2.76 | 0.53 |
| 2:Q:114:LYS:O | 2:Q:147:ASN:ND2 | 2.41 | 0.53 |
| 4:1:243:PRO:O | 4:Y:291:LYS:HE2 | 2.07 | 0.53 |
| 1:A:32:PHE:CD1 | 1:A:83:PRO:HD3 | 2.44 | 0.53 |
| 1:A:493:HIS:ND1 | 1:A:514:ASP:OD2 | 2.41 | 0.53 |
| 1:A:823:PHE:HE1 | 2:B:161:GLU:N | 2.06 | 0.53 |
| 1:A:836:PHE:CE2 | 2:B:160:GLY:C | 2.82 | 0.53 |
| 1:D:493:HIS:ND1 | 1:D:514:ASP:OD2 | 2.41 | 0.53 |
| 2:E:156:VAL:HA | 2:E:159:HIS:O | 2.07 | 0.53 |
| 1:G:792:ALA:CB | 3:I:42:THR:N | 2.70 | 0.53 |
| 1:J:126:VAL:HG13 | 1:J:675:ILE:HG22 | 1.90 | 0.53 |
| 1:J:638:GLY:HA2 | 4:W:345:ILE:H | 1.72 | 0.53 |
| 1:P:78:PHE:HB3 | 1:P:98:HIS:NE2 | 2.22 | 0.53 |
| 1:P:135:TYR:HD2 | 1:P:191:ARG:HG2 | 1.73 | 0.53 |
| 1:P:135:TYR:HD2 | 1:P:191:ARG:HD3 | 1.73 | 0.53 |
| 1:P:277:PHE:CG | 1:P:278:GLN:N | 2.76 | 0.53 |
| 1:P:571:ALA:O | 1:P:572:LYS:CB | 2.56 | 0.53 |
| 1:P:798:LEU:HD13 | 3:R:126:LEU:HD11 | 1.75 | 0.53 |
| 1:P:817:GLN:HG2 | 2:Q:127:ARG:CG | 2.38 | 0.53 |
| 1:P:818:TYR:OH | 2:Q:127:ARG:NH2 | 2.35 | 0.53 |
| 2:Q:112:ILE:C | 2:Q:147:ASN:O | 2.42 | 0.53 |
| 4:1:243:PRO:C | 4:Y:291:LYS:CG | 2.77 | 0.53 |
| 4:2:203:THR:CG2 | 4:Z:287:ILE:CG2 | 2.73 | 0.53 |
| 4:X:185:LEU:HD23 | 4:X:306:TYR:OH | 2.09 | 0.53 |
| 1:A:538:GLU:CG | 4:8:351:THR:C | 2.74 | 0.53 |
| 1:A:553:MLY:CE | 4:V:45:VAL:CA | 2.49 | 0.53 |
| 1:D:218:LEU:N | 1:D:221:GLN:HG2 | 2.24 | 0.53 |
| 1:D:649:VAL:HA | 1:D:649:VAL:HG22 | 1.80 | 0.53 |
| 1:D:732:ILE:HG23 | 1:D:747:LEU:CD1 | 1.04 | 0.53 |
| 1:G:753:VAL:O | 1:G:779:ARG:HD3 | 2.06 | 0.53 |
| 1:J:135:TYR:HD2 | 1:J:191:ARG:HG2 | 1.73 | 0.53 |
| 1:J:599:ASN:CG | 1:J:649:VAL:H | 2.12 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:22:LYS:O | 1:M:26:GLU:N | 2.30 | 0.53 |
| 1:M:739:ASP:CB | 1:M:742:LYS:CB | 2.81 | 0.53 |
| 2:N:114:LYS:O | 2:N:147:ASN:ND2 | 2.41 | 0.53 |
| 1:P:149:GLN:CB | 1:P:716:LEU:HD11 | 2.39 | 0.53 |
| 1:P:599:ASN:CG | 1:P:649:VAL:H | 2.12 | 0.53 |
| 1:P:642:LYS:CG | 4:1:22:ALA:HA | 2.37 | 0.53 |
| 1:P:818:TYR:CG | 2:Q:127:ARG:NH1 | 2.75 | 0.53 |
| 1:A:135:TYR:CD2 | 1:A:191:ARG:HG2 | 2.44 | 0.53 |
| 1:D:769:ALA:O | 1:D:774:LEU:CB | 2.56 | 0.53 |
| 3:F:92:ARG:HA | 3:F:139:TYR:OH | 2.09 | 0.53 |
| 1:G:98:HIS:HB3 | 1:G:100:PRO:CD | 2.25 | 0.53 |
| 1:J:38:VAL:CB | 1:J:52:ILE:HD11 | 2.38 | 0.53 |
| 1:J:251:ARG:HB2 | 1:J:264:ASP:HB2 | 1.91 | 0.53 |
| 1:J:584:TYR:CD1 | 1:J:585:ALA:N | 2.77 | 0.53 |
| 1:J:642:LYS:CG | 4:W:22:ALA:HA | 2.37 | 0.53 |
| 1:J:756:THR:HG23 | 1:J:779:ARG:HD2 | 1.91 | 0.53 |
| 1:J:791:GLN:HB3 | 3:L:116:GLU:CD | 2.29 | 0.53 |
| 1:J:796:GLY:N | 3:L:35:ARG:NE | 2.56 | 0.53 |
| 1:M:38:VAL:CB | 1:M:52:ILE:HD11 | 2.38 | 0.53 |
| 1:M:98:HIS:HB3 | 1:M:100:PRO:CD | 2.25 | 0.53 |
| 1:M:154:HIS:CE1 | 1:M:156:PHE:HD2 | 2.26 | 0.53 |
| 1:M:493:HIS:ND1 | 1:M:514:ASP:OD2 | 2.41 | 0.53 |
| 1:M:579:PHE:HE1 | 1:M:581:LEU:HD13 | 1.72 | 0.53 |
| 1:M:642:LYS:CA | 4:Z:22:ALA:C | 2.70 | 0.53 |
| 1:M:791:GLN:O | 1:M:794:CYS:HB2 | 2.08 | 0.53 |
| 2:N:146:GLY:O | 2:N:147:ASN:ND2 | 2.41 | 0.53 |
| 1:P:38:VAL:CB | 1:P:52:ILE:HD11 | 2.38 | 0.53 |
| 1:P:553:MLY:N | 4:3:49:GLN:HG3 | 2.07 | 0.53 |
| 4:4:185:LEU:HD23 | 4:4:306:TYR:OH | 2.09 | 0.53 |
| 4:7:185:LEU:HD23 | 4:7:306:TYR:OH | 2.09 | 0.53 |
| 4:Z:185:LEU:HD23 | 4:Z:306:TYR:OH | 2.09 | 0.53 |
| 3:C:92:ARG:HA | 3:C:139:TYR:OH | 2.09 | 0.53 |
| 1:D:42:HIS:HB3 | 1:D:45:GLN:O | 2.09 | 0.53 |
| 1:D:529:PRO:HB2 | 4:9:354:GLN:HA | 1.91 | 0.53 |
| 1:D:579:PHE:CD2 | 1:D:592:ILE:HD11 | 2.40 | 0.53 |
| 1:D:636:LYS:HB2 | 4:9:334:GLU:OE1 | 2.09 | 0.53 |
| 1:D:642:LYS:CG | 4:9:22:ALA:HA | 2.37 | 0.53 |
| 1:D:661:MET:O | 1:D:665:ARG:HG3 | 2.09 | 0.53 |
| 1:G:32:PHE:CD1 | 1:G:83:PRO:HD3 | 2.44 | 0.53 |
| 1:G:404:PRO:HG3 | 1:G:417:GLU:HG3 | 1.91 | 0.53 |
| 2:H:114:LYS:N | 2:H:146:GLY:O | 2.40 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:H:156:VAL:HA | 2:H:159:HIS:O | 2.07 | 0.53 |
| 1:J:661:MET:O | 1:J:665:ARG:HG3 | 2.09 | 0.53 |
| 1:J:765:VAL:HG12 | 1:J:766:PHE:N | 2.22 | 0.53 |
| 1:M:599:ASN:CG | 1:M:649:VAL:H | 2.12 | 0.53 |
| 1:M:795:ARG:CZ | 3:O:116:GLU:CB | 2.74 | 0.53 |
| 1:M:796:GLY:HA2 | 3:O:35:ARG:CG | 2.39 | 0.53 |
| 1:P:584:TYR:CD1 | 1:P:585:ALA:N | 2.77 | 0.53 |
| 1:P:817:GLN:OE1 | 2:Q:127:ARG:HD2 | 2.09 | 0.53 |
| 1:P:821:ARG:NH2 | 2:Q:127:ARG:NE | 2.56 | 0.53 |
| 2:Q:129:THR:O | 2:Q:133:ILE:HG13 | 2.09 | 0.53 |
| 4:2:185:LEU:HD23 | 4:2:306:TYR:OH | 2.09 | 0.53 |
| 1:A:502:GLU:HG2 | 1:A:766:PHE:CD1 | 2.43 | 0.53 |
| 1:A:556:ASP:CA | 4:V:49:GLN:O | 2.52 | 0.53 |
| 1:A:721:LYS:C | 1:A:736:GLN:OE1 | 2.46 | 0.53 |
| 1:D:154:HIS:CE1 | 1:D:156:PHE:HD2 | 2.27 | 0.53 |
| 1:D:507:GLY:O | 1:D:762:HIS:CD2 | 2.62 | 0.53 |
| 1:G:42:HIS:HB3 | 1:G:45:GLN:O | 2.09 | 0.53 |
| 1:G:571:ALA:O | 1:G:572:LYS:CB | 2.56 | 0.53 |
| 1:J:154:HIS:CE1 | 1:J:156:PHE:HD2 | 2.26 | 0.53 |
| 1:J:218:LEU:N | 1:J:221:GLN:HG2 | 2.24 | 0.53 |
| 1:J:649:VAL:HA | 1:J:649:VAL:HG22 | 1.80 | 0.53 |
| 1:M:831:TRP:HE1 | 2:N:67:MET:HG2 | 1.74 | 0.53 |
| 1:P:530:MET:HE3 | 4:1:354:GLN:HG2 | 1.82 | 0.53 |
| 4:2:324:THR:CB | 4:4:244:ASP:CA | 2.82 | 0.53 |
| 4:4:324:THR:H | 4:6:244:ASP:HA | 1.73 | 0.53 |
| 4:Y:185:LEU:HD23 | 4:Y:306:TYR:OH | 2.09 | 0.53 |
| 1:A:277:PHE:CG | 1:A:278:GLN:N | 2.76 | 0.53 |
| 1:A:404:PRO:HG3 | 1:A:417:GLU:HG3 | 1.91 | 0.53 |
| 1:A:584:TYR:CD1 | 1:A:585:ALA:N | 2.77 | 0.53 |
| 1:A:797:PHE:CE1 | 3:C:149:VAL:HG12 | 2.44 | 0.53 |
| 1:A:815:CYS:SG | 2:B:92:ASP:CB | 2.92 | 0.53 |
| 1:D:539:GLU:OE2 | 4:W:45:VAL:C | 2.47 | 0.53 |
| 1:D:640:LYS:C | 4:9:23:GLY:CA | 2.64 | 0.53 |
| 1:D:724:TYR:CA | 1:D:782:MLY:CE | 2.86 | 0.53 |
| 1:G:135:TYR:CD2 | 1:G:191:ARG:HG2 | 2.44 | 0.53 |
| 1:G:493:HIS:ND1 | 1:G:514:ASP:OD2 | 2.41 | 0.53 |
| 1:G:599:ASN:CG | 1:G:649:VAL:H | 2.12 | 0.53 |
| 1:G:732:ILE:HG23 | 1:G:747:LEU:CD1 | 1.04 | 0.53 |
| 3:I:92:ARG:HA | 3:I:139:TYR:OH | 2.09 | 0.53 |
| 1:J:553:MLY:CE | 4:Y:45:VAL:CG1 | 2.78 | 0.53 |
| 1:J:561:LYS:HE2 | 4:Y:48:GLY:HA3 | 1.88 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:839:MLY:HH21 | 2:K:158:THR:CG2 | 2.39 | 0.53 |
| 1:M:42:HIS:HB3 | 1:M:45:GLN:O | 2.09 | 0.53 |
| 1:M:215:GLN:CA | 1:M:340:ILE:CG2 | 2.63 | 0.53 |
| 1:M:642:LYS:HG2 | 4:Z:22:ALA:C | 2.27 | 0.53 |
| 1:M:661:MET:O | 1:M:665:ARG:HG3 | 2.09 | 0.53 |
| 2:N:114:LYS:N | 2:N:146:GLY:O | 2.40 | 0.53 |
| 1:P:42:HIS:HB3 | 1:P:45:GLN:O | 2.09 | 0.53 |
| 1:P:491:PHE:HD1 | 1:P:671:PHE:CE2 | 2.27 | 0.53 |
| 4:3:185:LEU:HD23 | 4:3:306:TYR:OH | 2.09 | 0.53 |
| 4:W:185:LEU:HD23 | 4:W:306:TYR:OH | 2.09 | 0.53 |
| 4:W:288:ASP:H | 4:Y:204:ALA:H | 1.56 | 0.53 |
| 1:A:42:HIS:HB3 | 1:A:45:GLN:O | 2.09 | 0.53 |
| 1:A:78:PHE:HB3 | 1:A:98:HIS:NE2 | 2.22 | 0.53 |
| 1:A:135:TYR:HD2 | 1:A:191:ARG:HD3 | 1.74 | 0.53 |
| 1:A:404:PRO:CG | 1:A:417:GLU:HG3 | 2.38 | 0.53 |
| 1:A:556:ASP:HB3 | 4:V:43:VAL:HG12 | 1.91 | 0.53 |
| 1:A:733:PRO:O | 1:A:737:PHE:CE1 | 2.53 | 0.53 |
| 1:A:797:PHE:HE1 | 3:C:146:ILE:CA | 1.92 | 0.53 |
| 1:A:833:MLY:HA | 2:B:161:GLU:OE1 | 2.09 | 0.53 |
| 1:D:634:GLY:N | 4:9:25:ASP:O | 2.31 | 0.53 |
| 1:D:747:LEU:HD11 | 1:D:782:MLY:CH2 | 2.34 | 0.53 |
| 1:G:135:TYR:HD2 | 1:G:191:ARG:HD3 | 1.73 | 0.53 |
| 1:G:156:PHE:HD1 | 1:G:195:TYR:CD1 | 2.27 | 0.53 |
| 1:G:202:SER:HA | 1:G:207:LYS:HE3 | 1.72 | 0.53 |
| 1:G:584:TYR:CD1 | 1:G:585:ALA:N | 2.77 | 0.53 |
| 1:G:661:MET:O | 1:G:665:ARG:HG3 | 2.09 | 0.53 |
| 2:H:137:TRP:CA | 2:H:145:ALA:CB | 2.82 | 0.53 |
| 1:J:220:ASP:O | 1:J:224:SER:N | 2.27 | 0.53 |
| 1:J:529:PRO:HB2 | 4:W:354:GLN:HA | 1.91 | 0.53 |
| 1:J:797:PHE:CE1 | 3:L:146:ILE:HD13 | 2.38 | 0.53 |
| 1:M:404:PRO:CG | 1:M:417:GLU:HG3 | 2.38 | 0.53 |
| 1:P:32:PHE:CD1 | 1:P:83:PRO:HD3 | 2.43 | 0.53 |
| 1:P:218:LEU:N | 1:P:221:GLN:HG2 | 2.24 | 0.53 |
| 1:P:295:MLY:HE2 | 1:P:332:MET:HE1 | 1.91 | 0.53 |
| 1:P:404:PRO:HG3 | 1:P:417:GLU:HG3 | 1.91 | 0.53 |
| 1:P:792:ALA:HB2 | 3:R:42:THR:CB | 2.38 | 0.53 |
| 4:2:288:ASP:CB | 4:4:203:THR:CG2 | 2.87 | 0.53 |
| 1:A:529:PRO:HB2 | 4:8:354:GLN:HA | 1.91 | 0.53 |
| 2:B:114:LYS:O | 2:B:147:ASN:ND2 | 2.41 | 0.53 |
| 1:D:135:TYR:CD2 | 1:D:191:ARG:HG2 | 2.44 | 0.53 |
| 1:D:556:ASP:HB3 | 4:W:43:VAL:HG12 | 1.91 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:819:ASN:OD1 | 2:E:92:ASP:N | 2.27 | 0.53 |
| 1:D:836:PHE:CZ | 2:E:160:GLY:N | 2.77 | 0.53 |
| 1:G:218:LEU:N | 1:G:221:GLN:HG2 | 2.24 | 0.53 |
| 1:G:292:MET:CE | 1:G:309:PRO:HA | 2.39 | 0.53 |
| 1:G:538:GLU:HG3 | 4:V:352:PHE:CA | 2.38 | 0.53 |
| 1:G:642:LYS:HG2 | 4:V:22:ALA:C | 2.27 | 0.53 |
| 3:I:53:PRO:HB2 | 3:I:55:LYS:HG3 | 1.91 | 0.53 |
| 1:J:277:PHE:CG | 1:J:278:GLN:N | 2.76 | 0.53 |
| 1:J:404:PRO:HG3 | 1:J:417:GLU:HG3 | 1.91 | 0.53 |
| 1:J:732:ILE:HG23 | 1:J:747:LEU:CD1 | 1.05 | 0.53 |
| 1:M:470:PHE:O | 1:M:473:ASN:ND2 | 2.40 | 0.53 |
| 1:M:584:TYR:CD1 | 1:M:585:ALA:N | 2.77 | 0.53 |
| 1:P:251:ARG:HB2 | 1:P:264:ASP:HB2 | 1.91 | 0.53 |
| 1:P:636:LYS:HB2 | 4:1:334:GLU:OE1 | 2.09 | 0.53 |
| 1:P:661:MET:O | 1:P:665:ARG:HG3 | 2.09 | 0.53 |
| 1:P:783:LEU:CB | 1:P:786:ILE:HD11 | 2.24 | 0.53 |
| 1:P:797:PHE:CD1 | 3:R:149:VAL:HG13 | 2.42 | 0.53 |
| 1:A:206:LYS:HD2 | 1:A:217:THR:CG2 | 2.17 | 0.52 |
| 1:A:837:MLY:NZ | 2:H:20:ASP:HB2 | 2.24 | 0.52 |
| 1:D:295:MLY:HE2 | 1:D:332:MET:HE1 | 1.91 | 0.52 |
| 1:D:507:GLY:HA3 | 1:D:762:HIS:N | 2.24 | 0.52 |
| 3:F:110:VAL:HG13 | 3:F:114:LEU:HD12 | 1.92 | 0.52 |
| 1:G:63:MLY:HG3 | 1:G:64:THR:H | 1.74 | 0.52 |
| 1:J:135:TYR:CD2 | 1:J:191:ARG:HG2 | 2.44 | 0.52 |
| 1:J:156:PHE:HD1 | 1:J:195:TYR:CD1 | 2.27 | 0.52 |
| 1:J:404:PRO:CG | 1:J:417:GLU:HG3 | 2.38 | 0.52 |
| 1:J:470:PHE:O | 1:J:473:ASN:ND2 | 2.40 | 0.52 |
| 1:M:197:ALA:O | 1:M:201:ALA:HB2 | 2.10 | 0.52 |
| 1:M:218:LEU:N | 1:M:221:GLN:HG2 | 2.24 | 0.52 |
| 4:8:180:LEU:HD22 | 4:8:267:ILE:HD11 | 1.91 | 0.52 |
| 4:9:185:LEU:HD23 | 4:9:306:TYR:OH | 2.09 | 0.52 |
| 1:A:599:ASN:CG | 1:A:649:VAL:H | 2.12 | 0.52 |
| 1:A:636:LYS:HB2 | 4:8:334:GLU:OE1 | 2.08 | 0.52 |
| 1:D:410:ASN:CG | 4:9:334:GLU:C | 2.65 | 0.52 |
| 1:D:470:PHE:O | 1:D:473:ASN:ND2 | 2.40 | 0.52 |
| 1:D:584:TYR:CD1 | 1:D:585:ALA:N | 2.77 | 0.52 |
| 1:D:791:GLN:O | 1:D:794:CYS:HB2 | 2.08 | 0.52 |
| 2:E:114:LYS:O | 2:E:147:ASN:ND2 | 2.42 | 0.52 |
| 1:G:640:LYS:C | 4:V:23:GLY:CA | 2.64 | 0.52 |
| 1:G:817:GLN:HE21 | 2:H:127:ARG:HB2 | 1.71 | 0.52 |
| 1:J:553:MLY:CE | 4:Y:45:VAL:HG11 | 2.32 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:404:PRO:HG3 | 1:M:417:GLU:HG3 | 1.91 | 0.52 |
| 1:M:529:PRO:HB2 | 4:Z:354:GLN:HA | 1.91 | 0.52 |
| 1:M:636:LYS:HB2 | 4:Z:334:GLU:OE1 | 2.09 | 0.52 |
| 3:O:92:ARG:HA | 3:O:139:TYR:OH | 2.08 | 0.52 |
| 1:P:135:TYR:CD2 | 1:P:191:ARG:HG2 | 2.44 | 0.52 |
| 4:1:205:GLU:OE1 | 4:Y:287:ILE:O | 2.26 | 0.52 |
| 4:6:185:LEU:HD23 | 4:6:306:TYR:OH | 2.09 | 0.52 |
| 4:Y:265:SER:HB3 | 4:Z:39:ARG:NH2 | 2.25 | 0.52 |
| 1:A:494:HIS:O | 1:A:498:LEU:HB2 | 2.09 | 0.52 |
| 1:D:599:ASN:CG | 1:D:649:VAL:H | 2.12 | 0.52 |
| 3:F:53:PRO:HB2 | 3:F:55:LYS:HG3 | 1.91 | 0.52 |
| 3:F:104:GLY:HA2 | 3:F:137:ILE:HD11 | 1.92 | 0.52 |
| 1:G:93:MET:CE | 1:G:764:MLY:HD2 | 2.40 | 0.52 |
| 1:G:795:ARG:HG3 | 3:I:116:GLU:OE2 | 2.09 | 0.52 |
| 1:G:817:GLN:CB | 2:H:127:ARG:HD2 | 2.39 | 0.52 |
| 2:H:114:LYS:O | 2:H:147:ASN:ND2 | 2.42 | 0.52 |
| 1:J:295:MLY:HE2 | 1:J:332:MET:HE1 | 1.91 | 0.52 |
| 1:J:491:PHE:HD1 | 1:J:671:PHE:CE2 | 2.27 | 0.52 |
| 1:J:579:PHE:CD2 | 1:J:592:ILE:HD11 | 2.40 | 0.52 |
| 1:M:135:TYR:HD2 | 1:M:191:ARG:HD3 | 1.73 | 0.52 |
| 1:M:292:MET:CE | 1:M:309:PRO:HA | 2.40 | 0.52 |
| 1:M:491:PHE:HD1 | 1:M:671:PHE:CE2 | 2.27 | 0.52 |
| 1:M:530:MET:HE3 | 4:Z:354:GLN:CB | 2.39 | 0.52 |
| 1:M:839:MLY:HH21 | 2:N:158:THR:CG2 | 2.39 | 0.52 |
| 1:P:292:MET:CE | 1:P:309:PRO:HA | 2.39 | 0.52 |
| 1:P:494:HIS:O | 1:P:498:LEU:HB2 | 2.09 | 0.52 |
| 1:P:529:PRO:HB2 | 4:1:354:GLN:HA | 1.91 | 0.52 |
| 1:A:538:GLU:HA | 4:8:349:LEU:CB | 2.39 | 0.52 |
| 1:A:661:MET:O | 1:A:665:ARG:HG3 | 2.09 | 0.52 |
| 2:B:121:LEU:CA | 2:B:128:PHE:CG | 2.89 | 0.52 |
| 3:C:53:PRO:HB2 | 3:C:55:LYS:HG3 | 1.91 | 0.52 |
| 3:C:110:VAL:HG13 | 3:C:114:LEU:HD12 | 1.92 | 0.52 |
| 1:D:41:VAL:HG13 | 1:D:42:HIS:N | 2.25 | 0.52 |
| 1:D:156:PHE:HD1 | 1:D:195:TYR:CD1 | 2.27 | 0.52 |
| 1:D:830:PRO:HB2 | 2:E:51:PHE:CE1 | 2.45 | 0.52 |
| 1:G:725:ARG:HG3 | 1:G:733:PRO:CA | 2.36 | 0.52 |
| 1:G:798:LEU:HD22 | 3:I:118:MET:CG | 2.40 | 0.52 |
| 3:I:110:VAL:HG13 | 3:I:114:LEU:HD12 | 1.92 | 0.52 |
| 1:J:135:TYR:HD2 | 1:J:191:ARG:HD3 | 1.73 | 0.52 |
| 1:M:649:VAL:CG1 | 1:M:649:VAL:HA | 2.35 | 0.52 |
| 1:M:785:GLU:C | 1:M:789:ALA:CB | 2.76 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:P:786:ILE:HG22 | 1:P:787:ILE:N | 2.24 | 0.52 |
| 4:2:285:CYS:O | 4:2:290:ARG:NH1 | 2.43 | 0.52 |
| 4:5:180:LEU:HD22 | 4:5:267:ILE:HD11 | 1.92 | 0.52 |
| 4:6:180:LEU:HD22 | 4:6:267:ILE:HD11 | 1.92 | 0.52 |
| 4:9:180:LEU:HD22 | 4:9:267:ILE:HD11 | 1.92 | 0.52 |
| 4:V:180:LEU:HD22 | 4:V:267:ILE:HD11 | 1.92 | 0.52 |
| 4:V:185:LEU:HD23 | 4:V:306:TYR:OH | 2.09 | 0.52 |
| 4:X:180:LEU:HD22 | 4:X:267:ILE:HD11 | 1.92 | 0.52 |
| 1:A:530:MET:HG2 | 4:8:354:GLN:HB2 | 0.57 | 0.52 |
| 1:D:109:ARG:HD3 | 1:D:117:THR:HB | 1.92 | 0.52 |
| 1:D:277:PHE:CG | 1:D:278:GLN:N | 2.76 | 0.52 |
| 1:D:292:MET:CE | 1:D:309:PRO:HA | 2.39 | 0.52 |
| 2:H:114:LYS:HA | 2:H:147:ASN:HD22 | 1.75 | 0.52 |
| 1:J:636:LYS:HB2 | 4:W:334:GLU:OE1 | 2.09 | 0.52 |
| 4:1:285:CYS:O | 4:1:290:ARG:NH1 | 2.43 | 0.52 |
| 4:2:180:LEU:HD22 | 4:2:267:ILE:HD11 | 1.92 | 0.52 |
| 4:3:180:LEU:HD22 | 4:3:267:ILE:HD11 | 1.92 | 0.52 |
| 4:4:180:LEU:HD22 | 4:4:267:ILE:HD11 | 1.92 | 0.52 |
| 4:V:324:THR:HG22 | 4:X:247:VAL:HG13 | 1.91 | 0.52 |
| 4:Z:180:LEU:HD22 | 4:Z:267:ILE:HD11 | 1.92 | 0.52 |
| 1:A:156:PHE:HD1 | 1:A:195:TYR:CD1 | 2.27 | 0.52 |
| 1:A:295:MLY:HE2 | 1:A:332:MET:HE1 | 1.90 | 0.52 |
| 1:A:839:MLY:HH13 | 2:B:159:HIS:CD2 | 2.45 | 0.52 |
| 1:D:40:VAL:HG13 | 1:D:41:VAL:O | 2.10 | 0.52 |
| 1:D:96:HIS:CE1 | 1:D:770:GLY:N | 2.78 | 0.52 |
| 1:G:41:VAL:HG13 | 1:G:42:HIS:N | 2.25 | 0.52 |
| 1:G:109:ARG:HD3 | 1:G:117:THR:HB | 1.91 | 0.52 |
| 1:G:277:PHE:CG | 1:G:278:GLN:N | 2.76 | 0.52 |
| 1:G:838:ILE:CG1 | 2:H:54:MET:CE | 2.86 | 0.52 |
| 1:J:798:LEU:HD12 | 3:L:126:LEU:HD11 | 1.75 | 0.52 |
| 2:K:114:LYS:HA | 2:K:147:ASN:HD22 | 1.74 | 0.52 |
| 1:M:63:MLY:HG3 | 1:M:64:THR:H | 1.75 | 0.52 |
| 1:M:156:PHE:HD1 | 1:M:195:TYR:CD1 | 2.27 | 0.52 |
| 1:M:206:LYS:HD2 | 1:M:217:THR:CG2 | 2.17 | 0.52 |
| 1:M:217:THR:C | 1:M:221:GLN:NE2 | 2.62 | 0.52 |
| 1:M:538:GLU:HG3 | 4:Z:352:PHE:CA | 2.38 | 0.52 |
| 1:M:786:ILE:CA | 1:M:787:ILE:N | 2.73 | 0.52 |
| 1:M:797:PHE:HE1 | 3:O:149:VAL:HG12 | 1.71 | 0.52 |
| 2:N:129:THR:O | 2:N:133:ILE:HG13 | 2.10 | 0.52 |
| 1:P:156:PHE:HD1 | 1:P:195:TYR:CD1 | 2.27 | 0.52 |
| 1:P:232:PHE:CE1 | 1:P:287:ILE:HD13 | 2.45 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:1:185:LEU:HD23 | 4:1:306:TYR:OH | 2.09 | 0.52 |
| 4:4:322:PRO:C | 4:6:244:ASP:HB2 | 2.30 | 0.52 |
| 4:Z:285:CYS:O | 4:Z:290:ARG:NH1 | 2.43 | 0.52 |
| 1:A:128:PRO:O | 1:A:129:TYR:HB2 | 2.09 | 0.52 |
| 1:A:197:ALA:O | 1:A:201:ALA:HB2 | 2.10 | 0.52 |
| 1:A:632:GLY:HA3 | 1:A:643:GLY:N | 2.17 | 0.52 |
| 1:D:22:LYS:O | 1:D:26:GLU:N | 2.29 | 0.52 |
| 1:D:128:PRO:O | 1:D:129:TYR:HB2 | 2.10 | 0.52 |
| 1:D:404:PRO:HG3 | 1:D:417:GLU:HG3 | 1.91 | 0.52 |
| 1:D:713:SER:CB | 1:D:775:LEU:CD2 | 2.88 | 0.52 |
| 1:G:197:ALA:O | 1:G:201:ALA:HB2 | 2.09 | 0.52 |
| 1:G:251:ARG:HB2 | 1:G:264:ASP:HB2 | 1.91 | 0.52 |
| 1:G:529:PRO:HB2 | 4:V:354:GLN:HA | 1.92 | 0.52 |
| 1:J:63:MLY:HG3 | 1:J:64:THR:H | 1.75 | 0.52 |
| 1:J:494:HIS:O | 1:J:498:LEU:HB2 | 2.09 | 0.52 |
| 1:J:836:PHE:CE1 | 2:K:160:GLY:N | 2.69 | 0.52 |
| 1:M:135:TYR:CD2 | 1:M:191:ARG:HG2 | 2.44 | 0.52 |
| 1:M:295:MLY:HE2 | 1:M:332:MET:HE1 | 1.91 | 0.52 |
| 1:M:836:PHE:CD1 | 2:N:159:HIS:CA | 2.90 | 0.52 |
| 1:P:154:HIS:CE1 | 1:P:156:PHE:HD2 | 2.26 | 0.52 |
| 2:Q:114:LYS:HA | 2:Q:147:ASN:HD22 | 1.74 | 0.52 |
| 4:4:285:CYS:O | 4:4:290:ARG:NH1 | 2.43 | 0.52 |
| 4:7:180:LEU:HD22 | 4:7:267:ILE:HD11 | 1.92 | 0.52 |
| 4:8:185:LEU:HD23 | 4:8:306:TYR:OH | 2.09 | 0.52 |
| 4:9:285:CYS:O | 4:9:290:ARG:NH1 | 2.43 | 0.52 |
| 4:V:285:CYS:O | 4:V:290:ARG:NH1 | 2.43 | 0.52 |
| 4:X:285:CYS:O | 4:X:290:ARG:NH1 | 2.43 | 0.52 |
| 4:X:287:ILE:H | 4:Z:202:THR:N | 2.07 | 0.52 |
| 4:Y:285:CYS:O | 4:Y:290:ARG:NH1 | 2.43 | 0.52 |
| 1:A:538:GLU:HG3 | 4:8:352:PHE:CA | 2.38 | 0.52 |
| 2:B:129:THR:O | 2:B:133:ILE:HG13 | 2.10 | 0.52 |
| 3:C:104:GLY:HA2 | 3:C:137:ILE:HD11 | 1.92 | 0.52 |
| 2:E:129:THR:O | 2:E:133:ILE:HG13 | 2.09 | 0.52 |
| 1:G:642:LYS:CA | 4:V:22:ALA:C | 2.70 | 0.52 |
| 3:L:110:VAL:HG13 | 3:L:114:LEU:HD12 | 1.92 | 0.52 |
| 1:P:109:ARG:HD3 | 1:P:117:THR:HB | 1.92 | 0.52 |
| 1:P:548:THR:HG21 | 4:3:47:MET:CB | 2.40 | 0.52 |
| 4:5:185:LEU:HD23 | 4:5:306:TYR:OH | 2.09 | 0.52 |
| 4:6:285:CYS:O | 4:6:290:ARG:NH1 | 2.43 | 0.52 |
| 4:8:285:CYS:O | 4:8:290:ARG:NH1 | 2.43 | 0.52 |
| 4:Y:180:LEU:HD22 | 4:Y:267:ILE:HD11 | 1.92 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:505:MLY:N | 1:A:762:HIS:CD2 | 2.77 | 0.52 |
| 1:A:732:ILE:H | 1:A:733:PRO:CD | 2.23 | 0.52 |
| 1:A:836:PHE:CE2 | 2:B:160:GLY:CA | 2.93 | 0.52 |
| 1:G:28:GLN:CD | 1:G:723:ARG:NH1 | 2.62 | 0.52 |
| 1:G:40:VAL:HG13 | 1:G:41:VAL:O | 2.10 | 0.52 |
| 1:G:838:ILE:HD13 | 2:H:33:VAL:CG1 | 2.40 | 0.52 |
| 1:J:538:GLU:HA | 4:W:349:LEU:CB | 2.40 | 0.52 |
| 1:M:195:TYR:CE2 | 1:M:199:ILE:CD1 | 2.93 | 0.52 |
| 1:M:251:ARG:HB2 | 1:M:264:ASP:HB2 | 1.91 | 0.52 |
| 1:M:793:ARG:HD3 | 3:O:40:ASN:ND2 | 2.25 | 0.52 |
| 1:P:63:MLY:HG3 | 1:P:64:THR:H | 1.75 | 0.52 |
| 4:1:180:LEU:HD22 | 4:1:267:ILE:HD11 | 1.92 | 0.52 |
| 4:W:180:LEU:HD22 | 4:W:267:ILE:HD11 | 1.92 | 0.52 |
| 1:A:251:ARG:HB2 | 1:A:264:ASP:HB2 | 1.91 | 0.52 |
| 1:A:292:MET:CE | 1:A:309:PRO:HA | 2.40 | 0.52 |
| 1:A:539:GLU:OE2 | 4:V:45:VAL:C | 2.48 | 0.52 |
| 1:A:555:TYR:N | 4:V:48:GLY:N | 2.58 | 0.52 |
| 2:B:114:LYS:N | 2:B:146:GLY:O | 2.40 | 0.52 |
| 1:D:538:GLU:HA | 4:9:349:LEU:CB | 2.39 | 0.52 |
| 2:E:117:LEU:CG | 2:E:147:ASN:OD1 | 2.52 | 0.52 |
| 1:G:553:MLY:CB | 4:X:45:VAL:O | 2.57 | 0.52 |
| 1:G:821:ARG:HH22 | 2:H:127:ARG:CD | 2.23 | 0.52 |
| 1:G:831:TRP:CZ3 | 2:H:34:ILE:HD13 | 2.45 | 0.52 |
| 1:G:838:ILE:HD13 | 2:H:33:VAL:HG11 | 1.92 | 0.52 |
| 2:H:121:LEU:CA | 2:H:128:PHE:CG | 2.89 | 0.52 |
| 1:J:135:TYR:HD2 | 1:J:191:ARG:CD | 2.23 | 0.52 |
| 1:J:221:GLN:HB2 | 1:J:449:LEU:HD11 | 1.92 | 0.52 |
| 1:M:109:ARG:O | 1:M:114:MET:N | 2.37 | 0.52 |
| 1:M:725:ARG:O | 1:M:729:ALA:HA | 2.10 | 0.52 |
| 1:P:93:MET:HE1 | 1:P:764:MLY:HD3 | 1.92 | 0.52 |
| 1:P:481:ASN:N | 1:P:481:ASN:ND2 | 2.51 | 0.52 |
| 1:P:538:GLU:HA | 4:1:349:LEU:CB | 2.40 | 0.52 |
| 1:A:212:GLY:O | 1:A:213:LYS:HB2 | 2.10 | 0.51 |
| 1:A:218:LEU:N | 1:A:221:GLN:HG2 | 2.24 | 0.51 |
| 1:A:221:GLN:HB2 | 1:A:449:LEU:HD11 | 1.93 | 0.51 |
| 1:D:135:TYR:HD2 | 1:D:191:ARG:CD | 2.23 | 0.51 |
| 1:D:212:GLY:O | 1:D:213:LYS:HB2 | 2.11 | 0.51 |
| 1:D:221:GLN:HB2 | 1:D:449:LEU:HD11 | 1.93 | 0.51 |
| 1:D:491:PHE:HD1 | 1:D:671:PHE:CE2 | 2.27 | 0.51 |
| 1:D:546:THR:CG2 | 1:D:548:THR:HB | 2.40 | 0.51 |
| 1:G:221:GLN:HB2 | 1:G:449:LEU:HD11 | 1.92 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:295:MLY:HE2 | 1:G:332:MET:HE1 | 1.91 | 0.51 |
| 1:J:42:HIS:HB3 | 1:J:45:GLN:O | 2.09 | 0.51 |
| 1:J:197:ALA:O | 1:J:201:ALA:HB2 | 2.09 | 0.51 |
| 1:J:725:ARG:O | 1:J:729:ALA:HA | 2.10 | 0.51 |
| 1:M:494:HIS:O | 1:M:498:LEU:HB2 | 2.09 | 0.51 |
| 1:M:553:MLY:N | 4:2:49:GLN:HG3 | 2.00 | 0.51 |
| 2:N:114:LYS:HA | 2:N:147:ASN:HD22 | 1.75 | 0.51 |
| 1:P:197:ALA:O | 1:P:201:ALA:HB2 | 2.09 | 0.51 |
| 1:P:640:LYS:CA | 1:P:645:SER:OG | 2.58 | 0.51 |
| 1:A:13:ALA:C | 1:A:15:PRO:HD2 | 2.31 | 0.51 |
| 1:A:63:MLY:HG3 | 1:A:64:THR:H | 1.75 | 0.51 |
| 1:A:836:PHE:CZ | 2:B:159:HIS:HA | 2.45 | 0.51 |
| 2:B:114:LYS:HA | 2:B:147:ASN:HD22 | 1.75 | 0.51 |
| 1:D:217:THR:C | 1:D:221:GLN:NE2 | 2.62 | 0.51 |
| 1:D:218:LEU:CD2 | 1:D:222:ILE:CG1 | 2.86 | 0.51 |
| 1:D:530:MET:HE3 | 4:9:354:GLN:CB | 2.40 | 0.51 |
| 1:D:578:HIS:O | 1:D:579:PHE:HB3 | 2.11 | 0.51 |
| 1:G:128:PRO:O | 1:G:129:TYR:HB2 | 2.10 | 0.51 |
| 1:G:494:HIS:O | 1:G:498:LEU:HB2 | 2.09 | 0.51 |
| 1:G:642:LYS:HB2 | 4:V:24:ASP:O | 1.89 | 0.51 |
| 1:G:755:HIS:N | 1:G:779:ARG:NE | 2.46 | 0.51 |
| 1:G:797:PHE:CD2 | 3:I:126:LEU:HD13 | 2.45 | 0.51 |
| 2:H:129:THR:O | 2:H:133:ILE:HG13 | 2.09 | 0.51 |
| 1:J:195:TYR:CE2 | 1:J:199:ILE:CD1 | 2.93 | 0.51 |
| 1:J:232:PHE:CE1 | 1:J:287:ILE:HD13 | 2.45 | 0.51 |
| 1:J:248:MLY:N | 1:J:463:ASP:O | 2.44 | 0.51 |
| 1:J:546:THR:CG2 | 1:J:548:THR:HB | 2.41 | 0.51 |
| 1:J:640:LYS:CA | 1:J:645:SER:OG | 2.58 | 0.51 |
| 1:J:792:ALA:HB2 | 3:L:42:THR:N | 2.03 | 0.51 |
| 2:K:114:LYS:O | 2:K:147:ASN:ND2 | 2.42 | 0.51 |
| 1:M:41:VAL:HG13 | 1:M:42:HIS:N | 2.25 | 0.51 |
| 1:M:109:ARG:HD3 | 1:M:117:THR:HB | 1.92 | 0.51 |
| 1:P:248:MLY:N | 1:P:463:ASP:O | 2.44 | 0.51 |
| 4:3:285:CYS:O | 4:3:290:ARG:NH1 | 2.43 | 0.51 |
| 4:7:287:ILE:HG22 | 4:9:204:ALA:HB3 | 1.91 | 0.51 |
| 4:W:285:CYS:O | 4:W:290:ARG:NH1 | 2.43 | 0.51 |
| 1:A:195:TYR:CE2 | 1:A:199:ILE:CD1 | 2.93 | 0.51 |
| 1:A:220:ASP:O | 1:A:224:SER:N | 2.27 | 0.51 |
| 1:A:491:PHE:HD1 | 1:A:671:PHE:CE2 | 2.27 | 0.51 |
| 1:D:251:ARG:HB2 | 1:D:264:ASP:HB2 | 1.91 | 0.51 |
| 1:D:494:HIS:O | 1:D:498:LEU:HB2 | 2.09 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:508:ILE:HA | 1:D:761:GLY:CA | 2.32 | 0.51 |
| 1:G:41:VAL:HG21 | 1:G:76:GLN:HG3 | 1.93 | 0.51 |
| 1:G:135:TYR:HD2 | 1:G:191:ARG:CD | 2.23 | 0.51 |
| 1:G:491:PHE:HD1 | 1:G:671:PHE:CE2 | 2.27 | 0.51 |
| 1:G:732:ILE:H | 1:G:733:PRO:CD | 2.23 | 0.51 |
| 3:I:104:GLY:HA2 | 3:I:137:ILE:HD11 | 1.92 | 0.51 |
| 1:J:559:LEU:HD23 | 1:J:559:LEU:C | 2.31 | 0.51 |
| 1:M:41:VAL:HG21 | 1:M:76:GLN:HG3 | 1.93 | 0.51 |
| 3:O:49:ILE:CA | 3:O:52:ASN:ND2 | 2.53 | 0.51 |
| 3:O:100:GLY:O | 3:O:138:ASN:HA | 2.11 | 0.51 |
| 1:P:578:HIS:O | 1:P:579:PHE:HB3 | 2.11 | 0.51 |
| 4:8:287:ILE:HG22 | 4:V:204:ALA:HB3 | 1.91 | 0.51 |
| 1:A:40:VAL:HG13 | 1:A:41:VAL:O | 2.10 | 0.51 |
| 1:A:725:ARG:O | 1:A:729:ALA:HA | 2.10 | 0.51 |
| 3:C:100:GLY:O | 3:C:138:ASN:HA | 2.11 | 0.51 |
| 1:D:197:ALA:O | 1:D:201:ALA:HB2 | 2.09 | 0.51 |
| 1:D:555:TYR:N | 4:W:48:GLY:N | 2.58 | 0.51 |
| 1:D:725:ARG:O | 1:D:729:ALA:HA | 2.10 | 0.51 |
| 1:D:732:ILE:H | 1:D:733:PRO:CD | 2.22 | 0.51 |
| 1:D:739:ASP:CB | 1:D:742:LYS:CB | 2.81 | 0.51 |
| 2:H:112:ILE:HG23 | 2:H:147:ASN:HB3 | 1.93 | 0.51 |
| 1:J:38:VAL:CG1 | 1:J:39:PHE:N | 2.74 | 0.51 |
| 1:M:40:VAL:HG13 | 1:M:41:VAL:O | 2.10 | 0.51 |
| 1:M:221:GLN:HB2 | 1:M:449:LEU:HD11 | 1.92 | 0.51 |
| 1:M:278:GLN:HG3 | 1:M:318:GLY:H | 1.76 | 0.51 |
| 1:M:530:MET:HG2 | 4:Z:354:GLN:HB2 | 0.57 | 0.51 |
| 3:O:110:VAL:HG13 | 3:O:114:LEU:HD12 | 1.91 | 0.51 |
| 1:P:40:VAL:HG13 | 1:P:41:VAL:O | 2.10 | 0.51 |
| 1:P:212:GLY:O | 1:P:213:LYS:HB2 | 2.10 | 0.51 |
| 1:P:546:THR:CG2 | 1:P:548:THR:HB | 2.41 | 0.51 |
| 2:Q:114:LYS:N | 2:Q:146:GLY:O | 2.40 | 0.51 |
| 3:R:53:PRO:HB2 | 3:R:55:LYS:HG3 | 1.91 | 0.51 |
| 4:2:203:THR:HB | 4:Z:287:ILE:HB | 1.91 | 0.51 |
| 4:2:287:ILE:HD13 | 4:4:203:THR:CA | 2.41 | 0.51 |
| 1:A:578:HIS:O | 1:A:579:PHE:HB3 | 2.10 | 0.51 |
| 1:A:797:PHE:CD1 | 3:C:149:VAL:CG1 | 2.93 | 0.51 |
| 1:D:408:VAL:CG1 | 4:9:332:PRO:HB3 | 2.41 | 0.51 |
| 1:D:798:LEU:HD13 | 3:F:126:LEU:CD1 | 2.19 | 0.51 |
| 1:G:195:TYR:CE2 | 1:G:199:ILE:CD1 | 2.93 | 0.51 |
| 1:G:538:GLU:HA | 4:V:349:LEU:CB | 2.40 | 0.51 |
| 1:G:636:LYS:HB2 | 4:V:334:GLU:OE1 | 2.09 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:642:LYS:HG2 | 4:V:21:PHE:C | 2.30 | 0.51 |
| 1:J:635:GLY:HA3 | 4:W:334:GLU:CG | 2.30 | 0.51 |
| 1:J:817:GLN:NE2 | 2:K:127:ARG:HB2 | 2.24 | 0.51 |
| 1:J:829:TRP:HZ3 | 2:K:84:PHE:CE1 | 2.28 | 0.51 |
| 1:J:838:ILE:CG1 | 2:K:54:MET:HE1 | 2.38 | 0.51 |
| 1:M:649:VAL:HA | 1:M:649:VAL:HG22 | 1.81 | 0.51 |
| 1:M:769:ALA:O | 1:M:770:GLY:HA3 | 2.08 | 0.51 |
| 1:P:38:VAL:CG1 | 1:P:39:PHE:N | 2.74 | 0.51 |
| 1:P:135:TYR:HD2 | 1:P:191:ARG:CD | 2.23 | 0.51 |
| 1:P:221:GLN:HB2 | 1:P:449:LEU:HD11 | 1.92 | 0.51 |
| 1:P:408:VAL:CG1 | 4:1:332:PRO:HB3 | 2.41 | 0.51 |
| 1:P:559:LEU:C | 1:P:559:LEU:HD23 | 2.31 | 0.51 |
| 3:R:100:GLY:O | 3:R:138:ASN:HA | 2.11 | 0.51 |
| 3:R:110:VAL:HG13 | 3:R:114:LEU:HD12 | 1.92 | 0.51 |
| 4:2:287:ILE:CG2 | 4:4:202:THR:CA | 2.82 | 0.51 |
| 1:A:218:LEU:N | 1:A:221:GLN:CG | 2.74 | 0.51 |
| 1:A:501:GLU:O | 1:A:762:HIS:CD2 | 2.64 | 0.51 |
| 1:A:502:GLU:HA | 1:A:761:GLY:C | 2.29 | 0.51 |
| 1:D:38:VAL:CG1 | 1:D:39:PHE:N | 2.74 | 0.51 |
| 1:D:400:ALA:HB1 | 1:D:606:THR:HG22 | 1.92 | 0.51 |
| 2:E:114:LYS:HA | 2:E:147:ASN:HD22 | 1.75 | 0.51 |
| 1:G:725:ARG:O | 1:G:729:ALA:HA | 2.10 | 0.51 |
| 1:J:128:PRO:O | 1:J:129:TYR:HB2 | 2.10 | 0.51 |
| 1:J:578:HIS:O | 1:J:579:PHE:HB3 | 2.11 | 0.51 |
| 3:L:53:PRO:HB2 | 3:L:55:LYS:HG3 | 1.91 | 0.51 |
| 1:M:128:PRO:O | 1:M:129:TYR:HB2 | 2.10 | 0.51 |
| 1:M:687:GLU:O | 1:M:691:VAL:HG23 | 2.11 | 0.51 |
| 1:M:795:ARG:NE | 3:O:116:GLU:OE2 | 2.41 | 0.51 |
| 3:O:53:PRO:HB2 | 3:O:55:LYS:HG3 | 1.91 | 0.51 |
| 1:P:41:VAL:HG21 | 1:P:76:GLN:HG3 | 1.93 | 0.51 |
| 1:P:291:ILE:HA | 1:P:331:LEU:CD1 | 2.39 | 0.51 |
| 1:P:687:GLU:O | 1:P:691:VAL:HG23 | 2.11 | 0.51 |
| 4:4:287:ILE:HG22 | 4:6:204:ALA:HB3 | 1.92 | 0.51 |
| 4:7:285:CYS:O | 4:7:290:ARG:NH1 | 2.43 | 0.51 |
| 1:A:232:PHE:CE1 | 1:A:287:ILE:HD13 | 2.44 | 0.51 |
| 1:A:278:GLN:HG3 | 1:A:318:GLY:H | 1.75 | 0.51 |
| 1:A:559:LEU:HD23 | 1:A:559:LEU:C | 2.31 | 0.51 |
| 1:A:592:ILE:O | 1:A:592:ILE:HG22 | 2.11 | 0.51 |
| 1:A:687:GLU:O | 1:A:691:VAL:HG23 | 2.11 | 0.51 |
| 1:D:41:VAL:HG21 | 1:D:76:GLN:HG3 | 1.92 | 0.51 |
| 1:D:63:MLY:HG3 | 1:D:64:THR:H | 1.75 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:592:ILE:O | 1:D:592:ILE:HG22 | 2.11 | 0.51 |
| 1:G:232:PHE:CE1 | 1:G:287:ILE:HD13 | 2.45 | 0.51 |
| 1:G:278:GLN:HG3 | 1:G:318:GLY:H | 1.76 | 0.51 |
| 1:G:640:LYS:CA | 1:G:645:SER:OG | 2.59 | 0.51 |
| 1:J:41:VAL:HG13 | 1:J:42:HIS:N | 2.25 | 0.51 |
| 1:J:109:ARG:HD3 | 1:J:117:THR:HB | 1.92 | 0.51 |
| 1:J:418:THR:O | 1:J:422:VAL:HG23 | 2.11 | 0.51 |
| 1:J:592:ILE:HG22 | 1:J:592:ILE:O | 2.11 | 0.51 |
| 1:J:642:LYS:HG2 | 4:W:22:ALA:C | 2.27 | 0.51 |
| 1:M:212:GLY:O | 1:M:213:LYS:HB2 | 2.11 | 0.51 |
| 1:M:642:LYS:HG2 | 4:Z:21:PHE:C | 2.29 | 0.51 |
| 1:M:642:LYS:HB2 | 4:Z:24:ASP:O | 1.89 | 0.51 |
| 1:M:732:ILE:HG23 | 1:M:747:LEU:HD12 | 0.95 | 0.51 |
| 1:P:218:LEU:N | 1:P:221:GLN:CG | 2.74 | 0.51 |
| 1:P:592:ILE:HG22 | 1:P:592:ILE:O | 2.10 | 0.51 |
| 1:P:725:ARG:HG3 | 1:P:733:PRO:CA | 2.36 | 0.51 |
| 3:R:104:GLY:HA2 | 3:R:137:ILE:HD11 | 1.91 | 0.51 |
| 4:1:287:ILE:HG21 | 4:3:204:ALA:H | 1.76 | 0.51 |
| 4:V:322:PRO:HB3 | 4:X:246:GLN:HG2 | 1.92 | 0.51 |
| 1:A:237:THR:O | 1:A:240:ASN:O | 2.29 | 0.51 |
| 1:A:400:ALA:HB1 | 1:A:606:THR:HG22 | 1.92 | 0.51 |
| 1:A:418:THR:O | 1:A:422:VAL:HG23 | 2.11 | 0.51 |
| 1:A:642:LYS:HB2 | 4:8:24:ASP:O | 1.88 | 0.51 |
| 1:A:813:ILE:HG21 | 2:B:127:ARG:CD | 2.23 | 0.51 |
| 1:D:13:ALA:C | 1:D:15:PRO:HD2 | 2.31 | 0.51 |
| 1:D:631:GLU:C | 4:9:25:ASP:HB2 | 2.32 | 0.51 |
| 1:D:632:GLY:HA3 | 1:D:643:GLY:N | 2.17 | 0.51 |
| 1:D:646:PHE:CE2 | 1:D:652:LEU:CD2 | 2.87 | 0.51 |
| 1:D:742:LYS:O | 1:D:745:GLU:HB2 | 2.10 | 0.51 |
| 1:G:93:MET:HE3 | 1:G:764:MLY:HD3 | 1.87 | 0.51 |
| 1:G:212:GLY:O | 1:G:213:LYS:HB2 | 2.11 | 0.51 |
| 1:G:218:LEU:N | 1:G:221:GLN:CG | 2.74 | 0.51 |
| 1:G:578:HIS:O | 1:G:579:PHE:HB3 | 2.10 | 0.51 |
| 1:G:733:PRO:O | 1:G:737:PHE:CE1 | 2.54 | 0.51 |
| 3:I:100:GLY:O | 3:I:138:ASN:HA | 2.11 | 0.51 |
| 1:J:13:ALA:C | 1:J:15:PRO:HD2 | 2.31 | 0.51 |
| 1:J:169:ASP:N | 1:J:169:ASP:OD1 | 2.44 | 0.51 |
| 2:K:129:THR:O | 2:K:133:ILE:HG13 | 2.09 | 0.51 |
| 3:L:104:GLY:HA2 | 3:L:137:ILE:HD11 | 1.92 | 0.51 |
| 1:M:418:THR:O | 1:M:422:VAL:HG23 | 2.11 | 0.51 |
| 1:M:829:TRP:HZ3 | 2:N:84:PHE:CE2 | 2.28 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:P:237:THR:O | 1:P:240:ASN:O | 2.29 | 0.51 |
| 1:P:631:GLU:C | 4:1:25:ASP:HB2 | 2.32 | 0.51 |
| 1:P:733:PRO:CA | 1:P:737:PHE:CE1 | 2.94 | 0.51 |
| 4:1:201:VAL:CB | 4:Y:287:ILE:CG1 | 2.87 | 0.51 |
| 4:5:285:CYS:O | 4:5:290:ARG:NH1 | 2.43 | 0.51 |
| 4:W:286:ASP:OD2 | 4:Y:203:THR:CG2 | 2.47 | 0.51 |
| 1:A:408:VAL:CG1 | 4:8:332:PRO:HB3 | 2.40 | 0.51 |
| 1:A:429:LEU:O | 1:A:433:VAL:HG23 | 2.11 | 0.51 |
| 1:A:752:ASP:O | 1:A:778:MET:SD | 2.69 | 0.51 |
| 2:B:117:LEU:CG | 2:B:147:ASN:OD1 | 2.52 | 0.51 |
| 1:D:169:ASP:OD1 | 1:D:169:ASP:N | 2.44 | 0.51 |
| 1:D:202:SER:HB2 | 1:D:207:LYS:NZ | 2.26 | 0.51 |
| 1:D:248:MLY:N | 1:D:463:ASP:O | 2.44 | 0.51 |
| 1:D:311:ASP:HB2 | 1:D:312:TYR:CE1 | 2.46 | 0.51 |
| 1:D:530:MET:HE3 | 4:9:355:MET:SD | 2.50 | 0.51 |
| 1:D:675:ILE:CG2 | 1:D:676:ILE:N | 2.74 | 0.51 |
| 3:F:100:GLY:O | 3:F:138:ASN:HA | 2.11 | 0.51 |
| 1:G:109:ARG:O | 1:G:114:MET:N | 2.37 | 0.51 |
| 1:G:206:LYS:HD2 | 1:G:217:THR:CG2 | 2.17 | 0.51 |
| 1:J:202:SER:HB2 | 1:J:207:LYS:NZ | 2.26 | 0.51 |
| 1:J:795:ARG:HH21 | 3:L:116:GLU:HG2 | 1.76 | 0.51 |
| 2:K:117:LEU:HG | 2:K:147:ASN:HB3 | 1.93 | 0.51 |
| 1:M:640:LYS:CA | 1:M:645:SER:OG | 2.58 | 0.51 |
| 1:M:785:GLU:C | 1:M:789:ALA:HB3 | 2.30 | 0.51 |
| 2:N:117:LEU:HG | 2:N:147:ASN:HB3 | 1.93 | 0.51 |
| 2:N:121:LEU:CA | 2:N:128:PHE:CG | 2.89 | 0.51 |
| 1:P:128:PRO:O | 1:P:129:TYR:HB2 | 2.10 | 0.51 |
| 1:P:418:THR:O | 1:P:422:VAL:HG23 | 2.11 | 0.51 |
| 1:A:642:LYS:CG | 4:8:22:ALA:CA | 2.81 | 0.51 |
| 1:A:643:GLY:N | 4:8:23:GLY:C | 2.55 | 0.51 |
| 1:A:820:VAL:HG21 | 2:B:136:MET:HE3 | 1.93 | 0.51 |
| 1:D:769:ALA:O | 1:D:774:LEU:CG | 2.56 | 0.51 |
| 2:E:121:LEU:CA | 2:E:128:PHE:CG | 2.89 | 0.51 |
| 1:G:202:SER:HB2 | 1:G:207:LYS:NZ | 2.26 | 0.51 |
| 1:G:237:THR:O | 1:G:240:ASN:O | 2.29 | 0.51 |
| 1:J:41:VAL:HG21 | 1:J:76:GLN:HG3 | 1.92 | 0.51 |
| 1:J:267:THR:HG21 | 1:J:438:PHE:HE2 | 1.76 | 0.51 |
| 1:J:311:ASP:HB2 | 1:J:312:TYR:CE1 | 2.46 | 0.51 |
| 1:M:135:TYR:HD2 | 1:M:191:ARG:CD | 2.23 | 0.51 |
| 1:M:642:LYS:CG | 4:Z:22:ALA:HA | 2.37 | 0.51 |
| 1:M:786:ILE:CB | 1:M:787:ILE:N | 2.74 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:P:202:SER:HB2 | 1:P:207:LYS:NZ | 2.26 | 0.51 |
| 1:P:725:ARG:O | 1:P:729:ALA:HA | 2.10 | 0.51 |
| 1:P:742:LYS:O | 1:P:745:GLU:HB2 | 2.11 | 0.51 |
| 4:9:287:ILE:HG22 | 4:W:204:ALA:HB3 | 1.92 | 0.51 |
| 1:A:248:MLY:N | 1:A:463:ASP:O | 2.44 | 0.50 |
| 1:A:642:LYS:HG2 | 4:8:21:PHE:C | 2.30 | 0.50 |
| 2:B:112:ILE:HG23 | 2:B:147:ASN:HB3 | 1.93 | 0.50 |
| 1:D:733:PRO:CA | 1:D:737:PHE:CE1 | 2.94 | 0.50 |
| 1:G:411:GLU:H | 4:V:333:PRO:CG | 2.24 | 0.50 |
| 1:G:559:LEU:HD23 | 1:G:559:LEU:C | 2.31 | 0.50 |
| 1:G:813:ILE:CG2 | 2:H:128:PHE:HZ | 2.14 | 0.50 |
| 1:G:813:ILE:HG22 | 2:H:128:PHE:CE1 | 2.44 | 0.50 |
| 1:J:212:GLY:O | 1:J:213:LYS:HB2 | 2.10 | 0.50 |
| 1:J:400:ALA:HB1 | 1:J:606:THR:HG22 | 1.93 | 0.50 |
| 1:J:429:LEU:O | 1:J:433:VAL:HG23 | 2.11 | 0.50 |
| 1:J:742:LYS:O | 1:J:745:GLU:HB2 | 2.10 | 0.50 |
| 1:M:232:PHE:CE1 | 1:M:287:ILE:HD13 | 2.45 | 0.50 |
| 1:M:578:HIS:O | 1:M:579:PHE:HB3 | 2.11 | 0.50 |
| 4:1:243:PRO:CB | 4:Y:291:LYS:HD2 | 2.37 | 0.50 |
| 1:A:41:VAL:HG13 | 1:A:42:HIS:N | 2.25 | 0.50 |
| 1:A:291:ILE:HA | 1:A:331:LEU:CD1 | 2.39 | 0.50 |
| 1:A:646:PHE:HE2 | 1:A:652:LEU:CG | 2.25 | 0.50 |
| 1:D:629:GLU:CB | 1:D:645:SER:N | 2.73 | 0.50 |
| 1:D:799:MET:SD | 3:F:32:ASP:OD2 | 2.69 | 0.50 |
| 1:G:149:GLN:CG | 1:G:716:LEU:HD11 | 2.41 | 0.50 |
| 1:G:248:MLY:N | 1:G:463:ASP:O | 2.44 | 0.50 |
| 1:G:592:ILE:HG22 | 1:G:592:ILE:O | 2.11 | 0.50 |
| 1:G:834:LEU:HD22 | 2:H:34:ILE:HD11 | 1.90 | 0.50 |
| 1:J:40:VAL:HG13 | 1:J:41:VAL:O | 2.10 | 0.50 |
| 1:J:237:THR:O | 1:J:240:ASN:O | 2.29 | 0.50 |
| 1:J:506:GLU:HG3 | 1:J:760:PHE:O | 2.11 | 0.50 |
| 1:J:629:GLU:CA | 1:J:643:GLY:C | 2.73 | 0.50 |
| 1:J:796:GLY:HA2 | 3:L:35:ARG:HG2 | 1.93 | 0.50 |
| 1:M:549:SER:HA | 4:2:43:VAL:CG1 | 2.39 | 0.50 |
| 1:P:267:THR:HG21 | 1:P:438:PHE:HE2 | 1.76 | 0.50 |
| 1:P:311:ASP:HB2 | 1:P:312:TYR:CE1 | 2.46 | 0.50 |
| 1:P:733:PRO:O | 1:P:737:PHE:CE1 | 2.53 | 0.50 |
| 1:A:41:VAL:HG21 | 1:A:76:GLN:HG3 | 1.93 | 0.50 |
| 1:A:135:TYR:HD2 | 1:A:191:ARG:CD | 2.23 | 0.50 |
| 1:A:217:THR:C | 1:A:221:GLN:NE2 | 2.62 | 0.50 |
| 1:D:635:GLY:HA3 | 4:9:334:GLU:CG | 2.30 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:346:ASP:O | 1:G:349:THR:HB | 2.11 | 0.50 |
| 1:G:646:PHE:HE2 | 1:G:652:LEU:CG | 2.25 | 0.50 |
| 1:G:823:PHE:HE1 | 2:H:160:GLY:CA | 2.23 | 0.50 |
| 1:J:646:PHE:HE2 | 1:J:652:LEU:CG | 2.25 | 0.50 |
| 1:M:237:THR:O | 1:M:240:ASN:O | 2.29 | 0.50 |
| 1:M:544:LYS:O | 4:2:45:VAL:HG13 | 2.11 | 0.50 |
| 1:P:41:VAL:HG13 | 1:P:42:HIS:N | 2.25 | 0.50 |
| 1:P:400:ALA:HB1 | 1:P:606:THR:HG22 | 1.93 | 0.50 |
| 1:P:739:ASP:CB | 1:P:742:LYS:CB | 2.81 | 0.50 |
| 1:A:505:MLY:CA | 1:A:762:HIS:NE2 | 2.74 | 0.50 |
| 1:A:631:GLU:C | 4:8:25:ASP:HB2 | 2.32 | 0.50 |
| 1:A:732:ILE:O | 1:A:736:GLN:HG3 | 2.12 | 0.50 |
| 1:A:733:PRO:CA | 1:A:737:PHE:CE1 | 2.95 | 0.50 |
| 1:A:742:LYS:O | 1:A:745:GLU:HB2 | 2.11 | 0.50 |
| 1:D:195:TYR:CE2 | 1:D:199:ILE:CD1 | 2.93 | 0.50 |
| 1:D:559:LEU:HD23 | 1:D:559:LEU:C | 2.31 | 0.50 |
| 1:D:640:LYS:CA | 1:D:645:SER:OG | 2.58 | 0.50 |
| 1:G:400:ALA:HB1 | 1:G:606:THR:HG22 | 1.93 | 0.50 |
| 1:G:418:THR:O | 1:G:422:VAL:HG23 | 2.11 | 0.50 |
| 1:G:631:GLU:C | 4:V:25:ASP:HB2 | 2.31 | 0.50 |
| 1:G:742:LYS:O | 1:G:745:GLU:HB2 | 2.10 | 0.50 |
| 1:J:218:LEU:CD2 | 1:J:222:ILE:CG1 | 2.86 | 0.50 |
| 1:J:530:MET:HA | 4:W:354:GLN:CD | 2.11 | 0.50 |
| 1:J:631:GLU:C | 4:W:25:ASP:HB2 | 2.32 | 0.50 |
| 1:J:687:GLU:O | 1:J:691:VAL:HG23 | 2.11 | 0.50 |
| 1:M:218:LEU:N | 1:M:221:GLN:CG | 2.74 | 0.50 |
| 1:M:732:ILE:H | 1:M:733:PRO:CD | 2.23 | 0.50 |
| 1:M:733:PRO:CA | 1:M:737:PHE:CE1 | 2.95 | 0.50 |
| 3:O:104:GLY:HA2 | 3:O:137:ILE:HD11 | 1.92 | 0.50 |
| 1:P:411:GLU:H | 4:1:333:PRO:CG | 2.24 | 0.50 |
| 1:P:530:MET:HG2 | 4:1:354:GLN:HB2 | 0.57 | 0.50 |
| 1:P:549:SER:CA | 4:3:47:MET:O | 2.59 | 0.50 |
| 4:1:205:GLU:CD | 4:Y:287:ILE:O | 2.48 | 0.50 |
| 1:A:109:ARG:HD3 | 1:A:117:THR:HB | 1.92 | 0.50 |
| 2:B:121:LEU:HA | 2:B:128:PHE:CD2 | 2.46 | 0.50 |
| 1:D:267:THR:HG21 | 1:D:438:PHE:HE2 | 1.76 | 0.50 |
| 1:D:429:LEU:O | 1:D:433:VAL:HG23 | 2.11 | 0.50 |
| 1:G:13:ALA:C | 1:G:15:PRO:HD2 | 2.31 | 0.50 |
| 1:J:732:ILE:H | 1:J:733:PRO:CD | 2.23 | 0.50 |
| 1:J:789:ALA:HB2 | 3:L:81:GLN:OE1 | 2.11 | 0.50 |
| 2:K:121:LEU:HA | 2:K:128:PHE:CD2 | 2.47 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:13:ALA:C | 1:M:15:PRO:HD2 | 2.31 | 0.50 |
| 1:M:38:VAL:CG1 | 1:M:39:PHE:N | 2.74 | 0.50 |
| 1:M:248:MLY:N | 1:M:463:ASP:O | 2.44 | 0.50 |
| 1:M:429:LEU:O | 1:M:433:VAL:HG23 | 2.12 | 0.50 |
| 1:M:640:LYS:C | 4:Z:23:GLY:CA | 2.64 | 0.50 |
| 1:M:793:ARG:NH1 | 3:O:40:ASN:HD21 | 2.01 | 0.50 |
| 1:P:836:PHE:CZ | 2:Q:159:HIS:HA | 2.26 | 0.50 |
| 2:Q:121:LEU:HA | 2:Q:128:PHE:CD2 | 2.47 | 0.50 |
| 1:A:202:SER:HB2 | 1:A:207:LYS:NZ | 2.26 | 0.50 |
| 1:A:546:THR:CG2 | 1:A:548:THR:HB | 2.41 | 0.50 |
| 1:A:640:LYS:CA | 1:A:645:SER:OG | 2.59 | 0.50 |
| 1:D:232:PHE:CE1 | 1:D:287:ILE:HD13 | 2.45 | 0.50 |
| 1:D:418:THR:O | 1:D:422:VAL:HG23 | 2.11 | 0.50 |
| 1:D:732:ILE:O | 1:D:736:GLN:HG3 | 2.11 | 0.50 |
| 1:D:800:ARG:HB3 | 3:F:149:VAL:CG1 | 2.41 | 0.50 |
| 1:G:38:VAL:CG1 | 1:G:39:PHE:N | 2.74 | 0.50 |
| 1:G:471:ASP:HB3 | 1:G:573:GLY:O | 2.12 | 0.50 |
| 1:G:538:GLU:OE1 | 4:V:351:THR:HB | 2.12 | 0.50 |
| 1:J:411:GLU:H | 4:W:333:PRO:CG | 2.24 | 0.50 |
| 1:J:795:ARG:CD | 3:L:43:ASN:H | 2.25 | 0.50 |
| 1:J:817:GLN:HG2 | 2:K:127:ARG:CD | 2.20 | 0.50 |
| 1:M:154:HIS:CD2 | 1:M:155:ILE:H | 2.30 | 0.50 |
| 1:M:471:ASP:HB3 | 1:M:573:GLY:O | 2.12 | 0.50 |
| 1:M:530:MET:HE3 | 4:Z:355:MET:SD | 2.51 | 0.50 |
| 1:M:724:TYR:CE1 | 1:M:772:LEU:HG | 2.44 | 0.50 |
| 1:P:195:TYR:CE2 | 1:P:199:ILE:CD1 | 2.93 | 0.50 |
| 1:P:629:GLU:CB | 1:P:645:SER:N | 2.74 | 0.50 |
| 1:P:757:GLN:HB2 | 1:P:772:LEU:HD11 | 1.94 | 0.50 |
| 4:1:205:GLU:OE1 | 4:Y:287:ILE:C | 2.49 | 0.50 |
| 1:A:22:LYS:O | 1:A:26:GLU:N | 2.30 | 0.50 |
| 1:A:38:VAL:CG1 | 1:A:39:PHE:N | 2.74 | 0.50 |
| 1:A:169:ASP:OD1 | 1:A:169:ASP:N | 2.44 | 0.50 |
| 1:A:707:CYS:SG | 1:A:714:ARG:NH1 | 2.85 | 0.50 |
| 1:D:237:THR:O | 1:D:240:ASN:O | 2.29 | 0.50 |
| 1:G:169:ASP:N | 1:G:169:ASP:OD1 | 2.44 | 0.50 |
| 1:G:546:THR:CG2 | 1:G:548:THR:HB | 2.41 | 0.50 |
| 1:G:675:ILE:CG2 | 1:G:676:ILE:N | 2.74 | 0.50 |
| 1:G:733:PRO:CA | 1:G:737:PHE:CE1 | 2.95 | 0.50 |
| 1:G:792:ALA:N | 3:I:42:THR:HG22 | 2.26 | 0.50 |
| 1:G:816:ILE:HD11 | 2:H:100:ALA:CB | 2.41 | 0.50 |
| 1:J:291:ILE:HA | 1:J:331:LEU:CD1 | 2.39 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:310:TYR:CE2 | 1:J:320:ILE:CD1 | 2.94 | 0.50 |
| 1:J:346:ASP:O | 1:J:349:THR:HB | 2.12 | 0.50 |
| 1:J:471:ASP:HB3 | 1:J:573:GLY:O | 2.12 | 0.50 |
| 2:K:114:LYS:N | 2:K:146:GLY:O | 2.40 | 0.50 |
| 1:M:202:SER:HB2 | 1:M:207:LYS:NZ | 2.26 | 0.50 |
| 1:M:311:ASP:HB2 | 1:M:312:TYR:CE1 | 2.46 | 0.50 |
| 1:M:400:ALA:HB1 | 1:M:606:THR:HG22 | 1.93 | 0.50 |
| 1:M:559:LEU:HD23 | 1:M:559:LEU:C | 2.31 | 0.50 |
| 1:M:715:VAL:O | 1:M:764:MLY:HB3 | 2.12 | 0.50 |
| 1:M:742:LYS:O | 1:M:745:GLU:HB2 | 2.10 | 0.50 |
| 1:M:795:ARG:NE | 3:O:116:GLU:HB3 | 2.26 | 0.50 |
| 1:P:154:HIS:CD2 | 1:P:155:ILE:H | 2.30 | 0.50 |
| 1:P:757:GLN:HG3 | 1:P:772:LEU:CD1 | 2.42 | 0.50 |
| 1:A:251:ARG:O | 1:A:263:ALA:HA | 2.12 | 0.50 |
| 1:A:754:ASP:H | 1:A:775:LEU:CD1 | 2.25 | 0.50 |
| 1:D:346:ASP:O | 1:D:349:THR:HB | 2.11 | 0.50 |
| 1:D:687:GLU:O | 1:D:691:VAL:HG23 | 2.11 | 0.50 |
| 1:D:715:VAL:O | 1:D:764:MLY:HB3 | 2.12 | 0.50 |
| 1:G:154:HIS:CD2 | 1:G:155:ILE:H | 2.30 | 0.50 |
| 1:G:291:ILE:HA | 1:G:331:LEU:CD1 | 2.39 | 0.50 |
| 1:G:687:GLU:O | 1:G:691:VAL:HG23 | 2.11 | 0.50 |
| 1:J:93:MET:SD | 1:J:716:LEU:HB2 | 2.52 | 0.50 |
| 1:J:409:GLY:N | 1:J:636:LYS:CD | 2.70 | 0.50 |
| 1:J:642:LYS:HG2 | 4:W:21:PHE:C | 2.30 | 0.50 |
| 1:J:733:PRO:CA | 1:J:737:PHE:CE1 | 2.94 | 0.50 |
| 1:M:411:GLU:H | 4:Z:333:PRO:CG | 2.24 | 0.50 |
| 1:M:631:GLU:C | 4:Z:25:ASP:HB2 | 2.32 | 0.50 |
| 1:P:22:LYS:O | 1:P:26:GLU:N | 2.29 | 0.50 |
| 1:P:217:THR:C | 1:P:221:GLN:NE2 | 2.62 | 0.50 |
| 1:P:646:PHE:HE2 | 1:P:652:LEU:CG | 2.25 | 0.50 |
| 2:Q:121:LEU:O | 2:Q:128:PHE:CG | 2.61 | 0.50 |
| 4:X:318:THR:HA | 4:X:327:ILE:HG12 | 1.94 | 0.50 |
| 1:A:154:HIS:CD2 | 1:A:155:ILE:H | 2.30 | 0.50 |
| 1:A:214:MET:HA | 1:A:340:ILE:CD1 | 2.42 | 0.50 |
| 1:A:267:THR:HG21 | 1:A:438:PHE:HE2 | 1.76 | 0.50 |
| 1:A:715:VAL:O | 1:A:764:MLY:HB3 | 2.12 | 0.50 |
| 2:B:140:PHE:HB3 | 2:B:144:VAL:HG12 | 1.94 | 0.50 |
| 1:D:218:LEU:N | 1:D:221:GLN:CG | 2.74 | 0.50 |
| 1:D:411:GLU:H | 4:9:333:PRO:CG | 2.24 | 0.50 |
| 1:D:712:PRO:HB2 | 1:D:771:LEU:CD2 | 2.42 | 0.50 |
| 1:G:804:ARG:NH2 | 3:I:149:VAL:HG23 | 2.27 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:J:218:LEU:N | 1:J:221:GLN:CG | 2.74 | 0.50 |
| 1:J:601:ASP:N | 1:J:602:PRO:CD | 2.75 | 0.50 |
| 1:J:642:LYS:HA | 4:W:22:ALA:C | 2.33 | 0.50 |
| 3:L:46:ILE:O | 3:L:50:LEU:CG | 2.47 | 0.50 |
| 1:M:267:THR:HG21 | 1:M:438:PHE:HE2 | 1.76 | 0.50 |
| 1:M:291:ILE:HA | 1:M:331:LEU:CD1 | 2.39 | 0.50 |
| 1:M:538:GLU:HA | 4:Z:349:LEU:CB | 2.40 | 0.50 |
| 1:P:169:ASP:N | 1:P:169:ASP:OD1 | 2.44 | 0.50 |
| 1:P:251:ARG:O | 1:P:263:ALA:HA | 2.12 | 0.50 |
| 1:P:278:GLN:HG3 | 1:P:318:GLY:H | 1.76 | 0.50 |
| 1:P:642:LYS:HG2 | 4:1:21:PHE:C | 2.30 | 0.50 |
| 1:P:839:MLY:HB2 | 1:P:840:PRO:HD3 | 1.94 | 0.50 |
| 4:2:287:ILE:CA | 4:4:202:THR:HB | 2.35 | 0.50 |
| 4:4:287:ILE:CG2 | 4:6:204:ALA:N | 2.68 | 0.50 |
| 1:A:149:GLN:CD | 1:A:716:LEU:CD2 | 2.49 | 0.49 |
| 1:A:311:ASP:HB2 | 1:A:312:TYR:CE1 | 2.46 | 0.49 |
| 1:A:346:ASP:O | 1:A:349:THR:HB | 2.11 | 0.49 |
| 1:A:498:LEU:CD2 | 1:A:764:MLY:CH2 | 2.71 | 0.49 |
| 1:A:799:MET:HE1 | 3:C:32:ASP:HB3 | 1.81 | 0.49 |
| 1:D:538:GLU:OE1 | 4:9:351:THR:HB | 2.12 | 0.49 |
| 1:D:823:PHE:CD1 | 2:E:160:GLY:HA2 | 2.44 | 0.49 |
| 1:G:530:MET:HG2 | 4:V:354:GLN:HB2 | 0.57 | 0.49 |
| 1:G:553:MLY:O | 4:X:46:GLY:HA3 | 2.12 | 0.49 |
| 1:G:642:LYS:CG | 4:V:22:ALA:HA | 2.37 | 0.49 |
| 1:J:646:PHE:CE2 | 1:J:652:LEU:CD2 | 2.87 | 0.49 |
| 1:J:818:TYR:CZ | 2:K:127:ARG:NH1 | 2.80 | 0.49 |
| 1:M:176:LEU:N | 1:M:176:LEU:CD1 | 2.75 | 0.49 |
| 1:M:346:ASP:O | 1:M:349:THR:HB | 2.12 | 0.49 |
| 1:M:408:VAL:CG1 | 4:Z:332:PRO:HB3 | 2.40 | 0.49 |
| 1:M:546:THR:CG2 | 1:M:548:THR:HB | 2.41 | 0.49 |
| 1:M:646:PHE:HE2 | 1:M:652:LEU:CG | 2.25 | 0.49 |
| 1:P:13:ALA:C | 1:P:15:PRO:HD2 | 2.32 | 0.49 |
| 1:P:795:ARG:HB2 | 3:R:35:ARG:CZ | 2.34 | 0.49 |
| 4:5:70:PRO:HG3 | 4:5:81:ASP:HB3 | 1.94 | 0.49 |
| 4:X:287:ILE:HD13 | 4:Z:205:GLU:HB2 | 1.93 | 0.49 |
| 1:A:411:GLU:H | 4:8:333:PRO:CG | 2.24 | 0.49 |
| 1:A:547:ASP:O | 1:A:550:PHE:HB3 | 2.12 | 0.49 |
| 1:A:739:ASP:CB | 1:A:742:LYS:CB | 2.81 | 0.49 |
| 1:A:819:ASN:OD1 | 2:B:92:ASP:N | 2.39 | 0.49 |
| 1:D:20:SER:HB3 | 1:D:23:GLU:OE1 | 2.13 | 0.49 |
| 1:D:97:LEU:HD13 | 1:D:97:LEU:N | 2.27 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:642:LYS:CB | 4:9:24:ASP:O | 2.60 | 0.49 |
| 2:E:112:ILE:HG23 | 2:E:147:ASN:HB3 | 1.92 | 0.49 |
| 1:G:601:ASP:N | 1:G:602:PRO:CD | 2.75 | 0.49 |
| 1:G:818:TYR:HE1 | 2:H:127:ARG:NH2 | 1.95 | 0.49 |
| 1:J:675:ILE:CG2 | 1:J:676:ILE:N | 2.74 | 0.49 |
| 1:J:839:MLY:N | 1:J:840:PRO:CD | 2.75 | 0.49 |
| 1:M:192:VAL:O | 1:M:195:TYR:HB3 | 2.12 | 0.49 |
| 1:M:251:ARG:O | 1:M:263:ALA:HA | 2.12 | 0.49 |
| 1:M:601:ASP:N | 1:M:602:PRO:CD | 2.75 | 0.49 |
| 1:P:429:LEU:O | 1:P:433:VAL:HG23 | 2.12 | 0.49 |
| 1:P:732:ILE:HG23 | 1:P:747:LEU:CD1 | 1.04 | 0.49 |
| 1:P:739:ASP:OD1 | 1:P:740:SER:N | 2.45 | 0.49 |
| 4:W:285:CYS:O | 4:Y:202:THR:HG22 | 2.12 | 0.49 |
| 4:Z:318:THR:HA | 4:Z:327:ILE:HG12 | 1.95 | 0.49 |
| 1:A:799:MET:SD | 3:C:32:ASP:CG | 2.89 | 0.49 |
| 1:D:154:HIS:CD2 | 1:D:155:ILE:H | 2.30 | 0.49 |
| 1:D:507:GLY:CA | 1:D:762:HIS:CD2 | 2.94 | 0.49 |
| 1:D:547:ASP:O | 1:D:550:PHE:HB3 | 2.12 | 0.49 |
| 1:D:831:TRP:CE2 | 2:E:51:PHE:CE2 | 3.00 | 0.49 |
| 2:E:140:PHE:HB3 | 2:E:144:VAL:HG12 | 1.94 | 0.49 |
| 1:G:547:ASP:O | 1:G:550:PHE:HB3 | 2.12 | 0.49 |
| 1:G:595:TRP:N | 1:G:595:TRP:CD1 | 2.80 | 0.49 |
| 1:G:715:VAL:O | 1:G:764:MLY:HB3 | 2.12 | 0.49 |
| 1:G:792:ALA:HB1 | 3:I:42:THR:HA | 1.92 | 0.49 |
| 1:G:797:PHE:HE2 | 3:I:126:LEU:CD2 | 2.05 | 0.49 |
| 1:G:834:LEU:CD2 | 2:H:34:ILE:CG1 | 2.90 | 0.49 |
| 2:H:149:ASP:CG | 2:H:150:TYR:N | 2.49 | 0.49 |
| 1:J:290:GLN:HG2 | 1:J:331:LEU:CA | 2.43 | 0.49 |
| 1:J:418:THR:CB | 1:J:421:GLU:HG3 | 2.37 | 0.49 |
| 1:J:576:GLU:CG | 1:J:577:ALA:N | 2.44 | 0.49 |
| 1:J:756:THR:O | 1:J:758:TYR:N | 2.45 | 0.49 |
| 2:K:112:ILE:HG23 | 2:K:147:ASN:HB3 | 1.93 | 0.49 |
| 1:M:169:ASP:N | 1:M:169:ASP:OD1 | 2.44 | 0.49 |
| 1:M:538:GLU:OE1 | 4:Z:351:THR:HB | 2.12 | 0.49 |
| 1:M:756:THR:O | 1:M:758:TYR:N | 2.46 | 0.49 |
| 1:M:839:MLY:HB2 | 1:M:840:PRO:HD3 | 1.95 | 0.49 |
| 2:N:93:PRO:O | 2:N:97:ILE:HG13 | 2.13 | 0.49 |
| 1:P:290:GLN:HG2 | 1:P:331:LEU:CA | 2.43 | 0.49 |
| 1:P:470:PHE:O | 1:P:473:ASN:ND2 | 2.40 | 0.49 |
| 1:P:543:PRO:CD | 4:1:146:GLY:O | 2.60 | 0.49 |
| 1:P:640:LYS:C | 4:1:23:GLY:CA | 2.64 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:P:675:ILE:CG2 | 1:P:676:ILE:N | 2.74 | 0.49 |
| 1:P:839:MLY:N | 1:P:840:PRO:CD | 2.75 | 0.49 |
| 4:1:201:VAL:HG23 | 4:Y:287:ILE:CB | 2.42 | 0.49 |
| 4:1:318:THR:HA | 4:1:327:ILE:HG12 | 1.95 | 0.49 |
| 4:2:318:THR:HA | 4:2:327:ILE:HG12 | 1.94 | 0.49 |
| 4:4:70:PRO:HG3 | 4:4:81:ASP:HB3 | 1.94 | 0.49 |
| 4:7:318:THR:HA | 4:7:327:ILE:HG12 | 1.94 | 0.49 |
| 4:9:70:PRO:HG3 | 4:9:81:ASP:HB3 | 1.94 | 0.49 |
| 1:A:471:ASP:HB3 | 1:A:573:GLY:O | 2.12 | 0.49 |
| 1:A:538:GLU:OE1 | 4:8:351:THR:HB | 2.12 | 0.49 |
| 1:A:735:GLY:O | 1:A:743:ALA:HA | 1.94 | 0.49 |
| 1:A:817:GLN:OE1 | 2:B:127:ARG:CZ | 2.27 | 0.49 |
| 1:D:128:PRO:O | 1:D:683:PRO:HB3 | 2.12 | 0.49 |
| 1:D:471:ASP:HB3 | 1:D:573:GLY:O | 2.12 | 0.49 |
| 1:D:724:TYR:HA | 1:D:782:MLY:CE | 2.42 | 0.49 |
| 2:E:121:LEU:O | 2:E:128:PHE:CG | 2.61 | 0.49 |
| 1:G:217:THR:C | 1:G:221:GLN:NE2 | 2.62 | 0.49 |
| 1:G:251:ARG:O | 1:G:263:ALA:HA | 2.13 | 0.49 |
| 1:G:429:LEU:O | 1:G:433:VAL:HG23 | 2.12 | 0.49 |
| 1:J:217:THR:C | 1:J:221:GLN:NE2 | 2.62 | 0.49 |
| 1:J:530:MET:HG2 | 4:W:354:GLN:HB2 | 0.57 | 0.49 |
| 1:J:732:ILE:O | 1:J:736:GLN:HG3 | 2.12 | 0.49 |
| 3:L:100:GLY:O | 3:L:138:ASN:HA | 2.11 | 0.49 |
| 1:M:547:ASP:O | 1:M:550:PHE:HB3 | 2.12 | 0.49 |
| 1:M:592:ILE:HG22 | 1:M:592:ILE:O | 2.11 | 0.49 |
| 1:M:642:LYS:HA | 4:Z:22:ALA:C | 2.33 | 0.49 |
| 2:N:112:ILE:HG23 | 2:N:147:ASN:HB3 | 1.93 | 0.49 |
| 1:P:149:GLN:HB3 | 1:P:716:LEU:CD1 | 2.43 | 0.49 |
| 1:P:218:LEU:CD2 | 1:P:222:ILE:CG1 | 2.86 | 0.49 |
| 1:P:346:ASP:O | 1:P:349:THR:HB | 2.12 | 0.49 |
| 2:Q:117:LEU:CB | 2:Q:147:ASN:ND2 | 2.35 | 0.49 |
| 4:2:203:THR:CB | 4:Z:287:ILE:CB | 2.83 | 0.49 |
| 4:3:318:THR:HA | 4:3:327:ILE:HG12 | 1.95 | 0.49 |
| 4:6:124:PHE:CZ | 4:6:132:MET:HG3 | 2.48 | 0.49 |
| 4:8:318:THR:HA | 4:8:327:ILE:HG12 | 1.95 | 0.49 |
| 4:9:318:THR:HA | 4:9:327:ILE:HG12 | 1.95 | 0.49 |
| 4:V:318:THR:HA | 4:V:327:ILE:HG12 | 1.94 | 0.49 |
| 4:W:318:THR:HA | 4:W:327:ILE:HG12 | 1.95 | 0.49 |
| 1:A:237:THR:HG22 | 1:A:238:VAL:N | 2.28 | 0.49 |
| 1:A:715:VAL:HG12 | 1:A:716:LEU:O | 2.13 | 0.49 |
| 1:A:739:ASP:OD1 | 1:A:740:SER:N | 2.45 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:93:PRO:O | 2:B:97:ILE:HG13 | 2.13 | 0.49 |
| 1:D:215:GLN:H | 1:D:340:ILE:CD1 | 2.20 | 0.49 |
| 1:D:332:MET:O | 1:D:336:SER:OG | 2.27 | 0.49 |
| 1:D:556:ASP:CA | 4:W:49:GLN:O | 2.52 | 0.49 |
| 1:G:408:VAL:CG1 | 4:V:332:PRO:HB3 | 2.41 | 0.49 |
| 1:G:538:GLU:HA | 4:V:351:THR:H | 1.77 | 0.49 |
| 1:G:754:ASP:HB2 | 1:G:776:GLU:CB | 2.41 | 0.49 |
| 1:G:839:MLY:N | 1:G:840:PRO:CD | 2.75 | 0.49 |
| 1:J:93:MET:HG2 | 1:J:715:VAL:CA | 2.30 | 0.49 |
| 1:J:103:LEU:C | 1:J:103:LEU:HD12 | 2.33 | 0.49 |
| 1:J:206:LYS:HD2 | 1:J:217:THR:CG2 | 2.17 | 0.49 |
| 1:J:538:GLU:OE1 | 4:W:351:THR:HB | 2.12 | 0.49 |
| 1:J:739:ASP:OD1 | 1:J:740:SER:N | 2.46 | 0.49 |
| 2:K:93:PRO:O | 2:K:97:ILE:HG13 | 2.13 | 0.49 |
| 1:M:97:LEU:HD13 | 1:M:97:LEU:N | 2.28 | 0.49 |
| 1:M:103:LEU:HD12 | 1:M:103:LEU:C | 2.33 | 0.49 |
| 1:M:629:GLU:CA | 1:M:643:GLY:C | 2.73 | 0.49 |
| 1:M:732:ILE:O | 1:M:736:GLN:HG3 | 2.11 | 0.49 |
| 1:P:793:ARG:NH1 | 3:R:40:ASN:HD21 | 1.94 | 0.49 |
| 1:P:831:TRP:NE1 | 2:Q:67:MET:HB3 | 2.24 | 0.49 |
| 2:Q:112:ILE:HG23 | 2:Q:147:ASN:HB3 | 1.93 | 0.49 |
| 4:4:287:ILE:CB | 4:6:204:ALA:H | 2.24 | 0.49 |
| 4:6:70:PRO:HG3 | 4:6:81:ASP:HB3 | 1.94 | 0.49 |
| 4:7:70:PRO:HG3 | 4:7:81:ASP:HB3 | 1.94 | 0.49 |
| 4:Y:318:THR:HA | 4:Y:327:ILE:HG12 | 1.95 | 0.49 |
| 1:A:543:PRO:CD | 4:8:146:GLY:O | 2.61 | 0.49 |
| 1:A:725:ARG:NE | 1:A:733:PRO:CB | 1.95 | 0.49 |
| 1:D:310:TYR:CE2 | 1:D:320:ILE:CD1 | 2.95 | 0.49 |
| 1:G:237:THR:HG22 | 1:G:238:VAL:N | 2.28 | 0.49 |
| 1:G:543:PRO:CD | 4:V:146:GLY:O | 2.61 | 0.49 |
| 1:G:793:ARG:O | 1:G:797:PHE:N | 2.39 | 0.49 |
| 1:G:817:GLN:HB3 | 2:H:127:ARG:HH11 | 1.77 | 0.49 |
| 2:H:117:LEU:HG | 2:H:147:ASN:HB3 | 1.94 | 0.49 |
| 1:J:128:PRO:O | 1:J:683:PRO:HB3 | 2.12 | 0.49 |
| 1:J:168:THR:HG22 | 1:J:169:ASP:OD1 | 2.12 | 0.49 |
| 1:J:292:MET:HE1 | 1:J:309:PRO:HD3 | 1.94 | 0.49 |
| 1:J:830:PRO:CB | 2:K:67:MET:HE1 | 2.42 | 0.49 |
| 1:M:168:THR:HG22 | 1:M:169:ASP:OD1 | 2.12 | 0.49 |
| 1:M:332:MET:O | 1:M:336:SER:OG | 2.27 | 0.49 |
| 1:M:739:ASP:OD1 | 1:M:740:SER:N | 2.45 | 0.49 |
| 3:O:50:LEU:O | 3:O:55:LYS:HB2 | 2.13 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:Q:139:ALA:C | 2:Q:141:PRO:HD3 | 2.33 | 0.49 |
| 3:R:50:LEU:O | 3:R:55:LYS:HB2 | 2.13 | 0.49 |
| 4:3:290:ARG:NH2 | 4:5:202:THR:HG21 | 1.60 | 0.49 |
| 4:4:124:PHE:CZ | 4:4:132:MET:HG3 | 2.48 | 0.49 |
| 4:5:318:THR:HA | 4:5:327:ILE:HG12 | 1.95 | 0.49 |
| 4:6:318:THR:HA | 4:6:327:ILE:HG12 | 1.94 | 0.49 |
| 4:7:124:PHE:CZ | 4:7:132:MET:HG3 | 2.48 | 0.49 |
| 4:W:124:PHE:CZ | 4:W:132:MET:HG3 | 2.48 | 0.49 |
| 1:A:51:THR:C | 1:A:62:VAL:HG13 | 2.32 | 0.49 |
| 1:A:410:ASN:HD22 | 4:8:336:LYS:HE2 | 1.78 | 0.49 |
| 1:A:502:GLU:O | 1:A:761:GLY:HA2 | 2.12 | 0.49 |
| 1:A:752:ASP:O | 1:A:778:MET:CB | 2.60 | 0.49 |
| 2:B:128:PHE:O | 2:B:133:ILE:HD11 | 2.13 | 0.49 |
| 1:D:291:ILE:HA | 1:D:331:LEU:CD1 | 2.40 | 0.49 |
| 1:D:530:MET:HG2 | 4:9:354:GLN:HB2 | 0.57 | 0.49 |
| 1:D:629:GLU:CA | 1:D:643:GLY:C | 2.73 | 0.49 |
| 1:D:642:LYS:HG2 | 4:9:21:PHE:C | 2.30 | 0.49 |
| 1:D:839:MLY:N | 1:D:840:PRO:CD | 2.75 | 0.49 |
| 1:G:311:ASP:HB2 | 1:G:312:TYR:CE1 | 2.46 | 0.49 |
| 1:G:732:ILE:O | 1:G:736:GLN:HG3 | 2.12 | 0.49 |
| 1:G:769:ALA:HB3 | 1:G:770:GLY:N | 2.04 | 0.49 |
| 1:J:192:VAL:O | 1:J:195:TYR:HB3 | 2.13 | 0.49 |
| 1:J:543:PRO:CD | 4:W:146:GLY:O | 2.61 | 0.49 |
| 1:J:715:VAL:O | 1:J:764:MLY:HB3 | 2.12 | 0.49 |
| 1:M:831:TRP:NE1 | 2:N:67:MET:HB3 | 2.25 | 0.49 |
| 1:P:64:THR:CG2 | 1:P:65:GLU:N | 2.75 | 0.49 |
| 1:P:471:ASP:HB3 | 1:P:573:GLY:O | 2.12 | 0.49 |
| 1:P:805:ALA:C | 1:P:807:VAL:N | 2.65 | 0.49 |
| 4:7:253:GLU:HA | 4:7:256:ARG:CG | 2.42 | 0.49 |
| 4:9:124:PHE:CZ | 4:9:132:MET:HG3 | 2.48 | 0.49 |
| 4:V:253:GLU:HA | 4:V:256:ARG:CG | 2.42 | 0.49 |
| 4:W:70:PRO:HG3 | 4:W:81:ASP:HB3 | 1.94 | 0.49 |
| 4:Z:70:PRO:HG3 | 4:Z:81:ASP:HB3 | 1.94 | 0.49 |
| 1:A:97:LEU:HD13 | 1:A:97:LEU:N | 2.28 | 0.49 |
| 1:A:502:GLU:O | 1:A:761:GLY:CA | 2.61 | 0.49 |
| 1:A:642:LYS:CG | 4:8:22:ALA:HA | 2.38 | 0.49 |
| 1:A:813:ILE:CG2 | 2:B:127:ARG:CB | 2.91 | 0.49 |
| 1:D:173:GLN:OE1 | 1:D:668:HIS:HB3 | 2.13 | 0.49 |
| 1:D:278:GLN:HG3 | 1:D:318:GLY:H | 1.75 | 0.49 |
| 1:D:637:LYS:HD2 | 4:9:144:ALA:HB3 | 1.21 | 0.49 |
| 3:I:50:LEU:O | 3:I:55:LYS:HB2 | 2.13 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:251:ARG:HB2 | 1:M:264:ASP:HB3 | 1.95 | 0.49 |
| 1:M:839:MLY:N | 1:M:840:PRO:CD | 2.75 | 0.49 |
| 1:P:192:VAL:O | 1:P:195:TYR:HB3 | 2.13 | 0.49 |
| 1:P:601:ASP:N | 1:P:602:PRO:CD | 2.75 | 0.49 |
| 1:P:642:LYS:HA | 4:1:22:ALA:C | 2.33 | 0.49 |
| 1:P:649:VAL:HA | 1:P:649:VAL:HG23 | 1.83 | 0.49 |
| 4:2:124:PHE:CZ | 4:2:132:MET:HG3 | 2.48 | 0.49 |
| 1:A:128:PRO:O | 1:A:683:PRO:HB3 | 2.12 | 0.49 |
| 1:A:173:GLN:OE1 | 1:A:668:HIS:HB3 | 2.13 | 0.49 |
| 1:A:601:ASP:N | 1:A:602:PRO:CD | 2.75 | 0.49 |
| 1:A:720:PHE:CD2 | 1:A:744:SER:HB3 | 2.48 | 0.49 |
| 1:A:836:PHE:CE2 | 2:B:160:GLY:O | 2.66 | 0.49 |
| 1:D:41:VAL:CG1 | 1:D:42:HIS:N | 2.75 | 0.49 |
| 1:D:251:ARG:O | 1:D:263:ALA:HA | 2.12 | 0.49 |
| 1:D:312:TYR:N | 1:D:312:TYR:CD1 | 2.80 | 0.49 |
| 1:D:601:ASP:N | 1:D:602:PRO:CD | 2.75 | 0.49 |
| 1:D:813:ILE:HG21 | 2:E:128:PHE:HE1 | 1.76 | 0.49 |
| 3:F:50:LEU:O | 3:F:55:LYS:HB2 | 2.13 | 0.49 |
| 1:G:64:THR:CG2 | 1:G:65:GLU:N | 2.76 | 0.49 |
| 1:G:97:LEU:HD13 | 1:G:97:LEU:N | 2.28 | 0.49 |
| 1:G:757:GLN:HB2 | 1:G:776:GLU:CG | 2.39 | 0.49 |
| 2:H:114:LYS:HG3 | 2:H:137:TRP:CZ2 | 2.48 | 0.49 |
| 2:H:121:LEU:HA | 2:H:128:PHE:CD2 | 2.47 | 0.49 |
| 1:J:64:THR:CG2 | 1:J:65:GLU:N | 2.75 | 0.49 |
| 1:J:214:MET:HA | 1:J:340:ILE:CD1 | 2.41 | 0.49 |
| 1:J:547:ASP:O | 1:J:550:PHE:HB3 | 2.12 | 0.49 |
| 1:J:640:LYS:C | 4:W:23:GLY:CA | 2.64 | 0.49 |
| 1:J:739:ASP:CB | 1:J:742:LYS:CB | 2.81 | 0.49 |
| 1:J:754:ASP:HB3 | 1:J:780:ASP:OD2 | 2.07 | 0.49 |
| 2:K:114:LYS:HG3 | 2:K:137:TRP:CZ2 | 2.48 | 0.49 |
| 1:M:206:LYS:CE | 1:M:217:THR:HG23 | 2.29 | 0.49 |
| 1:M:405:ARG:HB2 | 1:M:414:THR:OG1 | 2.13 | 0.49 |
| 1:M:418:THR:CB | 1:M:421:GLU:HG3 | 2.37 | 0.49 |
| 1:M:543:PRO:CD | 4:Z:146:GLY:O | 2.61 | 0.49 |
| 1:P:332:MET:O | 1:P:336:SER:OG | 2.27 | 0.49 |
| 1:P:405:ARG:HB2 | 1:P:414:THR:OG1 | 2.13 | 0.49 |
| 1:P:791:GLN:HE22 | 3:R:116:GLU:N | 2.10 | 0.49 |
| 2:Q:117:LEU:HG | 2:Q:147:ASN:HB3 | 1.93 | 0.49 |
| 4:4:213:LYS:O | 4:4:217:CYS:HB2 | 2.13 | 0.49 |
| 4:4:318:THR:HA | 4:4:327:ILE:HG12 | 1.94 | 0.49 |
| 1:A:20:SER:HB3 | 1:A:23:GLU:OE1 | 2.13 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:192:VAL:O | 1:A:195:TYR:HB3 | 2.13 | 0.49 |
| 1:A:290:GLN:HG2 | 1:A:331:LEU:CA | 2.43 | 0.49 |
| 1:A:757:GLN:O | 1:A:771:LEU:HD22 | 2.12 | 0.49 |
| 1:A:839:MLY:N | 1:A:840:PRO:CD | 2.75 | 0.49 |
| 1:D:51:THR:C | 1:D:62:VAL:HG13 | 2.32 | 0.49 |
| 1:D:64:THR:CG2 | 1:D:65:GLU:N | 2.75 | 0.49 |
| 1:D:168:THR:HG22 | 1:D:169:ASP:OD1 | 2.12 | 0.49 |
| 2:E:114:LYS:HG3 | 2:E:137:TRP:CZ2 | 2.48 | 0.49 |
| 1:G:51:THR:C | 1:G:62:VAL:HG13 | 2.32 | 0.49 |
| 1:G:192:VAL:O | 1:G:195:TYR:HB3 | 2.13 | 0.49 |
| 1:G:332:MET:O | 1:G:336:SER:OG | 2.27 | 0.49 |
| 1:G:739:ASP:OD1 | 1:G:740:SER:N | 2.45 | 0.49 |
| 2:H:140:PHE:HB3 | 2:H:144:VAL:HG12 | 1.94 | 0.49 |
| 1:J:20:SER:HB3 | 1:J:23:GLU:OE1 | 2.13 | 0.49 |
| 1:J:154:HIS:CD2 | 1:J:155:ILE:H | 2.30 | 0.49 |
| 1:J:715:VAL:HG12 | 1:J:716:LEU:O | 2.12 | 0.49 |
| 2:K:121:LEU:O | 2:K:128:PHE:CG | 2.61 | 0.49 |
| 2:K:140:PHE:HB3 | 2:K:144:VAL:HG12 | 1.94 | 0.49 |
| 1:M:64:THR:CG2 | 1:M:65:GLU:N | 2.75 | 0.49 |
| 1:M:173:GLN:OE1 | 1:M:668:HIS:HB3 | 2.13 | 0.49 |
| 1:M:715:VAL:HG12 | 1:M:716:LEU:O | 2.13 | 0.49 |
| 1:M:720:PHE:CD2 | 1:M:744:SER:HB3 | 2.48 | 0.49 |
| 2:N:140:PHE:HB3 | 2:N:144:VAL:HG12 | 1.94 | 0.49 |
| 1:P:168:THR:HG22 | 1:P:169:ASP:OD1 | 2.12 | 0.49 |
| 1:P:499:GLU:OE1 | 1:P:499:GLU:HA | 2.13 | 0.49 |
| 1:P:538:GLU:HA | 4:1:351:THR:H | 1.77 | 0.49 |
| 1:P:547:ASP:O | 1:P:550:PHE:HB3 | 2.12 | 0.49 |
| 1:P:715:VAL:O | 1:P:764:MLY:HB3 | 2.12 | 0.49 |
| 1:P:732:ILE:O | 1:P:736:GLN:HG3 | 2.12 | 0.49 |
| 1:P:756:THR:O | 1:P:758:TYR:N | 2.45 | 0.49 |
| 2:Q:114:LYS:HG3 | 2:Q:137:TRP:CZ2 | 2.48 | 0.49 |
| 4:1:287:ILE:CB | 4:3:203:THR:CB | 2.85 | 0.49 |
| 4:2:70:PRO:HG3 | 4:2:81:ASP:HB3 | 1.94 | 0.49 |
| 4:2:148:THR:OG1 | 4:4:45:VAL:CG2 | 2.61 | 0.49 |
| 4:3:70:PRO:HG3 | 4:3:81:ASP:HB3 | 1.94 | 0.49 |
| 4:Y:70:PRO:HG3 | 4:Y:81:ASP:HB3 | 1.94 | 0.49 |
| 4:Y:124:PHE:CZ | 4:Y:132:MET:HG3 | 2.48 | 0.49 |
| 1:A:251:ARG:HB2 | 1:A:264:ASP:HB3 | 1.95 | 0.48 |
| 1:A:405:ARG:HB2 | 1:A:414:THR:OG1 | 2.13 | 0.48 |
| 1:D:192:VAL:O | 1:D:195:TYR:HB3 | 2.13 | 0.48 |
| 1:D:290:GLN:HG2 | 1:D:331:LEU:CA | 2.43 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:507:GLY:C | 1:D:762:HIS:N | 2.65 | 0.48 |
| 1:D:543:PRO:CD | 4:9:146:GLY:O | 2.61 | 0.48 |
| 1:D:715:VAL:HG12 | 1:D:716:LEU:O | 2.12 | 0.48 |
| 1:D:739:ASP:OD1 | 1:D:740:SER:N | 2.45 | 0.48 |
| 1:D:756:THR:O | 1:D:758:TYR:N | 2.45 | 0.48 |
| 1:D:767:PHE:O | 1:D:771:LEU:HD21 | 2.13 | 0.48 |
| 2:E:163:ALA:C | 2:K:21:GLU:HB3 | 2.33 | 0.48 |
| 1:G:103:LEU:C | 1:G:103:LEU:HD12 | 2.33 | 0.48 |
| 1:G:290:GLN:HG2 | 1:G:331:LEU:CA | 2.43 | 0.48 |
| 1:G:405:ARG:HB2 | 1:G:414:THR:OG1 | 2.13 | 0.48 |
| 1:G:410:ASN:HD22 | 4:V:336:LYS:HE2 | 1.78 | 0.48 |
| 1:G:732:ILE:HG23 | 1:G:747:LEU:HD12 | 0.94 | 0.48 |
| 1:G:756:THR:O | 1:G:758:TYR:N | 2.46 | 0.48 |
| 1:J:798:LEU:HD12 | 1:J:798:LEU:HA | 1.36 | 0.48 |
| 1:M:128:PRO:O | 1:M:683:PRO:HB3 | 2.12 | 0.48 |
| 1:M:595:TRP:N | 1:M:595:TRP:CD1 | 2.80 | 0.48 |
| 1:P:20:SER:HB3 | 1:P:23:GLU:OE1 | 2.13 | 0.48 |
| 1:P:97:LEU:HD21 | 1:P:712:PRO:CA | 2.42 | 0.48 |
| 1:P:292:MET:HE1 | 1:P:309:PRO:HD3 | 1.95 | 0.48 |
| 1:P:409:GLY:N | 1:P:636:LYS:CD | 2.70 | 0.48 |
| 1:P:701:LEU:HD12 | 1:P:701:LEU:HA | 1.55 | 0.48 |
| 2:Q:93:PRO:O | 2:Q:97:ILE:HG13 | 2.13 | 0.48 |
| 4:1:124:PHE:CZ | 4:1:132:MET:HG3 | 2.48 | 0.48 |
| 4:3:124:PHE:CZ | 4:3:132:MET:HG3 | 2.48 | 0.48 |
| 4:8:198:TYR:CZ | 4:8:248:ILE:HG13 | 2.48 | 0.48 |
| 4:9:198:TYR:CZ | 4:9:248:ILE:HG13 | 2.48 | 0.48 |
| 4:W:198:TYR:CZ | 4:W:248:ILE:HG13 | 2.48 | 0.48 |
| 4:X:70:PRO:HG3 | 4:X:81:ASP:HB3 | 1.94 | 0.48 |
| 1:A:732:ILE:HG21 | 1:A:747:LEU:CD1 | 0.64 | 0.48 |
| 1:A:836:PHE:CE1 | 2:B:159:HIS:HA | 2.49 | 0.48 |
| 2:B:114:LYS:HG3 | 2:B:137:TRP:CZ2 | 2.48 | 0.48 |
| 2:B:117:LEU:HG | 2:B:147:ASN:HB3 | 1.93 | 0.48 |
| 1:D:103:LEU:C | 1:D:103:LEU:HD12 | 2.33 | 0.48 |
| 1:G:20:SER:HB3 | 1:G:23:GLU:OE1 | 2.12 | 0.48 |
| 1:G:251:ARG:HB2 | 1:G:264:ASP:HB3 | 1.95 | 0.48 |
| 1:G:267:THR:HG21 | 1:G:438:PHE:HE2 | 1.77 | 0.48 |
| 1:G:715:VAL:HG12 | 1:G:716:LEU:O | 2.13 | 0.48 |
| 1:J:173:GLN:OE1 | 1:J:668:HIS:HB3 | 2.13 | 0.48 |
| 1:J:839:MLY:HB2 | 1:J:840:PRO:HD3 | 1.94 | 0.48 |
| 1:M:538:GLU:HA | 4:Z:351:THR:H | 1.77 | 0.48 |
| 1:P:128:PRO:O | 1:P:683:PRO:HB3 | 2.12 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:P:720:PHE:CD2 | 1:P:744:SER:HB3 | 2.48 | 0.48 |
| 1:P:829:TRP:CZ3 | 2:Q:84:PHE:CE1 | 3.01 | 0.48 |
| 4:1:70:PRO:HG3 | 4:1:81:ASP:HB3 | 1.94 | 0.48 |
| 4:1:198:TYR:CZ | 4:1:248:ILE:HG13 | 2.48 | 0.48 |
| 4:3:198:TYR:CZ | 4:3:248:ILE:HG13 | 2.48 | 0.48 |
| 4:7:198:TYR:CZ | 4:7:248:ILE:HG13 | 2.48 | 0.48 |
| 4:8:70:PRO:HG3 | 4:8:81:ASP:HB3 | 1.94 | 0.48 |
| 4:Y:198:TYR:CZ | 4:Y:248:ILE:HG13 | 2.48 | 0.48 |
| 4:Z:198:TYR:CZ | 4:Z:248:ILE:HG13 | 2.48 | 0.48 |
| 1:A:168:THR:HG22 | 1:A:169:ASP:OD1 | 2.12 | 0.48 |
| 1:A:709:LYS:C | 1:A:710:GLY:N | 2.67 | 0.48 |
| 1:A:723:ARG:HH11 | 1:A:723:ARG:HG3 | 1.78 | 0.48 |
| 1:A:839:MLY:HB2 | 1:A:840:PRO:HD3 | 1.94 | 0.48 |
| 1:D:418:THR:CB | 1:D:421:GLU:HG3 | 2.37 | 0.48 |
| 1:D:839:MLY:HB2 | 1:D:840:PRO:HD3 | 1.94 | 0.48 |
| 1:G:168:THR:HG22 | 1:G:169:ASP:OD1 | 2.12 | 0.48 |
| 1:M:314:TYR:CZ | 1:M:362:GLY:HA2 | 2.48 | 0.48 |
| 1:M:404:PRO:HD2 | 1:M:415:MLY:O | 2.13 | 0.48 |
| 1:M:508:ILE:HD11 | 1:M:766:PHE:CD1 | 2.48 | 0.48 |
| 1:M:530:MET:CE | 4:Z:354:GLN:HG3 | 2.35 | 0.48 |
| 1:M:723:ARG:HH11 | 1:M:723:ARG:HG3 | 1.79 | 0.48 |
| 2:N:114:LYS:HG3 | 2:N:137:TRP:CZ2 | 2.48 | 0.48 |
| 2:N:128:PHE:O | 2:N:133:ILE:HD11 | 2.13 | 0.48 |
| 2:N:130:PRO:O | 2:N:131:GLU:C | 2.52 | 0.48 |
| 1:P:202:SER:HA | 1:P:207:LYS:NZ | 2.22 | 0.48 |
| 1:P:538:GLU:OE1 | 4:1:351:THR:HB | 2.12 | 0.48 |
| 1:P:640:LYS:HB3 | 1:P:645:SER:CB | 2.41 | 0.48 |
| 2:Q:128:PHE:O | 2:Q:133:ILE:HD11 | 2.13 | 0.48 |
| 4:1:173:HIS:CD2 | 4:2:268:GLY:HA3 | 2.48 | 0.48 |
| 4:X:120:THR:HG21 | 4:X:370:VAL:HG11 | 1.95 | 0.48 |
| 4:X:198:TYR:CZ | 4:X:248:ILE:HG13 | 2.48 | 0.48 |
| 4:Z:120:THR:HG21 | 4:Z:370:VAL:HG11 | 1.95 | 0.48 |
| 1:A:642:LYS:CB | 4:8:24:ASP:O | 2.59 | 0.48 |
| 1:A:707:CYS:SG | 1:A:714:ARG:CZ | 3.02 | 0.48 |
| 1:D:136:ASN:HA | 1:D:137:PRO:HD3 | 1.49 | 0.48 |
| 1:D:642:LYS:HA | 4:9:22:ALA:C | 2.33 | 0.48 |
| 1:D:733:PRO:O | 1:D:737:PHE:CE1 | 2.54 | 0.48 |
| 1:D:793:ARG:NH2 | 3:F:147:MET:HE3 | 2.27 | 0.48 |
| 1:G:41:VAL:CG1 | 1:G:42:HIS:N | 2.75 | 0.48 |
| 1:G:629:GLU:CA | 1:G:643:GLY:C | 2.73 | 0.48 |
| 2:H:121:LEU:O | 2:H:128:PHE:CG | 2.61 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:312:TYR:N | 1:J:312:TYR:CD1 | 2.81 | 0.48 |
| 1:J:499:GLU:OE1 | 1:J:499:GLU:HA | 2.13 | 0.48 |
| 1:J:538:GLU:HA | 4:W:351:THR:H | 1.77 | 0.48 |
| 1:J:756:THR:HG23 | 1:J:779:ARG:CD | 2.43 | 0.48 |
| 1:J:829:TRP:HZ3 | 2:K:84:PHE:CE2 | 2.32 | 0.48 |
| 1:M:51:THR:C | 1:M:62:VAL:HG13 | 2.32 | 0.48 |
| 1:M:290:GLN:HG2 | 1:M:331:LEU:CA | 2.43 | 0.48 |
| 1:M:550:PHE:CE2 | 1:M:592:ILE:CG2 | 2.97 | 0.48 |
| 1:M:795:ARG:NE | 3:O:118:MET:HE1 | 2.27 | 0.48 |
| 1:P:103:LEU:C | 1:P:103:LEU:HD12 | 2.33 | 0.48 |
| 1:P:404:PRO:HD2 | 1:P:415:MLY:O | 2.13 | 0.48 |
| 1:P:530:MET:CE | 4:1:354:GLN:HG3 | 2.35 | 0.48 |
| 1:P:795:ARG:NE | 3:R:118:MET:HE1 | 2.28 | 0.48 |
| 1:P:798:LEU:HD12 | 1:P:798:LEU:HA | 1.36 | 0.48 |
| 2:Q:130:PRO:O | 2:Q:131:GLU:C | 2.52 | 0.48 |
| 4:1:243:PRO:O | 4:Y:291:LYS:HG3 | 2.13 | 0.48 |
| 4:2:253:GLU:HA | 4:2:256:ARG:CG | 2.42 | 0.48 |
| 4:3:322:PRO:C | 4:5:244:ASP:HB2 | 2.33 | 0.48 |
| 4:5:120:THR:HG21 | 4:5:370:VAL:HG11 | 1.95 | 0.48 |
| 4:5:198:TYR:CZ | 4:5:248:ILE:HG13 | 2.48 | 0.48 |
| 4:6:120:THR:HG21 | 4:6:370:VAL:HG11 | 1.95 | 0.48 |
| 4:8:120:THR:HG21 | 4:8:370:VAL:HG11 | 1.95 | 0.48 |
| 4:8:213:LYS:O | 4:8:217:CYS:HB2 | 2.13 | 0.48 |
| 4:V:120:THR:HG21 | 4:V:370:VAL:HG11 | 1.95 | 0.48 |
| 1:A:689:GLU:O | 1:A:689:GLU:HG2 | 2.14 | 0.48 |
| 1:A:813:ILE:HG21 | 2:B:127:ARG:HB2 | 1.94 | 0.48 |
| 1:D:409:GLY:N | 1:D:636:LYS:CD | 2.71 | 0.48 |
| 1:D:797:PHE:CE2 | 3:F:126:LEU:HD21 | 2.35 | 0.48 |
| 1:G:128:PRO:O | 1:G:683:PRO:HB3 | 2.12 | 0.48 |
| 1:G:173:GLN:OE1 | 1:G:668:HIS:HB3 | 2.13 | 0.48 |
| 1:G:218:LEU:HD22 | 1:G:222:ILE:HG13 | 1.95 | 0.48 |
| 1:G:314:TYR:CZ | 1:G:362:GLY:HA2 | 2.48 | 0.48 |
| 1:J:93:MET:HA | 1:J:714:ARG:N | 2.25 | 0.48 |
| 1:J:97:LEU:HD13 | 1:J:97:LEU:N | 2.28 | 0.48 |
| 1:J:314:TYR:CZ | 1:J:362:GLY:HA2 | 2.48 | 0.48 |
| 1:J:793:ARG:HA | 3:L:40:ASN:HB3 | 1.95 | 0.48 |
| 1:P:51:THR:C | 1:P:62:VAL:HG13 | 2.33 | 0.48 |
| 1:P:173:GLN:OE1 | 1:P:668:HIS:HB3 | 2.13 | 0.48 |
| 1:P:642:LYS:HB2 | 4:1:24:ASP:O | 1.88 | 0.48 |
| 1:P:689:GLU:O | 1:P:689:GLU:HG2 | 2.14 | 0.48 |
| 1:P:715:VAL:HG12 | 1:P:716:LEU:O | 2.12 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:P:732:ILE:H | 1:P:733:PRO:CD | 2.23 | 0.48 |
| 2:Q:144:VAL:HG12 | 2:Q:153:ILE:HD11 | 1.76 | 0.48 |
| 4:1:247:VAL:HG23 | 4:Y:324:THR:HG21 | 1.92 | 0.48 |
| 4:4:198:TYR:CZ | 4:4:248:ILE:HG13 | 2.48 | 0.48 |
| 4:7:120:THR:HG21 | 4:7:370:VAL:HG11 | 1.95 | 0.48 |
| 4:V:198:TYR:CZ | 4:V:248:ILE:HG13 | 2.48 | 0.48 |
| 4:Y:213:LYS:O | 4:Y:217:CYS:HB2 | 2.13 | 0.48 |
| 1:A:64:THR:CG2 | 1:A:65:GLU:N | 2.76 | 0.48 |
| 1:A:312:TYR:N | 1:A:312:TYR:CD1 | 2.81 | 0.48 |
| 1:A:418:THR:CB | 1:A:421:GLU:HG3 | 2.37 | 0.48 |
| 1:D:237:THR:HG22 | 1:D:238:VAL:N | 2.28 | 0.48 |
| 1:D:251:ARG:HB2 | 1:D:264:ASP:HB3 | 1.94 | 0.48 |
| 1:D:617:MLY:O | 1:D:620:ALA:HB3 | 2.14 | 0.48 |
| 1:D:800:ARG:HD2 | 3:F:149:VAL:C | 2.32 | 0.48 |
| 2:E:128:PHE:O | 2:E:133:ILE:HD11 | 2.13 | 0.48 |
| 1:G:720:PHE:CD2 | 1:G:744:SER:HB3 | 2.48 | 0.48 |
| 1:G:723:ARG:HH11 | 1:G:723:ARG:HG3 | 1.79 | 0.48 |
| 1:G:817:GLN:CD | 2:H:127:ARG:CB | 2.78 | 0.48 |
| 2:H:93:PRO:O | 2:H:97:ILE:HG13 | 2.12 | 0.48 |
| 1:J:248:MLY:HE2 | 1:J:250:ILE:HD11 | 1.96 | 0.48 |
| 1:J:637:LYS:HD2 | 4:W:144:ALA:HB3 | 1.20 | 0.48 |
| 1:M:214:MET:HA | 1:M:340:ILE:CD1 | 2.41 | 0.48 |
| 1:M:831:TRP:CZ3 | 2:N:34:ILE:HD13 | 2.40 | 0.48 |
| 1:P:635:GLY:HA3 | 4:1:334:GLU:CG | 2.30 | 0.48 |
| 1:P:723:ARG:HH11 | 1:P:723:ARG:HG3 | 1.78 | 0.48 |
| 4:3:120:THR:HG21 | 4:3:370:VAL:HG11 | 1.95 | 0.48 |
| 4:6:198:TYR:CZ | 4:6:248:ILE:HG13 | 2.48 | 0.48 |
| 1:A:595:TRP:N | 1:A:595:TRP:CD1 | 2.80 | 0.48 |
| 1:A:756:THR:O | 1:A:758:TYR:N | 2.46 | 0.48 |
| 1:D:134:VAL:C | 1:D:136:ASN:H | 2.16 | 0.48 |
| 1:D:314:TYR:CZ | 1:D:362:GLY:HA2 | 2.48 | 0.48 |
| 1:D:410:ASN:HD22 | 4:9:336:LYS:HE2 | 1.78 | 0.48 |
| 1:D:499:GLU:OE1 | 1:D:499:GLU:HA | 2.13 | 0.48 |
| 1:D:732:ILE:H | 1:D:733:PRO:HD2 | 1.74 | 0.48 |
| 2:E:112:ILE:CG2 | 2:E:147:ASN:O | 2.62 | 0.48 |
| 1:G:550:PHE:CE2 | 1:G:592:ILE:CG2 | 2.96 | 0.48 |
| 1:G:689:GLU:O | 1:G:689:GLU:HG2 | 2.14 | 0.48 |
| 1:G:739:ASP:CB | 1:G:742:LYS:CB | 2.81 | 0.48 |
| 2:H:130:PRO:O | 2:H:131:GLU:C | 2.52 | 0.48 |
| 1:J:768:MLY:HB2 | 1:J:773:GLY:HA3 | 1.33 | 0.48 |
| 1:M:499:GLU:HA | 1:M:499:GLU:OE1 | 2.13 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:791:GLN:HE22 | 3:O:116:GLU:N | 2.11 | 0.48 |
| 1:M:839:MLY:HH13 | 2:N:159:HIS:HD2 | 1.78 | 0.48 |
| 1:P:10:PHE:CD2 | 1:P:17:LEU:HD23 | 2.49 | 0.48 |
| 1:P:310:TYR:CE2 | 1:P:320:ILE:CD1 | 2.94 | 0.48 |
| 1:P:602:PRO:O | 1:P:603:LEU:HD12 | 2.14 | 0.48 |
| 1:P:803:TYR:HE2 | 3:R:17:PHE:CZ | 2.30 | 0.48 |
| 2:Q:140:PHE:HB3 | 2:Q:144:VAL:HG12 | 1.94 | 0.48 |
| 4:2:198:TYR:CZ | 4:2:248:ILE:HG13 | 2.48 | 0.48 |
| 4:4:287:ILE:HG21 | 4:6:204:ALA:N | 2.28 | 0.48 |
| 4:5:213:LYS:O | 4:5:217:CYS:HB2 | 2.13 | 0.48 |
| 4:8:124:PHE:CZ | 4:8:132:MET:HG3 | 2.48 | 0.48 |
| 4:V:124:PHE:CZ | 4:V:132:MET:HG3 | 2.48 | 0.48 |
| 4:V:285:CYS:O | 4:X:202:THR:HG22 | 2.13 | 0.48 |
| 1:A:154:HIS:CE1 | 1:A:156:PHE:CE2 | 3.02 | 0.48 |
| 1:A:550:PHE:CE2 | 1:A:592:ILE:CG2 | 2.96 | 0.48 |
| 1:D:602:PRO:O | 1:D:603:LEU:HD12 | 2.14 | 0.48 |
| 1:D:836:PHE:HZ | 2:E:160:GLY:H | 1.61 | 0.48 |
| 2:E:163:ALA:C | 2:K:22:THR:OG1 | 2.52 | 0.48 |
| 1:G:84:MLY:CH2 | 1:G:720:PHE:HA | 2.40 | 0.48 |
| 1:G:84:MLY:HH22 | 1:G:723:ARG:CB | 2.40 | 0.48 |
| 1:G:136:ASN:O | 1:G:139:VAL:N | 2.47 | 0.48 |
| 1:G:312:TYR:N | 1:G:312:TYR:CD1 | 2.81 | 0.48 |
| 1:G:418:THR:CB | 1:G:421:GLU:HG3 | 2.37 | 0.48 |
| 1:G:530:MET:CE | 4:V:354:GLN:HG3 | 2.34 | 0.48 |
| 1:G:617:MLY:O | 1:G:620:ALA:HB3 | 2.14 | 0.48 |
| 1:G:725:ARG:NE | 1:G:733:PRO:CB | 1.95 | 0.48 |
| 1:G:839:MLY:HB2 | 1:G:840:PRO:HD3 | 1.94 | 0.48 |
| 2:H:128:PHE:O | 2:H:133:ILE:HD11 | 2.13 | 0.48 |
| 1:J:10:PHE:CD2 | 1:J:17:LEU:HD23 | 2.49 | 0.48 |
| 1:J:251:ARG:O | 1:J:263:ALA:HA | 2.12 | 0.48 |
| 1:J:278:GLN:HG3 | 1:J:318:GLY:H | 1.76 | 0.48 |
| 1:J:404:PRO:HD2 | 1:J:415:MLY:O | 2.13 | 0.48 |
| 1:J:405:ARG:HB2 | 1:J:414:THR:OG1 | 2.13 | 0.48 |
| 1:J:546:THR:CG2 | 1:J:547:ASP:N | 2.77 | 0.48 |
| 1:M:642:LYS:CB | 4:Z:24:ASP:O | 2.60 | 0.48 |
| 1:M:821:ARG:HH22 | 2:N:127:ARG:CD | 2.15 | 0.48 |
| 1:P:546:THR:CG2 | 1:P:547:ASP:N | 2.77 | 0.48 |
| 1:P:836:PHE:CD1 | 2:Q:159:HIS:CA | 2.92 | 0.48 |
| 4:1:299:MET:HE2 | 4:1:331:ALA:HB2 | 1.95 | 0.48 |
| 4:5:253:GLU:HA | 4:5:256:ARG:CG | 2.42 | 0.48 |
| 4:7:213:LYS:O | 4:7:217:CYS:HB2 | 2.13 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:7:250:ILE:HG23 | 4:7:253:GLU:HG2 | 1.96 | 0.48 |
| 4:8:250:ILE:HG23 | 4:8:253:GLU:HG2 | 1.96 | 0.48 |
| 4:9:120:THR:HG21 | 4:9:370:VAL:HG11 | 1.95 | 0.48 |
| 4:V:285:CYS:O | 4:X:202:THR:CG2 | 2.62 | 0.48 |
| 4:W:213:LYS:O | 4:W:217:CYS:HB2 | 2.13 | 0.48 |
| 4:X:213:LYS:O | 4:X:217:CYS:HB2 | 2.13 | 0.48 |
| 1:A:314:TYR:CZ | 1:A:362:GLY:HA2 | 2.48 | 0.48 |
| 1:D:689:GLU:O | 1:D:689:GLU:HG2 | 2.14 | 0.48 |
| 1:D:720:PHE:CD2 | 1:D:744:SER:HB3 | 2.49 | 0.48 |
| 1:D:725:ARG:NE | 1:D:733:PRO:CB | 1.95 | 0.48 |
| 2:E:130:PRO:O | 2:E:131:GLU:C | 2.52 | 0.48 |
| 1:G:406:VAL:CG1 | 1:G:407:GLY:N | 2.77 | 0.48 |
| 1:G:642:LYS:HA | 4:V:22:ALA:C | 2.33 | 0.48 |
| 1:J:136:ASN:O | 1:J:139:VAL:N | 2.47 | 0.48 |
| 1:J:251:ARG:HB2 | 1:J:264:ASP:HB3 | 1.95 | 0.48 |
| 1:J:406:VAL:CG1 | 1:J:407:GLY:N | 2.77 | 0.48 |
| 1:J:617:MLY:O | 1:J:620:ALA:HB3 | 2.14 | 0.48 |
| 1:J:797:PHE:HZ | 3:L:146:ILE:HD13 | 1.44 | 0.48 |
| 2:K:112:ILE:CG2 | 2:K:147:ASN:O | 2.62 | 0.48 |
| 2:K:130:PRO:O | 2:K:131:GLU:C | 2.52 | 0.48 |
| 1:M:617:MLY:O | 1:M:620:ALA:HB3 | 2.14 | 0.48 |
| 1:M:689:GLU:O | 1:M:689:GLU:HG2 | 2.14 | 0.48 |
| 1:P:97:LEU:HD13 | 1:P:97:LEU:N | 2.27 | 0.48 |
| 1:P:136:ASN:O | 1:P:139:VAL:N | 2.47 | 0.48 |
| 1:P:206:LYS:HD2 | 1:P:217:THR:CG2 | 2.17 | 0.48 |
| 1:P:251:ARG:HB2 | 1:P:264:ASP:HB3 | 1.95 | 0.48 |
| 1:P:617:MLY:O | 1:P:620:ALA:HB3 | 2.14 | 0.48 |
| 1:P:821:ARG:CZ | 2:Q:127:ARG:CD | 2.91 | 0.48 |
| 1:P:838:ILE:C | 1:P:840:PRO:HD2 | 2.35 | 0.48 |
| 4:1:213:LYS:O | 4:1:217:CYS:HB2 | 2.13 | 0.48 |
| 4:9:213:LYS:O | 4:9:217:CYS:HB2 | 2.13 | 0.48 |
| 4:V:250:ILE:HG23 | 4:V:253:GLU:HG2 | 1.96 | 0.48 |
| 4:X:124:PHE:CZ | 4:X:132:MET:HG3 | 2.48 | 0.48 |
| 4:Z:213:LYS:O | 4:Z:217:CYS:HB2 | 2.13 | 0.48 |
| 1:A:752:ASP:CB | 1:A:782:MLY:HD3 | 2.44 | 0.48 |
| 1:A:798:LEU:HD21 | 3:C:126:LEU:CD1 | 2.38 | 0.48 |
| 1:A:817:GLN:CG | 2:B:127:ARG:HB3 | 2.44 | 0.48 |
| 1:D:214:MET:HA | 1:D:340:ILE:CD1 | 2.42 | 0.48 |
| 1:D:218:LEU:HA | 1:D:221:GLN:H | 1.79 | 0.48 |
| 1:D:221:GLN:HG2 | 1:D:221:GLN:H | 1.47 | 0.48 |
| 1:D:405:ARG:HB2 | 1:D:414:THR:OG1 | 2.13 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:530:MET:CE | 4:9:354:GLN:HG3 | 2.35 | 0.48 |
| 1:D:595:TRP:N | 1:D:595:TRP:CD1 | 2.80 | 0.48 |
| 1:D:646:PHE:HE2 | 1:D:652:LEU:CG | 2.25 | 0.48 |
| 2:E:93:PRO:O | 2:E:97:ILE:HG13 | 2.13 | 0.48 |
| 1:G:106:LEU:HD12 | 1:G:117:THR:HG21 | 1.96 | 0.48 |
| 1:G:154:HIS:CE1 | 1:G:156:PHE:CE2 | 3.02 | 0.48 |
| 1:G:289:TYR:OH | 1:G:315:VAL:O | 2.27 | 0.48 |
| 1:G:292:MET:HE1 | 1:G:309:PRO:HD3 | 1.95 | 0.48 |
| 1:G:499:GLU:OE1 | 1:G:499:GLU:HA | 2.13 | 0.48 |
| 1:G:762:HIS:CD2 | 1:G:762:HIS:N | 2.78 | 0.48 |
| 1:G:796:GLY:CA | 3:I:35:ARG:NE | 2.77 | 0.48 |
| 1:G:796:GLY:N | 3:I:35:ARG:NH2 | 2.62 | 0.48 |
| 1:G:797:PHE:CE1 | 3:I:146:ILE:CB | 2.97 | 0.48 |
| 1:G:835:PHE:CD1 | 2:H:30:ALA:HB2 | 2.48 | 0.48 |
| 1:J:51:THR:C | 1:J:62:VAL:HG13 | 2.32 | 0.48 |
| 1:J:237:THR:HG22 | 1:J:238:VAL:N | 2.28 | 0.48 |
| 1:J:595:TRP:N | 1:J:595:TRP:CD1 | 2.80 | 0.48 |
| 1:J:804:ARG:HH22 | 3:L:149:VAL:HA | 1.78 | 0.48 |
| 1:J:819:ASN:OD1 | 2:K:90:GLY:O | 2.30 | 0.48 |
| 1:M:542:PHE:CD2 | 4:Z:143:TYR:CD1 | 3.02 | 0.48 |
| 1:M:546:THR:CG2 | 1:M:547:ASP:N | 2.77 | 0.48 |
| 1:P:134:VAL:C | 1:P:136:ASN:H | 2.16 | 0.48 |
| 1:P:406:VAL:CG1 | 1:P:407:GLY:N | 2.77 | 0.48 |
| 1:P:576:GLU:CG | 1:P:577:ALA:N | 2.44 | 0.48 |
| 1:P:595:TRP:CD1 | 1:P:595:TRP:N | 2.80 | 0.48 |
| 4:2:213:LYS:O | 4:2:217:CYS:HB2 | 2.13 | 0.48 |
| 4:3:290:ARG:NH1 | 4:5:202:THR:CG2 | 2.75 | 0.48 |
| 4:4:250:ILE:HG23 | 4:4:253:GLU:HG2 | 1.96 | 0.48 |
| 4:V:70:PRO:HG3 | 4:V:81:ASP:HB3 | 1.94 | 0.48 |
| 4:W:120:THR:HG21 | 4:W:370:VAL:HG11 | 1.95 | 0.48 |
| 4:Z:250:ILE:HG23 | 4:Z:253:GLU:HG2 | 1.96 | 0.48 |
| 4:Z:253:GLU:HA | 4:Z:256:ARG:CG | 2.42 | 0.48 |
| 1:A:404:PRO:HD2 | 1:A:415:MLY:O | 2.13 | 0.47 |
| 1:A:546:THR:CG2 | 1:A:547:ASP:N | 2.77 | 0.47 |
| 1:A:578:HIS:HB3 | 1:A:592:ILE:CD1 | 2.38 | 0.47 |
| 1:A:617:MLY:O | 1:A:620:ALA:HB3 | 2.14 | 0.47 |
| 1:A:675:ILE:CG2 | 1:A:676:ILE:N | 2.74 | 0.47 |
| 1:A:793:ARG:O | 1:A:797:PHE:N | 2.40 | 0.47 |
| 2:B:139:ALA:C | 2:B:141:PRO:HD3 | 2.33 | 0.47 |
| 1:D:10:PHE:CD2 | 1:D:17:LEU:HD23 | 2.49 | 0.47 |
| 1:D:538:GLU:HA | 4:9:351:THR:H | 1.78 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:E:121:LEU:HA | 2:E:128:PHE:CD2 | 2.46 | 0.47 |
| 1:G:564:ASN:HD22 | 1:G:582:VAL:HB | 1.79 | 0.47 |
| 1:J:22:LYS:O | 1:J:26:GLU:N | 2.29 | 0.47 |
| 1:J:798:LEU:HD22 | 3:L:118:MET:SD | 2.53 | 0.47 |
| 1:J:839:MLY:HH11 | 2:K:158:THR:HG22 | 1.96 | 0.47 |
| 3:L:50:LEU:O | 3:L:55:LYS:HB2 | 2.13 | 0.47 |
| 1:M:106:LEU:HD12 | 1:M:117:THR:HG21 | 1.96 | 0.47 |
| 1:M:154:HIS:CE1 | 1:M:156:PHE:CE2 | 3.02 | 0.47 |
| 1:M:218:LEU:HA | 1:M:221:GLN:H | 1.79 | 0.47 |
| 1:M:312:TYR:N | 1:M:312:TYR:CD1 | 2.81 | 0.47 |
| 1:P:218:LEU:HA | 1:P:221:GLN:H | 1.79 | 0.47 |
| 1:P:550:PHE:CE2 | 1:P:592:ILE:CG2 | 2.97 | 0.47 |
| 4:5:250:ILE:HG23 | 4:5:253:GLU:HG2 | 1.96 | 0.47 |
| 4:9:250:ILE:HG23 | 4:9:253:GLU:HG2 | 1.96 | 0.47 |
| 1:A:568:PRO:HD3 | 1:A:579:PHE:HA | 1.97 | 0.47 |
| 1:A:629:GLU:CB | 1:A:645:SER:N | 2.74 | 0.47 |
| 1:A:753:VAL:CB | 1:A:775:LEU:HG | 2.30 | 0.47 |
| 1:A:836:PHE:CD2 | 2:B:161:GLU:HG2 | 2.50 | 0.47 |
| 1:A:838:ILE:C | 1:A:840:PRO:HD2 | 2.35 | 0.47 |
| 1:D:248:MLY:HE2 | 1:D:250:ILE:HD11 | 1.96 | 0.47 |
| 1:D:404:PRO:HD2 | 1:D:415:MLY:O | 2.13 | 0.47 |
| 1:D:406:VAL:CG1 | 1:D:407:GLY:N | 2.77 | 0.47 |
| 1:D:538:GLU:CD | 4:9:355:MET:HE3 | 2.31 | 0.47 |
| 1:D:732:ILE:HD13 | 1:D:782:MLY:HH21 | 1.95 | 0.47 |
| 1:G:148:ARG:NE | 1:G:764:MLY:CH2 | 2.71 | 0.47 |
| 1:G:310:TYR:CE2 | 1:G:320:ILE:CD1 | 2.94 | 0.47 |
| 1:G:404:PRO:HD2 | 1:G:415:MLY:O | 2.13 | 0.47 |
| 1:G:636:LYS:O | 4:V:144:ALA:HB1 | 2.14 | 0.47 |
| 1:G:637:LYS:HD2 | 4:V:144:ALA:HB3 | 1.20 | 0.47 |
| 1:G:724:TYR:HD1 | 1:G:727:LEU:CD1 | 2.27 | 0.47 |
| 1:G:795:ARG:CZ | 3:I:116:GLU:OE1 | 2.57 | 0.47 |
| 2:H:139:ALA:C | 2:H:141:PRO:HD3 | 2.33 | 0.47 |
| 2:H:144:VAL:HG12 | 2:H:153:ILE:HD11 | 1.75 | 0.47 |
| 1:J:292:MET:CE | 1:J:309:PRO:HA | 2.39 | 0.47 |
| 1:J:720:PHE:CD2 | 1:J:744:SER:HB3 | 2.48 | 0.47 |
| 1:J:769:ALA:HB2 | 1:J:770:GLY:HA2 | 1.92 | 0.47 |
| 2:K:117:LEU:CG | 2:K:147:ASN:OD1 | 2.52 | 0.47 |
| 2:K:128:PHE:O | 2:K:133:ILE:HD11 | 2.13 | 0.47 |
| 1:M:10:PHE:CD2 | 1:M:17:LEU:HD23 | 2.49 | 0.47 |
| 1:M:20:SER:HB3 | 1:M:23:GLU:OE1 | 2.13 | 0.47 |
| 1:M:202:SER:HA | 1:M:207:LYS:NZ | 2.22 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:546:THR:HG21 | 4:2:47:MET:CA | 2.26 | 0.47 |
| 1:M:602:PRO:O | 1:M:603:LEU:HD12 | 2.14 | 0.47 |
| 1:M:632:GLY:HA3 | 1:M:643:GLY:N | 2.17 | 0.47 |
| 1:M:732:ILE:HG23 | 1:M:747:LEU:CD1 | 1.05 | 0.47 |
| 1:M:765:VAL:CG1 | 1:M:766:PHE:N | 2.77 | 0.47 |
| 1:P:248:MLY:HE2 | 1:P:250:ILE:HD11 | 1.95 | 0.47 |
| 1:P:312:TYR:N | 1:P:312:TYR:CD1 | 2.81 | 0.47 |
| 1:P:542:PHE:CD2 | 4:1:143:TYR:CD1 | 3.02 | 0.47 |
| 1:P:544:LYS:HD2 | 4:1:147:ARG:CB | 2.36 | 0.47 |
| 1:P:568:PRO:HD3 | 1:P:579:PHE:HA | 1.96 | 0.47 |
| 4:1:247:VAL:N | 4:Y:324:THR:CB | 2.77 | 0.47 |
| 4:1:287:ILE:HB | 4:3:203:THR:HB | 1.92 | 0.47 |
| 4:2:250:ILE:HG23 | 4:2:253:GLU:HG2 | 1.96 | 0.47 |
| 4:3:213:LYS:O | 4:3:217:CYS:HB2 | 2.13 | 0.47 |
| 4:5:124:PHE:CZ | 4:5:132:MET:HG3 | 2.48 | 0.47 |
| 4:6:250:ILE:HG23 | 4:6:253:GLU:HG2 | 1.96 | 0.47 |
| 4:8:253:GLU:HA | 4:8:256:ARG:CG | 2.42 | 0.47 |
| 4:V:213:LYS:O | 4:V:217:CYS:HB2 | 2.14 | 0.47 |
| 4:W:250:ILE:HG23 | 4:W:253:GLU:HG2 | 1.96 | 0.47 |
| 4:Y:253:GLU:HA | 4:Y:256:ARG:CG | 2.42 | 0.47 |
| 1:A:218:LEU:CD2 | 1:A:222:ILE:CG1 | 2.85 | 0.47 |
| 1:A:346:ASP:O | 1:A:350:ALA:N | 2.46 | 0.47 |
| 3:C:50:LEU:O | 3:C:55:LYS:HB2 | 2.13 | 0.47 |
| 1:D:542:PHE:CD2 | 4:9:143:TYR:CD1 | 3.02 | 0.47 |
| 1:G:122:PHE:CE2 | 1:G:700:VAL:HA | 2.50 | 0.47 |
| 1:G:546:THR:CG2 | 1:G:547:ASP:N | 2.77 | 0.47 |
| 1:G:701:LEU:HD12 | 1:G:701:LEU:HA | 1.55 | 0.47 |
| 1:J:640:LYS:HD2 | 1:J:646:PHE:O | 2.15 | 0.47 |
| 1:M:215:GLN:H | 1:M:340:ILE:CD1 | 2.21 | 0.47 |
| 1:M:564:ASN:HD22 | 1:M:582:VAL:HB | 1.79 | 0.47 |
| 1:M:635:GLY:HA3 | 4:Z:334:GLU:CG | 2.30 | 0.47 |
| 1:M:640:LYS:HD2 | 1:M:646:PHE:O | 2.14 | 0.47 |
| 1:M:732:ILE:HG21 | 1:M:747:LEU:CD1 | 0.63 | 0.47 |
| 1:M:834:LEU:CD1 | 2:N:51:PHE:CD1 | 2.95 | 0.47 |
| 2:N:160:GLY:O | 2:N:161:GLU:HG2 | 2.15 | 0.47 |
| 1:P:314:TYR:CZ | 1:P:362:GLY:HA2 | 2.48 | 0.47 |
| 1:P:642:LYS:CB | 4:1:24:ASP:O | 2.60 | 0.47 |
| 1:P:821:ARG:HH22 | 2:Q:127:ARG:CD | 2.21 | 0.47 |
| 4:7:287:ILE:HA | 4:9:202:THR:HG21 | 1.59 | 0.47 |
| 4:X:250:ILE:HG23 | 4:X:253:GLU:HG2 | 1.96 | 0.47 |
| 4:X:253:GLU:HA | 4:X:256:ARG:CG | 2.42 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:Y:120:THR:HG21 | 4:Y:370:VAL:HG11 | 1.95 | 0.47 |
| 4:Z:124:PHE:CZ | 4:Z:132:MET:HG3 | 2.48 | 0.47 |
| 1:A:103:LEU:C | 1:A:103:LEU:HD12 | 2.33 | 0.47 |
| 1:A:122:PHE:CE2 | 1:A:700:VAL:HA | 2.49 | 0.47 |
| 1:A:214:MET:C | 1:A:340:ILE:CD1 | 2.82 | 0.47 |
| 1:A:310:TYR:CE2 | 1:A:320:ILE:CD1 | 2.94 | 0.47 |
| 1:A:406:VAL:CG1 | 1:A:407:GLY:N | 2.77 | 0.47 |
| 1:A:732:ILE:H | 1:A:733:PRO:HD2 | 1.74 | 0.47 |
| 1:A:765:VAL:CG1 | 1:A:766:PHE:N | 2.77 | 0.47 |
| 1:D:546:THR:CG2 | 1:D:547:ASP:N | 2.77 | 0.47 |
| 1:D:783:LEU:HA | 1:D:786:ILE:HB | 1.97 | 0.47 |
| 1:D:831:TRP:NE1 | 2:E:51:PHE:CE2 | 2.83 | 0.47 |
| 2:E:160:GLY:O | 2:E:161:GLU:HG2 | 2.15 | 0.47 |
| 1:G:708:ARG:CA | 1:G:712:PRO:HG3 | 2.30 | 0.47 |
| 1:G:765:VAL:CG1 | 1:G:766:PHE:N | 2.77 | 0.47 |
| 1:J:41:VAL:CG1 | 1:J:42:HIS:N | 2.75 | 0.47 |
| 1:J:292:MET:HE3 | 1:J:309:PRO:CA | 2.43 | 0.47 |
| 1:J:538:GLU:CD | 4:W:355:MET:HE3 | 2.30 | 0.47 |
| 1:J:542:PHE:CD2 | 4:W:143:TYR:CD1 | 3.02 | 0.47 |
| 1:J:602:PRO:O | 1:J:603:LEU:HD12 | 2.14 | 0.47 |
| 1:J:765:VAL:CG1 | 1:J:766:PHE:N | 2.77 | 0.47 |
| 1:J:829:TRP:CH2 | 2:K:84:PHE:CE1 | 3.03 | 0.47 |
| 1:M:237:THR:HG22 | 1:M:238:VAL:N | 2.28 | 0.47 |
| 1:M:818:TYR:OH | 2:N:127:ARG:NH2 | 2.42 | 0.47 |
| 1:P:765:VAL:CG1 | 1:P:766:PHE:N | 2.77 | 0.47 |
| 2:Q:160:GLY:O | 2:Q:161:GLU:HG2 | 2.14 | 0.47 |
| 4:3:250:ILE:HG23 | 4:3:253:GLU:HG2 | 1.96 | 0.47 |
| 4:4:120:THR:HG21 | 4:4:370:VAL:HG11 | 1.95 | 0.47 |
| 4:6:213:LYS:O | 4:6:217:CYS:HB2 | 2.13 | 0.47 |
| 4:Y:250:ILE:HG23 | 4:Y:253:GLU:HG2 | 1.96 | 0.47 |
| 1:A:10:PHE:CD2 | 1:A:17:LEU:HD23 | 2.49 | 0.47 |
| 1:A:248:MLY:HE2 | 1:A:250:ILE:HD11 | 1.95 | 0.47 |
| 1:A:499:GLU:OE1 | 1:A:499:GLU:HA | 2.13 | 0.47 |
| 2:B:112:ILE:CG2 | 2:B:147:ASN:O | 2.62 | 0.47 |
| 3:C:53:PRO:O | 3:C:55:LYS:HG3 | 2.15 | 0.47 |
| 1:D:640:LYS:HB3 | 1:D:645:SER:CB | 2.42 | 0.47 |
| 1:D:765:VAL:CG1 | 1:D:766:PHE:N | 2.77 | 0.47 |
| 1:D:800:ARG:CG | 3:F:149:VAL:HG22 | 2.44 | 0.47 |
| 1:G:134:VAL:C | 1:G:136:ASN:H | 2.17 | 0.47 |
| 1:G:218:LEU:HA | 1:G:221:GLN:H | 1.79 | 0.47 |
| 1:G:248:MLY:HE2 | 1:G:250:ILE:HD11 | 1.95 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:578:HIS:HB3 | 1:G:592:ILE:CD1 | 2.38 | 0.47 |
| 1:G:602:PRO:O | 1:G:603:LEU:HD12 | 2.14 | 0.47 |
| 2:H:160:GLY:O | 2:H:161:GLU:HG2 | 2.15 | 0.47 |
| 1:J:550:PHE:CE2 | 1:J:592:ILE:CG2 | 2.97 | 0.47 |
| 1:J:568:PRO:HD3 | 1:J:579:PHE:HA | 1.96 | 0.47 |
| 1:J:640:LYS:HB3 | 1:J:645:SER:CB | 2.42 | 0.47 |
| 1:J:642:LYS:HG3 | 4:W:23:GLY:CA | 2.32 | 0.47 |
| 1:J:689:GLU:O | 1:J:689:GLU:HG2 | 2.14 | 0.47 |
| 1:J:838:ILE:C | 1:J:840:PRO:HD2 | 2.35 | 0.47 |
| 1:M:295:MLY:HG3 | 1:M:332:MET:HE2 | 1.94 | 0.47 |
| 1:M:449:LEU:HA | 1:M:449:LEU:HD12 | 1.60 | 0.47 |
| 1:M:675:ILE:CG2 | 1:M:676:ILE:N | 2.74 | 0.47 |
| 4:1:250:ILE:HG23 | 4:1:253:GLU:HG2 | 1.96 | 0.47 |
| 4:V:162:ASN:OD1 | 4:V:277:THR:HG22 | 2.15 | 0.47 |
| 1:A:406:VAL:CG1 | 1:A:407:GLY:H | 2.28 | 0.47 |
| 1:A:524:GLU:HB3 | 1:A:528:MLY:HG2 | 1.96 | 0.47 |
| 1:A:542:PHE:CD2 | 4:8:143:TYR:CD1 | 3.02 | 0.47 |
| 1:A:553:MLY:NZ | 4:V:45:VAL:CA | 2.58 | 0.47 |
| 2:B:160:GLY:O | 2:B:161:GLU:HG2 | 2.14 | 0.47 |
| 1:D:122:PHE:CE2 | 1:D:700:VAL:HA | 2.50 | 0.47 |
| 1:D:154:HIS:CE1 | 1:D:156:PHE:CE2 | 3.02 | 0.47 |
| 1:D:214:MET:C | 1:D:340:ILE:CD1 | 2.82 | 0.47 |
| 1:D:295:MLY:HG3 | 1:D:332:MET:HE2 | 1.94 | 0.47 |
| 1:D:795:ARG:NH2 | 3:F:116:GLU:HG2 | 2.22 | 0.47 |
| 1:G:798:LEU:HA | 1:G:798:LEU:HD12 | 1.36 | 0.47 |
| 3:I:53:PRO:O | 3:I:55:LYS:HG3 | 2.15 | 0.47 |
| 1:J:94:MET:C | 1:J:713:SER:CB | 2.55 | 0.47 |
| 1:J:410:ASN:HD22 | 4:W:336:LYS:HE2 | 1.78 | 0.47 |
| 1:J:643:GLY:CA | 4:W:24:ASP:OD1 | 2.62 | 0.47 |
| 1:J:795:ARG:CG | 3:L:116:GLU:OE2 | 2.63 | 0.47 |
| 1:M:568:PRO:HD3 | 1:M:579:PHE:HA | 1.96 | 0.47 |
| 1:P:41:VAL:CG1 | 1:P:42:HIS:N | 2.75 | 0.47 |
| 1:P:629:GLU:CA | 1:P:643:GLY:C | 2.73 | 0.47 |
| 1:P:640:LYS:HD2 | 1:P:646:PHE:O | 2.15 | 0.47 |
| 2:Q:117:LEU:CG | 2:Q:147:ASN:OD1 | 2.53 | 0.47 |
| 4:1:120:THR:HG21 | 4:1:370:VAL:HG11 | 1.95 | 0.47 |
| 4:1:244:ASP:CG | 4:Y:325:MET:SD | 2.89 | 0.47 |
| 4:8:162:ASN:OD1 | 4:8:277:THR:HG22 | 2.15 | 0.47 |
| 4:9:324:THR:O | 4:W:244:ASP:HA | 2.08 | 0.47 |
| 4:W:162:ASN:OD1 | 4:W:277:THR:HG22 | 2.15 | 0.47 |
| 4:W:299:MET:HE2 | 4:W:331:ALA:HB2 | 1.95 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:W:325:MET:SD | 4:Y:244:ASP:OD2 | 2.73 | 0.47 |
| 1:A:636:LYS:O | 4:8:144:ALA:HB1 | 2.15 | 0.47 |
| 1:A:640:LYS:HD2 | 1:A:646:PHE:O | 2.15 | 0.47 |
| 1:A:642:LYS:HA | 4:8:22:ALA:C | 2.34 | 0.47 |
| 1:A:783:LEU:HA | 1:A:786:ILE:HB | 1.97 | 0.47 |
| 1:A:801:VAL:N | 3:C:149:VAL:HG21 | 2.30 | 0.47 |
| 2:B:130:PRO:O | 2:B:131:GLU:C | 2.52 | 0.47 |
| 1:D:188:ASN:ND2 | 1:D:674:CYS:SG | 2.88 | 0.47 |
| 1:D:550:PHE:CE2 | 1:D:592:ILE:CG2 | 2.97 | 0.47 |
| 1:D:795:ARG:HH21 | 3:F:116:GLU:HG2 | 1.76 | 0.47 |
| 1:D:800:ARG:HB3 | 3:F:149:VAL:HG13 | 1.96 | 0.47 |
| 1:D:838:ILE:C | 1:D:840:PRO:HD2 | 2.34 | 0.47 |
| 1:G:640:LYS:HD2 | 1:G:646:PHE:O | 2.15 | 0.47 |
| 1:G:732:ILE:H | 1:G:733:PRO:HD2 | 1.74 | 0.47 |
| 1:G:820:VAL:HG11 | 2:H:136:MET:HE1 | 1.92 | 0.47 |
| 1:G:829:TRP:HZ3 | 2:H:84:PHE:CE2 | 2.27 | 0.47 |
| 2:H:112:ILE:CG2 | 2:H:147:ASN:O | 2.62 | 0.47 |
| 1:J:106:LEU:HD12 | 1:J:117:THR:HG21 | 1.96 | 0.47 |
| 1:J:122:PHE:CE2 | 1:J:700:VAL:HA | 2.50 | 0.47 |
| 1:J:214:MET:C | 1:J:340:ILE:CD1 | 2.82 | 0.47 |
| 1:J:564:ASN:HD22 | 1:J:582:VAL:HB | 1.79 | 0.47 |
| 1:J:636:LYS:O | 4:W:144:ALA:HB1 | 2.14 | 0.47 |
| 1:J:642:LYS:CB | 4:W:24:ASP:O | 2.60 | 0.47 |
| 2:K:160:GLY:O | 2:K:161:GLU:HG2 | 2.14 | 0.47 |
| 3:L:53:PRO:O | 3:L:55:LYS:HG3 | 2.15 | 0.47 |
| 1:M:310:TYR:CE2 | 1:M:320:ILE:CD1 | 2.94 | 0.47 |
| 1:M:410:ASN:HD22 | 4:Z:336:LYS:HE2 | 1.78 | 0.47 |
| 1:M:578:HIS:HB3 | 1:M:592:ILE:CD1 | 2.38 | 0.47 |
| 1:M:733:PRO:O | 1:M:737:PHE:CE1 | 2.53 | 0.47 |
| 2:N:112:ILE:CG2 | 2:N:147:ASN:O | 2.62 | 0.47 |
| 2:N:121:LEU:HA | 2:N:128:PHE:CD2 | 2.46 | 0.47 |
| 1:P:214:MET:HA | 1:P:340:ILE:CD1 | 2.41 | 0.47 |
| 1:P:218:LEU:HD22 | 1:P:222:ILE:HG13 | 1.95 | 0.47 |
| 1:P:237:THR:HG22 | 1:P:238:VAL:N | 2.28 | 0.47 |
| 1:P:564:ASN:HD22 | 1:P:582:VAL:HB | 1.80 | 0.47 |
| 1:P:646:PHE:CE2 | 1:P:652:LEU:CD2 | 2.87 | 0.47 |
| 1:P:695:LEU:HB3 | 1:P:701:LEU:HD22 | 1.97 | 0.47 |
| 1:P:715:VAL:HG11 | 1:P:720:PHE:CD1 | 2.49 | 0.47 |
| 1:P:732:ILE:H | 1:P:733:PRO:HD2 | 1.74 | 0.47 |
| 3:R:53:PRO:O | 3:R:55:LYS:HG3 | 2.15 | 0.47 |
| 4:1:162:ASN:OD1 | 4:1:277:THR:HG22 | 2.15 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:2:120:THR:HG21 | 4:2:370:VAL:HG11 | 1.95 | 0.47 |
| 4:7:299:MET:HE2 | 4:7:331:ALA:HB2 | 1.96 | 0.47 |
| 4:X:287:ILE:CD1 | 4:Z:205:GLU:HG2 | 2.44 | 0.47 |
| 1:A:106:LEU:HD12 | 1:A:117:THR:HG21 | 1.96 | 0.47 |
| 1:A:218:LEU:HA | 1:A:221:GLN:H | 1.79 | 0.47 |
| 1:A:400:ALA:HB1 | 1:A:606:THR:CG2 | 2.45 | 0.47 |
| 1:A:602:PRO:O | 1:A:603:LEU:HD12 | 2.14 | 0.47 |
| 1:A:664:LEU:HD12 | 1:A:664:LEU:HA | 1.53 | 0.47 |
| 1:D:292:MET:HE1 | 1:D:309:PRO:CG | 2.45 | 0.47 |
| 1:D:640:LYS:HD2 | 1:D:646:PHE:O | 2.15 | 0.47 |
| 1:G:354:LEU:HD12 | 1:G:354:LEU:HA | 1.56 | 0.47 |
| 1:G:568:PRO:HD3 | 1:G:579:PHE:HA | 1.97 | 0.47 |
| 1:G:830:PRO:HG3 | 2:H:67:MET:HE2 | 1.96 | 0.47 |
| 1:J:106:LEU:HD12 | 1:J:106:LEU:HA | 1.80 | 0.47 |
| 1:J:436:MLY:HE3 | 1:J:626:TYR:HE1 | 1.77 | 0.47 |
| 1:J:567:LYS:HZ1 | 4:Y:92:ASN:ND2 | 2.05 | 0.47 |
| 1:J:695:LEU:HB3 | 1:J:701:LEU:HD22 | 1.97 | 0.47 |
| 1:J:830:PRO:CB | 2:K:67:MET:CE | 2.93 | 0.47 |
| 3:L:50:LEU:O | 3:L:53:PRO:CD | 2.63 | 0.47 |
| 1:M:248:MLY:HE2 | 1:M:250:ILE:HD11 | 1.96 | 0.47 |
| 1:M:346:ASP:O | 1:M:350:ALA:N | 2.46 | 0.47 |
| 1:M:725:ARG:NE | 1:M:733:PRO:CB | 1.95 | 0.47 |
| 1:M:791:GLN:OE1 | 3:O:116:GLU:N | 2.44 | 0.47 |
| 1:M:817:GLN:HB3 | 2:N:127:ARG:HD3 | 1.91 | 0.47 |
| 1:M:838:ILE:C | 1:M:840:PRO:HD2 | 2.35 | 0.47 |
| 1:P:406:VAL:CG1 | 1:P:407:GLY:H | 2.28 | 0.47 |
| 1:P:410:ASN:HD22 | 4:1:336:LYS:HE2 | 1.78 | 0.47 |
| 1:P:810:ARG:HG2 | 1:P:810:ARG:NH1 | 2.29 | 0.47 |
| 2:Q:112:ILE:CG2 | 2:Q:147:ASN:O | 2.62 | 0.47 |
| 4:3:162:ASN:OD1 | 4:3:277:THR:HG22 | 2.15 | 0.47 |
| 4:5:162:ASN:OD1 | 4:5:277:THR:HG22 | 2.15 | 0.47 |
| 4:8:290:ARG:HH22 | 4:V:202:THR:CG2 | 2.17 | 0.47 |
| 1:A:149:GLN:CB | 1:A:719:ASP:CA | 2.79 | 0.47 |
| 1:A:311:ASP:CB | 1:A:312:TYR:CE1 | 2.98 | 0.47 |
| 1:A:354:LEU:HD12 | 1:A:354:LEU:HA | 1.56 | 0.47 |
| 1:A:506:GLU:OE1 | 1:A:761:GLY:N | 2.48 | 0.47 |
| 1:A:529:PRO:HB2 | 4:8:354:GLN:HB3 | 1.97 | 0.47 |
| 1:A:629:GLU:CA | 1:A:643:GLY:C | 2.73 | 0.47 |
| 1:A:715:VAL:HG11 | 1:A:720:PHE:CD1 | 2.50 | 0.47 |
| 3:C:50:LEU:O | 3:C:53:PRO:CD | 2.63 | 0.47 |
| 1:D:106:LEU:HD12 | 1:D:117:THR:HG21 | 1.96 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:400:ALA:HB1 | 1:D:606:THR:CG2 | 2.45 | 0.47 |
| 1:D:813:ILE:HG22 | 2:E:127:ARG:HD2 | 1.97 | 0.47 |
| 2:E:117:LEU:HG | 2:E:147:ASN:HB3 | 1.94 | 0.47 |
| 1:G:30:MLY:HB3 | 1:G:31:PRO:HD2 | 1.97 | 0.47 |
| 1:G:214:MET:C | 1:G:340:ILE:CD1 | 2.82 | 0.47 |
| 1:G:311:ASP:CB | 1:G:312:TYR:CE1 | 2.98 | 0.47 |
| 1:G:400:ALA:HB1 | 1:G:606:THR:CG2 | 2.45 | 0.47 |
| 1:G:406:VAL:CG1 | 1:G:407:GLY:H | 2.28 | 0.47 |
| 1:G:795:ARG:HB3 | 3:I:35:ARG:NH1 | 2.27 | 0.47 |
| 1:G:817:GLN:NE2 | 2:H:128:PHE:HE1 | 2.06 | 0.47 |
| 1:G:838:ILE:C | 1:G:840:PRO:HD2 | 2.34 | 0.47 |
| 1:J:134:VAL:C | 1:J:136:ASN:H | 2.16 | 0.47 |
| 1:J:559:LEU:HD23 | 1:J:560:GLY:N | 2.30 | 0.47 |
| 1:J:757:GLN:HA | 1:J:776:GLU:CB | 2.45 | 0.47 |
| 1:M:218:LEU:CD2 | 1:M:222:ILE:CG1 | 2.85 | 0.47 |
| 1:M:799:MET:CE | 3:O:32:ASP:HB3 | 2.41 | 0.47 |
| 1:P:154:HIS:CE1 | 1:P:156:PHE:CE2 | 3.02 | 0.47 |
| 1:P:732:ILE:CG2 | 1:P:747:LEU:HD11 | 1.26 | 0.47 |
| 1:P:792:ALA:HB2 | 3:R:42:THR:CA | 2.45 | 0.47 |
| 1:P:806:MET:CB | 1:P:807:VAL:N | 2.76 | 0.47 |
| 3:R:50:LEU:O | 3:R:53:PRO:CD | 2.63 | 0.47 |
| 4:2:162:ASN:OD1 | 4:2:277:THR:HG22 | 2.15 | 0.47 |
| 4:6:162:ASN:OD1 | 4:6:277:THR:HG22 | 2.15 | 0.47 |
| 4:8:287:ILE:CB | 4:V:204:ALA:H | 2.13 | 0.47 |
| 4:X:162:ASN:OD1 | 4:X:277:THR:HG22 | 2.15 | 0.47 |
| 1:A:188:ASN:ND2 | 1:A:674:CYS:SG | 2.88 | 0.47 |
| 1:A:218:LEU:HD22 | 1:A:222:ILE:HG13 | 1.95 | 0.47 |
| 3:C:62:ALA:O | 3:C:63:ILE:HG13 | 2.13 | 0.47 |
| 1:D:568:PRO:HD3 | 1:D:579:PHE:HA | 1.97 | 0.47 |
| 1:D:642:LYS:HG3 | 4:9:23:GLY:CA | 2.31 | 0.47 |
| 1:G:10:PHE:CD2 | 1:G:17:LEU:HD23 | 2.49 | 0.47 |
| 1:G:84:MLY:HA | 1:G:723:ARG:NH1 | 2.30 | 0.47 |
| 1:G:93:MET:SD | 1:G:715:VAL:C | 2.93 | 0.47 |
| 1:G:188:ASN:ND2 | 1:G:674:CYS:SG | 2.89 | 0.47 |
| 1:G:218:LEU:CD2 | 1:G:222:ILE:CG1 | 2.85 | 0.47 |
| 1:G:524:GLU:HB3 | 1:G:528:MLY:HG2 | 1.96 | 0.47 |
| 1:J:83:PRO:C | 1:J:723:ARG:NH2 | 2.69 | 0.47 |
| 1:J:176:LEU:N | 1:J:176:LEU:CD1 | 2.75 | 0.47 |
| 1:J:715:VAL:CG1 | 1:J:720:PHE:HB2 | 2.45 | 0.47 |
| 1:M:406:VAL:CG1 | 1:M:407:GLY:N | 2.77 | 0.47 |
| 1:M:436:MLY:HE3 | 1:M:626:TYR:HE1 | 1.77 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:524:GLU:HB3 | 1:M:528:MLY:HG2 | 1.96 | 0.47 |
| 1:M:559:LEU:HD23 | 1:M:560:GLY:N | 2.30 | 0.47 |
| 1:M:637:LYS:HD2 | 4:Z:144:ALA:HB3 | 1.21 | 0.47 |
| 1:M:701:LEU:HD12 | 1:M:701:LEU:HA | 1.55 | 0.47 |
| 1:M:709:LYS:O | 1:M:768:MLY:CH1 | 2.63 | 0.47 |
| 1:M:724:TYR:HD1 | 1:M:727:LEU:CD1 | 2.27 | 0.47 |
| 1:P:106:LEU:HD12 | 1:P:117:THR:HG21 | 1.96 | 0.47 |
| 1:P:214:MET:C | 1:P:340:ILE:CD1 | 2.82 | 0.47 |
| 1:P:715:VAL:CG1 | 1:P:720:PHE:HB2 | 2.45 | 0.47 |
| 1:P:786:ILE:O | 1:P:790:THR:N | 2.48 | 0.47 |
| 1:P:791:GLN:NE2 | 3:R:116:GLU:N | 2.58 | 0.47 |
| 1:P:795:ARG:NE | 3:R:116:GLU:OE2 | 2.46 | 0.47 |
| 4:1:166:TYR:OH | 4:3:64:ILE:HD13 | 2.15 | 0.47 |
| 4:1:253:GLU:HA | 4:1:256:ARG:CG | 2.42 | 0.47 |
| 4:3:290:ARG:NE | 4:5:202:THR:HG21 | 2.15 | 0.47 |
| 4:Y:162:ASN:OD1 | 4:Y:277:THR:HG22 | 2.15 | 0.47 |
| 1:A:754:ASP:H | 1:A:775:LEU:HD11 | 1.80 | 0.46 |
| 2:E:163:ALA:O | 2:K:21:GLU:CA | 2.63 | 0.46 |
| 1:G:93:MET:HE1 | 1:G:764:MLY:HD2 | 1.96 | 0.46 |
| 1:G:206:LYS:CE | 1:G:217:THR:HG23 | 2.30 | 0.46 |
| 1:G:519:LEU:N | 1:G:519:LEU:CD1 | 2.77 | 0.46 |
| 1:G:715:VAL:CG1 | 1:G:720:PHE:HB2 | 2.45 | 0.46 |
| 1:G:783:LEU:N | 1:G:783:LEU:CD1 | 2.78 | 0.46 |
| 1:G:829:TRP:HZ3 | 2:H:84:PHE:CD1 | 2.32 | 0.46 |
| 1:J:218:LEU:HA | 1:J:221:GLN:H | 1.80 | 0.46 |
| 1:M:82:PRO:HG2 | 1:M:85:TYR:CE2 | 2.50 | 0.46 |
| 1:M:311:ASP:CB | 1:M:312:TYR:CE1 | 2.98 | 0.46 |
| 1:M:714:ARG:HD3 | 1:M:766:PHE:CE2 | 2.50 | 0.46 |
| 1:M:791:GLN:NE2 | 3:O:116:GLU:N | 2.61 | 0.46 |
| 1:M:817:GLN:HG2 | 2:N:127:ARG:CG | 2.45 | 0.46 |
| 1:M:831:TRP:NE1 | 2:N:67:MET:CG | 2.78 | 0.46 |
| 3:O:50:LEU:O | 3:O:53:PRO:CD | 2.63 | 0.46 |
| 1:P:418:THR:CB | 1:P:421:GLU:HG3 | 2.37 | 0.46 |
| 1:P:559:LEU:HD23 | 1:P:560:GLY:N | 2.30 | 0.46 |
| 4:4:288:ASP:OD2 | 4:6:203:THR:OG1 | 2.33 | 0.46 |
| 1:A:496:PHE:CE2 | 1:A:514:ASP:HA | 2.50 | 0.46 |
| 1:D:311:ASP:CB | 1:D:312:TYR:CE1 | 2.98 | 0.46 |
| 1:D:436:MLY:HE3 | 1:D:626:TYR:HE1 | 1.77 | 0.46 |
| 1:D:564:ASN:HD22 | 1:D:582:VAL:HB | 1.79 | 0.46 |
| 1:D:695:LEU:HB3 | 1:D:701:LEU:HD22 | 1.97 | 0.46 |
| 1:D:714:ARG:HD3 | 1:D:766:PHE:CE2 | 2.50 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:797:PHE:HD1 | 3:F:146:ILE:O | 1.99 | 0.46 |
| 1:D:804:ARG:NH2 | 3:F:149:VAL:HA | 2.30 | 0.46 |
| 2:E:114:LYS:N | 2:E:146:GLY:O | 2.40 | 0.46 |
| 3:F:53:PRO:O | 3:F:55:LYS:HG3 | 2.15 | 0.46 |
| 1:G:97:LEU:HD22 | 1:G:712:PRO:CB | 2.25 | 0.46 |
| 1:G:97:LEU:HD12 | 1:G:97:LEU:HA | 1.68 | 0.46 |
| 1:G:332:MET:H | 1:G:332:MET:HG2 | 1.52 | 0.46 |
| 1:G:664:LEU:HD12 | 1:G:664:LEU:HA | 1.53 | 0.46 |
| 1:G:695:LEU:HB3 | 1:G:701:LEU:HD22 | 1.97 | 0.46 |
| 1:G:784:ALA:O | 1:G:788:THR:CA | 2.61 | 0.46 |
| 1:G:821:ARG:NH2 | 2:H:127:ARG:CD | 2.78 | 0.46 |
| 1:J:642:LYS:HA | 4:W:21:PHE:C | 2.36 | 0.46 |
| 1:J:732:ILE:CG2 | 1:J:747:LEU:HD12 | 0.35 | 0.46 |
| 1:M:122:PHE:CE2 | 1:M:700:VAL:HA | 2.50 | 0.46 |
| 1:M:278:GLN:HE21 | 1:M:278:GLN:HB3 | 1.42 | 0.46 |
| 1:M:292:MET:HE1 | 1:M:309:PRO:HD3 | 1.97 | 0.46 |
| 1:M:400:ALA:HB1 | 1:M:606:THR:CG2 | 2.45 | 0.46 |
| 1:M:406:VAL:CG1 | 1:M:407:GLY:H | 2.28 | 0.46 |
| 1:M:540:CYS:N | 4:Z:349:LEU:HD11 | 2.31 | 0.46 |
| 1:P:538:GLU:OE1 | 4:1:355:MET:HE3 | 2.15 | 0.46 |
| 1:P:543:PRO:HD2 | 4:1:146:GLY:O | 2.15 | 0.46 |
| 1:P:714:ARG:HD3 | 1:P:766:PHE:CE2 | 2.50 | 0.46 |
| 1:P:724:TYR:HD1 | 1:P:727:LEU:CD1 | 2.27 | 0.46 |
| 4:2:203:THR:CA | 4:Z:287:ILE:HG21 | 2.45 | 0.46 |
| 4:6:299:MET:HE2 | 4:6:331:ALA:HB2 | 1.97 | 0.46 |
| 4:9:287:ILE:HA | 4:W:202:THR:HG21 | 1.59 | 0.46 |
| 4:Z:162:ASN:OD1 | 4:Z:277:THR:HG22 | 2.15 | 0.46 |
| 1:A:87:MLY:HD3 | 1:A:87:MLY:HH12 | 1.62 | 0.46 |
| 1:A:543:PRO:HD2 | 4:8:146:GLY:O | 2.15 | 0.46 |
| 1:A:831:TRP:CE3 | 2:B:34:ILE:HG12 | 2.47 | 0.46 |
| 1:D:723:ARG:HH11 | 1:D:723:ARG:HG3 | 1.79 | 0.46 |
| 3:F:52:ASN:CB | 3:F:53:PRO:CD | 2.92 | 0.46 |
| 1:G:42:HIS:O | 1:G:45:GLN:O | 2.33 | 0.46 |
| 1:G:732:ILE:CG2 | 1:G:747:LEU:CD1 | 0.65 | 0.46 |
| 1:G:834:LEU:HD23 | 2:H:34:ILE:HD11 | 1.95 | 0.46 |
| 1:J:154:HIS:CE1 | 1:J:156:PHE:CE2 | 3.02 | 0.46 |
| 1:J:265:ILE:CG2 | 1:J:266:GLU:N | 2.79 | 0.46 |
| 1:J:543:PRO:HD2 | 4:W:146:GLY:O | 2.16 | 0.46 |
| 1:J:839:MLY:HH13 | 2:K:159:HIS:HD2 | 1.80 | 0.46 |
| 2:K:140:PHE:HA | 2:K:141:PRO:HD2 | 1.56 | 0.46 |
| 1:M:543:PRO:CD | 4:Z:143:TYR:O | 2.64 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:543:PRO:HD2 | 4:Z:146:GLY:O | 2.16 | 0.46 |
| 1:M:636:LYS:O | 4:Z:144:ALA:HB1 | 2.14 | 0.46 |
| 1:M:640:LYS:C | 4:Z:23:GLY:C | 2.74 | 0.46 |
| 1:M:642:LYS:HA | 4:Z:21:PHE:C | 2.36 | 0.46 |
| 1:M:732:ILE:CG2 | 1:M:747:LEU:HD12 | 0.35 | 0.46 |
| 1:P:374:GLN:NE2 | 1:P:403:TYR:CE1 | 2.84 | 0.46 |
| 1:P:728:ASN:OD1 | 3:R:93:VAL:HG11 | 2.14 | 0.46 |
| 4:2:6:THR:HG22 | 4:2:101:HIS:HA | 1.98 | 0.46 |
| 4:4:253:GLU:HA | 4:4:256:ARG:CG | 2.42 | 0.46 |
| 4:7:162:ASN:OD1 | 4:7:277:THR:HG22 | 2.15 | 0.46 |
| 4:9:162:ASN:OD1 | 4:9:277:THR:HG22 | 2.15 | 0.46 |
| 4:X:6:THR:HG22 | 4:X:101:HIS:HA | 1.98 | 0.46 |
| 4:X:299:MET:HE2 | 4:X:331:ALA:HB2 | 1.97 | 0.46 |
| 1:A:82:PRO:HG2 | 1:A:85:TYR:CE2 | 2.50 | 0.46 |
| 1:A:206:LYS:CE | 1:A:217:THR:HG23 | 2.29 | 0.46 |
| 1:A:502:GLU:OE1 | 1:A:763:THR:N | 2.48 | 0.46 |
| 1:A:559:LEU:HD23 | 1:A:560:GLY:N | 2.30 | 0.46 |
| 1:A:564:ASN:HD22 | 1:A:582:VAL:HB | 1.79 | 0.46 |
| 1:A:752:ASP:OD2 | 1:A:782:MLY:HG2 | 2.15 | 0.46 |
| 1:D:218:LEU:HD22 | 1:D:222:ILE:HG13 | 1.95 | 0.46 |
| 1:D:374:GLN:NE2 | 1:D:403:TYR:CE1 | 2.84 | 0.46 |
| 1:G:82:PRO:HG2 | 1:G:85:TYR:CE2 | 2.50 | 0.46 |
| 1:G:496:PHE:CE2 | 1:G:514:ASP:HA | 2.50 | 0.46 |
| 1:G:817:GLN:CB | 2:H:127:ARG:CD | 2.93 | 0.46 |
| 1:J:218:LEU:HD22 | 1:J:222:ILE:HG13 | 1.95 | 0.46 |
| 1:J:354:LEU:HD12 | 1:J:354:LEU:HA | 1.56 | 0.46 |
| 1:J:639:GLY:CA | 4:W:344:SER:O | 2.39 | 0.46 |
| 1:J:732:ILE:H | 1:J:733:PRO:HD2 | 1.74 | 0.46 |
| 1:M:42:HIS:O | 1:M:45:GLN:O | 2.33 | 0.46 |
| 1:M:519:LEU:N | 1:M:519:LEU:CD1 | 2.77 | 0.46 |
| 1:M:695:LEU:HB3 | 1:M:701:LEU:HD22 | 1.97 | 0.46 |
| 1:M:715:VAL:CG1 | 1:M:720:PHE:HB2 | 2.45 | 0.46 |
| 1:M:793:ARG:O | 1:M:797:PHE:N | 2.39 | 0.46 |
| 1:P:87:MLY:HH12 | 1:P:87:MLY:HD3 | 1.61 | 0.46 |
| 1:P:221:GLN:HG2 | 1:P:221:GLN:H | 1.47 | 0.46 |
| 1:P:549:SER:CB | 4:3:43:VAL:HG11 | 2.45 | 0.46 |
| 4:Z:6:THR:HG22 | 4:Z:101:HIS:HA | 1.98 | 0.46 |
| 1:A:640:LYS:HB3 | 1:A:645:SER:CB | 2.42 | 0.46 |
| 1:A:732:ILE:CG2 | 1:A:747:LEU:CD1 | 0.65 | 0.46 |
| 1:A:798:LEU:HD12 | 1:A:798:LEU:HA | 1.37 | 0.46 |
| 1:A:800:ARG:O | 3:C:149:VAL:HG21 | 2.09 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:361:TYR:O | 1:D:364:LEU:HB2 | 2.16 | 0.46 |
| 1:D:793:ARG:NH2 | 3:F:147:MET:HE1 | 2.29 | 0.46 |
| 1:G:559:LEU:HD23 | 1:G:560:GLY:N | 2.30 | 0.46 |
| 1:J:311:ASP:CB | 1:J:312:TYR:CE1 | 2.98 | 0.46 |
| 1:J:374:GLN:NE2 | 1:J:403:TYR:CE1 | 2.84 | 0.46 |
| 1:J:400:ALA:HB1 | 1:J:606:THR:CG2 | 2.45 | 0.46 |
| 1:J:406:VAL:CG1 | 1:J:407:GLY:H | 2.28 | 0.46 |
| 1:J:701:LEU:HD12 | 1:J:701:LEU:HA | 1.55 | 0.46 |
| 1:J:733:PRO:O | 1:J:737:PHE:CE1 | 2.53 | 0.46 |
| 1:M:188:ASN:ND2 | 1:M:674:CYS:SG | 2.88 | 0.46 |
| 1:M:214:MET:C | 1:M:340:ILE:CD1 | 2.82 | 0.46 |
| 1:M:782:MLY:O | 1:M:786:ILE:CD1 | 2.63 | 0.46 |
| 1:P:530:MET:HA | 4:1:354:GLN:CD | 2.11 | 0.46 |
| 1:P:642:LYS:HA | 4:1:21:PHE:C | 2.36 | 0.46 |
| 4:2:322:PRO:HB2 | 4:4:244:ASP:CB | 2.26 | 0.46 |
| 1:A:42:HIS:O | 1:A:45:GLN:O | 2.33 | 0.46 |
| 1:A:448:GLN:C | 1:A:450:ASP:H | 2.19 | 0.46 |
| 1:A:543:PRO:CD | 4:8:143:TYR:O | 2.63 | 0.46 |
| 1:A:637:LYS:HD2 | 4:8:144:ALA:HB3 | 1.21 | 0.46 |
| 1:A:732:ILE:HG23 | 1:A:747:LEU:HD12 | 0.94 | 0.46 |
| 1:D:42:HIS:O | 1:D:45:GLN:O | 2.33 | 0.46 |
| 1:D:524:GLU:HB3 | 1:D:528:MLY:HG2 | 1.97 | 0.46 |
| 1:D:642:LYS:HA | 4:9:21:PHE:C | 2.36 | 0.46 |
| 1:D:664:LEU:HD12 | 1:D:664:LEU:HA | 1.53 | 0.46 |
| 1:D:724:TYR:HD1 | 1:D:727:LEU:CD1 | 2.27 | 0.46 |
| 1:D:747:LEU:HD21 | 1:D:782:MLY:HH11 | 1.90 | 0.46 |
| 2:E:139:ALA:C | 2:E:141:PRO:HD3 | 2.33 | 0.46 |
| 1:G:530:MET:HE3 | 4:V:354:GLN:CG | 2.42 | 0.46 |
| 1:G:629:GLU:HG2 | 1:G:643:GLY:C | 2.36 | 0.46 |
| 1:J:188:ASN:ND2 | 1:J:674:CYS:SG | 2.88 | 0.46 |
| 1:J:496:PHE:CE2 | 1:J:514:ASP:HA | 2.50 | 0.46 |
| 1:J:543:PRO:CD | 4:W:143:TYR:O | 2.64 | 0.46 |
| 1:J:798:LEU:CG | 3:L:126:LEU:HD11 | 2.37 | 0.46 |
| 1:M:361:TYR:O | 1:M:364:LEU:HB2 | 2.16 | 0.46 |
| 1:M:374:GLN:NE2 | 1:M:403:TYR:CE1 | 2.84 | 0.46 |
| 1:M:529:PRO:HB2 | 4:Z:354:GLN:HB3 | 1.98 | 0.46 |
| 2:N:144:VAL:HG12 | 2:N:153:ILE:HD13 | 1.92 | 0.46 |
| 1:P:188:ASN:ND2 | 1:P:674:CYS:SG | 2.88 | 0.46 |
| 1:P:664:LEU:HD12 | 1:P:664:LEU:HA | 1.52 | 0.46 |
| 4:4:162:ASN:OD1 | 4:4:277:THR:HG22 | 2.15 | 0.46 |
| 1:A:361:TYR:O | 1:A:364:LEU:HB2 | 2.16 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:783:LEU:N | 1:A:783:LEU:CD1 | 2.79 | 0.46 |
| 1:D:543:PRO:HD2 | 4:9:146:GLY:O | 2.15 | 0.46 |
| 1:D:642:LYS:HB2 | 4:9:24:ASP:O | 1.88 | 0.46 |
| 1:D:810:ARG:HG2 | 1:D:810:ARG:NH1 | 2.29 | 0.46 |
| 2:E:88:LEU:HB3 | 2:E:91:ALA:HB2 | 1.98 | 0.46 |
| 1:G:542:PHE:CD2 | 4:V:143:TYR:CD1 | 3.03 | 0.46 |
| 1:G:543:PRO:CD | 4:V:143:TYR:O | 2.64 | 0.46 |
| 1:J:361:TYR:O | 1:J:364:LEU:HB2 | 2.16 | 0.46 |
| 1:J:524:GLU:HB3 | 1:J:528:MLY:HG2 | 1.96 | 0.46 |
| 1:M:97:LEU:HD12 | 1:M:97:LEU:HA | 1.68 | 0.46 |
| 1:M:335:ASP:OD1 | 1:M:348:MLY:NZ | 2.49 | 0.46 |
| 2:N:88:LEU:HB3 | 2:N:91:ALA:HB2 | 1.98 | 0.46 |
| 1:P:637:LYS:HD2 | 4:1:144:ALA:HB3 | 1.20 | 0.46 |
| 1:P:643:GLY:CA | 4:1:24:ASP:OD1 | 2.62 | 0.46 |
| 4:5:299:MET:HE2 | 4:5:331:ALA:HB2 | 1.96 | 0.46 |
| 4:8:6:THR:HG22 | 4:8:101:HIS:HA | 1.98 | 0.46 |
| 4:V:190:MET:O | 4:V:194:THR:HG23 | 2.16 | 0.46 |
| 4:Z:299:MET:HE2 | 4:Z:331:ALA:HB2 | 1.98 | 0.46 |
| 1:A:519:LEU:N | 1:A:519:LEU:CD1 | 2.77 | 0.46 |
| 1:A:629:GLU:HG2 | 1:A:643:GLY:C | 2.35 | 0.46 |
| 1:A:640:LYS:C | 4:8:23:GLY:C | 2.74 | 0.46 |
| 1:A:695:LEU:HB3 | 1:A:701:LEU:HD22 | 1.97 | 0.46 |
| 2:B:114:LYS:CG | 2:B:146:GLY:HA2 | 2.46 | 0.46 |
| 1:D:218:LEU:HA | 1:D:221:GLN:HG3 | 1.71 | 0.46 |
| 1:D:346:ASP:O | 1:D:350:ALA:N | 2.46 | 0.46 |
| 1:D:559:LEU:HD23 | 1:D:560:GLY:N | 2.30 | 0.46 |
| 1:D:793:ARG:CZ | 3:F:87:PHE:HE1 | 2.29 | 0.46 |
| 2:E:114:LYS:CG | 2:E:146:GLY:HA2 | 2.46 | 0.46 |
| 1:G:330:GLU:H | 1:G:330:GLU:HG2 | 1.55 | 0.46 |
| 1:G:346:ASP:O | 1:G:350:ALA:N | 2.46 | 0.46 |
| 1:J:139:VAL:HG12 | 1:J:143:TYR:HD2 | 1.81 | 0.46 |
| 1:J:418:THR:CG2 | 1:J:419:VAL:N | 2.79 | 0.46 |
| 1:J:714:ARG:HD3 | 1:J:766:PHE:CE2 | 2.50 | 0.46 |
| 1:J:725:ARG:NE | 1:J:733:PRO:CB | 1.95 | 0.46 |
| 2:K:88:LEU:HB3 | 2:K:91:ALA:HB2 | 1.98 | 0.46 |
| 2:K:137:TRP:CA | 2:K:145:ALA:HB2 | 2.37 | 0.46 |
| 1:M:292:MET:HE1 | 1:M:309:PRO:CG | 2.46 | 0.46 |
| 1:M:448:GLN:C | 1:M:450:ASP:H | 2.19 | 0.46 |
| 1:P:265:ILE:CG2 | 1:P:266:GLU:N | 2.79 | 0.46 |
| 1:P:322:VAL:HB | 1:P:325:ILE:HG13 | 1.98 | 0.46 |
| 1:P:529:PRO:HB2 | 4:1:354:GLN:HB3 | 1.98 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:P:640:LYS:C | 4:1:23:GLY:C | 2.74 | 0.46 |
| 4:1:287:ILE:HG21 | 4:3:203:THR:CA | 2.43 | 0.46 |
| 4:9:299:MET:HE2 | 4:9:331:ALA:HB2 | 1.96 | 0.46 |
| 4:V:6:THR:HG22 | 4:V:101:HIS:HA | 1.98 | 0.46 |
| 1:A:206:LYS:HD3 | 1:A:217:THR:OG1 | 2.16 | 0.46 |
| 1:A:701:LEU:HA | 1:A:701:LEU:HD12 | 1.54 | 0.46 |
| 1:A:715:VAL:CG1 | 1:A:720:PHE:HB2 | 2.45 | 0.46 |
| 1:D:89:GLU:CD | 1:D:153:PRO:HD2 | 2.36 | 0.46 |
| 1:D:210:GLN:C | 1:D:211:SER:HG | 2.15 | 0.46 |
| 1:D:265:ILE:CG2 | 1:D:266:GLU:N | 2.78 | 0.46 |
| 1:D:406:VAL:CG1 | 1:D:407:GLY:H | 2.28 | 0.46 |
| 1:G:265:ILE:CG2 | 1:G:266:GLU:N | 2.79 | 0.46 |
| 1:G:374:GLN:NE2 | 1:G:403:TYR:CE1 | 2.84 | 0.46 |
| 1:G:449:LEU:HD12 | 1:G:449:LEU:HA | 1.60 | 0.46 |
| 1:G:714:ARG:HD3 | 1:G:766:PHE:CE2 | 2.51 | 0.46 |
| 1:G:715:VAL:HG11 | 1:G:720:PHE:CD1 | 2.50 | 0.46 |
| 3:I:50:LEU:O | 3:I:53:PRO:CD | 2.63 | 0.46 |
| 1:J:629:GLU:CB | 1:J:645:SER:N | 2.73 | 0.46 |
| 2:K:114:LYS:CG | 2:K:146:GLY:HA2 | 2.46 | 0.46 |
| 1:M:136:ASN:O | 1:M:139:VAL:N | 2.47 | 0.46 |
| 1:M:265:ILE:CG2 | 1:M:266:GLU:N | 2.79 | 0.46 |
| 1:M:797:PHE:HD1 | 3:O:149:VAL:HG13 | 1.80 | 0.46 |
| 1:M:819:ASN:CB | 2:N:90:GLY:O | 2.58 | 0.46 |
| 1:P:89:GLU:CD | 1:P:153:PRO:HD2 | 2.37 | 0.46 |
| 1:P:122:PHE:CE2 | 1:P:700:VAL:HA | 2.50 | 0.46 |
| 1:P:335:ASP:OD1 | 1:P:348:MLY:NZ | 2.49 | 0.46 |
| 1:P:640:LYS:C | 1:P:645:SER:HG | 2.14 | 0.46 |
| 4:5:366:GLY:O | 4:5:369:ILE:HG22 | 2.16 | 0.46 |
| 4:8:190:MET:O | 4:8:194:THR:HG23 | 2.16 | 0.46 |
| 4:8:366:GLY:O | 4:8:369:ILE:HG22 | 2.16 | 0.46 |
| 4:9:253:GLU:HA | 4:9:256:ARG:CG | 2.42 | 0.46 |
| 4:V:366:GLY:O | 4:V:369:ILE:HG22 | 2.16 | 0.46 |
| 1:A:292:MET:HE1 | 1:A:309:PRO:CG | 2.45 | 0.46 |
| 1:A:408:VAL:HG22 | 1:A:636:LYS:HG2 | 1.51 | 0.46 |
| 1:A:540:CYS:N | 4:8:349:LEU:HD11 | 2.31 | 0.46 |
| 1:D:496:PHE:CE2 | 1:D:514:ASP:HA | 2.50 | 0.46 |
| 1:D:543:PRO:CD | 4:9:143:TYR:O | 2.64 | 0.46 |
| 1:D:715:VAL:CG1 | 1:D:720:PHE:HB2 | 2.46 | 0.46 |
| 1:G:206:LYS:HD3 | 1:G:217:THR:OG1 | 2.16 | 0.46 |
| 1:G:214:MET:HA | 1:G:340:ILE:CD1 | 2.41 | 0.46 |
| 1:G:278:GLN:HE21 | 1:G:278:GLN:HB3 | 1.42 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:529:PRO:HB2 | 4:V:354:GLN:HB3 | 1.98 | 0.46 |
| 1:G:540:CYS:N | 4:V:349:LEU:HD11 | 2.31 | 0.46 |
| 1:J:179:GLY:O | 1:J:185:LYS:HE2 | 2.17 | 0.46 |
| 1:J:485:GLU:OE1 | 1:J:583:HIS:ND1 | 2.49 | 0.46 |
| 1:M:97:LEU:HD21 | 1:M:712:PRO:HB3 | 1.98 | 0.46 |
| 1:M:322:VAL:HB | 1:M:325:ILE:HG13 | 1.98 | 0.46 |
| 1:M:659:MLY:HH22 | 1:M:659:MLY:HD2 | 1.42 | 0.46 |
| 1:P:400:ALA:HB1 | 1:P:606:THR:CG2 | 2.45 | 0.46 |
| 2:Q:144:VAL:HG12 | 2:Q:153:ILE:HD13 | 1.92 | 0.46 |
| 4:2:366:GLY:O | 4:2:369:ILE:HG22 | 2.16 | 0.46 |
| 4:8:324:THR:N | 4:V:245:GLY:CA | 2.69 | 0.46 |
| 1:A:30:MLY:HB3 | 1:A:31:PRO:HD2 | 1.97 | 0.45 |
| 1:A:136:ASN:HA | 1:A:137:PRO:HD3 | 1.50 | 0.45 |
| 1:A:218:LEU:HA | 1:A:221:GLN:HG3 | 1.71 | 0.45 |
| 1:A:265:ILE:CG2 | 1:A:266:GLU:N | 2.79 | 0.45 |
| 1:A:464:ILE:CG2 | 1:A:465:ALA:N | 2.79 | 0.45 |
| 1:D:82:PRO:HG2 | 1:D:85:TYR:CE2 | 2.51 | 0.45 |
| 1:D:88:ILE:HG21 | 1:D:88:ILE:HD12 | 1.78 | 0.45 |
| 1:D:326:ASP:O | 1:D:330:GLU:HG2 | 2.16 | 0.45 |
| 1:D:793:ARG:HH21 | 3:F:147:MET:HE3 | 1.73 | 0.45 |
| 1:G:99:GLU:N | 1:G:100:PRO:CD | 2.79 | 0.45 |
| 1:G:292:MET:HE1 | 1:G:309:PRO:CG | 2.47 | 0.45 |
| 1:G:335:ASP:OD1 | 1:G:348:MLY:NZ | 2.49 | 0.45 |
| 1:G:543:PRO:HD2 | 4:V:146:GLY:O | 2.15 | 0.45 |
| 1:G:817:GLN:CG | 2:H:128:PHE:CE1 | 2.98 | 0.45 |
| 1:J:42:HIS:O | 1:J:45:GLN:O | 2.33 | 0.45 |
| 1:J:136:ASN:HA | 1:J:137:PRO:HD3 | 1.49 | 0.45 |
| 1:J:540:CYS:N | 4:W:349:LEU:HD11 | 2.31 | 0.45 |
| 1:J:783:LEU:N | 1:J:783:LEU:CD1 | 2.78 | 0.45 |
| 1:M:89:GLU:CD | 1:M:153:PRO:HD2 | 2.37 | 0.45 |
| 1:M:629:GLU:HG2 | 1:M:643:GLY:C | 2.35 | 0.45 |
| 1:M:720:PHE:CE1 | 1:M:772:LEU:HD21 | 2.50 | 0.45 |
| 1:M:732:ILE:CG2 | 1:M:747:LEU:CD1 | 0.65 | 0.45 |
| 1:M:783:LEU:CD1 | 1:M:783:LEU:N | 2.78 | 0.45 |
| 1:P:793:ARG:CZ | 3:R:40:ASN:ND2 | 2.71 | 0.45 |
| 1:P:804:ARG:O | 1:P:808:GLU:HG3 | 2.16 | 0.45 |
| 1:P:835:PHE:O | 1:P:839:MLY:N | 2.49 | 0.45 |
| 2:Q:112:ILE:O | 2:Q:148:VAL:HA | 2.17 | 0.45 |
| 4:4:6:THR:HG22 | 4:4:101:HIS:HA | 1.98 | 0.45 |
| 4:5:6:THR:HG22 | 4:5:101:HIS:HA | 1.97 | 0.45 |
| 4:X:290:ARG:NH2 | 4:Z:201:VAL:HG21 | 2.30 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:X:366:GLY:O | 4:X:369:ILE:HG22 | 2.16 | 0.45 |
| 1:A:136:ASN:O | 1:A:139:VAL:N | 2.47 | 0.45 |
| 1:A:714:ARG:HD3 | 1:A:766:PHE:CE2 | 2.51 | 0.45 |
| 1:D:411:GLU:H | 4:9:333:PRO:HB2 | 1.80 | 0.45 |
| 1:D:530:MET:HA | 4:9:354:GLN:CD | 2.11 | 0.45 |
| 1:D:639:GLY:CA | 4:9:344:SER:O | 2.40 | 0.45 |
| 1:D:732:ILE:CG2 | 1:D:747:LEU:CD1 | 0.65 | 0.45 |
| 1:D:818:TYR:HB3 | 2:E:90:GLY:H | 1.77 | 0.45 |
| 2:E:162:ASP:O | 2:K:21:GLU:HB3 | 2.13 | 0.45 |
| 1:G:640:LYS:HB3 | 1:G:645:SER:CB | 2.42 | 0.45 |
| 1:G:817:GLN:NE2 | 2:H:128:PHE:CD1 | 2.77 | 0.45 |
| 1:J:335:ASP:OD1 | 1:J:348:MLY:NZ | 2.49 | 0.45 |
| 1:J:529:PRO:HB2 | 4:W:354:GLN:HB3 | 1.98 | 0.45 |
| 1:J:540:CYS:C | 4:W:349:LEU:HD21 | 2.36 | 0.45 |
| 2:K:144:VAL:HG12 | 2:K:153:ILE:HD11 | 1.75 | 0.45 |
| 1:M:410:ASN:HA | 4:Z:334:GLU:HB3 | 1.29 | 0.45 |
| 1:M:835:PHE:O | 1:M:839:MLY:N | 2.49 | 0.45 |
| 2:N:121:LEU:O | 2:N:128:PHE:CG | 2.61 | 0.45 |
| 2:N:139:ALA:C | 2:N:141:PRO:HD3 | 2.33 | 0.45 |
| 3:O:53:PRO:O | 3:O:55:LYS:HG3 | 2.15 | 0.45 |
| 1:P:206:LYS:HD3 | 1:P:217:THR:OG1 | 2.16 | 0.45 |
| 3:R:49:ILE:CA | 3:R:52:ASN:ND2 | 2.54 | 0.45 |
| 4:2:324:THR:OG1 | 4:4:244:ASP:HB3 | 2.16 | 0.45 |
| 4:3:287:ILE:HG13 | 4:5:202:THR:HG22 | 1.89 | 0.45 |
| 4:4:299:MET:HE2 | 4:4:331:ALA:HB2 | 1.98 | 0.45 |
| 4:6:190:MET:O | 4:6:194:THR:HG23 | 2.16 | 0.45 |
| 4:Z:366:GLY:O | 4:Z:369:ILE:HG22 | 2.16 | 0.45 |
| 1:A:99:GLU:N | 1:A:100:PRO:CD | 2.79 | 0.45 |
| 1:G:410:ASN:HA | 4:V:334:GLU:HB3 | 1.29 | 0.45 |
| 1:G:835:PHE:O | 1:G:839:MLY:N | 2.49 | 0.45 |
| 1:J:82:PRO:HG2 | 1:J:85:TYR:CE2 | 2.51 | 0.45 |
| 1:J:89:GLU:CD | 1:J:153:PRO:HD2 | 2.37 | 0.45 |
| 1:J:186:THR:O | 1:J:190:MLY:HG2 | 2.17 | 0.45 |
| 1:J:667:THR:O | 1:J:669:PRO:HD3 | 2.17 | 0.45 |
| 1:M:99:GLU:N | 1:M:100:PRO:CD | 2.80 | 0.45 |
| 1:M:723:ARG:CG | 1:M:723:ARG:NH1 | 2.79 | 0.45 |
| 1:M:829:TRP:CZ2 | 2:N:87:LYS:CE | 2.78 | 0.45 |
| 1:P:82:PRO:HG2 | 1:P:85:TYR:CE2 | 2.50 | 0.45 |
| 1:P:311:ASP:CB | 1:P:312:TYR:CE1 | 2.98 | 0.45 |
| 1:P:485:GLU:OE1 | 1:P:583:HIS:ND1 | 2.49 | 0.45 |
| 1:P:488:GLN:O | 1:P:491:PHE:HB3 | 2.17 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:P:524:GLU:HB3 | 1:P:528:MLY:HG2 | 1.97 | 0.45 |
| 2:Q:137:TRP:CZ3 | 2:Q:145:ALA:N | 2.81 | 0.45 |
| 4:4:190:MET:O | 4:4:194:THR:HG23 | 2.16 | 0.45 |
| 4:V:223:PHE:CD2 | 4:V:259:GLU:HG3 | 2.52 | 0.45 |
| 4:Y:6:THR:HG22 | 4:Y:101:HIS:HA | 1.98 | 0.45 |
| 4:Z:223:PHE:CD2 | 4:Z:259:GLU:HG3 | 2.51 | 0.45 |
| 1:A:89:GLU:CD | 1:A:153:PRO:HD2 | 2.37 | 0.45 |
| 1:A:322:VAL:CG1 | 1:A:325:ILE:HD11 | 2.47 | 0.45 |
| 1:A:330:GLU:O | 1:A:333:ALA:HB3 | 2.17 | 0.45 |
| 1:A:374:GLN:NE2 | 1:A:403:TYR:CE1 | 2.84 | 0.45 |
| 1:A:642:LYS:NZ | 4:8:340:TRP:O | 2.50 | 0.45 |
| 1:A:768:MLY:HB3 | 1:A:771:LEU:CG | 2.43 | 0.45 |
| 1:A:835:PHE:O | 1:A:839:MLY:N | 2.49 | 0.45 |
| 2:B:137:TRP:CA | 2:B:145:ALA:CB | 2.82 | 0.45 |
| 1:D:322:VAL:HB | 1:D:325:ILE:HG13 | 1.98 | 0.45 |
| 1:D:529:PRO:HB2 | 4:9:354:GLN:HB3 | 1.98 | 0.45 |
| 1:D:732:ILE:HD12 | 1:D:782:MLY:CH1 | 2.46 | 0.45 |
| 1:D:793:ARG:NH2 | 3:F:87:PHE:HE1 | 2.15 | 0.45 |
| 2:E:112:ILE:O | 2:E:148:VAL:HA | 2.17 | 0.45 |
| 1:G:568:PRO:CG | 1:G:578:HIS:H | 2.30 | 0.45 |
| 1:J:448:GLN:C | 1:J:450:ASP:H | 2.19 | 0.45 |
| 1:J:723:ARG:CG | 1:J:723:ARG:NH1 | 2.79 | 0.45 |
| 1:J:725:ARG:CG | 1:J:733:PRO:HA | 2.43 | 0.45 |
| 1:J:835:PHE:O | 1:J:839:MLY:N | 2.49 | 0.45 |
| 1:M:30:MLY:HB3 | 1:M:31:PRO:HD2 | 1.97 | 0.45 |
| 1:M:326:ASP:O | 1:M:330:GLU:HG2 | 2.16 | 0.45 |
| 1:M:408:VAL:HG22 | 1:M:636:LYS:HG2 | 1.51 | 0.45 |
| 1:M:612:GLN:NE2 | 1:M:627:GLY:H | 2.15 | 0.45 |
| 1:M:753:VAL:CG1 | 1:M:771:LEU:HD11 | 2.44 | 0.45 |
| 1:M:795:ARG:HH22 | 3:O:116:GLU:HG2 | 1.74 | 0.45 |
| 1:M:795:ARG:NH1 | 3:O:116:GLU:OE2 | 2.46 | 0.45 |
| 1:P:139:VAL:HG12 | 1:P:143:TYR:HD2 | 1.81 | 0.45 |
| 1:P:186:THR:O | 1:P:190:MLY:HG2 | 2.17 | 0.45 |
| 1:P:278:GLN:HE21 | 1:P:278:GLN:HB3 | 1.42 | 0.45 |
| 1:P:411:GLU:H | 4:1:333:PRO:HB2 | 1.81 | 0.45 |
| 1:P:540:CYS:N | 4:1:349:LEU:HD11 | 2.31 | 0.45 |
| 1:P:636:LYS:O | 4:1:144:ALA:HB1 | 2.14 | 0.45 |
| 4:1:32:PRO:HB2 | 4:1:34:ILE:HD11 | 1.98 | 0.45 |
| 4:2:190:MET:O | 4:2:194:THR:HG23 | 2.16 | 0.45 |
| 4:3:366:GLY:O | 4:3:369:ILE:HG22 | 2.16 | 0.45 |
| 4:5:223:PHE:CD2 | 4:5:259:GLU:HG3 | 2.52 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:W:6:THR:HG22 | 4:W:101:HIS:HA | 1.98 | 0.45 |
| 1:A:149:GLN:CB | 1:A:719:ASP:CG | 2.83 | 0.45 |
| 2:B:112:ILE:O | 2:B:148:VAL:HA | 2.17 | 0.45 |
| 1:D:139:VAL:HG12 | 1:D:143:TYR:HD2 | 1.81 | 0.45 |
| 1:D:144:ARG:HA | 1:D:144:ARG:HD2 | 1.78 | 0.45 |
| 1:D:206:LYS:HD3 | 1:D:217:THR:OG1 | 2.16 | 0.45 |
| 1:D:411:GLU:H | 4:9:333:PRO:CB | 2.30 | 0.45 |
| 1:D:464:ILE:CG2 | 1:D:465:ALA:N | 2.80 | 0.45 |
| 1:D:485:GLU:OE1 | 1:D:583:HIS:ND1 | 2.49 | 0.45 |
| 1:D:642:LYS:NZ | 4:9:340:TRP:O | 2.50 | 0.45 |
| 1:D:794:CYS:O | 1:D:797:PHE:HB3 | 2.17 | 0.45 |
| 1:D:813:ILE:CG1 | 2:E:128:PHE:CE1 | 3.00 | 0.45 |
| 1:D:823:PHE:HE1 | 2:E:161:GLU:N | 2.14 | 0.45 |
| 1:G:330:GLU:O | 1:G:333:ALA:HB3 | 2.17 | 0.45 |
| 1:G:361:TYR:O | 1:G:364:LEU:HB2 | 2.16 | 0.45 |
| 1:G:464:ILE:CG2 | 1:G:465:ALA:N | 2.80 | 0.45 |
| 1:G:642:LYS:HB3 | 4:V:24:ASP:HB2 | 1.38 | 0.45 |
| 1:G:836:PHE:CE2 | 2:H:160:GLY:N | 2.77 | 0.45 |
| 2:H:88:LEU:HB3 | 2:H:91:ALA:HB2 | 1.98 | 0.45 |
| 2:H:112:ILE:O | 2:H:148:VAL:HA | 2.17 | 0.45 |
| 1:J:30:MLY:HB3 | 1:J:31:PRO:HD2 | 1.97 | 0.45 |
| 1:J:326:ASP:O | 1:J:330:GLU:HG2 | 2.16 | 0.45 |
| 1:M:783:LEU:O | 1:M:786:ILE:HG13 | 2.17 | 0.45 |
| 1:M:794:CYS:O | 1:M:797:PHE:HB3 | 2.17 | 0.45 |
| 1:P:418:THR:CG2 | 1:P:419:VAL:N | 2.79 | 0.45 |
| 1:P:449:LEU:HD12 | 1:P:449:LEU:HA | 1.61 | 0.45 |
| 1:P:464:ILE:CG2 | 1:P:465:ALA:N | 2.80 | 0.45 |
| 1:P:543:PRO:CD | 4:1:143:TYR:O | 2.64 | 0.45 |
| 4:2:299:MET:HE2 | 4:2:331:ALA:HB2 | 1.99 | 0.45 |
| 4:3:223:PHE:CD2 | 4:3:259:GLU:HG3 | 2.52 | 0.45 |
| 4:7:366:GLY:O | 4:7:369:ILE:HG22 | 2.16 | 0.45 |
| 4:8:223:PHE:CD2 | 4:8:259:GLU:HG3 | 2.52 | 0.45 |
| 4:9:190:MET:O | 4:9:194:THR:HG23 | 2.16 | 0.45 |
| 4:9:287:ILE:CB | 4:W:204:ALA:H | 2.13 | 0.45 |
| 4:W:32:PRO:HB2 | 4:W:34:ILE:HD11 | 1.98 | 0.45 |
| 4:X:291:LYS:HE3 | 4:Z:243:PRO:CD | 2.43 | 0.45 |
| 4:Y:32:PRO:HB2 | 4:Y:34:ILE:HD11 | 1.98 | 0.45 |
| 4:Z:171:LEU:HA | 4:Z:172:PRO:HD2 | 1.84 | 0.45 |
| 1:A:139:VAL:HG12 | 1:A:143:TYR:HD2 | 1.81 | 0.45 |
| 1:A:163:TYR:O | 1:A:166:MET:HB3 | 2.17 | 0.45 |
| 1:A:612:GLN:NE2 | 1:A:627:GLY:H | 2.14 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:642:LYS:HA | 4:8:21:PHE:C | 2.36 | 0.45 |
| 2:B:88:LEU:HB3 | 2:B:91:ALA:HB2 | 1.97 | 0.45 |
| 1:D:179:GLY:O | 1:D:185:LYS:HE2 | 2.17 | 0.45 |
| 1:D:206:LYS:CE | 1:D:217:THR:HG23 | 2.30 | 0.45 |
| 1:D:418:THR:CG2 | 1:D:419:VAL:N | 2.79 | 0.45 |
| 1:D:727:LEU:CD1 | 1:D:782:MLY:HG2 | 2.34 | 0.45 |
| 1:D:732:ILE:HG21 | 1:D:747:LEU:CD1 | 0.64 | 0.45 |
| 1:D:762:HIS:N | 1:D:762:HIS:CD2 | 2.79 | 0.45 |
| 1:D:783:LEU:N | 1:D:783:LEU:CD1 | 2.78 | 0.45 |
| 1:G:14:ALA:N | 1:G:15:PRO:HD2 | 2.32 | 0.45 |
| 1:G:642:LYS:NZ | 4:V:340:TRP:O | 2.50 | 0.45 |
| 1:J:206:LYS:HD3 | 1:J:217:THR:OG1 | 2.16 | 0.45 |
| 1:J:295:MLY:CG | 1:J:332:MET:HE1 | 2.45 | 0.45 |
| 1:J:332:MET:O | 1:J:336:SER:OG | 2.27 | 0.45 |
| 1:J:556:ASP:HB3 | 4:Y:47:MET:HB2 | 1.00 | 0.45 |
| 1:J:793:ARG:O | 1:J:797:PHE:N | 2.39 | 0.45 |
| 1:J:795:ARG:HD2 | 3:L:43:ASN:H | 1.79 | 0.45 |
| 2:K:139:ALA:C | 2:K:141:PRO:HD3 | 2.33 | 0.45 |
| 1:M:173:GLN:HG3 | 1:M:670:HIS:HD2 | 1.82 | 0.45 |
| 1:M:548:THR:CG2 | 4:2:47:MET:HB3 | 2.44 | 0.45 |
| 1:P:29:ASN:OD1 | 1:P:723:ARG:NH2 | 2.50 | 0.45 |
| 1:P:42:HIS:O | 1:P:45:GLN:O | 2.33 | 0.45 |
| 1:P:578:HIS:HB3 | 1:P:592:ILE:CD1 | 2.38 | 0.45 |
| 1:P:757:GLN:CG | 1:P:772:LEU:HD11 | 2.46 | 0.45 |
| 4:1:190:MET:O | 4:1:194:THR:HG23 | 2.16 | 0.45 |
| 4:2:32:PRO:HB2 | 4:2:34:ILE:HD11 | 1.98 | 0.45 |
| 4:5:190:MET:O | 4:5:194:THR:HG23 | 2.16 | 0.45 |
| 4:7:190:MET:O | 4:7:194:THR:HG23 | 2.16 | 0.45 |
| 4:X:190:MET:O | 4:X:194:THR:HG23 | 2.16 | 0.45 |
| 4:X:223:PHE:CD2 | 4:X:259:GLU:HG3 | 2.51 | 0.45 |
| 1:A:292:MET:HE1 | 1:A:309:PRO:HD3 | 1.98 | 0.45 |
| 1:A:296:MLY:O | 1:A:299:LEU:HB2 | 2.17 | 0.45 |
| 1:A:443:ILE:HG22 | 1:A:444:ARG:N | 2.29 | 0.45 |
| 1:A:476:GLU:OE2 | 1:A:598:MLY:HH13 | 2.17 | 0.45 |
| 1:A:759:ALA:O | 1:A:766:PHE:N | 2.32 | 0.45 |
| 2:B:121:LEU:O | 2:B:128:PHE:CG | 2.61 | 0.45 |
| 1:D:640:LYS:C | 4:9:23:GLY:C | 2.74 | 0.45 |
| 1:D:793:ARG:CZ | 3:F:87:PHE:CE1 | 3.00 | 0.45 |
| 1:G:92:ALA:O | 1:G:713:SER:HA | 2.16 | 0.45 |
| 1:G:675:ILE:HG23 | 1:G:676:ILE:N | 2.32 | 0.45 |
| 1:J:408:VAL:CG1 | 4:W:332:PRO:HB3 | 2.41 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:464:ILE:CG2 | 1:J:465:ALA:N | 2.80 | 0.45 |
| 1:J:488:GLN:O | 1:J:491:PHE:HB3 | 2.17 | 0.45 |
| 1:J:510:TRP:CZ2 | 1:J:772:LEU:HD11 | 2.51 | 0.45 |
| 1:J:629:GLU:HG2 | 1:J:643:GLY:C | 2.35 | 0.45 |
| 1:J:725:ARG:HH21 | 1:J:733:PRO:HB2 | 1.82 | 0.45 |
| 1:M:322:VAL:CG1 | 1:M:325:ILE:HD11 | 2.47 | 0.45 |
| 1:M:464:ILE:CG2 | 1:M:465:ALA:N | 2.80 | 0.45 |
| 1:M:725:ARG:CG | 1:M:733:PRO:CA | 2.95 | 0.45 |
| 1:M:725:ARG:HH21 | 1:M:733:PRO:HB2 | 1.82 | 0.45 |
| 1:P:55:MLY:HH23 | 1:P:60:VAL:HG22 | 1.99 | 0.45 |
| 1:P:179:GLY:O | 1:P:185:LYS:HE2 | 2.17 | 0.45 |
| 1:P:296:MLY:O | 1:P:299:LEU:HB2 | 2.17 | 0.45 |
| 1:P:326:ASP:O | 1:P:330:GLU:HG2 | 2.16 | 0.45 |
| 1:P:639:GLY:CA | 4:1:344:SER:O | 2.39 | 0.45 |
| 1:P:667:THR:O | 1:P:669:PRO:HD3 | 2.17 | 0.45 |
| 4:2:287:ILE:HG23 | 4:4:202:THR:CG2 | 2.28 | 0.45 |
| 4:3:32:PRO:HB2 | 4:3:34:ILE:HD11 | 1.98 | 0.45 |
| 4:4:223:PHE:CD2 | 4:4:259:GLU:HG3 | 2.52 | 0.45 |
| 4:6:6:THR:HG22 | 4:6:101:HIS:HA | 1.98 | 0.45 |
| 4:9:6:THR:HG22 | 4:9:101:HIS:HA | 1.98 | 0.45 |
| 4:W:190:MET:O | 4:W:194:THR:HG23 | 2.16 | 0.45 |
| 4:Z:190:MET:O | 4:Z:194:THR:HG23 | 2.16 | 0.45 |
| 1:A:195:TYR:CE2 | 1:A:199:ILE:HD12 | 2.52 | 0.45 |
| 1:A:488:GLN:O | 1:A:491:PHE:HB3 | 2.17 | 0.45 |
| 1:A:597:GLU:O | 1:A:600:MLY:N | 2.50 | 0.45 |
| 1:A:794:CYS:O | 1:A:797:PHE:HB3 | 2.17 | 0.45 |
| 1:D:37:SER:O | 1:D:38:VAL:HG23 | 2.17 | 0.45 |
| 1:D:335:ASP:OD1 | 1:D:348:MLY:NZ | 2.49 | 0.45 |
| 1:D:476:GLU:OE2 | 1:D:598:MLY:HH13 | 2.16 | 0.45 |
| 1:D:519:LEU:N | 1:D:519:LEU:CD1 | 2.77 | 0.45 |
| 1:D:725:ARG:HH21 | 1:D:733:PRO:HB2 | 1.81 | 0.45 |
| 1:D:726:VAL:CG1 | 1:D:785:GLU:HB3 | 2.46 | 0.45 |
| 1:D:775:LEU:HD12 | 1:D:775:LEU:HA | 1.71 | 0.45 |
| 1:G:89:GLU:CD | 1:G:153:PRO:HD2 | 2.36 | 0.45 |
| 1:G:448:GLN:C | 1:G:450:ASP:H | 2.19 | 0.45 |
| 1:G:476:GLU:OE2 | 1:G:598:MLY:HH13 | 2.16 | 0.45 |
| 1:G:642:LYS:HA | 4:V:21:PHE:C | 2.36 | 0.45 |
| 1:G:725:ARG:HH21 | 1:G:733:PRO:HB2 | 1.81 | 0.45 |
| 1:G:794:CYS:O | 1:G:797:PHE:HB3 | 2.17 | 0.45 |
| 2:H:137:TRP:CZ3 | 2:H:145:ALA:N | 2.81 | 0.45 |
| 1:J:55:MLY:HH23 | 1:J:60:VAL:HG22 | 1.99 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:202:SER:HA | 1:J:207:LYS:NZ | 2.22 | 0.45 |
| 1:J:278:GLN:HE21 | 1:J:278:GLN:HB3 | 1.42 | 0.45 |
| 1:J:322:VAL:HB | 1:J:325:ILE:HG13 | 1.98 | 0.45 |
| 1:J:476:GLU:OE2 | 1:J:598:MLY:HH13 | 2.16 | 0.45 |
| 1:J:664:LEU:HD12 | 1:J:664:LEU:HA | 1.52 | 0.45 |
| 1:J:724:TYR:HD1 | 1:J:727:LEU:CD1 | 2.27 | 0.45 |
| 1:J:732:ILE:HG23 | 1:J:747:LEU:HD12 | 0.95 | 0.45 |
| 1:M:35:MLY:N | 1:M:777:GLU:OE2 | 2.49 | 0.45 |
| 1:M:139:VAL:HG12 | 1:M:143:TYR:HD2 | 1.81 | 0.45 |
| 1:M:568:PRO:CG | 1:M:578:HIS:H | 2.30 | 0.45 |
| 1:M:640:LYS:HB3 | 1:M:645:SER:CB | 2.42 | 0.45 |
| 1:P:508:ILE:CD1 | 1:P:759:ALA:HB2 | 2.45 | 0.45 |
| 1:P:642:LYS:NZ | 4:1:340:TRP:O | 2.50 | 0.45 |
| 1:P:747:LEU:C | 1:P:749:GLY:H | 2.20 | 0.45 |
| 1:P:839:MLY:HH13 | 2:Q:159:HIS:CD2 | 2.50 | 0.45 |
| 4:6:366:GLY:O | 4:6:369:ILE:HG22 | 2.16 | 0.45 |
| 4:7:6:THR:HG22 | 4:7:101:HIS:HA | 1.98 | 0.45 |
| 4:9:32:PRO:HB2 | 4:9:34:ILE:HD11 | 1.98 | 0.45 |
| 4:Y:171:LEU:HA | 4:Y:172:PRO:HD2 | 1.84 | 0.45 |
| 1:A:14:ALA:N | 1:A:15:PRO:HD2 | 2.32 | 0.45 |
| 1:A:411:GLU:H | 4:8:333:PRO:CB | 2.30 | 0.45 |
| 1:A:501:GLU:O | 1:A:762:HIS:CE1 | 2.69 | 0.45 |
| 1:A:673:ARG:HD2 | 1:A:673:ARG:HA | 1.79 | 0.45 |
| 1:A:797:PHE:CG | 3:C:146:ILE:CG2 | 2.91 | 0.45 |
| 1:D:55:MLY:HH23 | 1:D:60:VAL:HG22 | 1.99 | 0.45 |
| 1:D:173:GLN:HG3 | 1:D:670:HIS:HD2 | 1.82 | 0.45 |
| 1:D:195:TYR:CE2 | 1:D:199:ILE:HD12 | 2.52 | 0.45 |
| 1:D:292:MET:HE1 | 1:D:309:PRO:CA | 2.47 | 0.45 |
| 1:D:540:CYS:N | 4:9:349:LEU:HD11 | 2.31 | 0.45 |
| 1:D:636:LYS:O | 4:9:144:ALA:HB1 | 2.14 | 0.45 |
| 1:D:725:ARG:CG | 1:D:733:PRO:CA | 2.95 | 0.45 |
| 1:G:148:ARG:HH22 | 1:G:764:MLY:HH11 | 1.77 | 0.45 |
| 1:G:226:ASN:N | 1:G:227:PRO:HD2 | 2.32 | 0.45 |
| 1:G:295:MLY:CG | 1:G:332:MET:HE1 | 2.46 | 0.45 |
| 1:G:640:LYS:C | 4:V:23:GLY:C | 2.75 | 0.45 |
| 1:G:725:ARG:HA | 1:G:732:ILE:HG22 | 1.99 | 0.45 |
| 1:G:795:ARG:HB3 | 3:I:35:ARG:NH2 | 2.29 | 0.45 |
| 1:G:838:ILE:HG13 | 2:H:54:MET:HE1 | 1.95 | 0.45 |
| 1:J:224:SER:O | 1:J:227:PRO:HD2 | 2.17 | 0.45 |
| 1:M:14:ALA:N | 1:M:15:PRO:HD2 | 2.32 | 0.45 |
| 1:M:226:ASN:N | 1:M:227:PRO:HD2 | 2.32 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:496:PHE:CE2 | 1:M:514:ASP:HA | 2.50 | 0.45 |
| 1:M:725:ARG:HA | 1:M:732:ILE:HG22 | 1.99 | 0.45 |
| 1:M:821:ARG:NH1 | 2:N:127:ARG:CZ | 2.80 | 0.45 |
| 1:P:103:LEU:HD22 | 1:P:692:LEU:HG | 1.98 | 0.45 |
| 1:P:226:ASN:HB2 | 1:P:227:PRO:CD | 2.47 | 0.45 |
| 1:P:486:MLY:HH22 | 1:P:527:GLU:CD | 2.37 | 0.45 |
| 1:P:496:PHE:CE2 | 1:P:514:ASP:HA | 2.50 | 0.45 |
| 1:P:725:ARG:CG | 1:P:733:PRO:CA | 2.95 | 0.45 |
| 1:P:732:ILE:HG21 | 1:P:747:LEU:CD1 | 0.63 | 0.45 |
| 4:1:223:PHE:CD2 | 4:1:259:GLU:HG3 | 2.52 | 0.45 |
| 4:3:6:THR:HG22 | 4:3:101:HIS:HA | 1.98 | 0.45 |
| 4:W:223:PHE:CD2 | 4:W:259:GLU:HG3 | 2.52 | 0.45 |
| 4:Y:223:PHE:CD2 | 4:Y:259:GLU:HG3 | 2.52 | 0.45 |
| 1:A:144:ARG:HA | 1:A:144:ARG:HD2 | 1.78 | 0.45 |
| 1:A:322:VAL:HA | 1:A:323:PRO:HD3 | 1.87 | 0.45 |
| 1:A:335:ASP:OD1 | 1:A:348:MLY:NZ | 2.49 | 0.45 |
| 1:A:568:PRO:CG | 1:A:578:HIS:H | 2.30 | 0.45 |
| 1:A:795:ARG:HD2 | 3:C:43:ASN:CG | 2.37 | 0.45 |
| 2:B:137:TRP:CZ3 | 2:B:145:ALA:N | 2.81 | 0.45 |
| 1:D:30:MLY:HB3 | 1:D:31:PRO:HD2 | 1.97 | 0.45 |
| 1:D:48:VAL:HA | 1:D:104:TYR:OH | 2.17 | 0.45 |
| 1:D:186:THR:O | 1:D:190:MLY:HG2 | 2.17 | 0.45 |
| 1:D:202:SER:HA | 1:D:207:LYS:NZ | 2.23 | 0.45 |
| 1:D:206:LYS:HD2 | 1:D:217:THR:CG2 | 2.17 | 0.45 |
| 1:D:296:MLY:O | 1:D:299:LEU:HB2 | 2.17 | 0.45 |
| 1:D:448:GLN:C | 1:D:450:ASP:H | 2.19 | 0.45 |
| 1:D:597:GLU:O | 1:D:600:MLY:N | 2.50 | 0.45 |
| 1:D:612:GLN:NE2 | 1:D:627:GLY:H | 2.14 | 0.45 |
| 3:F:50:LEU:O | 3:F:53:PRO:CD | 2.63 | 0.45 |
| 1:G:173:GLN:HG3 | 1:G:670:HIS:HD2 | 1.82 | 0.45 |
| 1:G:667:THR:O | 1:G:669:PRO:HD3 | 2.16 | 0.45 |
| 1:J:173:GLN:HG3 | 1:J:670:HIS:HD2 | 1.82 | 0.45 |
| 1:J:348:MLY:HH12 | 1:J:348:MLY:HD2 | 1.81 | 0.45 |
| 1:J:642:LYS:NZ | 4:W:340:TRP:O | 2.50 | 0.45 |
| 1:J:710:GLY:HA2 | 1:J:772:LEU:HD21 | 1.81 | 0.45 |
| 1:M:330:GLU:O | 1:M:333:ALA:HB3 | 2.16 | 0.45 |
| 1:P:37:SER:O | 1:P:38:VAL:HG23 | 2.17 | 0.45 |
| 1:P:361:TYR:O | 1:P:364:LEU:HB2 | 2.16 | 0.45 |
| 4:1:6:THR:HG22 | 4:1:101:HIS:HA | 1.98 | 0.45 |
| 4:1:201:VAL:CB | 4:Y:287:ILE:HG13 | 2.46 | 0.45 |
| 4:1:366:GLY:O | 4:1:369:ILE:HG22 | 2.16 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:6:223:PHE:CD2 | 4:6:259:GLU:HG3 | 2.52 | 0.45 |
| 4:6:253:GLU:HA | 4:6:256:ARG:CG | 2.42 | 0.45 |
| 4:7:223:PHE:CD2 | 4:7:259:GLU:HG3 | 2.52 | 0.45 |
| 4:8:299:MET:HE2 | 4:8:331:ALA:HB2 | 1.99 | 0.45 |
| 1:A:103:LEU:HD22 | 1:A:692:LEU:HG | 1.98 | 0.44 |
| 1:A:538:GLU:HA | 4:8:351:THR:H | 1.78 | 0.44 |
| 1:A:813:ILE:CD1 | 2:B:128:PHE:CE1 | 2.91 | 0.44 |
| 1:D:224:SER:O | 1:D:227:PRO:HD2 | 2.17 | 0.44 |
| 1:D:322:VAL:CG1 | 1:D:325:ILE:HD11 | 2.47 | 0.44 |
| 1:D:530:MET:CB | 4:9:354:GLN:CB | 2.95 | 0.44 |
| 3:F:69:LEU:HB3 | 3:F:70:PRO:HD3 | 1.99 | 0.44 |
| 1:G:91:MET:CE | 1:G:119:SER:HB2 | 2.47 | 0.44 |
| 1:G:186:THR:O | 1:G:190:MLY:HG2 | 2.17 | 0.44 |
| 1:G:195:TYR:CE2 | 1:G:199:ILE:HD12 | 2.52 | 0.44 |
| 1:G:322:VAL:HB | 1:G:325:ILE:HG13 | 1.98 | 0.44 |
| 1:G:597:GLU:O | 1:G:600:MLY:N | 2.50 | 0.44 |
| 1:G:642:LYS:CB | 4:V:24:ASP:O | 2.60 | 0.44 |
| 1:G:823:PHE:CE1 | 2:H:160:GLY:HA2 | 2.46 | 0.44 |
| 1:J:99:GLU:N | 1:J:100:PRO:CD | 2.80 | 0.44 |
| 1:J:103:LEU:HD22 | 1:J:692:LEU:HG | 1.98 | 0.44 |
| 1:J:296:MLY:O | 1:J:299:LEU:HB2 | 2.17 | 0.44 |
| 1:J:332:MET:H | 1:J:332:MET:HG2 | 1.52 | 0.44 |
| 1:J:346:ASP:O | 1:J:350:ALA:N | 2.46 | 0.44 |
| 1:J:640:LYS:C | 4:W:23:GLY:C | 2.74 | 0.44 |
| 1:J:673:ARG:HA | 1:J:673:ARG:HD2 | 1.79 | 0.44 |
| 1:M:136:ASN:HA | 1:M:137:PRO:HD3 | 1.50 | 0.44 |
| 1:M:163:TYR:O | 1:M:166:MET:HB3 | 2.17 | 0.44 |
| 1:M:296:MLY:O | 1:M:299:LEU:HB2 | 2.17 | 0.44 |
| 1:M:411:GLU:H | 4:Z:333:PRO:HB2 | 1.81 | 0.44 |
| 1:M:725:ARG:CG | 1:M:733:PRO:HA | 2.43 | 0.44 |
| 1:P:30:MLY:HB3 | 1:P:31:PRO:HD2 | 1.97 | 0.44 |
| 1:P:709:LYS:C | 1:P:710:GLY:CA | 2.85 | 0.44 |
| 1:P:783:LEU:HD12 | 1:P:786:ILE:HD11 | 1.93 | 0.44 |
| 4:4:366:GLY:O | 4:4:369:ILE:HG22 | 2.17 | 0.44 |
| 4:5:32:PRO:HB2 | 4:5:34:ILE:HD11 | 1.98 | 0.44 |
| 4:9:223:PHE:CD2 | 4:9:259:GLU:HG3 | 2.52 | 0.44 |
| 4:V:223:PHE:HB3 | 4:V:259:GLU:OE2 | 2.18 | 0.44 |
| 4:V:286:ASP:HA | 4:X:202:THR:HG22 | 1.63 | 0.44 |
| 4:V:290:ARG:NH1 | 4:X:202:THR:CG2 | 2.81 | 0.44 |
| 4:W:253:GLU:HA | 4:W:256:ARG:CG | 2.42 | 0.44 |
| 4:X:32:PRO:HB2 | 4:X:34:ILE:HD11 | 1.98 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:Y:366:GLY:O | 4:Y:369:ILE:HG22 | 2.16 | 0.44 |
| 1:A:541:MET:HB3 | 4:8:345:ILE:HG22 | 2.00 | 0.44 |
| 1:A:625:THR:H | 1:A:625:THR:HG22 | 1.48 | 0.44 |
| 1:A:725:ARG:HA | 1:A:732:ILE:HG22 | 1.99 | 0.44 |
| 1:A:827:MLY:HH21 | 2:B:139:ALA:CB | 2.47 | 0.44 |
| 1:D:103:LEU:HD22 | 1:D:692:LEU:HG | 1.98 | 0.44 |
| 1:D:136:ASN:O | 1:D:139:VAL:N | 2.47 | 0.44 |
| 1:D:354:LEU:HA | 1:D:354:LEU:HD12 | 1.56 | 0.44 |
| 1:D:747:LEU:C | 1:D:749:GLY:H | 2.21 | 0.44 |
| 1:G:411:GLU:H | 4:V:333:PRO:CB | 2.30 | 0.44 |
| 1:G:418:THR:CG2 | 1:G:419:VAL:N | 2.79 | 0.44 |
| 1:G:755:HIS:CB | 1:G:779:ARG:HH22 | 2.19 | 0.44 |
| 1:G:829:TRP:CZ3 | 2:H:84:PHE:CD1 | 3.00 | 0.44 |
| 1:J:14:ALA:N | 1:J:15:PRO:HD2 | 2.32 | 0.44 |
| 1:J:37:SER:O | 1:J:38:VAL:HG23 | 2.17 | 0.44 |
| 1:J:48:VAL:HA | 1:J:104:TYR:OH | 2.18 | 0.44 |
| 1:J:493:HIS:O | 1:J:496:PHE:HB3 | 2.17 | 0.44 |
| 1:J:711:PHE:HB3 | 1:J:766:PHE:HB3 | 2.00 | 0.44 |
| 1:J:794:CYS:O | 1:J:797:PHE:HB3 | 2.17 | 0.44 |
| 2:K:129:THR:HG23 | 2:K:132:GLU:OE1 | 2.17 | 0.44 |
| 1:M:103:LEU:HD22 | 1:M:692:LEU:HG | 1.98 | 0.44 |
| 1:M:667:THR:O | 1:M:669:PRO:HD3 | 2.16 | 0.44 |
| 1:P:346:ASP:O | 1:P:350:ALA:N | 2.45 | 0.44 |
| 1:P:476:GLU:OE2 | 1:P:598:MLY:HH13 | 2.17 | 0.44 |
| 1:P:725:ARG:CG | 1:P:733:PRO:HA | 2.43 | 0.44 |
| 1:P:757:GLN:CB | 1:P:772:LEU:HD11 | 2.47 | 0.44 |
| 2:Q:88:LEU:HB3 | 2:Q:91:ALA:HB2 | 1.98 | 0.44 |
| 4:2:223:PHE:CD2 | 4:2:259:GLU:HG3 | 2.52 | 0.44 |
| 4:7:32:PRO:HB2 | 4:7:34:ILE:HD11 | 1.98 | 0.44 |
| 4:W:366:GLY:O | 4:W:369:ILE:HG22 | 2.16 | 0.44 |
| 4:Z:32:PRO:HB2 | 4:Z:34:ILE:HD11 | 1.98 | 0.44 |
| 1:A:41:VAL:CG1 | 1:A:42:HIS:N | 2.76 | 0.44 |
| 1:A:214:MET:CA | 1:A:340:ILE:HD11 | 2.46 | 0.44 |
| 1:A:226:ASN:N | 1:A:227:PRO:HD2 | 2.32 | 0.44 |
| 1:A:322:VAL:HB | 1:A:325:ILE:HG13 | 1.98 | 0.44 |
| 1:A:326:ASP:O | 1:A:330:GLU:HG2 | 2.16 | 0.44 |
| 1:A:530:MET:HE3 | 4:8:355:MET:SD | 2.57 | 0.44 |
| 1:A:689:GLU:HA | 1:A:692:LEU:HB2 | 2.00 | 0.44 |
| 1:A:715:VAL:HG12 | 1:A:720:PHE:HB2 | 2.00 | 0.44 |
| 1:A:797:PHE:CE1 | 3:C:146:ILE:CG2 | 3.00 | 0.44 |
| 1:D:14:ALA:N | 1:D:15:PRO:HD2 | 2.32 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:99:GLU:N | 1:D:100:PRO:CD | 2.80 | 0.44 |
| 1:D:320:ILE:O | 1:D:320:ILE:HG22 | 2.18 | 0.44 |
| 1:G:37:SER:O | 1:G:38:VAL:HG23 | 2.17 | 0.44 |
| 1:G:84:MLY:CD | 1:G:724:TYR:OH | 2.66 | 0.44 |
| 1:G:139:VAL:HG12 | 1:G:143:TYR:HD2 | 1.81 | 0.44 |
| 1:G:488:GLN:O | 1:G:491:PHE:HB3 | 2.17 | 0.44 |
| 1:G:819:ASN:HD21 | 2:H:92:ASP:CA | 2.30 | 0.44 |
| 3:I:69:LEU:HB3 | 3:I:70:PRO:HD3 | 2.00 | 0.44 |
| 1:J:195:TYR:CE2 | 1:J:199:ILE:HD12 | 2.52 | 0.44 |
| 2:K:112:ILE:O | 2:K:148:VAL:HA | 2.16 | 0.44 |
| 1:M:179:GLY:O | 1:M:185:LYS:HE2 | 2.17 | 0.44 |
| 1:M:642:LYS:NZ | 4:Z:340:TRP:O | 2.50 | 0.44 |
| 1:M:715:VAL:HG11 | 1:M:720:PHE:CD1 | 2.50 | 0.44 |
| 1:M:797:PHE:CD1 | 3:O:149:VAL:HG13 | 2.44 | 0.44 |
| 1:P:64:THR:HB | 1:P:68:GLU:N | 2.33 | 0.44 |
| 1:P:408:VAL:HG22 | 1:P:636:LYS:HG2 | 1.52 | 0.44 |
| 1:P:436:MLY:HE3 | 1:P:626:TYR:HE1 | 1.78 | 0.44 |
| 1:P:448:GLN:C | 1:P:450:ASP:H | 2.19 | 0.44 |
| 1:P:544:LYS:HD3 | 4:3:45:VAL:CG2 | 2.42 | 0.44 |
| 1:P:732:ILE:CG2 | 1:P:747:LEU:HD12 | 0.35 | 0.44 |
| 1:P:829:TRP:O | 1:P:832:MET:N | 2.50 | 0.44 |
| 4:2:287:ILE:C | 4:4:203:THR:HG22 | 2.35 | 0.44 |
| 4:4:32:PRO:HB2 | 4:4:34:ILE:HD11 | 1.99 | 0.44 |
| 4:9:290:ARG:HH22 | 4:W:202:THR:CG2 | 2.17 | 0.44 |
| 4:Y:190:MET:O | 4:Y:194:THR:HG23 | 2.16 | 0.44 |
| 1:A:179:GLY:O | 1:A:185:LYS:HE2 | 2.17 | 0.44 |
| 1:A:599:ASN:CG | 1:A:649:VAL:CB | 2.80 | 0.44 |
| 1:A:675:ILE:HG23 | 1:A:676:ILE:N | 2.32 | 0.44 |
| 1:A:831:TRP:CH2 | 2:B:50:THR:HG22 | 2.25 | 0.44 |
| 3:C:69:LEU:HB3 | 3:C:70:PRO:HD3 | 2.00 | 0.44 |
| 1:D:106:LEU:HD12 | 1:D:106:LEU:HA | 1.80 | 0.44 |
| 1:D:278:GLN:HE21 | 1:D:278:GLN:HB3 | 1.42 | 0.44 |
| 1:D:667:THR:O | 1:D:669:PRO:HD3 | 2.17 | 0.44 |
| 1:D:813:ILE:HG12 | 2:E:128:PHE:CZ | 2.53 | 0.44 |
| 1:G:64:THR:HB | 1:G:68:GLU:N | 2.32 | 0.44 |
| 1:G:224:SER:O | 1:G:227:PRO:HD2 | 2.17 | 0.44 |
| 1:G:485:GLU:HA | 1:G:584:TYR:HE2 | 1.82 | 0.44 |
| 1:G:725:ARG:CG | 1:G:733:PRO:CA | 2.95 | 0.44 |
| 1:G:754:ASP:C | 1:G:776:GLU:OE2 | 2.55 | 0.44 |
| 1:J:97:LEU:HD12 | 1:J:97:LEU:HA | 1.67 | 0.44 |
| 1:M:206:LYS:HD3 | 1:M:217:THR:OG1 | 2.16 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:418:THR:CG2 | 1:M:419:VAL:N | 2.79 | 0.44 |
| 1:M:476:GLU:OE2 | 1:M:598:MLY:HH13 | 2.17 | 0.44 |
| 1:M:486:MLY:HH22 | 1:M:527:GLU:CD | 2.37 | 0.44 |
| 1:M:639:GLY:H | 4:Z:344:SER:HB3 | 1.82 | 0.44 |
| 1:M:675:ILE:HG23 | 1:M:676:ILE:N | 2.33 | 0.44 |
| 2:N:112:ILE:O | 2:N:148:VAL:HA | 2.17 | 0.44 |
| 1:P:48:VAL:HA | 1:P:104:TYR:OH | 2.18 | 0.44 |
| 1:P:215:GLN:CA | 1:P:340:ILE:CG2 | 2.62 | 0.44 |
| 1:P:295:MLY:CG | 1:P:332:MET:HE1 | 2.46 | 0.44 |
| 1:P:330:GLU:O | 1:P:333:ALA:HB3 | 2.16 | 0.44 |
| 1:P:354:LEU:HA | 1:P:354:LEU:HD12 | 1.56 | 0.44 |
| 1:P:493:HIS:O | 1:P:496:PHE:HB3 | 2.18 | 0.44 |
| 1:P:597:GLU:O | 1:P:600:MLY:N | 2.50 | 0.44 |
| 1:P:794:CYS:O | 1:P:797:PHE:HB3 | 2.17 | 0.44 |
| 1:P:797:PHE:CG | 3:R:146:ILE:HG23 | 2.53 | 0.44 |
| 1:P:804:ARG:O | 1:P:808:GLU:N | 2.49 | 0.44 |
| 3:R:69:LEU:HB3 | 3:R:70:PRO:HD3 | 2.00 | 0.44 |
| 4:3:190:MET:O | 4:3:194:THR:HG23 | 2.16 | 0.44 |
| 4:6:223:PHE:HB3 | 4:6:259:GLU:OE2 | 2.18 | 0.44 |
| 1:A:193:ILE:HD11 | 1:A:250:ILE:CD1 | 2.48 | 0.44 |
| 1:D:17:LEU:HA | 1:D:17:LEU:HD12 | 1.67 | 0.44 |
| 1:D:410:ASN:HA | 4:9:334:GLU:HB3 | 1.29 | 0.44 |
| 2:E:129:THR:HG23 | 2:E:132:GLU:OE1 | 2.18 | 0.44 |
| 2:E:149:ASP:CG | 2:E:150:TYR:N | 2.49 | 0.44 |
| 1:G:103:LEU:HD22 | 1:G:692:LEU:HG | 1.98 | 0.44 |
| 1:G:326:ASP:O | 1:G:330:GLU:HG2 | 2.16 | 0.44 |
| 1:G:689:GLU:HA | 1:G:692:LEU:HB2 | 2.00 | 0.44 |
| 1:G:692:LEU:O | 1:G:696:ARG:HG3 | 2.18 | 0.44 |
| 1:G:723:ARG:NH1 | 1:G:723:ARG:CG | 2.80 | 0.44 |
| 1:G:759:ALA:O | 1:G:766:PHE:N | 2.32 | 0.44 |
| 2:H:114:LYS:CG | 2:H:146:GLY:HA2 | 2.46 | 0.44 |
| 1:J:410:ASN:HA | 4:W:334:GLU:HB3 | 1.29 | 0.44 |
| 1:J:536:LEU:HA | 1:J:536:LEU:HD12 | 1.69 | 0.44 |
| 1:J:659:MLY:HD2 | 1:J:659:MLY:HH22 | 1.42 | 0.44 |
| 1:J:756:THR:C | 1:J:776:GLU:CD | 2.69 | 0.44 |
| 1:J:795:ARG:HE | 3:L:116:GLU:HB3 | 1.83 | 0.44 |
| 1:J:810:ARG:HG2 | 1:J:810:ARG:NH1 | 2.29 | 0.44 |
| 1:M:506:GLU:HG2 | 1:M:766:PHE:HE1 | 1.82 | 0.44 |
| 1:M:692:LEU:O | 1:M:696:ARG:HG3 | 2.18 | 0.44 |
| 1:M:747:LEU:C | 1:M:749:GLY:H | 2.21 | 0.44 |
| 1:M:786:ILE:C | 1:M:787:ILE:N | 2.71 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:836:PHE:CD1 | 2:N:160:GLY:N | 2.85 | 0.44 |
| 1:P:155:ILE:HG22 | 1:P:156:PHE:N | 2.33 | 0.44 |
| 1:P:485:GLU:HA | 1:P:584:TYR:HE2 | 1.83 | 0.44 |
| 1:P:639:GLY:H | 4:1:344:SER:HB3 | 1.83 | 0.44 |
| 1:P:829:TRP:CZ2 | 2:Q:87:LYS:CE | 2.75 | 0.44 |
| 3:R:62:ALA:O | 3:R:63:ILE:HG13 | 2.14 | 0.44 |
| 4:4:287:ILE:HG22 | 4:6:204:ALA:H | 1.74 | 0.44 |
| 4:6:32:PRO:HB2 | 4:6:34:ILE:HD11 | 1.98 | 0.44 |
| 4:7:223:PHE:HB3 | 4:7:259:GLU:OE2 | 2.18 | 0.44 |
| 4:8:32:PRO:HB2 | 4:8:34:ILE:HD11 | 1.98 | 0.44 |
| 1:A:37:SER:O | 1:A:38:VAL:HG23 | 2.17 | 0.44 |
| 1:A:48:VAL:HA | 1:A:104:TYR:OH | 2.18 | 0.44 |
| 1:A:123:CYS:CB | 1:A:158:ILE:HD13 | 2.48 | 0.44 |
| 1:A:186:THR:O | 1:A:190:MLY:HG2 | 2.17 | 0.44 |
| 1:A:493:HIS:O | 1:A:496:PHE:HB3 | 2.18 | 0.44 |
| 1:A:639:GLY:H | 4:8:344:SER:HB3 | 1.82 | 0.44 |
| 1:A:725:ARG:CG | 1:A:733:PRO:CA | 2.95 | 0.44 |
| 1:D:176:LEU:N | 1:D:176:LEU:CD1 | 2.75 | 0.44 |
| 1:G:163:TYR:O | 1:G:166:MET:HB3 | 2.17 | 0.44 |
| 1:G:296:MLY:O | 1:G:299:LEU:HB2 | 2.17 | 0.44 |
| 1:G:715:VAL:HG12 | 1:G:720:PHE:HB2 | 2.00 | 0.44 |
| 1:G:728:ASN:HD21 | 3:I:114:LEU:HD23 | 1.67 | 0.44 |
| 2:H:129:THR:HG23 | 2:H:132:GLU:OE1 | 2.18 | 0.44 |
| 1:J:320:ILE:O | 1:J:320:ILE:HG22 | 2.18 | 0.44 |
| 1:J:485:GLU:HA | 1:J:584:TYR:HE2 | 1.83 | 0.44 |
| 1:J:642:LYS:HB2 | 4:W:24:ASP:O | 1.89 | 0.44 |
| 1:J:797:PHE:HE2 | 3:L:126:LEU:HD13 | 1.82 | 0.44 |
| 2:K:137:TRP:CA | 2:K:145:ALA:CB | 2.82 | 0.44 |
| 1:M:37:SER:O | 1:M:38:VAL:HG23 | 2.17 | 0.44 |
| 1:M:123:CYS:CB | 1:M:158:ILE:HD13 | 2.48 | 0.44 |
| 1:M:186:THR:O | 1:M:190:MLY:HG2 | 2.17 | 0.44 |
| 1:M:485:GLU:HA | 1:M:584:TYR:HE2 | 1.83 | 0.44 |
| 1:M:689:GLU:HA | 1:M:692:LEU:HB2 | 2.00 | 0.44 |
| 1:M:715:VAL:HG12 | 1:M:720:PHE:HB2 | 2.00 | 0.44 |
| 1:M:817:GLN:HG3 | 2:N:128:PHE:HE1 | 1.81 | 0.44 |
| 1:P:97:LEU:HD12 | 1:P:97:LEU:HA | 1.67 | 0.44 |
| 1:P:123:CYS:CB | 1:P:158:ILE:HD13 | 2.48 | 0.44 |
| 1:P:173:GLN:HG3 | 1:P:670:HIS:HD2 | 1.82 | 0.44 |
| 1:P:193:ILE:HD11 | 1:P:250:ILE:CD1 | 2.48 | 0.44 |
| 3:R:50:LEU:O | 3:R:53:PRO:HG2 | 2.18 | 0.44 |
| 4:2:223:PHE:HB3 | 4:2:259:GLU:OE2 | 2.18 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:3:253:GLU:HA | 4:3:256:ARG:CG | 2.42 | 0.44 |
| 1:A:224:SER:O | 1:A:227:PRO:HD2 | 2.17 | 0.44 |
| 1:A:667:THR:O | 1:A:669:PRO:HD3 | 2.16 | 0.44 |
| 1:A:692:LEU:O | 1:A:696:ARG:HG3 | 2.18 | 0.44 |
| 1:A:797:PHE:CE2 | 3:C:126:LEU:CD2 | 2.89 | 0.44 |
| 1:D:95:THR:O | 1:D:770:GLY:N | 2.51 | 0.44 |
| 1:D:174:SER:OG | 1:D:669:PRO:HA | 2.18 | 0.44 |
| 1:D:516:GLY:O | 1:D:518:ASP:N | 2.51 | 0.44 |
| 1:D:536:LEU:HA | 1:D:536:LEU:HD12 | 1.69 | 0.44 |
| 1:D:643:GLY:CA | 4:9:24:ASP:OD1 | 2.62 | 0.44 |
| 1:D:711:PHE:HB3 | 1:D:766:PHE:HB3 | 2.00 | 0.44 |
| 1:D:829:TRP:O | 1:D:832:MET:N | 2.50 | 0.44 |
| 3:F:122:GLU:HA | 3:F:125:GLU:OE1 | 2.18 | 0.44 |
| 1:G:123:CYS:CB | 1:G:158:ILE:HD13 | 2.48 | 0.44 |
| 1:G:193:ILE:HD11 | 1:G:250:ILE:CD1 | 2.48 | 0.44 |
| 1:G:322:VAL:CG1 | 1:G:325:ILE:HD11 | 2.47 | 0.44 |
| 2:H:144:VAL:HG12 | 2:H:153:ILE:HD13 | 1.92 | 0.44 |
| 1:J:88:ILE:HG21 | 1:J:88:ILE:HD12 | 1.78 | 0.44 |
| 1:J:330:GLU:O | 1:J:333:ALA:HB3 | 2.17 | 0.44 |
| 1:J:519:LEU:N | 1:J:519:LEU:CD1 | 2.77 | 0.44 |
| 1:J:597:GLU:O | 1:J:600:MLY:N | 2.50 | 0.44 |
| 1:J:675:ILE:HG23 | 1:J:676:ILE:N | 2.33 | 0.44 |
| 1:J:747:LEU:C | 1:J:749:GLY:N | 2.71 | 0.44 |
| 1:J:792:ALA:HB2 | 3:L:42:THR:H | 1.77 | 0.44 |
| 1:J:829:TRP:O | 1:J:832:MET:N | 2.50 | 0.44 |
| 1:M:35:MLY:HE2 | 1:M:777:GLU:CD | 2.37 | 0.44 |
| 1:M:193:ILE:HD11 | 1:M:250:ILE:CD1 | 2.48 | 0.44 |
| 1:M:485:GLU:OE1 | 1:M:583:HIS:ND1 | 2.49 | 0.44 |
| 1:M:488:GLN:O | 1:M:491:PHE:HB3 | 2.17 | 0.44 |
| 1:M:810:ARG:HG2 | 1:M:810:ARG:NH1 | 2.29 | 0.44 |
| 3:O:101:THR:HA | 3:O:137:ILE:O | 2.18 | 0.44 |
| 1:P:35:MLY:HH22 | 1:P:777:GLU:OE1 | 2.18 | 0.44 |
| 1:P:224:SER:O | 1:P:227:PRO:HD2 | 2.17 | 0.44 |
| 1:P:411:GLU:H | 4:1:333:PRO:CB | 2.30 | 0.44 |
| 1:P:568:PRO:CG | 1:P:578:HIS:H | 2.30 | 0.44 |
| 1:P:725:ARG:CZ | 1:P:737:PHE:CZ | 3.01 | 0.44 |
| 4:5:223:PHE:HB3 | 4:5:259:GLU:OE2 | 2.18 | 0.44 |
| 4:7:193:LEU:O | 4:7:198:TYR:HD2 | 2.01 | 0.44 |
| 4:8:223:PHE:HB3 | 4:8:259:GLU:OE2 | 2.18 | 0.44 |
| 4:9:223:PHE:HB3 | 4:9:259:GLU:OE2 | 2.18 | 0.44 |
| 4:V:32:PRO:HB2 | 4:V:34:ILE:HD11 | 1.98 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:215:GLN:H | 1:A:340:ILE:CD1 | 2.21 | 0.44 |
| 1:A:506:GLU:HG3 | 1:A:760:PHE:HD1 | 1.49 | 0.44 |
| 1:A:711:PHE:HB3 | 1:A:766:PHE:HB3 | 1.99 | 0.44 |
| 1:A:725:ARG:CG | 1:A:733:PRO:HA | 2.43 | 0.44 |
| 1:A:753:VAL:HG12 | 1:A:775:LEU:HG | 0.47 | 0.44 |
| 3:C:50:LEU:O | 3:C:53:PRO:HG2 | 2.18 | 0.44 |
| 1:D:155:ILE:HG22 | 1:D:156:PHE:N | 2.33 | 0.44 |
| 1:D:629:GLU:HG2 | 1:D:643:GLY:C | 2.35 | 0.44 |
| 1:D:692:LEU:O | 1:D:696:ARG:HG3 | 2.18 | 0.44 |
| 1:G:791:GLN:NE2 | 3:I:116:GLU:N | 2.64 | 0.44 |
| 1:G:817:GLN:CD | 2:H:127:ARG:CG | 2.86 | 0.44 |
| 1:G:834:LEU:HD12 | 2:H:51:PHE:CD1 | 2.52 | 0.44 |
| 1:J:93:MET:SD | 1:J:715:VAL:HA | 2.57 | 0.44 |
| 1:J:123:CYS:CB | 1:J:158:ILE:HD13 | 2.48 | 0.44 |
| 1:J:144:ARG:HA | 1:J:144:ARG:HD2 | 1.78 | 0.44 |
| 1:J:215:GLN:H | 1:J:340:ILE:CD1 | 2.20 | 0.44 |
| 1:J:226:ASN:HB2 | 1:J:227:PRO:CD | 2.47 | 0.44 |
| 1:J:322:VAL:CG1 | 1:J:325:ILE:HD11 | 2.47 | 0.44 |
| 1:J:568:PRO:CG | 1:J:578:HIS:H | 2.30 | 0.44 |
| 1:J:578:HIS:HB3 | 1:J:592:ILE:CD1 | 2.38 | 0.44 |
| 1:J:639:GLY:H | 4:W:344:SER:HB3 | 1.83 | 0.44 |
| 1:J:692:LEU:O | 1:J:696:ARG:HG3 | 2.18 | 0.44 |
| 1:J:725:ARG:CG | 1:J:733:PRO:CA | 2.95 | 0.44 |
| 2:K:144:VAL:HG12 | 2:K:153:ILE:HD13 | 1.92 | 0.44 |
| 1:M:266:GLU:OE1 | 1:M:659:MLY:NZ | 2.51 | 0.44 |
| 1:M:411:GLU:H | 4:Z:333:PRO:CB | 2.30 | 0.44 |
| 1:M:787:ILE:HG23 | 1:M:791:GLN:HG3 | 2.00 | 0.44 |
| 3:O:62:ALA:O | 3:O:63:ILE:CB | 2.63 | 0.44 |
| 3:O:119:THR:O | 3:O:123:VAL:HG23 | 2.18 | 0.44 |
| 3:O:122:GLU:HA | 3:O:125:GLU:OE1 | 2.18 | 0.44 |
| 1:P:715:VAL:HG12 | 1:P:720:PHE:HB2 | 2.00 | 0.44 |
| 1:P:725:ARG:HA | 1:P:732:ILE:HG22 | 1.99 | 0.44 |
| 1:P:725:ARG:HH21 | 1:P:733:PRO:HB2 | 1.82 | 0.44 |
| 2:Q:114:LYS:CG | 2:Q:146:GLY:HA2 | 2.46 | 0.44 |
| 3:R:122:GLU:HA | 3:R:125:GLU:OE1 | 2.18 | 0.44 |
| 4:2:43:VAL:O | 4:Z:167:GLU:OE2 | 2.35 | 0.44 |
| 4:4:193:LEU:O | 4:4:198:TYR:HD2 | 2.01 | 0.44 |
| 4:6:193:LEU:O | 4:6:198:TYR:HD2 | 2.01 | 0.44 |
| 4:9:324:THR:N | 4:W:245:GLY:CA | 2.69 | 0.44 |
| 4:W:220:ALA:HB3 | 4:W:223:PHE:CD1 | 2.53 | 0.44 |
| 1:A:485:GLU:HA | 1:A:584:TYR:HE2 | 1.83 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:486:MLY:HH22 | 1:A:527:GLU:CD | 2.37 | 0.44 |
| 1:A:723:ARG:CG | 1:A:723:ARG:NH1 | 2.80 | 0.44 |
| 1:A:724:TYR:HD1 | 1:A:727:LEU:CD1 | 2.27 | 0.44 |
| 1:A:813:ILE:HG23 | 2:B:128:PHE:CE1 | 2.53 | 0.44 |
| 2:B:129:THR:HG23 | 2:B:132:GLU:OE1 | 2.18 | 0.44 |
| 2:B:140:PHE:HA | 2:B:141:PRO:HD2 | 1.57 | 0.44 |
| 3:C:119:THR:O | 3:C:123:VAL:HG23 | 2.18 | 0.44 |
| 1:D:123:CYS:CB | 1:D:158:ILE:HD13 | 2.48 | 0.44 |
| 1:D:348:MLY:HH12 | 1:D:348:MLY:HD2 | 1.81 | 0.44 |
| 1:D:568:PRO:CG | 1:D:578:HIS:H | 2.30 | 0.44 |
| 1:D:675:ILE:HG23 | 1:D:676:ILE:N | 2.32 | 0.44 |
| 1:D:725:ARG:HA | 1:D:732:ILE:HG22 | 2.00 | 0.44 |
| 1:D:800:ARG:HH22 | 3:F:40:ASN:HD21 | 1.18 | 0.44 |
| 1:D:835:PHE:O | 1:D:839:MLY:N | 2.49 | 0.44 |
| 1:G:179:GLY:O | 1:G:185:LYS:HE2 | 2.17 | 0.44 |
| 1:G:725:ARG:CZ | 1:G:737:PHE:CZ | 3.01 | 0.44 |
| 1:G:787:ILE:HG23 | 1:G:791:GLN:HG3 | 2.00 | 0.44 |
| 1:J:163:TYR:O | 1:J:166:MET:HB3 | 2.17 | 0.44 |
| 1:J:789:ALA:HA | 3:L:81:GLN:NE2 | 2.33 | 0.44 |
| 1:M:134:VAL:C | 1:M:136:ASN:H | 2.16 | 0.44 |
| 1:M:218:LEU:HD22 | 1:M:222:ILE:HG13 | 1.95 | 0.44 |
| 1:M:409:GLY:N | 1:M:636:LYS:CD | 2.70 | 0.44 |
| 1:M:597:GLU:O | 1:M:600:MLY:N | 2.51 | 0.44 |
| 1:M:762:HIS:CD2 | 1:M:762:HIS:N | 2.78 | 0.44 |
| 1:M:768:MLY:O | 1:M:770:GLY:N | 2.51 | 0.44 |
| 1:M:786:ILE:C | 1:M:790:THR:H | 2.21 | 0.44 |
| 1:M:795:ARG:CB | 3:O:35:ARG:HH22 | 2.07 | 0.44 |
| 3:O:48:LYS:HA | 3:O:48:LYS:HD3 | 1.17 | 0.44 |
| 3:O:69:LEU:HB3 | 3:O:70:PRO:HD3 | 1.99 | 0.44 |
| 1:P:320:ILE:O | 1:P:320:ILE:HG22 | 2.18 | 0.44 |
| 1:P:519:LEU:N | 1:P:519:LEU:CD1 | 2.77 | 0.44 |
| 1:P:529:PRO:HB3 | 4:1:354:GLN:HA | 2.00 | 0.44 |
| 1:P:552:ASN:CB | 4:3:49:GLN:H | 2.28 | 0.44 |
| 1:P:629:GLU:HG2 | 1:P:643:GLY:C | 2.35 | 0.44 |
| 1:P:725:ARG:NE | 1:P:733:PRO:CB | 1.95 | 0.44 |
| 4:1:220:ALA:HB3 | 4:1:223:PHE:CD1 | 2.53 | 0.44 |
| 4:1:243:PRO:CA | 4:Y:291:LYS:HD2 | 2.48 | 0.44 |
| 4:V:299:MET:HE2 | 4:V:331:ALA:HB2 | 2.00 | 0.44 |
| 1:A:64:THR:HB | 1:A:68:GLU:N | 2.33 | 0.43 |
| 1:A:166:MET:CE | 1:A:254:PHE:CD2 | 3.01 | 0.43 |
| 1:A:266:GLU:OE1 | 1:A:659:MLY:NZ | 2.51 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:485:GLU:OE2 | 1:A:584:TYR:N | 2.50 | 0.43 |
| 1:A:496:PHE:HB2 | 1:A:515:PHE:CD2 | 2.53 | 0.43 |
| 3:C:101:THR:HA | 3:C:137:ILE:O | 2.18 | 0.43 |
| 1:D:391:GLY:HA3 | 1:D:616:VAL:HG23 | 2.01 | 0.43 |
| 1:D:439:LEU:N | 1:D:439:LEU:CD1 | 2.81 | 0.43 |
| 1:D:725:ARG:CZ | 1:D:737:PHE:CZ | 3.01 | 0.43 |
| 1:D:799:MET:HE1 | 3:F:32:ASP:CB | 2.33 | 0.43 |
| 1:D:819:ASN:N | 2:E:90:GLY:C | 2.71 | 0.43 |
| 1:G:40:VAL:HG23 | 1:G:76:GLN:O | 2.18 | 0.43 |
| 1:G:496:PHE:HB2 | 1:G:515:PHE:CD2 | 2.53 | 0.43 |
| 1:G:820:VAL:CG1 | 2:H:136:MET:HE1 | 2.48 | 0.43 |
| 3:I:119:THR:O | 3:I:123:VAL:HG23 | 2.18 | 0.43 |
| 1:J:411:GLU:H | 4:W:333:PRO:CB | 2.30 | 0.43 |
| 1:M:476:GLU:CD | 1:M:476:GLU:H | 2.22 | 0.43 |
| 1:M:519:LEU:HD12 | 1:M:519:LEU:H | 1.83 | 0.43 |
| 1:P:14:ALA:N | 1:P:15:PRO:HD2 | 2.32 | 0.43 |
| 1:P:97:LEU:HD21 | 1:P:712:PRO:HA | 1.99 | 0.43 |
| 1:P:99:GLU:N | 1:P:100:PRO:CD | 2.80 | 0.43 |
| 1:P:175:ILE:C | 1:P:176:LEU:HD12 | 2.39 | 0.43 |
| 1:P:516:GLY:O | 1:P:518:ASP:N | 2.51 | 0.43 |
| 1:P:540:CYS:C | 4:1:349:LEU:HD21 | 2.36 | 0.43 |
| 1:P:759:ALA:O | 1:P:766:PHE:N | 2.32 | 0.43 |
| 1:P:816:ILE:HD11 | 2:Q:100:ALA:CB | 2.45 | 0.43 |
| 4:1:193:LEU:O | 4:1:198:TYR:HD2 | 2.01 | 0.43 |
| 4:9:220:ALA:HB3 | 4:9:223:PHE:CD1 | 2.53 | 0.43 |
| 4:V:205:GLU:O | 4:V:208:ILE:HG22 | 2.18 | 0.43 |
| 4:Z:205:GLU:O | 4:Z:208:ILE:HG22 | 2.18 | 0.43 |
| 1:A:55:MLY:HH23 | 1:A:60:VAL:HG22 | 1.99 | 0.43 |
| 1:A:93:MET:CE | 1:A:716:LEU:H | 2.31 | 0.43 |
| 1:A:109:ARG:CD | 1:A:117:THR:HB | 2.48 | 0.43 |
| 1:A:725:ARG:HH21 | 1:A:733:PRO:HB2 | 1.81 | 0.43 |
| 1:D:175:ILE:C | 1:D:176:LEU:HD12 | 2.39 | 0.43 |
| 1:D:217:THR:HG22 | 1:D:218:LEU:N | 2.34 | 0.43 |
| 1:D:322:VAL:CG1 | 1:D:325:ILE:HG13 | 2.49 | 0.43 |
| 1:D:330:GLU:O | 1:D:333:ALA:HB3 | 2.17 | 0.43 |
| 1:D:488:GLN:O | 1:D:491:PHE:HB3 | 2.17 | 0.43 |
| 1:D:549:SER:C | 4:W:45:VAL:O | 2.57 | 0.43 |
| 1:D:831:TRP:HD1 | 2:E:67:MET:SD | 2.33 | 0.43 |
| 1:G:166:MET:CE | 1:G:254:PHE:CD2 | 3.01 | 0.43 |
| 1:G:476:GLU:H | 1:G:476:GLU:CD | 2.22 | 0.43 |
| 1:J:439:LEU:N | 1:J:439:LEU:CD1 | 2.81 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:516:GLY:O | 1:J:518:ASP:N | 2.51 | 0.43 |
| 1:J:783:LEU:HA | 1:J:786:ILE:HB | 2.00 | 0.43 |
| 1:M:48:VAL:HA | 1:M:104:TYR:OH | 2.18 | 0.43 |
| 1:M:64:THR:HB | 1:M:68:GLU:N | 2.32 | 0.43 |
| 1:M:530:MET:HA | 4:Z:354:GLN:CD | 2.12 | 0.43 |
| 1:M:775:LEU:HD12 | 1:M:775:LEU:HA | 1.71 | 0.43 |
| 1:P:322:VAL:CG1 | 1:P:325:ILE:HD11 | 2.47 | 0.43 |
| 1:P:443:ILE:HG22 | 1:P:444:ARG:N | 2.29 | 0.43 |
| 1:P:496:PHE:HB2 | 1:P:515:PHE:CD2 | 2.54 | 0.43 |
| 1:P:673:ARG:HD2 | 1:P:673:ARG:HA | 1.79 | 0.43 |
| 1:P:692:LEU:O | 1:P:696:ARG:HG3 | 2.18 | 0.43 |
| 1:P:795:ARG:HE | 3:R:116:GLU:HB3 | 1.83 | 0.43 |
| 1:P:798:LEU:CD2 | 3:R:122:GLU:HB3 | 2.47 | 0.43 |
| 1:P:829:TRP:CH2 | 2:Q:84:PHE:CE1 | 3.06 | 0.43 |
| 1:P:834:LEU:CD1 | 2:Q:51:PHE:CD1 | 2.97 | 0.43 |
| 3:R:101:THR:HA | 3:R:137:ILE:O | 2.18 | 0.43 |
| 4:1:223:PHE:HB3 | 4:1:259:GLU:OE2 | 2.18 | 0.43 |
| 4:2:322:PRO:CA | 4:4:244:ASP:HB2 | 2.47 | 0.43 |
| 4:3:193:LEU:O | 4:3:198:TYR:HD2 | 2.01 | 0.43 |
| 4:7:220:ALA:HB3 | 4:7:223:PHE:CD1 | 2.53 | 0.43 |
| 1:A:14:ALA:HB3 | 1:A:15:PRO:CD | 2.46 | 0.43 |
| 1:A:295:MLY:CG | 1:A:332:MET:HE1 | 2.46 | 0.43 |
| 1:A:409:GLY:N | 1:A:636:LYS:CD | 2.70 | 0.43 |
| 1:A:418:THR:CG2 | 1:A:419:VAL:N | 2.79 | 0.43 |
| 1:A:516:GLY:O | 1:A:518:ASP:N | 2.51 | 0.43 |
| 1:A:541:MET:HG2 | 4:8:345:ILE:HG22 | 2.00 | 0.43 |
| 1:A:823:PHE:HE1 | 2:B:161:GLU:H | 1.64 | 0.43 |
| 1:D:201:ALA:O | 1:D:202:SER:OG | 2.36 | 0.43 |
| 1:D:309:PRO:C | 1:D:311:ASP:H | 2.22 | 0.43 |
| 1:D:493:HIS:O | 1:D:496:PHE:HB3 | 2.18 | 0.43 |
| 1:D:507:GLY:CA | 1:D:762:HIS:ND1 | 2.77 | 0.43 |
| 1:D:541:MET:HB3 | 4:9:345:ILE:HG22 | 2.00 | 0.43 |
| 1:D:715:VAL:HG12 | 1:D:720:PHE:HB2 | 2.00 | 0.43 |
| 1:G:48:VAL:HA | 1:G:104:TYR:OH | 2.18 | 0.43 |
| 1:G:55:MLY:HH23 | 1:G:60:VAL:HG22 | 1.99 | 0.43 |
| 1:G:93:MET:CA | 1:G:714:ARG:H | 2.00 | 0.43 |
| 1:G:148:ARG:HH21 | 1:G:764:MLY:CH2 | 2.28 | 0.43 |
| 1:G:155:ILE:HG22 | 1:G:156:PHE:N | 2.33 | 0.43 |
| 1:G:221:GLN:HG2 | 1:G:221:GLN:H | 1.47 | 0.43 |
| 1:G:639:GLY:H | 4:V:344:SER:HB3 | 1.83 | 0.43 |
| 1:G:747:LEU:C | 1:G:749:GLY:H | 2.20 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:H:140:PHE:HA | 2:H:141:PRO:HD2 | 1.57 | 0.43 |
| 1:J:64:THR:HB | 1:J:68:GLU:N | 2.33 | 0.43 |
| 1:J:91:MET:CE | 1:J:119:SER:HB2 | 2.48 | 0.43 |
| 1:J:174:SER:OG | 1:J:669:PRO:HA | 2.18 | 0.43 |
| 1:J:175:ILE:C | 1:J:176:LEU:HD12 | 2.38 | 0.43 |
| 1:J:214:MET:CA | 1:J:340:ILE:HD11 | 2.45 | 0.43 |
| 1:J:226:ASN:N | 1:J:227:PRO:HD2 | 2.32 | 0.43 |
| 1:J:292:MET:CE | 1:J:309:PRO:CA | 2.97 | 0.43 |
| 1:J:391:GLY:HA3 | 1:J:616:VAL:HG23 | 2.01 | 0.43 |
| 1:J:505:MLY:HG3 | 1:J:762:HIS:NE2 | 2.33 | 0.43 |
| 1:J:725:ARG:HA | 1:J:732:ILE:HG22 | 1.99 | 0.43 |
| 3:L:48:LYS:HA | 3:L:48:LYS:HD3 | 1.17 | 0.43 |
| 3:L:101:THR:HA | 3:L:137:ILE:O | 2.18 | 0.43 |
| 1:M:40:VAL:HG23 | 1:M:76:GLN:O | 2.19 | 0.43 |
| 1:M:166:MET:CE | 1:M:254:PHE:CD2 | 3.01 | 0.43 |
| 1:M:224:SER:O | 1:M:227:PRO:HD2 | 2.17 | 0.43 |
| 1:M:246:PHE:HB3 | 1:M:270:LEU:HD12 | 2.01 | 0.43 |
| 1:M:493:HIS:O | 1:M:496:PHE:HB3 | 2.18 | 0.43 |
| 1:M:541:MET:CE | 4:Z:346:LEU:HD12 | 2.48 | 0.43 |
| 1:M:711:PHE:HB3 | 1:M:766:PHE:HB3 | 2.00 | 0.43 |
| 1:M:725:ARG:CZ | 1:M:737:PHE:CE1 | 3.02 | 0.43 |
| 3:O:50:LEU:O | 3:O:53:PRO:HG2 | 2.19 | 0.43 |
| 1:P:64:THR:CG2 | 1:P:65:GLU:H | 2.32 | 0.43 |
| 1:P:534:SER:HB2 | 4:1:354:GLN:HE22 | 1.56 | 0.43 |
| 1:P:732:ILE:HG23 | 1:P:747:LEU:HD12 | 0.95 | 0.43 |
| 4:2:203:THR:HG22 | 4:Z:287:ILE:HG22 | 1.86 | 0.43 |
| 4:4:205:GLU:O | 4:4:208:ILE:HG22 | 2.18 | 0.43 |
| 4:4:287:ILE:HB | 4:6:204:ALA:H | 1.83 | 0.43 |
| 4:W:223:PHE:HB3 | 4:W:259:GLU:OE2 | 2.18 | 0.43 |
| 4:X:205:GLU:O | 4:X:208:ILE:HG22 | 2.19 | 0.43 |
| 1:A:64:THR:CG2 | 1:A:65:GLU:H | 2.32 | 0.43 |
| 1:A:155:ILE:HG22 | 1:A:156:PHE:N | 2.33 | 0.43 |
| 1:A:204:GLU:N | 1:A:207:LYS:HE3 | 2.23 | 0.43 |
| 1:A:791:GLN:OE1 | 3:C:116:GLU:N | 2.50 | 0.43 |
| 2:B:149:ASP:CG | 2:B:150:TYR:N | 2.49 | 0.43 |
| 3:C:122:GLU:HA | 3:C:125:GLU:OE1 | 2.18 | 0.43 |
| 1:D:193:ILE:HD11 | 1:D:250:ILE:CD1 | 2.48 | 0.43 |
| 1:D:226:ASN:N | 1:D:227:PRO:HD2 | 2.32 | 0.43 |
| 1:D:642:LYS:HB3 | 4:9:24:ASP:HB2 | 1.37 | 0.43 |
| 2:E:140:PHE:HA | 2:E:141:PRO:HD2 | 1.57 | 0.43 |
| 1:G:14:ALA:N | 1:G:15:PRO:CD | 2.81 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:486:MLY:HH22 | 1:G:527:GLU:CD | 2.37 | 0.43 |
| 1:G:516:GLY:O | 1:G:518:ASP:N | 2.51 | 0.43 |
| 1:G:540:CYS:C | 4:V:349:LEU:HD21 | 2.36 | 0.43 |
| 1:G:725:ARG:CZ | 1:G:737:PHE:CE1 | 3.01 | 0.43 |
| 1:J:411:GLU:H | 4:W:333:PRO:HB2 | 1.81 | 0.43 |
| 1:J:538:GLU:CA | 4:W:351:THR:N | 2.68 | 0.43 |
| 1:J:541:MET:HB3 | 4:W:345:ILE:HG22 | 2.00 | 0.43 |
| 1:J:789:ALA:CB | 3:L:81:GLN:OE1 | 2.66 | 0.43 |
| 1:M:14:ALA:HB3 | 1:M:15:PRO:CD | 2.46 | 0.43 |
| 1:M:123:CYS:HB2 | 1:M:158:ILE:HD13 | 2.00 | 0.43 |
| 1:M:195:TYR:CE2 | 1:M:199:ILE:HD12 | 2.52 | 0.43 |
| 1:M:226:ASN:HB2 | 1:M:227:PRO:CD | 2.47 | 0.43 |
| 1:M:354:LEU:HD12 | 1:M:354:LEU:HA | 1.56 | 0.43 |
| 1:M:485:GLU:OE2 | 1:M:584:TYR:N | 2.50 | 0.43 |
| 1:M:725:ARG:CZ | 1:M:737:PHE:CZ | 3.01 | 0.43 |
| 1:M:732:ILE:H | 1:M:733:PRO:HD2 | 1.74 | 0.43 |
| 2:N:140:PHE:HA | 2:N:141:PRO:HD2 | 1.57 | 0.43 |
| 1:P:14:ALA:N | 1:P:15:PRO:CD | 2.82 | 0.43 |
| 1:P:218:LEU:HA | 1:P:221:GLN:HG3 | 1.71 | 0.43 |
| 1:P:292:MET:HE1 | 1:P:309:PRO:CG | 2.48 | 0.43 |
| 1:P:786:ILE:C | 1:P:789:ALA:H | 2.21 | 0.43 |
| 1:P:795:ARG:HH22 | 3:R:116:GLU:HG2 | 1.77 | 0.43 |
| 2:Q:129:THR:HG23 | 2:Q:132:GLU:OE1 | 2.17 | 0.43 |
| 3:R:119:THR:O | 3:R:123:VAL:HG23 | 2.18 | 0.43 |
| 4:2:193:LEU:O | 4:2:198:TYR:HD2 | 2.01 | 0.43 |
| 4:9:366:GLY:O | 4:9:369:ILE:HG22 | 2.16 | 0.43 |
| 4:V:149:THR:HA | 4:V:165:ILE:O | 2.19 | 0.43 |
| 4:Y:220:ALA:HB3 | 4:Y:223:PHE:CD1 | 2.53 | 0.43 |
| 4:Z:220:ALA:HB3 | 4:Z:223:PHE:CD1 | 2.53 | 0.43 |
| 1:A:221:GLN:HG2 | 1:A:221:GLN:H | 1.47 | 0.43 |
| 1:A:246:PHE:HB3 | 1:A:270:LEU:HD12 | 2.01 | 0.43 |
| 1:A:292:MET:CE | 1:A:309:PRO:CA | 2.97 | 0.43 |
| 1:A:408:VAL:HA | 1:A:636:LYS:HG3 | 1.03 | 0.43 |
| 1:A:485:GLU:OE1 | 1:A:583:HIS:ND1 | 2.49 | 0.43 |
| 1:A:747:LEU:C | 1:A:749:GLY:H | 2.21 | 0.43 |
| 1:D:109:ARG:CD | 1:D:117:THR:HB | 2.49 | 0.43 |
| 1:D:229:LEU:HD12 | 1:D:229:LEU:HA | 1.75 | 0.43 |
| 1:D:296:MLY:HH11 | 1:D:348:MLY:CH2 | 2.48 | 0.43 |
| 1:D:408:VAL:HG22 | 1:D:636:LYS:HG2 | 1.51 | 0.43 |
| 1:D:725:ARG:CZ | 1:D:737:PHE:CE1 | 3.02 | 0.43 |
| 1:D:795:ARG:NH2 | 3:F:116:GLU:HB3 | 2.28 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:F:119:THR:O | 3:F:123:VAL:HG23 | 2.18 | 0.43 |
| 1:G:391:GLY:HA3 | 1:G:616:VAL:HG23 | 2.01 | 0.43 |
| 1:G:541:MET:HB3 | 4:V:345:ILE:HG22 | 2.01 | 0.43 |
| 1:G:711:PHE:HB3 | 1:G:766:PHE:HB3 | 2.00 | 0.43 |
| 1:G:791:GLN:NE2 | 3:I:116:GLU:H | 2.16 | 0.43 |
| 1:G:818:TYR:CB | 2:H:90:GLY:HA3 | 2.42 | 0.43 |
| 3:I:101:THR:HA | 3:I:137:ILE:O | 2.18 | 0.43 |
| 1:J:14:ALA:N | 1:J:15:PRO:CD | 2.82 | 0.43 |
| 1:J:95:THR:CA | 1:J:713:SER:HB3 | 2.48 | 0.43 |
| 1:J:322:VAL:CG1 | 1:J:325:ILE:HG13 | 2.49 | 0.43 |
| 1:J:529:PRO:HB3 | 4:W:354:GLN:HA | 2.00 | 0.43 |
| 3:L:69:LEU:HB3 | 3:L:70:PRO:HD3 | 1.99 | 0.43 |
| 1:M:109:ARG:CD | 1:M:117:THR:HB | 2.49 | 0.43 |
| 1:M:129:TYR:HD1 | 1:M:129:TYR:HA | 1.65 | 0.43 |
| 1:M:218:LEU:HA | 1:M:221:GLN:HG3 | 1.71 | 0.43 |
| 1:M:516:GLY:O | 1:M:518:ASP:N | 2.51 | 0.43 |
| 1:M:541:MET:HG2 | 4:Z:345:ILE:HG22 | 2.00 | 0.43 |
| 2:N:129:THR:HG23 | 2:N:132:GLU:OE1 | 2.18 | 0.43 |
| 2:N:137:TRP:CZ3 | 2:N:145:ALA:N | 2.81 | 0.43 |
| 1:P:14:ALA:HB3 | 1:P:15:PRO:CD | 2.46 | 0.43 |
| 1:P:123:CYS:HB2 | 1:P:158:ILE:HD13 | 2.00 | 0.43 |
| 1:P:136:ASN:HA | 1:P:137:PRO:HD3 | 1.49 | 0.43 |
| 1:P:163:TYR:O | 1:P:166:MET:HB3 | 2.17 | 0.43 |
| 1:P:195:TYR:CE2 | 1:P:199:ILE:HD12 | 2.52 | 0.43 |
| 1:P:229:LEU:HD12 | 1:P:229:LEU:HA | 1.76 | 0.43 |
| 1:P:292:MET:HE3 | 1:P:309:PRO:CA | 2.45 | 0.43 |
| 1:P:410:ASN:HA | 4:1:334:GLU:HB3 | 1.29 | 0.43 |
| 1:P:783:LEU:CD1 | 1:P:783:LEU:N | 2.78 | 0.43 |
| 4:3:223:PHE:HB3 | 4:3:259:GLU:OE2 | 2.18 | 0.43 |
| 4:5:220:ALA:HB3 | 4:5:223:PHE:CD1 | 2.53 | 0.43 |
| 4:9:193:LEU:O | 4:9:198:TYR:HD2 | 2.01 | 0.43 |
| 4:X:220:ALA:HB3 | 4:X:223:PHE:CD1 | 2.53 | 0.43 |
| 4:X:223:PHE:HB3 | 4:X:259:GLU:OE2 | 2.18 | 0.43 |
| 4:Y:223:PHE:HB3 | 4:Y:259:GLU:OE2 | 2.18 | 0.43 |
| 1:A:173:GLN:HG3 | 1:A:670:HIS:HD2 | 1.82 | 0.43 |
| 1:A:174:SER:OG | 1:A:669:PRO:HA | 2.18 | 0.43 |
| 1:A:295:MLY:HG3 | 1:A:332:MET:HE2 | 2.00 | 0.43 |
| 1:A:322:VAL:CG1 | 1:A:325:ILE:HG13 | 2.49 | 0.43 |
| 1:A:391:GLY:HA3 | 1:A:616:VAL:HG23 | 2.00 | 0.43 |
| 1:A:762:HIS:CD2 | 1:A:762:HIS:N | 2.78 | 0.43 |
| 1:D:266:GLU:OE1 | 1:D:659:MLY:NZ | 2.51 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:534:SER:CB | 4:9:351:THR:HA | 2.49 | 0.43 |
| 1:D:673:ARG:HD2 | 1:D:673:ARG:HA | 1.79 | 0.43 |
| 3:F:50:LEU:O | 3:F:53:PRO:HG2 | 2.19 | 0.43 |
| 1:G:14:ALA:HB3 | 1:G:15:PRO:CD | 2.46 | 0.43 |
| 1:G:109:ARG:CD | 1:G:117:THR:HB | 2.48 | 0.43 |
| 1:G:292:MET:CE | 1:G:309:PRO:CA | 2.97 | 0.43 |
| 1:G:493:HIS:O | 1:G:496:PHE:HB3 | 2.18 | 0.43 |
| 1:G:816:ILE:HD11 | 2:H:100:ALA:HB3 | 2.00 | 0.43 |
| 3:I:122:GLU:HA | 3:I:125:GLU:OE1 | 2.18 | 0.43 |
| 1:J:40:VAL:HG23 | 1:J:76:GLN:O | 2.19 | 0.43 |
| 1:J:109:ARG:CD | 1:J:117:THR:HB | 2.49 | 0.43 |
| 1:J:201:ALA:O | 1:J:202:SER:OG | 2.36 | 0.43 |
| 1:J:292:MET:HE1 | 1:J:309:PRO:CG | 2.48 | 0.43 |
| 1:J:408:VAL:HG22 | 1:J:636:LYS:HG2 | 1.52 | 0.43 |
| 1:J:715:VAL:HG11 | 1:J:720:PHE:CD1 | 2.50 | 0.43 |
| 1:J:715:VAL:HG12 | 1:J:720:PHE:HB2 | 2.00 | 0.43 |
| 1:J:732:ILE:CG2 | 1:J:747:LEU:CD1 | 0.65 | 0.43 |
| 1:J:787:ILE:HG21 | 1:J:787:ILE:HD13 | 1.67 | 0.43 |
| 1:M:217:THR:HG22 | 1:M:218:LEU:N | 2.34 | 0.43 |
| 1:M:391:GLY:HA3 | 1:M:616:VAL:HG23 | 2.01 | 0.43 |
| 1:M:506:GLU:HG2 | 1:M:766:PHE:CE1 | 2.54 | 0.43 |
| 1:M:727:LEU:CD2 | 1:M:775:LEU:HG | 2.44 | 0.43 |
| 1:M:795:ARG:CG | 3:O:35:ARG:HH12 | 2.30 | 0.43 |
| 2:N:149:ASP:CG | 2:N:150:TYR:N | 2.49 | 0.43 |
| 1:P:292:MET:CE | 1:P:309:PRO:CA | 2.97 | 0.43 |
| 1:P:322:VAL:CG1 | 1:P:325:ILE:HG13 | 2.49 | 0.43 |
| 4:5:149:THR:HA | 4:5:165:ILE:O | 2.19 | 0.43 |
| 4:6:149:THR:HA | 4:6:165:ILE:O | 2.19 | 0.43 |
| 4:6:205:GLU:O | 4:6:208:ILE:HG22 | 2.18 | 0.43 |
| 4:7:149:THR:HA | 4:7:165:ILE:O | 2.19 | 0.43 |
| 1:A:14:ALA:N | 1:A:15:PRO:CD | 2.81 | 0.43 |
| 1:A:530:MET:CB | 4:8:354:GLN:CB | 2.95 | 0.43 |
| 1:D:64:THR:HB | 1:D:68:GLU:N | 2.33 | 0.43 |
| 1:D:151:ALA:HB1 | 1:D:152:PRO:HD2 | 2.01 | 0.43 |
| 1:D:163:TYR:O | 1:D:166:MET:HB3 | 2.17 | 0.43 |
| 1:D:295:MLY:CE | 1:D:332:MET:CE | 2.97 | 0.43 |
| 1:D:400:ALA:CB | 1:D:606:THR:HG22 | 2.49 | 0.43 |
| 1:D:485:GLU:HA | 1:D:584:TYR:HE2 | 1.83 | 0.43 |
| 1:D:540:CYS:C | 4:9:349:LEU:HD21 | 2.37 | 0.43 |
| 1:D:639:GLY:H | 4:9:344:SER:HB3 | 1.83 | 0.43 |
| 2:E:137:TRP:CZ3 | 2:E:145:ALA:N | 2.81 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:439:LEU:N | 1:G:439:LEU:CD1 | 2.81 | 0.43 |
| 1:G:443:ILE:HG22 | 1:G:444:ARG:N | 2.29 | 0.43 |
| 1:G:485:GLU:OE1 | 1:G:583:HIS:ND1 | 2.49 | 0.43 |
| 1:G:536:LEU:HA | 1:G:536:LEU:HD12 | 1.69 | 0.43 |
| 1:J:151:ALA:HB1 | 1:J:152:PRO:HD2 | 2.01 | 0.43 |
| 1:J:193:ILE:HD11 | 1:J:250:ILE:CD1 | 2.48 | 0.43 |
| 1:J:206:LYS:CE | 1:J:217:THR:HG23 | 2.30 | 0.43 |
| 1:J:218:LEU:HA | 1:J:221:GLN:HG3 | 1.71 | 0.43 |
| 1:J:747:LEU:C | 1:J:749:GLY:H | 2.20 | 0.43 |
| 3:L:119:THR:O | 3:L:123:VAL:HG23 | 2.18 | 0.43 |
| 3:L:122:GLU:HA | 3:L:125:GLU:OE1 | 2.18 | 0.43 |
| 1:M:14:ALA:N | 1:M:15:PRO:CD | 2.81 | 0.43 |
| 1:M:55:MLY:HH23 | 1:M:60:VAL:HG22 | 1.99 | 0.43 |
| 1:M:292:MET:CE | 1:M:309:PRO:CA | 2.97 | 0.43 |
| 1:M:496:PHE:HB2 | 1:M:515:PHE:CD2 | 2.53 | 0.43 |
| 1:M:530:MET:CB | 4:Z:354:GLN:CB | 2.95 | 0.43 |
| 1:M:544:LYS:HD2 | 4:Z:147:ARG:CB | 2.36 | 0.43 |
| 1:P:93:MET:CE | 1:P:764:MLY:HD3 | 2.49 | 0.43 |
| 1:P:109:ARG:CD | 1:P:117:THR:HB | 2.49 | 0.43 |
| 1:P:217:THR:HG22 | 1:P:218:LEU:N | 2.34 | 0.43 |
| 1:P:226:ASN:N | 1:P:227:PRO:HD2 | 2.32 | 0.43 |
| 1:P:246:PHE:HB3 | 1:P:270:LEU:HD12 | 2.01 | 0.43 |
| 1:P:391:GLY:HA3 | 1:P:616:VAL:HG23 | 2.01 | 0.43 |
| 1:P:725:ARG:CZ | 1:P:737:PHE:CE1 | 3.02 | 0.43 |
| 4:2:322:PRO:HB3 | 4:4:244:ASP:HB3 | 1.77 | 0.43 |
| 4:4:149:THR:HA | 4:4:165:ILE:O | 2.19 | 0.43 |
| 4:4:223:PHE:HB3 | 4:4:259:GLU:OE2 | 2.18 | 0.43 |
| 4:6:220:ALA:HB3 | 4:6:223:PHE:CD1 | 2.53 | 0.43 |
| 4:X:193:LEU:O | 4:X:198:TYR:HD2 | 2.01 | 0.43 |
| 4:Z:149:THR:HA | 4:Z:165:ILE:O | 2.19 | 0.43 |
| 1:A:439:LEU:N | 1:A:439:LEU:CD1 | 2.81 | 0.43 |
| 1:A:502:GLU:HA | 1:A:762:HIS:N | 2.34 | 0.43 |
| 1:A:536:LEU:HA | 1:A:536:LEU:HD12 | 1.69 | 0.43 |
| 1:D:40:VAL:HG23 | 1:D:76:GLN:O | 2.19 | 0.43 |
| 1:D:64:THR:CG2 | 1:D:65:GLU:H | 2.32 | 0.43 |
| 1:D:659:MLY:HD2 | 1:D:659:MLY:HH22 | 1.42 | 0.43 |
| 1:D:787:ILE:HG23 | 1:D:791:GLN:HG3 | 2.01 | 0.43 |
| 1:G:195:TYR:CD2 | 1:G:199:ILE:HD13 | 2.54 | 0.43 |
| 1:G:217:THR:HG22 | 1:G:218:LEU:N | 2.34 | 0.43 |
| 1:G:322:VAL:CG1 | 1:G:325:ILE:HG13 | 2.49 | 0.43 |
| 1:G:400:ALA:CB | 1:G:606:THR:HG22 | 2.49 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:442:VAL:O | 1:G:445:ILE:HB | 2.19 | 0.43 |
| 1:J:294:ASN:OD1 | 1:J:307:THR:HG21 | 2.19 | 0.43 |
| 1:J:496:PHE:HB2 | 1:J:515:PHE:CD2 | 2.54 | 0.43 |
| 1:J:541:MET:HG2 | 4:W:345:ILE:HG22 | 2.00 | 0.43 |
| 1:M:169:ASP:O | 1:M:170:ARG:HB2 | 2.19 | 0.43 |
| 1:M:201:ALA:O | 1:M:202:SER:OG | 2.36 | 0.43 |
| 1:M:540:CYS:C | 4:Z:349:LEU:HD21 | 2.36 | 0.43 |
| 1:M:541:MET:HB3 | 4:Z:345:ILE:HG22 | 2.00 | 0.43 |
| 1:M:643:GLY:CA | 4:Z:24:ASP:OD1 | 2.62 | 0.43 |
| 1:M:747:LEU:C | 1:M:749:GLY:N | 2.71 | 0.43 |
| 1:M:787:ILE:HG21 | 1:M:787:ILE:HD13 | 1.67 | 0.43 |
| 1:M:829:TRP:CZ3 | 2:N:84:PHE:CE1 | 3.07 | 0.43 |
| 1:P:17:LEU:HA | 1:P:17:LEU:HD12 | 1.68 | 0.43 |
| 1:P:144:ARG:HD2 | 1:P:144:ARG:HA | 1.78 | 0.43 |
| 1:P:195:TYR:CD2 | 1:P:199:ILE:HD13 | 2.54 | 0.43 |
| 1:P:400:ALA:CB | 1:P:606:THR:HG22 | 2.49 | 0.43 |
| 1:P:500:GLN:HB2 | 1:P:512:PHE:CZ | 2.54 | 0.43 |
| 1:P:675:ILE:HG23 | 1:P:676:ILE:N | 2.33 | 0.43 |
| 1:P:711:PHE:HB3 | 1:P:766:PHE:HB3 | 1.99 | 0.43 |
| 1:P:732:ILE:CG2 | 1:P:747:LEU:CD1 | 0.65 | 0.43 |
| 1:P:793:ARG:O | 1:P:797:PHE:N | 2.39 | 0.43 |
| 1:P:795:ARG:CD | 3:R:35:ARG:HH12 | 2.30 | 0.43 |
| 4:4:217:CYS:C | 4:4:218:TYR:HD1 | 2.23 | 0.43 |
| 4:4:322:PRO:HB2 | 4:6:244:ASP:HB2 | 1.83 | 0.43 |
| 4:V:193:LEU:O | 4:V:198:TYR:HD2 | 2.01 | 0.43 |
| 4:X:149:THR:HA | 4:X:165:ILE:O | 2.19 | 0.43 |
| 4:Z:223:PHE:HB3 | 4:Z:259:GLU:OE2 | 2.18 | 0.43 |
| 1:A:278:GLN:HE21 | 1:A:278:GLN:HB3 | 1.42 | 0.43 |
| 1:A:295:MLY:CE | 1:A:332:MET:CE | 2.96 | 0.43 |
| 1:A:449:LEU:HD12 | 1:A:449:LEU:HA | 1.60 | 0.43 |
| 1:A:506:GLU:OE1 | 1:A:760:PHE:C | 2.47 | 0.43 |
| 1:A:541:MET:CE | 4:8:346:LEU:HD12 | 2.48 | 0.43 |
| 1:A:550:PHE:C | 4:V:46:GLY:CA | 2.87 | 0.43 |
| 1:A:795:ARG:CB | 3:C:35:ARG:HH12 | 1.76 | 0.43 |
| 1:D:86:ASP:OD2 | 1:D:87:MLY:HH22 | 2.19 | 0.43 |
| 1:D:292:MET:CE | 1:D:309:PRO:CA | 2.97 | 0.43 |
| 1:D:486:MLY:HH22 | 1:D:527:GLU:CD | 2.37 | 0.43 |
| 1:D:500:GLN:HB2 | 1:D:512:PHE:CZ | 2.54 | 0.43 |
| 1:G:174:SER:OG | 1:G:669:PRO:HA | 2.18 | 0.43 |
| 1:G:226:ASN:HB2 | 1:G:227:PRO:CD | 2.48 | 0.43 |
| 1:G:229:LEU:HD12 | 1:G:229:LEU:HA | 1.75 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:246:PHE:HB3 | 1:G:270:LEU:HD12 | 2.01 | 0.43 |
| 1:G:266:GLU:OE1 | 1:G:659:MLY:NZ | 2.51 | 0.43 |
| 1:G:436:MLY:HE3 | 1:G:626:TYR:HE1 | 1.77 | 0.43 |
| 1:J:537:GLU:OE1 | 4:W:350:SER:HA | 2.19 | 0.43 |
| 1:J:725:ARG:CZ | 1:J:737:PHE:CE1 | 3.02 | 0.43 |
| 1:J:829:TRP:HH2 | 2:K:83:MET:HE3 | 1.84 | 0.43 |
| 1:M:62:VAL:HG12 | 1:M:63:MLY:N | 2.34 | 0.43 |
| 1:M:174:SER:OG | 1:M:669:PRO:HA | 2.19 | 0.43 |
| 1:M:195:TYR:CD2 | 1:M:199:ILE:HD13 | 2.54 | 0.43 |
| 1:M:538:GLU:CD | 4:Z:355:MET:HE1 | 2.29 | 0.43 |
| 1:M:725:ARG:CZ | 1:M:733:PRO:CB | 2.83 | 0.43 |
| 1:P:141:LEU:HD12 | 1:P:141:LEU:N | 2.32 | 0.43 |
| 1:P:151:ALA:HB1 | 1:P:152:PRO:HD2 | 2.01 | 0.43 |
| 1:P:266:GLU:OE1 | 1:P:659:MLY:NZ | 2.51 | 0.43 |
| 1:P:330:GLU:HG2 | 1:P:330:GLU:H | 1.54 | 0.43 |
| 1:P:537:GLU:OE1 | 4:1:350:SER:HA | 2.19 | 0.43 |
| 1:P:659:MLY:HD2 | 1:P:659:MLY:HH22 | 1.42 | 0.43 |
| 4:1:287:ILE:CB | 4:3:203:THR:HB | 2.47 | 0.43 |
| 4:5:193:LEU:O | 4:5:198:TYR:HD2 | 2.01 | 0.43 |
| 4:9:149:THR:HA | 4:9:165:ILE:O | 2.19 | 0.43 |
| 4:Z:193:LEU:O | 4:Z:198:TYR:HD2 | 2.02 | 0.43 |
| 1:A:332:MET:O | 1:A:336:SER:OG | 2.27 | 0.43 |
| 1:A:410:ASN:HA | 4:8:334:GLU:HB3 | 1.30 | 0.43 |
| 1:A:442:VAL:O | 1:A:445:ILE:HB | 2.19 | 0.43 |
| 1:A:445:ILE:HG22 | 1:A:449:LEU:HD22 | 2.01 | 0.43 |
| 1:D:578:HIS:HB3 | 1:D:592:ILE:CD1 | 2.38 | 0.43 |
| 1:D:713:SER:H | 1:D:771:LEU:HD23 | 1.40 | 0.43 |
| 1:D:727:LEU:HD21 | 1:D:782:MLY:HG2 | 2.01 | 0.43 |
| 1:G:169:ASP:O | 1:G:170:ARG:HB2 | 2.19 | 0.43 |
| 1:G:541:MET:CE | 4:V:346:LEU:HD12 | 2.48 | 0.43 |
| 1:J:17:LEU:HA | 1:J:17:LEU:HD12 | 1.68 | 0.43 |
| 1:J:141:LEU:HD12 | 1:J:141:LEU:N | 2.32 | 0.43 |
| 1:J:217:THR:HG22 | 1:J:218:LEU:N | 2.34 | 0.43 |
| 1:J:266:GLU:OE1 | 1:J:659:MLY:NZ | 2.51 | 0.43 |
| 1:J:296:MLY:HH11 | 1:J:348:MLY:CH2 | 2.48 | 0.43 |
| 1:J:534:SER:CB | 4:W:351:THR:HA | 2.49 | 0.43 |
| 1:J:541:MET:N | 4:W:349:LEU:CD2 | 2.69 | 0.43 |
| 1:J:612:GLN:NE2 | 1:J:627:GLY:H | 2.14 | 0.43 |
| 1:J:787:ILE:HG23 | 1:J:791:GLN:HG3 | 2.01 | 0.43 |
| 1:J:797:PHE:HE2 | 3:L:126:LEU:CD2 | 2.24 | 0.43 |
| 2:K:112:ILE:O | 2:K:148:VAL:N | 2.50 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:64:THR:CG2 | 1:M:65:GLU:H | 2.32 | 0.43 |
| 1:M:322:VAL:CG1 | 1:M:325:ILE:HG13 | 2.49 | 0.43 |
| 1:M:724:TYR:HB3 | 1:M:727:LEU:CD1 | 2.49 | 0.43 |
| 1:P:169:ASP:O | 1:P:170:ARG:HB2 | 2.19 | 0.43 |
| 1:P:295:MLY:CE | 1:P:332:MET:CE | 2.97 | 0.43 |
| 1:P:689:GLU:HA | 1:P:692:LEU:HB2 | 2.00 | 0.43 |
| 1:P:712:PRO:HB2 | 1:P:713:SER:H | 1.61 | 0.43 |
| 1:P:769:ALA:C | 1:P:770:GLY:CA | 2.84 | 0.43 |
| 4:3:220:ALA:HB3 | 4:3:223:PHE:CD1 | 2.53 | 0.43 |
| 4:5:205:GLU:O | 4:5:208:ILE:HG22 | 2.18 | 0.43 |
| 1:A:549:SER:C | 4:V:45:VAL:O | 2.56 | 0.42 |
| 1:A:732:ILE:CG2 | 1:A:747:LEU:HD12 | 0.35 | 0.42 |
| 1:A:787:ILE:HG23 | 1:A:791:GLN:HG3 | 2.00 | 0.42 |
| 1:D:141:LEU:HD12 | 1:D:141:LEU:N | 2.32 | 0.42 |
| 1:D:173:GLN:HG3 | 1:D:670:HIS:CD2 | 2.54 | 0.42 |
| 1:D:496:PHE:HB2 | 1:D:515:PHE:CD2 | 2.54 | 0.42 |
| 1:D:541:MET:HG2 | 4:9:345:ILE:HG22 | 2.00 | 0.42 |
| 1:D:715:VAL:HG11 | 1:D:720:PHE:CD1 | 2.50 | 0.42 |
| 1:D:747:LEU:C | 1:D:749:GLY:N | 2.71 | 0.42 |
| 3:F:101:THR:HA | 3:F:137:ILE:O | 2.18 | 0.42 |
| 1:G:129:TYR:HD1 | 1:G:129:TYR:HA | 1.65 | 0.42 |
| 1:G:309:PRO:C | 1:G:311:ASP:H | 2.22 | 0.42 |
| 1:G:576:GLU:CG | 1:G:577:ALA:N | 2.44 | 0.42 |
| 1:G:659:MLY:HH22 | 1:G:659:MLY:HD2 | 1.42 | 0.42 |
| 3:I:63:ILE:CG2 | 3:I:64:THR:H | 2.32 | 0.42 |
| 1:J:86:ASP:OD2 | 1:J:87:MLY:HH22 | 2.19 | 0.42 |
| 1:J:486:MLY:HH22 | 1:J:527:GLU:CD | 2.37 | 0.42 |
| 1:J:530:MET:CE | 4:W:354:GLN:CB | 2.96 | 0.42 |
| 1:J:689:GLU:HA | 1:J:692:LEU:HB2 | 2.00 | 0.42 |
| 1:J:725:ARG:CZ | 1:J:737:PHE:CZ | 3.01 | 0.42 |
| 2:K:149:ASP:OD2 | 2:K:150:TYR:CA | 2.64 | 0.42 |
| 1:M:173:GLN:HG3 | 1:M:670:HIS:CD2 | 2.54 | 0.42 |
| 1:M:175:ILE:C | 1:M:176:LEU:HD12 | 2.39 | 0.42 |
| 1:M:400:ALA:CB | 1:M:606:THR:HG22 | 2.49 | 0.42 |
| 1:P:91:MET:CE | 1:P:119:SER:HB2 | 2.48 | 0.42 |
| 1:P:106:LEU:HD12 | 1:P:106:LEU:HA | 1.80 | 0.42 |
| 1:P:174:SER:OG | 1:P:669:PRO:HA | 2.18 | 0.42 |
| 1:P:176:LEU:N | 1:P:176:LEU:CD1 | 2.75 | 0.42 |
| 1:P:201:ALA:O | 1:P:202:SER:OG | 2.36 | 0.42 |
| 1:P:476:GLU:CD | 1:P:476:GLU:H | 2.22 | 0.42 |
| 1:P:546:THR:HB | 4:3:47:MET:C | 2.39 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:P:791:GLN:HE22 | 3:R:116:GLU:H | 1.61 | 0.42 |
| 1:P:819:ASN:CB | 2:Q:90:GLY:O | 2.61 | 0.42 |
| 3:R:63:ILE:CG2 | 3:R:64:THR:H | 2.32 | 0.42 |
| 4:1:149:THR:HA | 4:1:165:ILE:O | 2.19 | 0.42 |
| 4:2:217:CYS:C | 4:2:218:TYR:HD1 | 2.23 | 0.42 |
| 4:7:205:GLU:O | 4:7:208:ILE:HG22 | 2.19 | 0.42 |
| 4:8:149:THR:HA | 4:8:165:ILE:O | 2.19 | 0.42 |
| 4:8:205:GLU:O | 4:8:208:ILE:HG22 | 2.19 | 0.42 |
| 4:8:206:ARG:O | 4:8:209:VAL:HG12 | 2.19 | 0.42 |
| 4:8:287:ILE:HA | 4:V:202:THR:HG21 | 1.59 | 0.42 |
| 4:V:220:ALA:HB3 | 4:V:223:PHE:CD1 | 2.53 | 0.42 |
| 4:W:193:LEU:O | 4:W:198:TYR:HD2 | 2.01 | 0.42 |
| 1:A:62:VAL:O | 1:A:69:THR:HA | 2.19 | 0.42 |
| 1:A:217:THR:HG22 | 1:A:218:LEU:N | 2.34 | 0.42 |
| 1:A:476:GLU:H | 1:A:476:GLU:CD | 2.22 | 0.42 |
| 1:A:541:MET:HG2 | 4:8:345:ILE:HG23 | 2.01 | 0.42 |
| 1:A:568:PRO:O | 1:A:570:PRO:HD3 | 2.19 | 0.42 |
| 1:A:725:ARG:CZ | 1:A:737:PHE:CZ | 3.01 | 0.42 |
| 1:A:823:PHE:HE1 | 2:B:160:GLY:C | 2.21 | 0.42 |
| 1:D:38:VAL:HG13 | 1:D:39:PHE:N | 2.34 | 0.42 |
| 1:D:294:ASN:OD1 | 1:D:307:THR:HG21 | 2.19 | 0.42 |
| 1:D:689:GLU:HA | 1:D:692:LEU:HB2 | 2.00 | 0.42 |
| 2:E:123:THR:HA | 3:F:19:ARG:HH12 | 1.84 | 0.42 |
| 3:F:63:ILE:CG2 | 3:F:64:THR:H | 2.32 | 0.42 |
| 1:G:295:MLY:HG3 | 1:G:332:MET:HE2 | 2.01 | 0.42 |
| 1:G:445:ILE:HG22 | 1:G:449:LEU:HD22 | 2.01 | 0.42 |
| 1:G:519:LEU:HD12 | 1:G:519:LEU:H | 1.83 | 0.42 |
| 1:G:625:THR:H | 1:G:625:THR:HG22 | 1.48 | 0.42 |
| 1:G:724:TYR:HB3 | 1:G:727:LEU:CD1 | 2.48 | 0.42 |
| 2:H:140:PHE:CD2 | 2:H:144:VAL:HG11 | 2.55 | 0.42 |
| 1:J:64:THR:CG2 | 1:J:65:GLU:H | 2.32 | 0.42 |
| 1:J:195:TYR:CD2 | 1:J:199:ILE:HD13 | 2.54 | 0.42 |
| 1:J:246:PHE:HB3 | 1:J:270:LEU:HD12 | 2.01 | 0.42 |
| 1:J:500:GLN:HB2 | 1:J:512:PHE:CZ | 2.54 | 0.42 |
| 1:J:813:ILE:HG22 | 2:K:128:PHE:CE1 | 2.40 | 0.42 |
| 1:J:830:PRO:HB3 | 2:K:67:MET:CE | 2.47 | 0.42 |
| 1:J:839:MLY:N | 1:J:840:PRO:HD2 | 2.34 | 0.42 |
| 1:M:155:ILE:HG22 | 1:M:156:PHE:N | 2.33 | 0.42 |
| 1:M:402:CYS:C | 1:M:404:PRO:HD3 | 2.40 | 0.42 |
| 1:M:724:TYR:CE2 | 1:M:772:LEU:HG | 2.52 | 0.42 |
| 1:M:821:ARG:CZ | 2:N:127:ARG:NE | 2.81 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:P:439:LEU:N | 1:P:439:LEU:CD1 | 2.81 | 0.42 |
| 1:P:817:GLN:HG3 | 2:Q:128:PHE:HE1 | 1.78 | 0.42 |
| 4:1:287:ILE:CG2 | 4:3:203:THR:N | 2.57 | 0.42 |
| 4:5:206:ARG:O | 4:5:209:VAL:HG12 | 2.20 | 0.42 |
| 1:A:149:GLN:CG | 1:A:716:LEU:HD23 | 2.44 | 0.42 |
| 1:A:195:TYR:CD2 | 1:A:199:ILE:HD13 | 2.54 | 0.42 |
| 1:A:400:ALA:CB | 1:A:606:THR:HG22 | 2.48 | 0.42 |
| 1:A:551:MLY:C | 4:V:47:MET:HA | 2.48 | 0.42 |
| 1:A:774:LEU:HD23 | 1:A:778:MET:HE3 | 2.01 | 0.42 |
| 1:A:823:PHE:CD1 | 2:B:160:GLY:HA3 | 2.51 | 0.42 |
| 1:D:107:MLY:CB | 1:D:686:MET:HE2 | 2.41 | 0.42 |
| 1:D:690:LEU:O | 1:D:694:GLN:HG3 | 2.20 | 0.42 |
| 1:G:271:GLU:OE1 | 1:G:274:ARG:NH1 | 2.53 | 0.42 |
| 1:G:320:ILE:O | 1:G:320:ILE:HG22 | 2.18 | 0.42 |
| 1:G:505:MLY:HD2 | 1:G:762:HIS:CD2 | 2.53 | 0.42 |
| 1:G:505:MLY:HH22 | 1:G:762:HIS:CE1 | 1.42 | 0.42 |
| 1:G:530:MET:CE | 4:V:354:GLN:CB | 2.95 | 0.42 |
| 1:J:62:VAL:HG12 | 1:J:63:MLY:N | 2.35 | 0.42 |
| 1:J:445:ILE:HG22 | 1:J:449:LEU:HD22 | 2.02 | 0.42 |
| 1:J:476:GLU:CD | 1:J:476:GLU:H | 2.22 | 0.42 |
| 2:K:137:TRP:CZ3 | 2:K:145:ALA:N | 2.81 | 0.42 |
| 1:M:41:VAL:CG1 | 1:M:42:HIS:N | 2.76 | 0.42 |
| 1:M:63:MLY:HH23 | 1:M:63:MLY:HD3 | 1.76 | 0.42 |
| 1:M:442:VAL:O | 1:M:445:ILE:HB | 2.19 | 0.42 |
| 1:M:747:LEU:O | 1:M:749:GLY:N | 2.53 | 0.42 |
| 1:M:798:LEU:HD12 | 1:M:798:LEU:HA | 1.36 | 0.42 |
| 1:M:817:GLN:CD | 2:N:127:ARG:CD | 2.74 | 0.42 |
| 1:P:86:ASP:OD2 | 1:P:87:MLY:HH22 | 2.19 | 0.42 |
| 1:P:406:VAL:O | 1:P:412:ALA:HA | 2.19 | 0.42 |
| 1:P:442:VAL:O | 1:P:445:ILE:HB | 2.19 | 0.42 |
| 1:P:530:MET:CE | 4:1:354:GLN:CB | 2.96 | 0.42 |
| 1:P:541:MET:HB3 | 4:1:345:ILE:HG22 | 2.00 | 0.42 |
| 1:P:692:LEU:HA | 1:P:692:LEU:HD23 | 1.85 | 0.42 |
| 1:P:791:GLN:OE1 | 3:R:116:GLU:N | 2.45 | 0.42 |
| 1:P:831:TRP:CH2 | 2:Q:47:LEU:HD23 | 2.40 | 0.42 |
| 4:1:205:GLU:O | 4:1:208:ILE:HG22 | 2.18 | 0.42 |
| 4:4:180:LEU:HD11 | 4:4:261:LEU:HD23 | 2.02 | 0.42 |
| 4:4:220:ALA:HB3 | 4:4:223:PHE:CD1 | 2.53 | 0.42 |
| 4:V:180:LEU:HD11 | 4:V:261:LEU:HD23 | 2.02 | 0.42 |
| 4:W:149:THR:HA | 4:W:165:ILE:O | 2.19 | 0.42 |
| 4:Y:193:LEU:O | 4:Y:198:TYR:HD2 | 2.01 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:Y:222:ASP:OD1 | 4:Y:224:GLU:HB3 | 2.20 | 0.42 |
| 1:A:40:VAL:HG23 | 1:A:76:GLN:O | 2.19 | 0.42 |
| 1:A:134:VAL:C | 1:A:136:ASN:H | 2.16 | 0.42 |
| 1:A:271:GLU:OE1 | 1:A:274:ARG:NH1 | 2.53 | 0.42 |
| 1:A:797:PHE:CE1 | 3:C:149:VAL:CG1 | 3.03 | 0.42 |
| 1:D:14:ALA:N | 1:D:15:PRO:CD | 2.81 | 0.42 |
| 1:D:62:VAL:HG12 | 1:D:63:MLY:N | 2.35 | 0.42 |
| 1:D:91:MET:CE | 1:D:119:SER:HB2 | 2.48 | 0.42 |
| 1:D:169:ASP:O | 1:D:170:ARG:HB2 | 2.19 | 0.42 |
| 1:D:330:GLU:HG2 | 1:D:330:GLU:H | 1.54 | 0.42 |
| 1:D:442:VAL:O | 1:D:445:ILE:HB | 2.19 | 0.42 |
| 1:D:529:PRO:HB3 | 4:9:354:GLN:HA | 2.00 | 0.42 |
| 1:D:553:MLY:CE | 4:W:45:VAL:CA | 2.49 | 0.42 |
| 1:D:733:PRO:CB | 1:D:737:PHE:CE1 | 3.02 | 0.42 |
| 1:D:787:ILE:HG21 | 1:D:787:ILE:HD13 | 1.67 | 0.42 |
| 1:G:64:THR:CG2 | 1:G:65:GLU:H | 2.32 | 0.42 |
| 1:G:107:MLY:CB | 1:G:686:MET:HE2 | 2.43 | 0.42 |
| 1:G:279:LEU:CB | 1:G:280:PRO:HD2 | 2.49 | 0.42 |
| 1:G:406:VAL:O | 1:G:412:ALA:HA | 2.19 | 0.42 |
| 1:G:553:MLY:CB | 4:X:46:GLY:HA3 | 2.49 | 0.42 |
| 3:I:48:LYS:HA | 3:I:48:LYS:HD3 | 1.17 | 0.42 |
| 3:I:52:ASN:CB | 3:I:53:PRO:HD3 | 2.28 | 0.42 |
| 1:J:402:CYS:C | 1:J:404:PRO:HD3 | 2.40 | 0.42 |
| 1:J:506:GLU:OE2 | 1:J:760:PHE:O | 2.37 | 0.42 |
| 3:L:62:ALA:O | 3:L:63:ILE:HG13 | 2.14 | 0.42 |
| 1:M:295:MLY:CE | 1:M:332:MET:CE | 2.97 | 0.42 |
| 1:M:537:GLU:OE1 | 4:Z:350:SER:HA | 2.19 | 0.42 |
| 1:P:40:VAL:HG23 | 1:P:76:GLN:O | 2.19 | 0.42 |
| 1:P:308:ASN:HA | 1:P:309:PRO:HD2 | 1.88 | 0.42 |
| 1:P:836:PHE:CD1 | 2:Q:160:GLY:N | 2.86 | 0.42 |
| 4:2:205:GLU:O | 4:2:208:ILE:HG22 | 2.19 | 0.42 |
| 4:3:217:CYS:C | 4:3:218:TYR:HD1 | 2.23 | 0.42 |
| 4:4:315:LYS:HD2 | 4:4:315:LYS:HA | 1.92 | 0.42 |
| 4:6:180:LEU:HD11 | 4:6:261:LEU:HD23 | 2.02 | 0.42 |
| 4:8:180:LEU:HD11 | 4:8:261:LEU:HD23 | 2.02 | 0.42 |
| 4:9:196:ARG:HH21 | 4:9:249:THR:HG23 | 1.85 | 0.42 |
| 4:9:217:CYS:C | 4:9:218:TYR:HD1 | 2.23 | 0.42 |
| 4:X:180:LEU:HD11 | 4:X:261:LEU:HD23 | 2.01 | 0.42 |
| 1:A:91:MET:CE | 1:A:119:SER:HB2 | 2.47 | 0.42 |
| 1:A:169:ASP:O | 1:A:170:ARG:HB2 | 2.19 | 0.42 |
| 1:A:309:PRO:C | 1:A:311:ASP:H | 2.22 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:436:MLY:HE3 | 1:A:626:TYR:HE1 | 1.77 | 0.42 |
| 1:A:529:PRO:HB3 | 4:8:354:GLN:HA | 2.00 | 0.42 |
| 1:A:690:LEU:O | 1:A:694:GLN:HG3 | 2.20 | 0.42 |
| 1:D:332:MET:H | 1:D:332:MET:HG2 | 1.52 | 0.42 |
| 1:D:712:PRO:HD2 | 1:D:771:LEU:HD13 | 2.01 | 0.42 |
| 1:D:725:ARG:CZ | 1:D:733:PRO:CB | 2.83 | 0.42 |
| 1:D:798:LEU:HD12 | 1:D:798:LEU:HA | 1.36 | 0.42 |
| 1:D:839:MLY:N | 1:D:840:PRO:HD2 | 2.35 | 0.42 |
| 1:G:93:MET:HE1 | 1:G:764:MLY:CD | 2.49 | 0.42 |
| 1:G:295:MLY:CE | 1:G:332:MET:CE | 2.97 | 0.42 |
| 1:G:503:TYR:OH | 1:G:711:PHE:CE2 | 2.57 | 0.42 |
| 1:G:568:PRO:O | 1:G:570:PRO:HD3 | 2.19 | 0.42 |
| 1:G:747:LEU:C | 1:G:749:GLY:N | 2.71 | 0.42 |
| 1:G:756:THR:HB | 1:G:757:GLN:H | 1.64 | 0.42 |
| 3:I:50:LEU:O | 3:I:53:PRO:HG2 | 2.18 | 0.42 |
| 1:J:56:GLU:HB2 | 1:J:59:MLY:CB | 2.30 | 0.42 |
| 1:J:149:GLN:HE21 | 1:J:149:GLN:HB2 | 1.71 | 0.42 |
| 1:J:406:VAL:O | 1:J:412:ALA:HA | 2.19 | 0.42 |
| 1:J:442:VAL:O | 1:J:445:ILE:HB | 2.19 | 0.42 |
| 1:J:568:PRO:O | 1:J:570:PRO:HD3 | 2.19 | 0.42 |
| 3:L:50:LEU:O | 3:L:53:PRO:HG2 | 2.18 | 0.42 |
| 1:M:279:LEU:CB | 1:M:280:PRO:HD2 | 2.49 | 0.42 |
| 1:M:568:PRO:O | 1:M:570:PRO:HD3 | 2.19 | 0.42 |
| 3:O:62:ALA:O | 3:O:63:ILE:HG13 | 2.14 | 0.42 |
| 3:O:63:ILE:CG2 | 3:O:64:THR:H | 2.32 | 0.42 |
| 1:P:38:VAL:HG13 | 1:P:39:PHE:N | 2.35 | 0.42 |
| 1:P:213:LYS:HA | 1:P:220:ASP:OD2 | 2.19 | 0.42 |
| 1:P:309:PRO:C | 1:P:311:ASP:H | 2.22 | 0.42 |
| 1:P:445:ILE:HG22 | 1:P:449:LEU:HD22 | 2.02 | 0.42 |
| 1:P:795:ARG:CG | 3:R:35:ARG:HH12 | 2.33 | 0.42 |
| 1:P:826:VAL:O | 1:P:828:HIS:N | 2.53 | 0.42 |
| 4:2:180:LEU:HD11 | 4:2:261:LEU:HD23 | 2.02 | 0.42 |
| 4:8:220:ALA:HB3 | 4:8:223:PHE:CD1 | 2.53 | 0.42 |
| 4:9:180:LEU:HD11 | 4:9:261:LEU:HD23 | 2.01 | 0.42 |
| 4:W:206:ARG:O | 4:W:209:VAL:HG12 | 2.20 | 0.42 |
| 4:W:217:CYS:C | 4:W:218:TYR:HD1 | 2.23 | 0.42 |
| 4:X:206:ARG:O | 4:X:209:VAL:HG12 | 2.20 | 0.42 |
| 4:Y:206:ARG:O | 4:Y:209:VAL:HG12 | 2.20 | 0.42 |
| 4:Z:206:ARG:O | 4:Z:209:VAL:HG12 | 2.20 | 0.42 |
| 1:A:540:CYS:C | 4:8:349:LEU:HD21 | 2.36 | 0.42 |
| 1:A:829:TRP:O | 1:A:832:MET:N | 2.50 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:445:ILE:HG22 | 1:D:449:LEU:HD22 | 2.02 | 0.42 |
| 1:D:541:MET:CE | 4:9:346:LEU:HD12 | 2.47 | 0.42 |
| 1:D:625:THR:H | 1:D:625:THR:HG22 | 1.48 | 0.42 |
| 1:D:701:LEU:HA | 1:D:701:LEU:HD12 | 1.55 | 0.42 |
| 1:D:826:VAL:O | 1:D:828:HIS:N | 2.53 | 0.42 |
| 1:D:842:LEU:N | 1:D:842:LEU:CD1 | 2.83 | 0.42 |
| 1:G:202:SER:HA | 1:G:207:LYS:NZ | 2.23 | 0.42 |
| 1:G:538:GLU:OE1 | 4:V:355:MET:HE3 | 2.19 | 0.42 |
| 1:J:84:MLY:HH21 | 1:J:720:PHE:O | 2.18 | 0.42 |
| 1:J:87:MLY:HD3 | 1:J:87:MLY:HH12 | 1.61 | 0.42 |
| 1:J:95:THR:CA | 1:J:713:SER:CB | 2.88 | 0.42 |
| 1:J:155:ILE:HG22 | 1:J:156:PHE:N | 2.33 | 0.42 |
| 1:J:400:ALA:CB | 1:J:606:THR:HG22 | 2.49 | 0.42 |
| 1:J:553:MLY:HE2 | 4:Y:45:VAL:HB | 2.01 | 0.42 |
| 1:J:791:GLN:HB3 | 3:L:116:GLU:OE2 | 2.19 | 0.42 |
| 1:M:174:SER:HA | 1:M:460:GLY:O | 2.20 | 0.42 |
| 1:M:289:TYR:OH | 1:M:315:VAL:O | 2.27 | 0.42 |
| 1:M:826:VAL:O | 1:M:828:HIS:N | 2.53 | 0.42 |
| 2:N:114:LYS:CG | 2:N:146:GLY:HA2 | 2.46 | 0.42 |
| 1:P:88:ILE:HG21 | 1:P:88:ILE:HD12 | 1.78 | 0.42 |
| 2:Q:140:PHE:CD2 | 2:Q:144:VAL:HG11 | 2.55 | 0.42 |
| 4:1:244:ASP:HA | 4:Y:291:LYS:HG3 | 1.53 | 0.42 |
| 4:1:315:LYS:HD2 | 4:1:315:LYS:HA | 1.92 | 0.42 |
| 4:2:206:ARG:O | 4:2:209:VAL:HG12 | 2.20 | 0.42 |
| 4:2:220:ALA:HB3 | 4:2:223:PHE:CD1 | 2.53 | 0.42 |
| 4:5:171:LEU:HA | 4:5:172:PRO:HD2 | 1.84 | 0.42 |
| 4:5:196:ARG:HH21 | 4:5:249:THR:HG23 | 1.85 | 0.42 |
| 4:6:315:LYS:HD2 | 4:6:315:LYS:HA | 1.92 | 0.42 |
| 4:8:193:LEU:O | 4:8:198:TYR:HD2 | 2.01 | 0.42 |
| 4:Y:180:LEU:HD11 | 4:Y:261:LEU:HD23 | 2.02 | 0.42 |
| 4:Y:217:CYS:C | 4:Y:218:TYR:HD1 | 2.23 | 0.42 |
| 1:A:294:ASN:OD1 | 1:A:307:THR:HG21 | 2.19 | 0.42 |
| 1:A:502:GLU:HG2 | 1:A:766:PHE:CE1 | 2.55 | 0.42 |
| 1:A:578:HIS:CD2 | 1:A:592:ILE:H | 2.38 | 0.42 |
| 1:A:744:SER:O | 1:A:748:LEU:HD12 | 2.20 | 0.42 |
| 1:A:797:PHE:CD2 | 1:A:798:LEU:HD12 | 2.55 | 0.42 |
| 2:B:140:PHE:CD2 | 2:B:144:VAL:HG11 | 2.54 | 0.42 |
| 1:D:56:GLU:HB2 | 1:D:59:MLY:CB | 2.30 | 0.42 |
| 1:D:129:TYR:HD1 | 1:D:129:TYR:HA | 1.66 | 0.42 |
| 1:D:246:PHE:HB3 | 1:D:270:LEU:HD12 | 2.01 | 0.42 |
| 1:D:533:PHE:HD1 | 1:D:533:PHE:HA | 1.79 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:568:PRO:O | 1:D:570:PRO:HD3 | 2.20 | 0.42 |
| 1:D:725:ARG:HA | 1:D:732:ILE:CG2 | 2.50 | 0.42 |
| 1:D:744:SER:O | 1:D:748:LEU:HD12 | 2.20 | 0.42 |
| 2:E:113:LYS:O | 2:E:147:ASN:HB2 | 2.20 | 0.42 |
| 1:G:174:SER:HA | 1:G:460:GLY:O | 2.20 | 0.42 |
| 1:G:409:GLY:N | 1:G:636:LYS:CD | 2.70 | 0.42 |
| 1:G:725:ARG:HA | 1:G:732:ILE:CG2 | 2.50 | 0.42 |
| 1:G:747:LEU:O | 1:G:749:GLY:N | 2.52 | 0.42 |
| 1:G:818:TYR:C | 2:H:90:GLY:HA3 | 2.40 | 0.42 |
| 1:J:11:GLY:O | 1:J:14:ALA:HB3 | 2.20 | 0.42 |
| 1:J:169:ASP:O | 1:J:170:ARG:HB2 | 2.19 | 0.42 |
| 1:J:213:LYS:HA | 1:J:220:ASP:OD2 | 2.19 | 0.42 |
| 1:J:295:MLY:CE | 1:J:332:MET:CE | 2.97 | 0.42 |
| 1:J:309:PRO:C | 1:J:311:ASP:H | 2.22 | 0.42 |
| 1:J:826:VAL:O | 1:J:828:HIS:N | 2.53 | 0.42 |
| 1:J:839:MLY:HH11 | 2:K:158:THR:CG2 | 2.48 | 0.42 |
| 1:M:135:TYR:HD2 | 1:M:191:ARG:CG | 2.33 | 0.42 |
| 1:M:309:PRO:C | 1:M:311:ASP:H | 2.22 | 0.42 |
| 1:M:673:ARG:HD2 | 1:M:673:ARG:HA | 1.79 | 0.42 |
| 1:M:803:TYR:HD2 | 3:O:17:PHE:CE2 | 2.37 | 0.42 |
| 1:P:62:VAL:HG12 | 1:P:63:MLY:N | 2.35 | 0.42 |
| 1:P:62:VAL:O | 1:P:69:THR:HA | 2.20 | 0.42 |
| 1:P:294:ASN:OD1 | 1:P:307:THR:HG21 | 2.19 | 0.42 |
| 1:P:642:LYS:HB3 | 4:1:24:ASP:HB2 | 1.37 | 0.42 |
| 2:Q:113:LYS:O | 2:Q:147:ASN:HB2 | 2.20 | 0.42 |
| 4:1:196:ARG:HH21 | 4:1:249:THR:HG23 | 1.85 | 0.42 |
| 4:1:206:ARG:O | 4:1:209:VAL:HG12 | 2.20 | 0.42 |
| 4:3:180:LEU:HD11 | 4:3:261:LEU:HD23 | 2.02 | 0.42 |
| 4:4:171:LEU:HA | 4:4:172:PRO:HD2 | 1.84 | 0.42 |
| 4:4:206:ARG:O | 4:4:209:VAL:HG12 | 2.20 | 0.42 |
| 4:5:180:LEU:HD11 | 4:5:261:LEU:HD23 | 2.02 | 0.42 |
| 4:5:222:ASP:OD1 | 4:5:224:GLU:HB3 | 2.20 | 0.42 |
| 4:6:222:ASP:OD1 | 4:6:224:GLU:HB3 | 2.20 | 0.42 |
| 4:7:180:LEU:HD11 | 4:7:261:LEU:HD23 | 2.02 | 0.42 |
| 4:7:196:ARG:HH21 | 4:7:249:THR:HG23 | 1.85 | 0.42 |
| 4:9:206:ARG:O | 4:9:209:VAL:HG12 | 2.20 | 0.42 |
| 4:V:206:ARG:O | 4:V:209:VAL:HG12 | 2.20 | 0.42 |
| 4:W:180:LEU:HD11 | 4:W:261:LEU:HD23 | 2.02 | 0.42 |
| 4:W:222:ASP:OD1 | 4:W:224:GLU:HB3 | 2.20 | 0.42 |
| 4:Y:149:THR:HA | 4:Y:165:ILE:O | 2.19 | 0.42 |
| 1:A:356:GLY:HA2 | 1:A:359:MET:HG3 | 2.02 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:406:VAL:O | 1:A:412:ALA:HA | 2.19 | 0.42 |
| 1:A:500:GLN:HB2 | 1:A:512:PHE:CZ | 2.54 | 0.42 |
| 1:A:534:SER:CB | 4:8:351:THR:HA | 2.49 | 0.42 |
| 1:A:747:LEU:O | 1:A:749:GLY:N | 2.53 | 0.42 |
| 2:B:113:LYS:O | 2:B:147:ASN:HB2 | 2.20 | 0.42 |
| 1:D:60:VAL:O | 1:D:72:VAL:N | 2.51 | 0.42 |
| 1:D:439:LEU:HA | 1:D:439:LEU:HD12 | 1.85 | 0.42 |
| 1:D:550:PHE:C | 4:W:46:GLY:CA | 2.88 | 0.42 |
| 1:D:578:HIS:CD2 | 1:D:592:ILE:H | 2.38 | 0.42 |
| 1:D:767:PHE:O | 1:D:771:LEU:CD2 | 2.67 | 0.42 |
| 1:D:792:ALA:CA | 3:F:42:THR:HG22 | 2.33 | 0.42 |
| 1:G:485:GLU:OE2 | 1:G:584:TYR:N | 2.50 | 0.42 |
| 1:G:529:PRO:HB3 | 4:V:354:GLN:HA | 2.01 | 0.42 |
| 1:G:578:HIS:CD2 | 1:G:592:ILE:H | 2.38 | 0.42 |
| 1:J:741:LYS:HG2 | 1:J:742:LYS:N | 2.35 | 0.42 |
| 1:J:747:LEU:O | 1:J:749:GLY:N | 2.53 | 0.42 |
| 1:J:775:LEU:HA | 1:J:775:LEU:HD12 | 1.71 | 0.42 |
| 1:M:25:ILE:HG23 | 1:M:29:ASN:HD22 | 1.85 | 0.42 |
| 1:M:320:ILE:O | 1:M:320:ILE:HG22 | 2.18 | 0.42 |
| 1:M:445:ILE:HG22 | 1:M:449:LEU:HD22 | 2.02 | 0.42 |
| 1:M:529:PRO:HB3 | 4:Z:354:GLN:HA | 2.00 | 0.42 |
| 1:M:578:HIS:CD2 | 1:M:592:ILE:H | 2.38 | 0.42 |
| 1:M:744:SER:O | 1:M:748:LEU:HD12 | 2.20 | 0.42 |
| 3:O:52:ASN:CB | 3:O:53:PRO:HD3 | 2.28 | 0.42 |
| 1:P:206:LYS:CE | 1:P:217:THR:HG23 | 2.30 | 0.42 |
| 1:P:462:LEU:HD11 | 1:P:464:ILE:CD1 | 2.50 | 0.42 |
| 1:P:530:MET:CB | 4:1:354:GLN:CB | 2.95 | 0.42 |
| 2:Q:112:ILE:O | 2:Q:148:VAL:N | 2.50 | 0.42 |
| 4:1:180:LEU:HD11 | 4:1:261:LEU:HD23 | 2.02 | 0.42 |
| 4:2:222:ASP:OD1 | 4:2:224:GLU:HB3 | 2.19 | 0.42 |
| 4:3:149:THR:HA | 4:3:165:ILE:O | 2.19 | 0.42 |
| 4:4:196:ARG:HH21 | 4:4:249:THR:HG23 | 1.85 | 0.42 |
| 4:7:217:CYS:C | 4:7:218:TYR:HD1 | 2.22 | 0.42 |
| 4:9:205:GLU:O | 4:9:208:ILE:HG22 | 2.19 | 0.42 |
| 4:W:205:GLU:O | 4:W:208:ILE:HG22 | 2.18 | 0.42 |
| 1:A:107:MLY:CB | 1:A:686:MET:HE2 | 2.43 | 0.42 |
| 1:A:151:ALA:HB1 | 1:A:152:PRO:HD2 | 2.01 | 0.42 |
| 1:A:202:SER:HA | 1:A:207:LYS:NZ | 2.22 | 0.42 |
| 1:A:335:ASP:O | 1:A:338:ILE:HB | 2.20 | 0.42 |
| 1:A:537:GLU:OE1 | 4:8:350:SER:HA | 2.19 | 0.42 |
| 1:A:810:ARG:HG2 | 1:A:810:ARG:NH1 | 2.29 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:839:MLY:N | 1:A:840:PRO:HD2 | 2.35 | 0.42 |
| 3:C:25:ILE:O | 3:C:63:ILE:CB | 2.66 | 0.42 |
| 1:D:369:MLY:HH22 | 1:D:369:MLY:HD3 | 1.79 | 0.42 |
| 1:D:507:GLY:C | 1:D:761:GLY:HA3 | 2.39 | 0.42 |
| 1:D:538:GLU:CA | 4:9:351:THR:N | 2.69 | 0.42 |
| 1:D:636:LYS:CB | 4:9:334:GLU:OE1 | 2.68 | 0.42 |
| 1:D:800:ARG:HG2 | 3:F:149:VAL:HG22 | 2.01 | 0.42 |
| 2:E:140:PHE:CD2 | 2:E:144:VAL:HG11 | 2.55 | 0.42 |
| 1:G:17:LEU:HA | 1:G:17:LEU:HD12 | 1.68 | 0.42 |
| 1:G:135:TYR:HD2 | 1:G:191:ARG:CG | 2.32 | 0.42 |
| 1:G:173:GLN:HG3 | 1:G:670:HIS:CD2 | 2.55 | 0.42 |
| 1:G:294:ASN:OD1 | 1:G:307:THR:HG21 | 2.19 | 0.42 |
| 1:G:530:MET:HA | 4:V:354:GLN:CD | 2.12 | 0.42 |
| 1:G:537:GLU:OE1 | 4:V:350:SER:HA | 2.20 | 0.42 |
| 1:G:725:ARG:CZ | 1:G:733:PRO:CB | 2.83 | 0.42 |
| 1:G:744:SER:O | 1:G:748:LEU:HD12 | 2.20 | 0.42 |
| 1:G:815:CYS:SG | 2:H:92:ASP:CG | 2.98 | 0.42 |
| 1:G:829:TRP:O | 1:G:832:MET:N | 2.50 | 0.42 |
| 1:J:38:VAL:HG13 | 1:J:39:PHE:N | 2.35 | 0.42 |
| 1:J:539:GLU:OE2 | 1:J:553:MLY:HD3 | 2.20 | 0.42 |
| 1:J:553:MLY:HH12 | 4:Y:45:VAL:HG11 | 2.01 | 0.42 |
| 1:J:636:LYS:CB | 4:W:334:GLU:OE1 | 2.68 | 0.42 |
| 2:K:140:PHE:CD2 | 2:K:144:VAL:HG11 | 2.55 | 0.42 |
| 1:M:86:ASP:OD2 | 1:M:87:MLY:HH22 | 2.19 | 0.42 |
| 1:M:538:GLU:OE1 | 4:Z:355:MET:HE3 | 2.18 | 0.42 |
| 1:M:836:PHE:CZ | 2:N:159:HIS:CA | 2.92 | 0.42 |
| 1:M:842:LEU:N | 1:M:842:LEU:CD1 | 2.83 | 0.42 |
| 1:P:534:SER:CB | 4:1:351:THR:HA | 2.49 | 0.42 |
| 1:P:541:MET:HG2 | 4:1:345:ILE:HG22 | 2.00 | 0.42 |
| 1:P:723:ARG:CG | 1:P:723:ARG:NH1 | 2.79 | 0.42 |
| 1:P:806:MET:HB2 | 1:P:807:VAL:N | 2.34 | 0.42 |
| 3:R:52:ASN:CB | 3:R:53:PRO:CD | 2.92 | 0.42 |
| 4:3:206:ARG:O | 4:3:209:VAL:HG12 | 2.20 | 0.42 |
| 4:4:322:PRO:CA | 4:6:244:ASP:HB2 | 2.49 | 0.42 |
| 4:5:193:LEU:HD11 | 4:5:250:ILE:HG13 | 2.02 | 0.42 |
| 4:8:217:CYS:C | 4:8:218:TYR:HD1 | 2.23 | 0.42 |
| 4:8:369:ILE:HG23 | 4:8:370:VAL:N | 2.35 | 0.42 |
| 4:V:222:ASP:OD1 | 4:V:224:GLU:HB3 | 2.19 | 0.42 |
| 4:V:369:ILE:HG23 | 4:V:370:VAL:N | 2.35 | 0.42 |
| 4:Y:315:LYS:HD2 | 4:Y:315:LYS:HA | 1.92 | 0.42 |
| 4:Z:180:LEU:HD11 | 4:Z:261:LEU:HD23 | 2.02 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:129:TYR:HD1 | 1:A:129:TYR:HA | 1.65 | 0.42 |
| 1:A:135:TYR:HD2 | 1:A:191:ARG:CG | 2.32 | 0.42 |
| 1:A:174:SER:HA | 1:A:460:GLY:O | 2.20 | 0.42 |
| 1:A:194:GLN:HE21 | 1:A:194:GLN:HB3 | 1.43 | 0.42 |
| 1:A:320:ILE:O | 1:A:320:ILE:HG22 | 2.18 | 0.42 |
| 1:A:725:ARG:HA | 1:A:732:ILE:CG2 | 2.50 | 0.42 |
| 1:A:733:PRO:CB | 1:A:737:PHE:CE1 | 3.03 | 0.42 |
| 1:A:826:VAL:O | 1:A:828:HIS:N | 2.53 | 0.42 |
| 1:D:195:TYR:CD2 | 1:D:199:ILE:HD13 | 2.54 | 0.42 |
| 1:D:214:MET:CA | 1:D:340:ILE:HD11 | 2.45 | 0.42 |
| 1:D:292:MET:HE1 | 1:D:309:PRO:HD3 | 2.02 | 0.42 |
| 1:D:402:CYS:C | 1:D:404:PRO:HD3 | 2.40 | 0.42 |
| 1:D:476:GLU:H | 1:D:476:GLU:CD | 2.22 | 0.42 |
| 1:D:692:LEU:HD23 | 1:D:692:LEU:HA | 1.84 | 0.42 |
| 1:D:747:LEU:O | 1:D:749:GLY:N | 2.53 | 0.42 |
| 1:G:195:TYR:CE2 | 1:G:199:ILE:HD13 | 2.55 | 0.42 |
| 1:G:462:LEU:HD11 | 1:G:464:ILE:CD1 | 2.50 | 0.42 |
| 1:G:530:MET:CB | 4:V:354:GLN:CB | 2.96 | 0.42 |
| 1:G:541:MET:HG2 | 4:V:345:ILE:HG23 | 2.02 | 0.42 |
| 1:J:14:ALA:HB3 | 1:J:15:PRO:CD | 2.46 | 0.42 |
| 1:J:60:VAL:O | 1:J:72:VAL:N | 2.51 | 0.42 |
| 1:J:798:LEU:CD2 | 3:L:118:MET:SD | 3.08 | 0.42 |
| 1:M:151:ALA:HB1 | 1:M:152:PRO:HD2 | 2.01 | 0.42 |
| 1:M:786:ILE:O | 1:M:790:THR:N | 2.53 | 0.42 |
| 1:P:11:GLY:O | 1:P:14:ALA:HB3 | 2.20 | 0.42 |
| 1:P:402:CYS:C | 1:P:404:PRO:HD3 | 2.40 | 0.42 |
| 1:P:541:MET:CE | 4:1:346:LEU:HD12 | 2.47 | 0.42 |
| 1:P:747:LEU:C | 1:P:749:GLY:N | 2.71 | 0.42 |
| 4:1:222:ASP:OD1 | 4:1:224:GLU:HB3 | 2.20 | 0.42 |
| 4:2:149:THR:HA | 4:2:165:ILE:O | 2.19 | 0.42 |
| 4:2:203:THR:HB | 4:Z:287:ILE:CB | 2.50 | 0.42 |
| 4:2:204:ALA:N | 4:Z:287:ILE:HG21 | 2.30 | 0.42 |
| 4:3:369:ILE:HG23 | 4:3:370:VAL:N | 2.35 | 0.42 |
| 4:5:217:CYS:C | 4:5:218:TYR:HD1 | 2.23 | 0.42 |
| 4:W:286:ASP:HA | 4:Y:202:THR:HG22 | 1.32 | 0.42 |
| 4:X:217:CYS:C | 4:X:218:TYR:HD1 | 2.23 | 0.42 |
| 1:A:86:ASP:OD2 | 1:A:87:MLY:HH22 | 2.19 | 0.41 |
| 1:A:173:GLN:HG3 | 1:A:670:HIS:CD2 | 2.54 | 0.41 |
| 1:A:462:LEU:HD11 | 1:A:464:ILE:CD1 | 2.50 | 0.41 |
| 1:A:747:LEU:C | 1:A:749:GLY:N | 2.72 | 0.41 |
| 1:A:809:ARG:HH12 | 2:B:124:GLY:HA2 | 1.81 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:166:MET:CE | 1:D:254:PHE:HB2 | 2.46 | 0.41 |
| 1:D:195:TYR:CE2 | 1:D:199:ILE:HD13 | 2.55 | 0.41 |
| 1:D:406:VAL:O | 1:D:412:ALA:HA | 2.20 | 0.41 |
| 1:D:528:MLY:HB2 | 1:D:529:PRO:HD2 | 2.02 | 0.41 |
| 1:D:641:LYS:CD | 1:D:647:GLN:CG | 2.72 | 0.41 |
| 2:E:139:ALA:O | 2:E:141:PRO:CD | 2.51 | 0.41 |
| 1:G:84:MLY:HD2 | 1:G:724:TYR:OH | 2.20 | 0.41 |
| 1:G:86:ASP:OD2 | 1:G:87:MLY:HH22 | 2.19 | 0.41 |
| 1:G:151:ALA:HB1 | 1:G:152:PRO:HD2 | 2.01 | 0.41 |
| 1:G:175:ILE:C | 1:G:176:LEU:HD12 | 2.39 | 0.41 |
| 1:G:402:CYS:C | 1:G:404:PRO:HD3 | 2.40 | 0.41 |
| 1:G:757:GLN:CB | 1:G:776:GLU:OE2 | 2.66 | 0.41 |
| 1:G:791:GLN:CD | 3:I:116:GLU:H | 2.24 | 0.41 |
| 1:G:826:VAL:O | 1:G:828:HIS:N | 2.53 | 0.41 |
| 1:G:839:MLY:N | 1:G:840:PRO:HD2 | 2.35 | 0.41 |
| 1:G:842:LEU:N | 1:G:842:LEU:CD1 | 2.83 | 0.41 |
| 1:J:25:ILE:HG23 | 1:J:29:ASN:HD22 | 1.85 | 0.41 |
| 1:J:62:VAL:O | 1:J:69:THR:HA | 2.20 | 0.41 |
| 1:J:221:GLN:HG2 | 1:J:221:GLN:H | 1.47 | 0.41 |
| 1:J:485:GLU:OE2 | 1:J:584:TYR:N | 2.50 | 0.41 |
| 1:J:842:LEU:N | 1:J:842:LEU:CD1 | 2.83 | 0.41 |
| 1:M:11:GLY:O | 1:M:14:ALA:HB3 | 2.20 | 0.41 |
| 1:M:62:VAL:O | 1:M:69:THR:HA | 2.20 | 0.41 |
| 1:M:195:TYR:CE2 | 1:M:199:ILE:HD13 | 2.55 | 0.41 |
| 1:M:229:LEU:HD12 | 1:M:229:LEU:HA | 1.75 | 0.41 |
| 1:M:271:GLU:OE1 | 1:M:274:ARG:NH1 | 2.53 | 0.41 |
| 1:M:335:ASP:O | 1:M:338:ILE:HB | 2.20 | 0.41 |
| 1:P:173:GLN:HG3 | 1:P:670:HIS:CD2 | 2.54 | 0.41 |
| 1:P:195:TYR:CE2 | 1:P:199:ILE:HD13 | 2.55 | 0.41 |
| 1:P:295:MLY:HG3 | 1:P:332:MET:HE2 | 2.00 | 0.41 |
| 1:P:471:ASP:CB | 1:P:573:GLY:O | 2.68 | 0.41 |
| 1:P:568:PRO:O | 1:P:570:PRO:HD3 | 2.19 | 0.41 |
| 1:P:839:MLY:N | 1:P:840:PRO:HD2 | 2.35 | 0.41 |
| 2:Q:137:TRP:CA | 2:Q:145:ALA:HB2 | 2.37 | 0.41 |
| 4:1:369:ILE:HG23 | 4:1:370:VAL:N | 2.35 | 0.41 |
| 4:6:193:LEU:HD11 | 4:6:250:ILE:HG13 | 2.02 | 0.41 |
| 4:6:217:CYS:C | 4:6:218:TYR:HD1 | 2.23 | 0.41 |
| 4:7:193:LEU:HD11 | 4:7:250:ILE:HG13 | 2.02 | 0.41 |
| 4:7:222:ASP:OD1 | 4:7:224:GLU:HB3 | 2.20 | 0.41 |
| 4:8:193:LEU:HD11 | 4:8:250:ILE:HG13 | 2.02 | 0.41 |
| 4:8:221:LEU:HA | 4:8:312:ARG:HG2 | 2.03 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:W:369:ILE:HG23 | 4:W:370:VAL:N | 2.35 | 0.41 |
| 4:X:193:LEU:HD11 | 4:X:250:ILE:HG13 | 2.02 | 0.41 |
| 4:X:369:ILE:HG23 | 4:X:370:VAL:N | 2.35 | 0.41 |
| 4:Y:205:GLU:O | 4:Y:208:ILE:HG22 | 2.18 | 0.41 |
| 1:A:725:ARG:CZ | 1:A:737:PHE:CE1 | 3.02 | 0.41 |
| 1:A:776:GLU:O | 1:A:780:ASP:N | 2.45 | 0.41 |
| 1:A:793:ARG:NH2 | 3:C:147:MET:HE3 | 2.26 | 0.41 |
| 1:D:25:ILE:HG23 | 1:D:29:ASN:HD22 | 1.85 | 0.41 |
| 1:D:62:VAL:O | 1:D:69:THR:HA | 2.20 | 0.41 |
| 1:D:537:GLU:OE1 | 4:9:350:SER:HA | 2.19 | 0.41 |
| 1:D:551:MLY:C | 4:W:47:MET:HA | 2.48 | 0.41 |
| 1:D:568:PRO:CG | 1:D:578:HIS:N | 2.83 | 0.41 |
| 1:G:25:ILE:HG23 | 1:G:29:ASN:HD22 | 1.85 | 0.41 |
| 1:G:62:VAL:O | 1:G:69:THR:HA | 2.20 | 0.41 |
| 1:G:335:ASP:O | 1:G:338:ILE:HB | 2.20 | 0.41 |
| 1:G:500:GLN:HB2 | 1:G:512:PHE:CZ | 2.54 | 0.41 |
| 1:G:741:LYS:HG2 | 1:G:742:LYS:N | 2.35 | 0.41 |
| 1:G:797:PHE:CD2 | 1:G:798:LEU:HD12 | 2.55 | 0.41 |
| 2:H:113:LYS:O | 2:H:147:ASN:HB2 | 2.20 | 0.41 |
| 2:H:141:PRO:CB | 2:H:142:PRO:HD3 | 2.48 | 0.41 |
| 1:J:84:MLY:HH12 | 1:J:715:VAL:HG21 | 2.02 | 0.41 |
| 1:M:34:ALA:HB3 | 1:M:777:GLU:CG | 2.50 | 0.41 |
| 1:M:38:VAL:HG13 | 1:M:39:PHE:N | 2.35 | 0.41 |
| 1:M:204:GLU:N | 1:M:207:LYS:HE3 | 2.23 | 0.41 |
| 1:M:500:GLN:HB2 | 1:M:512:PHE:CZ | 2.54 | 0.41 |
| 1:M:534:SER:CB | 4:Z:351:THR:HA | 2.49 | 0.41 |
| 2:N:139:ALA:O | 2:N:141:PRO:CD | 2.51 | 0.41 |
| 1:P:541:MET:HG2 | 4:1:345:ILE:HG23 | 2.02 | 0.41 |
| 1:P:625:THR:H | 1:P:625:THR:HG22 | 1.48 | 0.41 |
| 1:P:741:LYS:HG2 | 1:P:742:LYS:N | 2.35 | 0.41 |
| 4:3:171:LEU:HA | 4:3:172:PRO:HD2 | 1.84 | 0.41 |
| 4:3:193:LEU:HD11 | 4:3:250:ILE:HG13 | 2.02 | 0.41 |
| 4:3:299:MET:HE2 | 4:3:331:ALA:HB2 | 2.00 | 0.41 |
| 4:4:148:THR:HG21 | 4:6:45:VAL:CG2 | 2.50 | 0.41 |
| 4:4:193:LEU:HD11 | 4:4:250:ILE:HG13 | 2.02 | 0.41 |
| 4:7:287:ILE:CB | 4:9:204:ALA:H | 2.13 | 0.41 |
| 4:8:222:ASP:OD1 | 4:8:224:GLU:HB3 | 2.20 | 0.41 |
| 4:Y:196:ARG:HH21 | 4:Y:249:THR:HG23 | 1.85 | 0.41 |
| 4:Y:226:GLU:HG3 | 4:Y:255:PHE:CE2 | 2.56 | 0.41 |
| 1:A:38:VAL:HG13 | 1:A:39:PHE:N | 2.35 | 0.41 |
| 1:A:402:CYS:C | 1:A:404:PRO:HD3 | 2.40 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:136:ASN:O | 1:D:138:MLY:N | 2.54 | 0.41 |
| 1:D:462:LEU:HD11 | 1:D:464:ILE:CD1 | 2.50 | 0.41 |
| 1:D:724:TYR:HB3 | 1:D:727:LEU:CD1 | 2.49 | 0.41 |
| 1:D:741:LYS:HG2 | 1:D:742:LYS:N | 2.35 | 0.41 |
| 1:D:797:PHE:CD2 | 1:D:798:LEU:HD12 | 2.55 | 0.41 |
| 1:D:818:TYR:HB2 | 2:E:90:GLY:HA3 | 0.58 | 0.41 |
| 1:G:62:VAL:HG12 | 1:G:63:MLY:N | 2.34 | 0.41 |
| 1:G:330:GLU:OE1 | 1:G:330:GLU:HA | 2.20 | 0.41 |
| 1:G:471:ASP:CB | 1:G:573:GLY:O | 2.68 | 0.41 |
| 1:G:632:GLY:HA3 | 1:G:643:GLY:N | 2.17 | 0.41 |
| 1:G:690:LEU:O | 1:G:694:GLN:HG3 | 2.20 | 0.41 |
| 1:G:754:ASP:C | 1:G:776:GLU:CD | 2.78 | 0.41 |
| 1:J:63:MLY:HD3 | 1:J:63:MLY:HH23 | 1.76 | 0.41 |
| 1:J:93:MET:CE | 1:J:716:LEU:HB2 | 2.50 | 0.41 |
| 1:J:530:MET:HE3 | 4:W:354:GLN:CG | 2.40 | 0.41 |
| 1:J:544:LYS:HD2 | 4:W:147:ARG:CB | 2.36 | 0.41 |
| 1:J:690:LEU:O | 1:J:694:GLN:HG3 | 2.20 | 0.41 |
| 1:M:406:VAL:O | 1:M:412:ALA:HA | 2.19 | 0.41 |
| 1:M:462:LEU:HD11 | 1:M:464:ILE:CD1 | 2.50 | 0.41 |
| 1:M:690:LEU:O | 1:M:694:GLN:HG3 | 2.20 | 0.41 |
| 1:M:725:ARG:HA | 1:M:732:ILE:CG2 | 2.50 | 0.41 |
| 1:M:785:GLU:C | 1:M:789:ALA:HB2 | 2.37 | 0.41 |
| 1:P:330:GLU:OE1 | 1:P:330:GLU:HA | 2.21 | 0.41 |
| 1:P:636:LYS:CB | 4:1:334:GLU:OE1 | 2.68 | 0.41 |
| 1:P:747:LEU:O | 1:P:749:GLY:N | 2.53 | 0.41 |
| 1:P:751:GLY:HA2 | 1:P:779:ARG:CZ | 2.48 | 0.41 |
| 2:Q:141:PRO:HB3 | 2:Q:142:PRO:CD | 2.49 | 0.41 |
| 3:R:96:LYS:H | 3:R:96:LYS:HG3 | 1.66 | 0.41 |
| 4:1:217:CYS:C | 4:1:218:TYR:HD1 | 2.23 | 0.41 |
| 4:2:193:LEU:HD11 | 4:2:250:ILE:HG13 | 2.02 | 0.41 |
| 4:6:226:GLU:HG3 | 4:6:255:PHE:CE2 | 2.56 | 0.41 |
| 4:7:369:ILE:HG23 | 4:7:370:VAL:N | 2.35 | 0.41 |
| 4:8:226:GLU:HG3 | 4:8:255:PHE:CE2 | 2.55 | 0.41 |
| 4:9:226:GLU:HG3 | 4:9:255:PHE:CE2 | 2.56 | 0.41 |
| 4:9:369:ILE:HG23 | 4:9:370:VAL:N | 2.35 | 0.41 |
| 4:V:221:LEU:HA | 4:V:312:ARG:HG2 | 2.03 | 0.41 |
| 4:V:226:GLU:HG3 | 4:V:255:PHE:CE2 | 2.55 | 0.41 |
| 4:Y:369:ILE:HG23 | 4:Y:370:VAL:N | 2.35 | 0.41 |
| 4:Z:193:LEU:HD11 | 4:Z:250:ILE:HG13 | 2.02 | 0.41 |
| 1:A:348:MLY:HH12 | 1:A:348:MLY:HD2 | 1.82 | 0.41 |
| 1:A:636:LYS:CB | 4:8:334:GLU:OE1 | 2.67 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:800:ARG:HH21 | 3:C:40:ASN:CG | 1.98 | 0.41 |
| 1:A:813:ILE:HG21 | 2:B:127:ARG:CG | 2.50 | 0.41 |
| 1:A:813:ILE:CG1 | 2:B:128:PHE:CE1 | 2.88 | 0.41 |
| 1:A:818:TYR:HB3 | 2:B:90:GLY:H | 1.81 | 0.41 |
| 1:D:97:LEU:HD12 | 1:D:97:LEU:HA | 1.67 | 0.41 |
| 1:D:330:GLU:OE1 | 1:D:330:GLU:HA | 2.21 | 0.41 |
| 1:D:793:ARG:O | 1:D:797:PHE:N | 2.39 | 0.41 |
| 1:D:799:MET:SD | 3:F:32:ASP:C | 2.98 | 0.41 |
| 1:G:136:ASN:O | 1:G:138:MLY:N | 2.54 | 0.41 |
| 2:H:149:ASP:OD2 | 2:H:150:TYR:CA | 2.65 | 0.41 |
| 1:J:129:TYR:HD1 | 1:J:129:TYR:HA | 1.65 | 0.41 |
| 1:J:217:THR:CA | 1:J:221:GLN:HE21 | 2.33 | 0.41 |
| 1:J:462:LEU:HD11 | 1:J:464:ILE:CD1 | 2.50 | 0.41 |
| 1:J:471:ASP:CB | 1:J:573:GLY:O | 2.68 | 0.41 |
| 1:J:578:HIS:CD2 | 1:J:592:ILE:H | 2.38 | 0.41 |
| 1:J:725:ARG:HA | 1:J:732:ILE:CG2 | 2.50 | 0.41 |
| 1:J:744:SER:O | 1:J:748:LEU:HD12 | 2.20 | 0.41 |
| 1:J:797:PHE:CD2 | 1:J:798:LEU:HD12 | 2.55 | 0.41 |
| 1:J:829:TRP:CH2 | 2:K:83:MET:HE3 | 2.56 | 0.41 |
| 1:M:60:VAL:O | 1:M:72:VAL:N | 2.51 | 0.41 |
| 1:M:295:MLY:CG | 1:M:332:MET:CE | 2.97 | 0.41 |
| 1:M:439:LEU:N | 1:M:439:LEU:CD1 | 2.81 | 0.41 |
| 1:M:642:LYS:HE2 | 4:Z:344:SER:HA | 1.56 | 0.41 |
| 1:M:800:ARG:HH22 | 3:O:40:ASN:ND2 | 2.17 | 0.41 |
| 1:P:63:MLY:HD3 | 1:P:63:MLY:HH23 | 1.76 | 0.41 |
| 1:P:539:GLU:OE2 | 1:P:553:MLY:HD3 | 2.20 | 0.41 |
| 1:P:544:LYS:HB3 | 4:3:45:VAL:CG2 | 2.42 | 0.41 |
| 1:P:578:HIS:CD2 | 1:P:592:ILE:H | 2.38 | 0.41 |
| 1:P:612:GLN:NE2 | 1:P:627:GLY:H | 2.14 | 0.41 |
| 1:P:725:ARG:HA | 1:P:732:ILE:CG2 | 2.50 | 0.41 |
| 3:R:48:LYS:HA | 3:R:48:LYS:HD3 | 1.17 | 0.41 |
| 4:3:196:ARG:HH21 | 4:3:249:THR:HG23 | 1.85 | 0.41 |
| 4:3:222:ASP:OD1 | 4:3:224:GLU:HB3 | 2.20 | 0.41 |
| 4:5:226:GLU:HG3 | 4:5:255:PHE:CE2 | 2.55 | 0.41 |
| 4:6:206:ARG:O | 4:6:209:VAL:HG12 | 2.20 | 0.41 |
| 4:7:226:GLU:HG3 | 4:7:255:PHE:CE2 | 2.56 | 0.41 |
| 4:V:193:LEU:HD11 | 4:V:250:ILE:HG13 | 2.02 | 0.41 |
| 4:V:287:ILE:HG13 | 4:X:202:THR:HG23 | 1.65 | 0.41 |
| 4:Y:193:LEU:HD11 | 4:Y:250:ILE:HG13 | 2.02 | 0.41 |
| 4:Z:217:CYS:C | 4:Z:218:TYR:HD1 | 2.23 | 0.41 |
| 1:A:836:PHE:CD1 | 2:B:159:HIS:HB2 | 2.43 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:166:MET:CE | 1:D:254:PHE:CD2 | 3.01 | 0.41 |
| 1:D:541:MET:HG2 | 4:9:345:ILE:HG23 | 2.01 | 0.41 |
| 3:F:56:GLU:OE1 | 3:F:59:ASN:ND2 | 2.54 | 0.41 |
| 1:G:11:GLY:O | 1:G:14:ALA:HB3 | 2.20 | 0.41 |
| 1:G:136:ASN:HA | 1:G:137:PRO:HD3 | 1.50 | 0.41 |
| 1:G:320:ILE:O | 1:G:320:ILE:CG2 | 2.68 | 0.41 |
| 1:G:534:SER:CB | 4:V:351:THR:HA | 2.50 | 0.41 |
| 1:G:629:GLU:CB | 1:G:645:SER:N | 2.74 | 0.41 |
| 1:J:541:MET:CE | 4:W:346:LEU:HD12 | 2.47 | 0.41 |
| 1:J:732:ILE:HG21 | 1:J:747:LEU:CD1 | 0.63 | 0.41 |
| 1:J:756:THR:HG23 | 1:J:776:GLU:CD | 2.35 | 0.41 |
| 3:L:56:GLU:OE1 | 3:L:59:ASN:ND2 | 2.54 | 0.41 |
| 1:M:296:MLY:HH11 | 1:M:348:MLY:CH2 | 2.48 | 0.41 |
| 1:M:464:ILE:HD13 | 1:M:464:ILE:HG21 | 1.69 | 0.41 |
| 3:O:25:ILE:O | 3:O:63:ILE:CB | 2.66 | 0.41 |
| 1:P:166:MET:CE | 1:P:254:PHE:HB2 | 2.46 | 0.41 |
| 1:P:508:ILE:CD1 | 1:P:759:ALA:CB | 2.71 | 0.41 |
| 1:P:568:PRO:CG | 1:P:578:HIS:N | 2.84 | 0.41 |
| 1:P:786:ILE:C | 1:P:789:ALA:HB3 | 2.40 | 0.41 |
| 4:1:193:LEU:HD11 | 4:1:250:ILE:HG13 | 2.02 | 0.41 |
| 4:3:205:GLU:O | 4:3:208:ILE:HG22 | 2.19 | 0.41 |
| 4:4:222:ASP:OD1 | 4:4:224:GLU:HB3 | 2.20 | 0.41 |
| 4:9:193:LEU:HD11 | 4:9:250:ILE:HG13 | 2.03 | 0.41 |
| 4:V:196:ARG:HH21 | 4:V:249:THR:HG23 | 1.85 | 0.41 |
| 4:W:193:LEU:HD11 | 4:W:250:ILE:HG13 | 2.02 | 0.41 |
| 1:A:175:ILE:C | 1:A:176:LEU:HD12 | 2.39 | 0.41 |
| 1:A:217:THR:CA | 1:A:221:GLN:HE21 | 2.33 | 0.41 |
| 1:A:629:GLU:HB3 | 1:A:643:GLY:C | 2.41 | 0.41 |
| 1:D:14:ALA:HB3 | 1:D:15:PRO:CD | 2.46 | 0.41 |
| 1:D:174:SER:HA | 1:D:460:GLY:O | 2.20 | 0.41 |
| 1:D:443:ILE:HG22 | 1:D:444:ARG:N | 2.29 | 0.41 |
| 1:G:296:MLY:HH11 | 1:G:348:MLY:CH2 | 2.48 | 0.41 |
| 1:G:466:GLY:CA | 1:G:484:ASN:HD21 | 2.32 | 0.41 |
| 1:G:810:ARG:HG2 | 1:G:810:ARG:NH1 | 2.28 | 0.41 |
| 1:G:834:LEU:CD1 | 2:H:51:PHE:CD1 | 3.03 | 0.41 |
| 3:I:56:GLU:OE1 | 3:I:59:ASN:ND2 | 2.54 | 0.41 |
| 1:J:166:MET:CE | 1:J:254:PHE:CD2 | 3.01 | 0.41 |
| 1:J:173:GLN:HG3 | 1:J:670:HIS:CD2 | 2.55 | 0.41 |
| 1:J:229:LEU:HD12 | 1:J:229:LEU:HA | 1.75 | 0.41 |
| 1:J:240:ASN:OD1 | 1:J:241:ASP:N | 2.52 | 0.41 |
| 1:J:449:LEU:N | 1:J:449:LEU:CD1 | 2.82 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:528:MLY:HB2 | 1:J:529:PRO:HD2 | 2.03 | 0.41 |
| 1:J:717:TYR:OH | 1:J:760:PHE:HB3 | 2.21 | 0.41 |
| 1:J:791:GLN:HE22 | 3:L:115:GLY:CA | 2.30 | 0.41 |
| 2:K:113:LYS:O | 2:K:147:ASN:HB2 | 2.20 | 0.41 |
| 2:K:141:PRO:HB3 | 2:K:142:PRO:CD | 2.49 | 0.41 |
| 1:M:294:ASN:OD1 | 1:M:307:THR:HG21 | 2.20 | 0.41 |
| 1:M:536:LEU:HA | 1:M:536:LEU:HD12 | 1.69 | 0.41 |
| 1:M:829:TRP:O | 1:M:832:MET:N | 2.50 | 0.41 |
| 1:P:135:TYR:HD2 | 1:P:191:ARG:CG | 2.33 | 0.41 |
| 1:P:166:MET:CE | 1:P:254:PHE:CD2 | 3.01 | 0.41 |
| 1:P:508:ILE:HD13 | 1:P:508:ILE:HG21 | 1.88 | 0.41 |
| 1:P:690:LEU:O | 1:P:694:GLN:HG3 | 2.20 | 0.41 |
| 1:P:744:SER:O | 1:P:748:LEU:HD12 | 2.20 | 0.41 |
| 1:P:787:ILE:HG23 | 1:P:791:GLN:HG3 | 2.01 | 0.41 |
| 4:3:221:LEU:HA | 4:3:312:ARG:HG2 | 2.03 | 0.41 |
| 4:6:369:ILE:HG23 | 4:6:370:VAL:N | 2.35 | 0.41 |
| 4:8:196:ARG:HH21 | 4:8:249:THR:HG23 | 1.85 | 0.41 |
| 4:W:227:MET:O | 4:W:230:ALA:HB3 | 2.21 | 0.41 |
| 4:Z:369:ILE:HG23 | 4:Z:370:VAL:N | 2.36 | 0.41 |
| 1:A:56:GLU:HB2 | 1:A:59:MLY:CB | 2.30 | 0.41 |
| 1:A:193:ILE:HD11 | 1:A:250:ILE:HD12 | 2.03 | 0.41 |
| 1:A:201:ALA:O | 1:A:202:SER:OG | 2.36 | 0.41 |
| 1:A:528:MLY:HB2 | 1:A:529:PRO:HD2 | 2.02 | 0.41 |
| 1:A:556:ASP:OD1 | 4:V:50:LYS:CG | 2.69 | 0.41 |
| 2:B:112:ILE:O | 2:B:148:VAL:N | 2.50 | 0.41 |
| 1:D:556:ASP:OD1 | 4:W:50:LYS:CG | 2.69 | 0.41 |
| 1:D:723:ARG:CG | 1:D:723:ARG:NH1 | 2.80 | 0.41 |
| 3:F:48:LYS:HD3 | 3:F:48:LYS:HA | 1.18 | 0.41 |
| 1:G:84:MLY:HH23 | 1:G:719:ASP:O | 2.19 | 0.41 |
| 1:G:322:VAL:HG12 | 1:G:325:ILE:HG13 | 2.03 | 0.41 |
| 1:G:636:LYS:CB | 4:V:334:GLU:OE1 | 2.68 | 0.41 |
| 1:G:732:ILE:HG21 | 1:G:747:LEU:CD1 | 0.64 | 0.41 |
| 1:G:733:PRO:CB | 1:G:737:PHE:CE1 | 3.02 | 0.41 |
| 1:G:812:SER:O | 1:G:816:ILE:HG13 | 2.21 | 0.41 |
| 1:G:817:GLN:NE2 | 2:H:127:ARG:CB | 2.73 | 0.41 |
| 1:J:369:MLY:HH22 | 1:J:369:MLY:HD3 | 1.79 | 0.41 |
| 1:J:443:ILE:HG22 | 1:J:444:ARG:N | 2.29 | 0.41 |
| 1:J:541:MET:HG2 | 4:W:345:ILE:HG23 | 2.02 | 0.41 |
| 1:M:141:LEU:HD12 | 1:M:141:LEU:N | 2.32 | 0.41 |
| 1:M:356:GLY:HA2 | 1:M:359:MET:HG3 | 2.02 | 0.41 |
| 1:M:539:GLU:OE2 | 1:M:553:MLY:HD3 | 2.20 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:629:GLU:CB | 1:M:645:SER:N | 2.74 | 0.41 |
| 1:M:797:PHE:CD2 | 1:M:798:LEU:HD12 | 2.55 | 0.41 |
| 1:M:818:TYR:CG | 2:N:127:ARG:NH1 | 2.81 | 0.41 |
| 2:N:140:PHE:CD2 | 2:N:144:VAL:HG11 | 2.54 | 0.41 |
| 1:P:60:VAL:O | 1:P:72:VAL:N | 2.51 | 0.41 |
| 1:P:174:SER:HA | 1:P:460:GLY:O | 2.20 | 0.41 |
| 1:P:240:ASN:OD1 | 1:P:241:ASP:N | 2.52 | 0.41 |
| 1:P:356:GLY:HA2 | 1:P:359:MET:HG3 | 2.02 | 0.41 |
| 1:P:411:GLU:HB2 | 1:P:412:ALA:H | 1.73 | 0.41 |
| 1:P:724:TYR:HB3 | 1:P:727:LEU:CD1 | 2.48 | 0.41 |
| 1:P:812:SER:O | 1:P:816:ILE:HG13 | 2.21 | 0.41 |
| 3:R:56:GLU:OE1 | 3:R:59:ASN:ND2 | 2.54 | 0.41 |
| 4:1:227:MET:O | 4:1:230:ALA:HB3 | 2.21 | 0.41 |
| 4:2:221:LEU:HA | 4:2:312:ARG:HG2 | 2.02 | 0.41 |
| 4:2:226:GLU:HG3 | 4:2:255:PHE:CE2 | 2.56 | 0.41 |
| 4:4:227:MET:O | 4:4:230:ALA:HB3 | 2.21 | 0.41 |
| 4:6:196:ARG:HH21 | 4:6:249:THR:HG23 | 1.85 | 0.41 |
| 4:7:206:ARG:O | 4:7:209:VAL:HG12 | 2.20 | 0.41 |
| 4:V:217:CYS:C | 4:V:218:TYR:HD1 | 2.23 | 0.41 |
| 4:V:315:LYS:HD2 | 4:V:315:LYS:HA | 1.92 | 0.41 |
| 4:Z:222:ASP:OD1 | 4:Z:224:GLU:HB3 | 2.19 | 0.41 |
| 1:A:11:GLY:O | 1:A:14:ALA:HB3 | 2.20 | 0.41 |
| 1:A:62:VAL:HG12 | 1:A:63:MLY:N | 2.34 | 0.41 |
| 1:A:136:ASN:O | 1:A:138:MLY:N | 2.54 | 0.41 |
| 1:A:195:TYR:CE2 | 1:A:199:ILE:HD13 | 2.55 | 0.41 |
| 1:A:471:ASP:CB | 1:A:573:GLY:O | 2.68 | 0.41 |
| 1:A:741:LYS:HG2 | 1:A:742:LYS:N | 2.35 | 0.41 |
| 2:B:150:TYR:HB3 | 2:B:151:LYS:HG3 | 2.03 | 0.41 |
| 1:D:11:GLY:O | 1:D:14:ALA:HB3 | 2.20 | 0.41 |
| 1:D:213:LYS:HA | 1:D:220:ASP:OD2 | 2.19 | 0.41 |
| 1:D:449:LEU:HD12 | 1:D:449:LEU:HA | 1.61 | 0.41 |
| 1:D:665:ARG:C | 1:D:667:THR:N | 2.74 | 0.41 |
| 1:G:38:VAL:HG13 | 1:G:39:PHE:N | 2.35 | 0.41 |
| 1:G:568:PRO:CG | 1:G:578:HIS:N | 2.84 | 0.41 |
| 1:G:612:GLN:NE2 | 1:G:627:GLY:H | 2.14 | 0.41 |
| 1:G:642:LYS:HE2 | 4:V:344:SER:HA | 1.56 | 0.41 |
| 1:G:819:ASN:CG | 2:H:92:ASP:HB3 | 2.23 | 0.41 |
| 1:G:821:ARG:HH21 | 2:H:127:ARG:HG2 | 1.64 | 0.41 |
| 1:J:136:ASN:O | 1:J:138:MLY:N | 2.54 | 0.41 |
| 1:J:356:GLY:HA2 | 1:J:359:MET:HG3 | 2.02 | 0.41 |
| 1:M:839:MLY:N | 1:M:840:PRO:HD2 | 2.35 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:N:113:LYS:O | 2:N:147:ASN:HB2 | 2.20 | 0.41 |
| 1:P:25:ILE:HG23 | 1:P:29:ASN:HD22 | 1.85 | 0.41 |
| 1:P:149:GLN:HE21 | 1:P:149:GLN:HB2 | 1.72 | 0.41 |
| 1:P:194:GLN:HE21 | 1:P:194:GLN:HB3 | 1.43 | 0.41 |
| 1:P:803:TYR:O | 1:P:807:VAL:HB | 2.21 | 0.41 |
| 4:1:226:GLU:HG3 | 4:1:255:PHE:CE2 | 2.56 | 0.41 |
| 4:4:287:ILE:CB | 4:6:203:THR:HG22 | 2.44 | 0.41 |
| 4:7:288:ASP:OD1 | 4:9:204:ALA:HA | 2.21 | 0.41 |
| 4:W:32:PRO:HB2 | 4:W:34:ILE:CD1 | 2.51 | 0.41 |
| 4:W:256:ARG:HH11 | 4:W:256:ARG:HD2 | 1.79 | 0.41 |
| 4:W:315:LYS:HD2 | 4:W:315:LYS:HA | 1.92 | 0.41 |
| 4:X:221:LEU:HA | 4:X:312:ARG:HG2 | 2.02 | 0.41 |
| 4:X:222:ASP:OD1 | 4:X:224:GLU:HB3 | 2.20 | 0.41 |
| 4:X:226:GLU:HG3 | 4:X:255:PHE:CE2 | 2.55 | 0.41 |
| 1:A:94:MET:HE1 | 1:A:101:ALA:CB | 2.50 | 0.41 |
| 1:A:296:MLY:HH11 | 1:A:348:MLY:CH2 | 2.48 | 0.41 |
| 1:A:322:VAL:HG12 | 1:A:325:ILE:HG13 | 2.03 | 0.41 |
| 1:A:568:PRO:CG | 1:A:578:HIS:N | 2.84 | 0.41 |
| 1:A:717:TYR:OH | 1:A:760:PHE:HB3 | 2.21 | 0.41 |
| 1:A:842:LEU:N | 1:A:842:LEU:CD1 | 2.83 | 0.41 |
| 2:B:149:ASP:OD2 | 2:B:150:TYR:CA | 2.64 | 0.41 |
| 3:C:48:LYS:HA | 3:C:48:LYS:HD3 | 1.17 | 0.41 |
| 3:C:62:ALA:O | 3:C:63:ILE:CB | 2.63 | 0.41 |
| 3:C:63:ILE:CG2 | 3:C:64:THR:H | 2.33 | 0.41 |
| 1:D:49:MLY:HH23 | 1:D:80:MET:CE | 2.51 | 0.41 |
| 1:D:63:MLY:HH23 | 1:D:63:MLY:HD3 | 1.76 | 0.41 |
| 1:D:135:TYR:HD2 | 1:D:191:ARG:CG | 2.33 | 0.41 |
| 1:D:193:ILE:HD11 | 1:D:250:ILE:HD12 | 2.03 | 0.41 |
| 1:D:193:ILE:CD1 | 1:D:250:ILE:HD13 | 2.51 | 0.41 |
| 1:D:279:LEU:CB | 1:D:280:PRO:HD2 | 2.49 | 0.41 |
| 1:D:485:GLU:OE1 | 1:D:583:HIS:HB3 | 2.21 | 0.41 |
| 1:D:708:ARG:O | 1:D:710:GLY:N | 2.52 | 0.41 |
| 1:D:797:PHE:HE2 | 3:F:126:LEU:HD22 | 0.43 | 0.41 |
| 1:D:812:SER:O | 1:D:816:ILE:HG13 | 2.21 | 0.41 |
| 3:F:62:ALA:O | 3:F:63:ILE:CB | 2.63 | 0.41 |
| 1:G:28:GLN:CB | 1:G:723:ARG:NH2 | 2.68 | 0.41 |
| 1:G:135:TYR:CD2 | 1:G:191:ARG:HD3 | 2.55 | 0.41 |
| 1:G:553:MLY:HA | 4:X:45:VAL:O | 2.21 | 0.41 |
| 1:G:629:GLU:HB3 | 1:G:643:GLY:C | 2.41 | 0.41 |
| 2:H:111:SER:OG | 2:H:148:VAL:CA | 2.69 | 0.41 |
| 3:I:95:ASP:OD1 | 3:I:139:TYR:HE1 | 2.04 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:174:SER:HA | 1:J:460:GLY:O | 2.20 | 0.41 |
| 1:J:193:ILE:HD11 | 1:J:250:ILE:HD12 | 2.03 | 0.41 |
| 1:J:195:TYR:CE2 | 1:J:199:ILE:HD13 | 2.55 | 0.41 |
| 1:J:330:GLU:OE1 | 1:J:330:GLU:HA | 2.21 | 0.41 |
| 1:J:335:ASP:O | 1:J:338:ILE:HB | 2.20 | 0.41 |
| 1:J:493:HIS:O | 1:J:496:PHE:N | 2.54 | 0.41 |
| 1:J:554:LEU:HD12 | 1:J:554:LEU:HA | 1.77 | 0.41 |
| 1:J:568:PRO:CG | 1:J:578:HIS:N | 2.84 | 0.41 |
| 1:J:657:LEU:HD12 | 1:J:657:LEU:O | 2.21 | 0.41 |
| 1:J:795:ARG:CD | 3:L:116:GLU:OE2 | 2.67 | 0.41 |
| 3:L:63:ILE:CG2 | 3:L:64:THR:H | 2.33 | 0.41 |
| 1:M:48:VAL:CG2 | 1:M:49:MLY:N | 2.84 | 0.41 |
| 1:M:193:ILE:HD11 | 1:M:250:ILE:HD12 | 2.03 | 0.41 |
| 1:M:217:THR:CA | 1:M:221:GLN:HE21 | 2.33 | 0.41 |
| 1:M:322:VAL:HG12 | 1:M:325:ILE:HG13 | 2.03 | 0.41 |
| 1:M:330:GLU:HA | 1:M:330:GLU:OE1 | 2.20 | 0.41 |
| 1:M:541:MET:HG2 | 4:Z:345:ILE:HG23 | 2.02 | 0.41 |
| 1:M:753:VAL:O | 1:M:755:HIS:ND1 | 2.54 | 0.41 |
| 1:M:812:SER:O | 1:M:816:ILE:HG13 | 2.21 | 0.41 |
| 3:O:56:GLU:OE1 | 3:O:59:ASN:ND2 | 2.54 | 0.41 |
| 1:P:51:THR:O | 1:P:62:VAL:CG1 | 2.64 | 0.41 |
| 1:P:193:ILE:CD1 | 1:P:250:ILE:HD13 | 2.51 | 0.41 |
| 1:P:204:GLU:N | 1:P:207:LYS:HE3 | 2.23 | 0.41 |
| 1:P:217:THR:CA | 1:P:221:GLN:HE21 | 2.33 | 0.41 |
| 1:P:408:VAL:HA | 1:P:636:LYS:HG2 | 1.14 | 0.41 |
| 1:P:485:GLU:OE1 | 1:P:583:HIS:HB3 | 2.21 | 0.41 |
| 1:P:493:HIS:O | 1:P:496:PHE:N | 2.54 | 0.41 |
| 1:P:543:PRO:CG | 4:1:146:GLY:O | 2.66 | 0.41 |
| 1:P:788:THR:O | 3:R:42:THR:HG21 | 2.21 | 0.41 |
| 3:R:95:ASP:OD1 | 3:R:139:TYR:HE1 | 2.03 | 0.41 |
| 4:1:144:ALA:HB2 | 4:1:342:GLY:CA | 2.51 | 0.41 |
| 4:2:148:THR:OG1 | 4:4:45:VAL:HG23 | 2.21 | 0.41 |
| 4:2:369:ILE:HG23 | 4:2:370:VAL:N | 2.36 | 0.41 |
| 4:3:32:PRO:HB2 | 4:3:34:ILE:CD1 | 2.51 | 0.41 |
| 4:3:227:MET:O | 4:3:230:ALA:HB3 | 2.21 | 0.41 |
| 4:4:324:THR:HG23 | 4:6:244:ASP:O | 2.17 | 0.41 |
| 4:6:32:PRO:HB2 | 4:6:34:ILE:CD1 | 2.51 | 0.41 |
| 4:6:144:ALA:HB2 | 4:6:342:GLY:CA | 2.51 | 0.41 |
| 4:7:32:PRO:HB2 | 4:7:34:ILE:CD1 | 2.51 | 0.41 |
| 4:7:315:LYS:HD2 | 4:7:315:LYS:HA | 1.93 | 0.41 |
| 4:8:288:ASP:OD1 | 4:V:204:ALA:HA | 2.21 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:8:315:LYS:HD2 | 4:8:315:LYS:HA | 1.92 | 0.41 |
| 4:8:324:THR:O | 4:V:244:ASP:HA | 2.09 | 0.41 |
| 4:9:32:PRO:HB2 | 4:9:34:ILE:CD1 | 2.51 | 0.41 |
| 4:9:222:ASP:OD1 | 4:9:224:GLU:HB3 | 2.20 | 0.41 |
| 4:9:227:MET:O | 4:9:230:ALA:HB3 | 2.21 | 0.41 |
| 4:9:288:ASP:OD1 | 4:W:204:ALA:HA | 2.21 | 0.41 |
| 4:V:144:ALA:HB2 | 4:V:342:GLY:CA | 2.51 | 0.41 |
| 4:W:196:ARG:HH21 | 4:W:249:THR:HG23 | 1.85 | 0.41 |
| 4:Y:32:PRO:HB2 | 4:Y:34:ILE:CD1 | 2.51 | 0.41 |
| 4:Z:226:GLU:HG3 | 4:Z:255:PHE:CE2 | 2.55 | 0.41 |
| 1:A:330:GLU:OE1 | 1:A:330:GLU:HA | 2.20 | 0.41 |
| 1:A:502:GLU:CD | 1:A:764:MLY:N | 2.70 | 0.41 |
| 1:A:823:PHE:CE1 | 2:B:156:VAL:HG12 | 2.56 | 0.41 |
| 1:D:335:ASP:O | 1:D:338:ILE:HB | 2.21 | 0.41 |
| 1:D:356:GLY:HA2 | 1:D:359:MET:HG3 | 2.02 | 0.41 |
| 1:D:724:TYR:CB | 1:D:782:MLY:HD3 | 2.51 | 0.41 |
| 1:D:753:VAL:O | 1:D:755:HIS:ND1 | 2.54 | 0.41 |
| 1:G:193:ILE:HD11 | 1:G:250:ILE:HD12 | 2.04 | 0.41 |
| 1:G:310:TYR:OH | 1:G:320:ILE:HD11 | 2.21 | 0.41 |
| 1:G:553:MLY:C | 4:X:46:GLY:HA3 | 2.50 | 0.41 |
| 1:G:556:ASP:OD1 | 4:X:47:MET:CE | 2.27 | 0.41 |
| 1:G:735:GLY:HA3 | 1:G:743:ALA:HA | 2.01 | 0.41 |
| 1:G:739:ASP:OD1 | 1:G:739:ASP:C | 2.58 | 0.41 |
| 1:G:753:VAL:O | 1:G:755:HIS:ND1 | 2.54 | 0.41 |
| 1:J:51:THR:O | 1:J:62:VAL:CG1 | 2.64 | 0.41 |
| 1:J:485:GLU:OE1 | 1:J:583:HIS:HB3 | 2.21 | 0.41 |
| 1:J:829:TRP:HA | 1:J:830:PRO:HD2 | 1.86 | 0.41 |
| 1:M:193:ILE:CD1 | 1:M:250:ILE:HD13 | 2.51 | 0.41 |
| 1:P:384:ASP:HA | 1:P:394:SER:OG | 2.21 | 0.41 |
| 1:P:717:TYR:OH | 1:P:760:PHE:HB3 | 2.21 | 0.41 |
| 2:Q:140:PHE:HA | 2:Q:141:PRO:HD2 | 1.56 | 0.41 |
| 4:2:32:PRO:HB2 | 4:2:34:ILE:CD1 | 2.51 | 0.41 |
| 4:2:324:THR:H | 4:4:244:ASP:HA | 1.86 | 0.41 |
| 4:4:32:PRO:HB2 | 4:4:34:ILE:CD1 | 2.51 | 0.41 |
| 4:6:227:MET:O | 4:6:230:ALA:HB3 | 2.21 | 0.41 |
| 4:8:227:MET:O | 4:8:230:ALA:HB3 | 2.21 | 0.41 |
| 4:W:144:ALA:HB2 | 4:W:342:GLY:CA | 2.51 | 0.41 |
| 4:W:221:LEU:HA | 4:W:312:ARG:HG2 | 2.02 | 0.41 |
| 4:W:226:GLU:HG3 | 4:W:255:PHE:CE2 | 2.56 | 0.41 |
| 4:Y:221:LEU:HA | 4:Y:312:ARG:HG2 | 2.02 | 0.41 |
| 4:Z:221:LEU:HA | 4:Z:312:ARG:HG2 | 2.02 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:237:THR:CG2 | 1:A:238:VAL:N | 2.84 | 0.40 |
| 1:A:502:GLU:HG2 | 1:A:766:PHE:HD1 | 1.86 | 0.40 |
| 1:A:541:MET:SD | 4:8:345:ILE:C | 2.95 | 0.40 |
| 1:A:543:PRO:CG | 4:8:146:GLY:O | 2.67 | 0.40 |
| 1:A:641:LYS:HG3 | 1:A:647:GLN:HG2 | 1.72 | 0.40 |
| 1:A:657:LEU:HD12 | 1:A:657:LEU:O | 2.21 | 0.40 |
| 1:A:791:GLN:NE2 | 3:C:115:GLY:CA | 2.55 | 0.40 |
| 3:C:11:LYS:HE2 | 3:C:11:LYS:HB3 | 1.83 | 0.40 |
| 1:D:194:GLN:HE21 | 1:D:194:GLN:HB3 | 1.43 | 0.40 |
| 1:D:322:VAL:HA | 1:D:323:PRO:HD3 | 1.87 | 0.40 |
| 1:G:97:LEU:HD21 | 1:G:712:PRO:C | 2.41 | 0.40 |
| 1:G:407:GLY:HA2 | 1:G:411:GLU:O | 2.21 | 0.40 |
| 1:G:485:GLU:OE1 | 1:G:583:HIS:HB3 | 2.21 | 0.40 |
| 1:G:502:GLU:OE2 | 1:G:760:PHE:O | 2.39 | 0.40 |
| 1:G:755:HIS:CG | 1:G:779:ARG:NH1 | 2.72 | 0.40 |
| 1:G:838:ILE:CD1 | 2:H:33:VAL:HG11 | 2.51 | 0.40 |
| 2:H:137:TRP:CA | 2:H:145:ALA:HB2 | 2.37 | 0.40 |
| 1:J:107:MLY:CB | 1:J:686:MET:HE2 | 2.43 | 0.40 |
| 1:J:193:ILE:CD1 | 1:J:250:ILE:HD13 | 2.51 | 0.40 |
| 1:J:398:LEU:HA | 1:J:398:LEU:HD12 | 1.84 | 0.40 |
| 1:J:553:MLY:HH13 | 4:Y:45:VAL:HG11 | 2.02 | 0.40 |
| 1:J:725:ARG:CZ | 1:J:733:PRO:CB | 2.83 | 0.40 |
| 3:L:95:ASP:OD1 | 3:L:139:TYR:HE1 | 2.03 | 0.40 |
| 1:M:49:MLY:HH23 | 1:M:80:MET:CE | 2.52 | 0.40 |
| 1:M:110:TYR:O | 1:M:113:TRP:N | 2.42 | 0.40 |
| 1:M:237:THR:CG2 | 1:M:238:VAL:N | 2.84 | 0.40 |
| 1:M:407:GLY:HA2 | 1:M:411:GLU:O | 2.21 | 0.40 |
| 1:M:466:GLY:CA | 1:M:484:ASN:HD21 | 2.32 | 0.40 |
| 1:M:471:ASP:CB | 1:M:573:GLY:O | 2.68 | 0.40 |
| 1:M:568:PRO:CG | 1:M:578:HIS:N | 2.84 | 0.40 |
| 1:M:831:TRP:NE1 | 2:N:67:MET:HG2 | 2.35 | 0.40 |
| 1:P:528:MLY:HB2 | 1:P:529:PRO:HD2 | 2.03 | 0.40 |
| 4:3:144:ALA:HB2 | 4:3:342:GLY:CA | 2.51 | 0.40 |
| 4:4:287:ILE:HG13 | 4:6:202:THR:HG22 | 2.03 | 0.40 |
| 4:5:227:MET:O | 4:5:230:ALA:HB3 | 2.21 | 0.40 |
| 4:6:75:ILE:HD12 | 4:6:75:ILE:HG23 | 1.93 | 0.40 |
| 4:6:221:LEU:HA | 4:6:312:ARG:HG2 | 2.02 | 0.40 |
| 4:V:120:THR:HG21 | 4:V:370:VAL:CG1 | 2.52 | 0.40 |
| 1:A:48:VAL:CG2 | 1:A:49:MLY:N | 2.84 | 0.40 |
| 1:A:242:ASN:OD1 | 1:A:286:HIS:NE2 | 2.49 | 0.40 |
| 1:A:752:ASP:OD2 | 1:A:782:MLY:CG | 2.69 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:140:PHE:HB3 | 2:B:144:VAL:HG11 | 2.03 | 0.40 |
| 3:C:95:ASP:OD1 | 3:C:139:TYR:HE1 | 2.04 | 0.40 |
| 1:D:72:VAL:O | 1:D:73:LYS:O | 2.40 | 0.40 |
| 1:D:322:VAL:HB | 1:D:325:ILE:CG1 | 2.51 | 0.40 |
| 1:D:485:GLU:OE2 | 1:D:584:TYR:N | 2.50 | 0.40 |
| 1:G:172:ASN:OD1 | 1:G:457:TYR:HA | 2.22 | 0.40 |
| 1:G:506:GLU:HG2 | 1:G:759:ALA:HB1 | 2.03 | 0.40 |
| 1:G:610:LEU:N | 1:G:610:LEU:CD1 | 2.85 | 0.40 |
| 1:J:135:TYR:HD2 | 1:J:191:ARG:CG | 2.33 | 0.40 |
| 1:J:303:LEU:O | 1:J:304:LEU:HB2 | 2.21 | 0.40 |
| 1:J:580:SER:O | 1:J:581:LEU:HD12 | 2.22 | 0.40 |
| 1:J:756:THR:HG21 | 1:J:779:ARG:HB3 | 2.03 | 0.40 |
| 1:M:91:MET:CE | 1:M:119:SER:HB2 | 2.47 | 0.40 |
| 1:M:636:LYS:CB | 4:Z:334:GLU:OE1 | 2.68 | 0.40 |
| 1:M:717:TYR:OH | 1:M:760:PHE:HB3 | 2.21 | 0.40 |
| 1:M:741:LYS:HG2 | 1:M:742:LYS:N | 2.35 | 0.40 |
| 2:N:150:TYR:HB3 | 2:N:151:LYS:HG3 | 2.04 | 0.40 |
| 1:P:49:MLY:HH23 | 1:P:80:MET:CE | 2.51 | 0.40 |
| 1:P:610:LEU:N | 1:P:610:LEU:CD1 | 2.84 | 0.40 |
| 1:P:797:PHE:CD2 | 1:P:798:LEU:HD12 | 2.55 | 0.40 |
| 2:Q:150:TYR:HB3 | 2:Q:151:LYS:HG3 | 2.03 | 0.40 |
| 4:1:167:GLU:OE1 | 4:3:43:VAL:N | 2.54 | 0.40 |
| 4:1:219:VAL:HG22 | 4:1:258:PRO:CB | 2.52 | 0.40 |
| 4:1:250:ILE:HG22 | 4:1:254:ARG:HB2 | 2.04 | 0.40 |
| 4:2:196:ARG:HH21 | 4:2:249:THR:HG23 | 1.85 | 0.40 |
| 4:3:120:THR:HG21 | 4:3:370:VAL:CG1 | 2.52 | 0.40 |
| 4:3:226:GLU:HG3 | 4:3:255:PHE:CE2 | 2.55 | 0.40 |
| 4:5:219:VAL:HG22 | 4:5:258:PRO:CB | 2.51 | 0.40 |
| 4:5:369:ILE:HG23 | 4:5:370:VAL:N | 2.35 | 0.40 |
| 4:8:32:PRO:HB2 | 4:8:34:ILE:CD1 | 2.51 | 0.40 |
| 4:9:144:ALA:HB2 | 4:9:342:GLY:CA | 2.51 | 0.40 |
| 4:Y:219:VAL:HG22 | 4:Y:258:PRO:CB | 2.52 | 0.40 |
| 4:Y:256:ARG:HH11 | 4:Y:256:ARG:HD2 | 1.79 | 0.40 |
| 4:Z:120:THR:HG21 | 4:Z:370:VAL:CG1 | 2.52 | 0.40 |
| 1:A:64:THR:OG1 | 1:A:68:GLU:HB3 | 2.22 | 0.40 |
| 1:A:172:ASN:OD1 | 1:A:457:TYR:HA | 2.22 | 0.40 |
| 1:A:176:LEU:N | 1:A:176:LEU:CD1 | 2.75 | 0.40 |
| 1:A:193:ILE:CD1 | 1:A:250:ILE:HD13 | 2.51 | 0.40 |
| 1:A:407:GLY:HA2 | 1:A:411:GLU:O | 2.21 | 0.40 |
| 1:A:659:MLY:HH22 | 1:A:659:MLY:HD2 | 1.42 | 0.40 |
| 3:C:56:GLU:OE1 | 3:C:59:ASN:ND2 | 2.54 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:110:TYR:O | 1:D:113:TRP:N | 2.42 | 0.40 |
| 1:D:217:THR:CA | 1:D:221:GLN:HE21 | 2.33 | 0.40 |
| 1:D:295:MLY:CD | 1:D:332:MET:HE2 | 2.52 | 0.40 |
| 1:D:544:LYS:HD2 | 4:9:147:ARG:CB | 2.37 | 0.40 |
| 2:E:140:PHE:HB3 | 2:E:144:VAL:HG11 | 2.03 | 0.40 |
| 2:E:149:ASP:OD2 | 2:E:150:TYR:CA | 2.65 | 0.40 |
| 3:F:49:ILE:HD13 | 3:F:49:ILE:HG21 | 1.89 | 0.40 |
| 1:G:322:VAL:HA | 1:G:323:PRO:HD3 | 1.87 | 0.40 |
| 1:G:356:GLY:HA2 | 1:G:359:MET:HG3 | 2.02 | 0.40 |
| 1:G:384:ASP:HA | 1:G:394:SER:OG | 2.21 | 0.40 |
| 1:G:795:ARG:N | 3:I:118:MET:HE1 | 2.16 | 0.40 |
| 1:J:172:ASN:OD1 | 1:J:457:TYR:HA | 2.21 | 0.40 |
| 1:J:755:HIS:HA | 1:J:758:TYR:CZ | 2.56 | 0.40 |
| 1:M:136:ASN:O | 1:M:138:MLY:N | 2.54 | 0.40 |
| 1:M:172:ASN:OD1 | 1:M:457:TYR:HA | 2.22 | 0.40 |
| 1:M:305:ILE:HG22 | 1:M:312:TYR:OH | 2.21 | 0.40 |
| 1:M:549:SER:HA | 4:2:47:MET:O | 2.08 | 0.40 |
| 1:M:629:GLU:HB3 | 1:M:643:GLY:C | 2.41 | 0.40 |
| 2:N:137:TRP:CA | 2:N:145:ALA:CB | 2.82 | 0.40 |
| 1:P:193:ILE:HD11 | 1:P:250:ILE:HD12 | 2.03 | 0.40 |
| 1:P:335:ASP:O | 1:P:338:ILE:HB | 2.21 | 0.40 |
| 1:P:449:LEU:N | 1:P:449:LEU:CD1 | 2.82 | 0.40 |
| 1:P:755:HIS:HA | 1:P:758:TYR:CZ | 2.56 | 0.40 |
| 1:P:788:THR:O | 3:R:42:THR:CG2 | 2.70 | 0.40 |
| 3:R:108:ARG:HH21 | 3:R:108:ARG:HD3 | 1.78 | 0.40 |
| 4:1:112:PRO:HG3 | 4:2:195:GLU:C | 2.38 | 0.40 |
| 4:2:144:ALA:HB2 | 4:2:342:GLY:CA | 2.51 | 0.40 |
| 4:2:203:THR:CB | 4:Z:287:ILE:CG1 | 2.99 | 0.40 |
| 4:2:250:ILE:HG22 | 4:2:254:ARG:HB2 | 2.04 | 0.40 |
| 4:4:369:ILE:HG23 | 4:4:370:VAL:N | 2.36 | 0.40 |
| 4:5:120:THR:HG21 | 4:5:370:VAL:CG1 | 2.52 | 0.40 |
| 4:5:250:ILE:HG22 | 4:5:254:ARG:HB2 | 2.04 | 0.40 |
| 4:7:144:ALA:HB2 | 4:7:342:GLY:CA | 2.51 | 0.40 |
| 4:7:221:LEU:HA | 4:7:312:ARG:HG2 | 2.02 | 0.40 |
| 4:8:144:ALA:HB2 | 4:8:342:GLY:CA | 2.51 | 0.40 |
| 4:8:219:VAL:HG22 | 4:8:258:PRO:CB | 2.51 | 0.40 |
| 4:W:219:VAL:HG22 | 4:W:258:PRO:CB | 2.52 | 0.40 |
| 4:X:32:PRO:HB2 | 4:X:34:ILE:CD1 | 2.51 | 0.40 |
| 4:X:144:ALA:HB2 | 4:X:342:GLY:CA | 2.51 | 0.40 |
| 4:X:219:VAL:HG22 | 4:X:258:PRO:CB | 2.51 | 0.40 |
| 4:X:227:MET:O | 4:X:230:ALA:HB3 | 2.21 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:Z:196:ARG:HH21 | 4:Z:249:THR:HG23 | 1.85 | 0.40 |
| 4:Z:219:VAL:HG22 | 4:Z:258:PRO:CB | 2.51 | 0.40 |
| 1:A:493:HIS:O | 1:A:496:PHE:N | 2.54 | 0.40 |
| 1:A:633:GLY:HA2 | 4:8:25:ASP:HA | 1.25 | 0.40 |
| 1:A:772:LEU:HA | 1:A:772:LEU:HD12 | 1.83 | 0.40 |
| 1:A:775:LEU:HD12 | 1:A:775:LEU:HA | 1.71 | 0.40 |
| 3:C:108:ARG:HH21 | 3:C:108:ARG:HD3 | 1.78 | 0.40 |
| 1:D:496:PHE:CG | 1:D:514:ASP:HA | 2.57 | 0.40 |
| 2:E:111:SER:OG | 2:E:148:VAL:CA | 2.69 | 0.40 |
| 3:F:96:LYS:H | 3:F:96:LYS:HG3 | 1.66 | 0.40 |
| 1:G:47:PHE:HE1 | 1:G:78:PHE:CE1 | 2.40 | 0.40 |
| 1:G:193:ILE:CD1 | 1:G:250:ILE:HD13 | 2.51 | 0.40 |
| 1:G:217:THR:CA | 1:G:221:GLN:HE21 | 2.34 | 0.40 |
| 1:G:493:HIS:O | 1:G:496:PHE:N | 2.54 | 0.40 |
| 2:H:63:GLU:O | 2:H:67:MET:HG3 | 2.22 | 0.40 |
| 1:J:72:VAL:O | 1:J:73:LYS:O | 2.39 | 0.40 |
| 1:J:166:MET:CE | 1:J:254:PHE:HB2 | 2.46 | 0.40 |
| 1:J:543:PRO:CG | 4:W:146:GLY:O | 2.66 | 0.40 |
| 1:J:692:LEU:HA | 1:J:692:LEU:HD23 | 1.85 | 0.40 |
| 1:J:812:SER:O | 1:J:816:ILE:HG13 | 2.21 | 0.40 |
| 2:K:139:ALA:O | 2:K:141:PRO:CD | 2.51 | 0.40 |
| 1:M:47:PHE:HE1 | 1:M:78:PHE:CE1 | 2.40 | 0.40 |
| 1:M:528:MLY:HB2 | 1:M:529:PRO:HD2 | 2.02 | 0.40 |
| 1:M:657:LEU:O | 1:M:657:LEU:HD12 | 2.21 | 0.40 |
| 1:M:817:GLN:OE1 | 2:N:127:ARG:HD2 | 2.16 | 0.40 |
| 2:N:141:PRO:HB3 | 2:N:142:PRO:CD | 2.49 | 0.40 |
| 1:P:136:ASN:O | 1:P:138:MLY:N | 2.54 | 0.40 |
| 1:P:172:ASN:OD1 | 1:P:457:TYR:HA | 2.21 | 0.40 |
| 1:P:305:ILE:HG22 | 1:P:312:TYR:OH | 2.22 | 0.40 |
| 1:P:599:ASN:OD1 | 1:P:649:VAL:C | 2.60 | 0.40 |
| 1:P:641:LYS:CE | 1:P:647:GLN:CB | 2.75 | 0.40 |
| 4:2:227:MET:O | 4:2:230:ALA:HB3 | 2.21 | 0.40 |
| 4:5:32:PRO:HB2 | 4:5:34:ILE:CD1 | 2.51 | 0.40 |
| 4:9:221:LEU:HA | 4:9:312:ARG:HG2 | 2.02 | 0.40 |
| 4:V:219:VAL:HG22 | 4:V:258:PRO:CB | 2.51 | 0.40 |
| 4:V:250:ILE:HG22 | 4:V:254:ARG:HB2 | 2.04 | 0.40 |
| 4:W:120:THR:HG21 | 4:W:370:VAL:CG1 | 2.52 | 0.40 |
| 4:X:120:THR:HG21 | 4:X:370:VAL:CG1 | 2.52 | 0.40 |
| 4:X:196:ARG:HH21 | 4:X:249:THR:HG23 | 1.85 | 0.40 |
| 4:Z:144:ALA:HB2 | 4:Z:342:GLY:CA | 2.51 | 0.40 |
| 4:Z:227:MET:O | 4:Z:230:ALA:HB3 | 2.21 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:97:LEU:HD12 | 1:A:97:LEU:HA | 1.67 | 0.40 |
| 1:A:400:ALA:CB | 1:A:606:THR:CG2 | 3.00 | 0.40 |
| 1:A:464:ILE:HD13 | 1:A:464:ILE:HG21 | 1.69 | 0.40 |
| 1:A:599:ASN:OD1 | 1:A:649:VAL:C | 2.60 | 0.40 |
| 1:A:610:LEU:N | 1:A:610:LEU:CD1 | 2.85 | 0.40 |
| 1:A:812:SER:O | 1:A:816:ILE:HG13 | 2.21 | 0.40 |
| 1:D:303:LEU:O | 1:D:304:LEU:HB2 | 2.21 | 0.40 |
| 1:D:554:LEU:N | 4:W:46:GLY:O | 2.52 | 0.40 |
| 1:D:800:ARG:HH22 | 3:F:40:ASN:CG | 1.93 | 0.40 |
| 2:E:141:PRO:CB | 2:E:142:PRO:HD3 | 2.48 | 0.40 |
| 1:G:49:MLY:HH23 | 1:G:80:MET:CE | 2.51 | 0.40 |
| 1:G:543:PRO:CG | 4:V:146:GLY:O | 2.66 | 0.40 |
| 1:G:554:LEU:HA | 1:G:554:LEU:HD12 | 1.77 | 0.40 |
| 1:G:792:ALA:H | 3:I:42:THR:HG22 | 1.86 | 0.40 |
| 1:J:305:ILE:HG22 | 1:J:312:TYR:OH | 2.22 | 0.40 |
| 1:J:407:GLY:HA2 | 1:J:411:GLU:O | 2.21 | 0.40 |
| 1:J:496:PHE:CG | 1:J:514:ASP:HA | 2.57 | 0.40 |
| 1:J:530:MET:CE | 4:W:354:GLN:HG3 | 2.35 | 0.40 |
| 1:J:544:LYS:N | 4:W:146:GLY:O | 2.55 | 0.40 |
| 2:K:150:TYR:HB3 | 2:K:151:LYS:HG3 | 2.03 | 0.40 |
| 1:M:544:LYS:N | 4:Z:146:GLY:O | 2.55 | 0.40 |
| 1:M:599:ASN:OD1 | 1:M:649:VAL:C | 2.60 | 0.40 |
| 1:M:769:ALA:O | 1:M:770:GLY:CA | 2.67 | 0.40 |
| 1:P:303:LEU:O | 1:P:304:LEU:HB2 | 2.21 | 0.40 |
| 1:P:435:GLU:O | 1:P:438:PHE:N | 2.55 | 0.40 |
| 1:P:544:LYS:N | 4:1:146:GLY:O | 2.55 | 0.40 |
| 1:P:769:ALA:C | 1:P:770:GLY:C | 2.67 | 0.40 |
| 4:4:226:GLU:HG3 | 4:4:255:PHE:CE2 | 2.56 | 0.40 |
| 4:5:144:ALA:HB2 | 4:5:342:GLY:CA | 2.51 | 0.40 |
| 4:6:219:VAL:HG22 | 4:6:258:PRO:CB | 2.52 | 0.40 |
| 4:9:219:VAL:HG22 | 4:9:258:PRO:CB | 2.52 | 0.40 |
| 4:9:315:LYS:HD2 | 4:9:315:LYS:HA | 1.92 | 0.40 |
| 4:Y:120:THR:HG21 | 4:Y:370:VAL:CG1 | 2.52 | 0.40 |
| 4:Y:144:ALA:HB2 | 4:Y:342:GLY:CA | 2.51 | 0.40 |
| 4:Y:250:ILE:HG22 | 4:Y:254:ARG:HB2 | 2.04 | 0.40 |
| 4:Z:32:PRO:HB2 | 4:Z:34:ILE:CD1 | 2.51 | 0.40 |

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|-----------|----------|-------------|-----|
| 1 | A | 789/840 (94%) | 652 (83%) | 111 (14%) | 26 (3%) | 4 | 26 |
| 1 | D | 789/840 (94%) | 651 (82%) | 112 (14%) | 26 (3%) | 4 | 26 |
| 1 | G | 791/840 (94%) | 650 (82%) | 114 (14%) | 27 (3%) | 3 | 26 |
| 1 | J | 791/840 (94%) | 652 (82%) | 112 (14%) | 27 (3%) | 3 | 26 |
| 1 | M | 788/840 (94%) | 651 (83%) | 110 (14%) | 27 (3%) | 3 | 26 |
| 1 | P | 787/840 (94%) | 651 (83%) | 109 (14%) | 27 (3%) | 3 | 26 |
| 2 | B | 143/145 (99%) | 126 (88%) | 9 (6%) | 8 (6%) | 2 | 19 |
| 2 | E | 143/145 (99%) | 126 (88%) | 9 (6%) | 8 (6%) | 2 | 19 |
| 2 | H | 143/145 (99%) | 126 (88%) | 9 (6%) | 8 (6%) | 2 | 19 |
| 2 | K | 143/145 (99%) | 126 (88%) | 9 (6%) | 8 (6%) | 2 | 19 |
| 2 | N | 143/145 (99%) | 126 (88%) | 9 (6%) | 8 (6%) | 2 | 19 |
| 2 | Q | 143/145 (99%) | 126 (88%) | 9 (6%) | 8 (6%) | 2 | 19 |
| 3 | C | 143/147 (97%) | 133 (93%) | 10 (7%) | 0 | 100 | 100 |
| 3 | F | 143/147 (97%) | 133 (93%) | 10 (7%) | 0 | 100 | 100 |
| 3 | I | 143/147 (97%) | 133 (93%) | 10 (7%) | 0 | 100 | 100 |
| 3 | L | 143/147 (97%) | 133 (93%) | 10 (7%) | 0 | 100 | 100 |
| 3 | O | 143/147 (97%) | 133 (93%) | 10 (7%) | 0 | 100 | 100 |
| 3 | R | 143/147 (97%) | 133 (93%) | 10 (7%) | 0 | 100 | 100 |
| 4 | 1 | 370/375 (99%) | 334 (90%) | 30 (8%) | 6 (2%) | 9 | 44 |
| 4 | 2 | 370/375 (99%) | 334 (90%) | 30 (8%) | 6 (2%) | 9 | 44 |
| 4 | 3 | 370/375 (99%) | 334 (90%) | 30 (8%) | 6 (2%) | 9 | 44 |
| 4 | 4 | 370/375 (99%) | 335 (90%) | 29 (8%) | 6 (2%) | 9 | 44 |
| 4 | 5 | 370/375 (99%) | 333 (90%) | 31 (8%) | 6 (2%) | 9 | 44 |
| 4 | 6 | 370/375 (99%) | 334 (90%) | 30 (8%) | 6 (2%) | 9 | 44 |
| 4 | 7 | 370/375 (99%) | 334 (90%) | 30 (8%) | 6 (2%) | 9 | 44 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-------------------|-------------|------------|----------|-------------|----|
| 4 | 8 | 370/375 (99%) | 333 (90%) | 31 (8%) | 6 (2%) | 9 | 44 |
| 4 | 9 | 370/375 (99%) | 334 (90%) | 30 (8%) | 6 (2%) | 9 | 44 |
| 4 | V | 370/375 (99%) | 335 (90%) | 29 (8%) | 6 (2%) | 9 | 44 |
| 4 | W | 370/375 (99%) | 334 (90%) | 30 (8%) | 6 (2%) | 9 | 44 |
| 4 | X | 370/375 (99%) | 335 (90%) | 29 (8%) | 6 (2%) | 9 | 44 |
| 4 | Y | 370/375 (99%) | 334 (90%) | 30 (8%) | 6 (2%) | 9 | 44 |
| 4 | Z | 370/375 (99%) | 334 (90%) | 30 (8%) | 6 (2%) | 9 | 44 |
| All | All | 11631/12042 (97%) | 10138 (87%) | 1201 (10%) | 292 (2%) | 9 | 32 |

All (292) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 73 | LYS |
| 1 | A | 202 | SER |
| 1 | A | 572 | LYS |
| 1 | A | 712 | PRO |
| 1 | A | 729 | ALA |
| 1 | A | 757 | GLN |
| 1 | A | 762 | HIS |
| 2 | B | 131 | GLU |
| 2 | B | 141 | PRO |
| 1 | D | 73 | LYS |
| 1 | D | 202 | SER |
| 1 | D | 572 | LYS |
| 1 | D | 712 | PRO |
| 1 | D | 729 | ALA |
| 1 | D | 757 | GLN |
| 1 | D | 762 | HIS |
| 2 | E | 131 | GLU |
| 2 | E | 141 | PRO |
| 1 | G | 73 | LYS |
| 1 | G | 202 | SER |
| 1 | G | 572 | LYS |
| 1 | G | 712 | PRO |
| 1 | G | 729 | ALA |
| 1 | G | 757 | GLN |
| 1 | G | 762 | HIS |
| 2 | H | 131 | GLU |
| 2 | H | 141 | PRO |
| 1 | J | 73 | LYS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | J | 202 | SER |
| 1 | J | 572 | LYS |
| 1 | J | 712 | PRO |
| 1 | J | 729 | ALA |
| 1 | J | 757 | GLN |
| 1 | J | 762 | HIS |
| 1 | J | 785 | GLU |
| 2 | K | 131 | GLU |
| 2 | K | 141 | PRO |
| 1 | M | 73 | LYS |
| 1 | M | 202 | SER |
| 1 | M | 572 | LYS |
| 1 | M | 712 | PRO |
| 1 | M | 729 | ALA |
| 1 | M | 757 | GLN |
| 1 | M | 762 | HIS |
| 2 | N | 131 | GLU |
| 2 | N | 141 | PRO |
| 1 | P | 73 | LYS |
| 1 | P | 202 | SER |
| 1 | P | 572 | LYS |
| 1 | P | 712 | PRO |
| 1 | P | 729 | ALA |
| 1 | P | 757 | GLN |
| 1 | P | 762 | HIS |
| 2 | Q | 131 | GLU |
| 2 | Q | 141 | PRO |
| 4 | 1 | 246 | GLN |
| 4 | 2 | 246 | GLN |
| 4 | 3 | 246 | GLN |
| 4 | 4 | 246 | GLN |
| 4 | 5 | 246 | GLN |
| 4 | 6 | 246 | GLN |
| 4 | 7 | 246 | GLN |
| 4 | 8 | 246 | GLN |
| 4 | 9 | 246 | GLN |
| 4 | V | 246 | GLN |
| 4 | W | 246 | GLN |
| 4 | X | 246 | GLN |
| 4 | Y | 246 | GLN |
| 4 | Z | 246 | GLN |
| 1 | A | 11 | GLY |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 21 | GLU |
| 1 | A | 219 | GLU |
| 1 | A | 517 | MET |
| 1 | A | 637 | LYS |
| 2 | B | 130 | PRO |
| 2 | B | 147 | ASN |
| 2 | B | 151 | LYS |
| 2 | B | 161 | GLU |
| 1 | D | 11 | GLY |
| 1 | D | 21 | GLU |
| 1 | D | 219 | GLU |
| 1 | D | 517 | MET |
| 1 | D | 637 | LYS |
| 2 | E | 130 | PRO |
| 2 | E | 147 | ASN |
| 2 | E | 151 | LYS |
| 2 | E | 161 | GLU |
| 1 | G | 11 | GLY |
| 1 | G | 21 | GLU |
| 1 | G | 219 | GLU |
| 1 | G | 517 | MET |
| 1 | G | 532 | ILE |
| 1 | G | 637 | LYS |
| 1 | G | 785 | GLU |
| 2 | H | 130 | PRO |
| 2 | H | 147 | ASN |
| 2 | H | 151 | LYS |
| 1 | J | 11 | GLY |
| 1 | J | 21 | GLU |
| 1 | J | 219 | GLU |
| 1 | J | 517 | MET |
| 1 | J | 637 | LYS |
| 2 | K | 130 | PRO |
| 2 | K | 147 | ASN |
| 2 | K | 151 | LYS |
| 1 | M | 11 | GLY |
| 1 | M | 21 | GLU |
| 1 | M | 219 | GLU |
| 1 | M | 517 | MET |
| 1 | M | 637 | LYS |
| 2 | N | 130 | PRO |
| 2 | N | 147 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | N | 151 | LYS |
| 2 | N | 161 | GLU |
| 1 | P | 11 | GLY |
| 1 | P | 21 | GLU |
| 1 | P | 219 | GLU |
| 1 | P | 517 | MET |
| 1 | P | 637 | LYS |
| 2 | Q | 130 | PRO |
| 2 | Q | 147 | ASN |
| 2 | Q | 151 | LYS |
| 4 | 1 | 274 | ILE |
| 4 | 2 | 274 | ILE |
| 4 | 3 | 274 | ILE |
| 4 | 4 | 274 | ILE |
| 4 | 5 | 274 | ILE |
| 4 | 6 | 274 | ILE |
| 4 | 7 | 274 | ILE |
| 4 | 8 | 274 | ILE |
| 4 | 9 | 274 | ILE |
| 4 | V | 274 | ILE |
| 4 | W | 274 | ILE |
| 4 | X | 274 | ILE |
| 4 | Y | 274 | ILE |
| 4 | Z | 274 | ILE |
| 1 | A | 58 | GLY |
| 1 | A | 294 | ASN |
| 1 | A | 532 | ILE |
| 1 | A | 644 | SER |
| 1 | D | 58 | GLY |
| 1 | D | 294 | ASN |
| 1 | D | 532 | ILE |
| 1 | D | 644 | SER |
| 1 | G | 58 | GLY |
| 1 | G | 294 | ASN |
| 1 | G | 644 | SER |
| 2 | H | 161 | GLU |
| 1 | J | 58 | GLY |
| 1 | J | 294 | ASN |
| 1 | J | 532 | ILE |
| 1 | J | 644 | SER |
| 2 | K | 161 | GLU |
| 1 | M | 58 | GLY |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | M | 294 | ASN |
| 1 | M | 532 | ILE |
| 1 | M | 644 | SER |
| 1 | P | 58 | GLY |
| 1 | P | 294 | ASN |
| 1 | P | 532 | ILE |
| 1 | P | 644 | SER |
| 2 | Q | 161 | GLU |
| 4 | 1 | 233 | SER |
| 4 | 2 | 233 | SER |
| 4 | 3 | 233 | SER |
| 4 | 4 | 233 | SER |
| 4 | 5 | 233 | SER |
| 4 | 6 | 233 | SER |
| 4 | 7 | 233 | SER |
| 4 | 8 | 233 | SER |
| 4 | 9 | 233 | SER |
| 4 | V | 233 | SER |
| 4 | W | 233 | SER |
| 4 | X | 233 | SER |
| 4 | Y | 233 | SER |
| 4 | Z | 233 | SER |
| 1 | A | 435 | GLU |
| 1 | A | 817 | GLN |
| 1 | D | 269 | LEU |
| 1 | D | 435 | GLU |
| 1 | D | 817 | GLN |
| 1 | G | 269 | LEU |
| 1 | G | 435 | GLU |
| 1 | G | 817 | GLN |
| 1 | J | 269 | LEU |
| 1 | J | 435 | GLU |
| 1 | J | 817 | GLN |
| 1 | M | 269 | LEU |
| 1 | M | 435 | GLU |
| 1 | M | 817 | GLN |
| 1 | P | 269 | LEU |
| 1 | P | 435 | GLU |
| 1 | P | 817 | GLN |
| 4 | 1 | 2 | GLU |
| 4 | 1 | 253 | GLU |
| 4 | 2 | 2 | GLU |

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Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4 | 2 | 253 | GLU |
| 4 | 3 | 2 | GLU |
| 4 | 4 | 2 | GLU |
| 4 | 5 | 2 | GLU |
| 4 | 6 | 2 | GLU |
| 4 | 7 | 2 | GLU |
| 4 | 8 | 2 | GLU |
| 4 | 8 | 253 | GLU |
| 4 | 9 | 2 | GLU |
| 4 | 9 | 253 | GLU |
| 4 | V | 2 | GLU |
| 4 | W | 2 | GLU |
| 4 | X | 2 | GLU |
| 4 | Y | 2 | GLU |
| 4 | Y | 253 | GLU |
| 4 | Z | 2 | GLU |
| 1 | A | 8 | ALA |
| 1 | A | 79 | SER |
| 1 | A | 269 | LEU |
| 1 | A | 578 | HIS |
| 2 | B | 140 | PHE |
| 1 | D | 8 | ALA |
| 1 | D | 556 | ASP |
| 1 | D | 578 | HIS |
| 2 | E | 140 | PHE |
| 1 | G | 8 | ALA |
| 1 | G | 79 | SER |
| 1 | G | 578 | HIS |
| 2 | H | 140 | PHE |
| 1 | J | 8 | ALA |
| 1 | J | 556 | ASP |
| 1 | J | 578 | HIS |
| 2 | K | 140 | PHE |
| 1 | M | 8 | ALA |
| 1 | M | 578 | HIS |
| 2 | N | 140 | PHE |
| 1 | P | 8 | ALA |
| 1 | P | 578 | HIS |
| 2 | Q | 140 | PHE |
| 4 | 3 | 253 | GLU |
| 4 | 4 | 253 | GLU |
| 4 | 5 | 253 | GLU |

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Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4 | 6 | 253 | GLU |
| 4 | 7 | 253 | GLU |
| 4 | V | 253 | GLU |
| 4 | W | 253 | GLU |
| 4 | X | 253 | GLU |
| 4 | Z | 253 | GLU |
| 1 | A | 199 | ILE |
| 1 | A | 556 | ASP |
| 2 | B | 142 | PRO |
| 1 | D | 79 | SER |
| 1 | D | 199 | ILE |
| 2 | E | 142 | PRO |
| 1 | G | 199 | ILE |
| 1 | G | 556 | ASP |
| 2 | H | 142 | PRO |
| 1 | J | 79 | SER |
| 1 | J | 199 | ILE |
| 2 | K | 142 | PRO |
| 1 | M | 79 | SER |
| 1 | M | 199 | ILE |
| 1 | M | 556 | ASP |
| 1 | M | 822 | SER |
| 2 | N | 142 | PRO |
| 1 | P | 79 | SER |
| 1 | P | 199 | ILE |
| 1 | P | 556 | ASP |
| 1 | P | 785 | GLU |
| 2 | Q | 142 | PRO |
| 1 | A | 840 | PRO |
| 1 | D | 287 | ILE |
| 1 | D | 840 | PRO |
| 1 | G | 287 | ILE |
| 1 | G | 840 | PRO |
| 1 | J | 840 | PRO |
| 1 | M | 840 | PRO |
| 1 | P | 287 | ILE |
| 1 | P | 840 | PRO |
| 4 | 1 | 242 | LEU |
| 4 | 2 | 242 | LEU |
| 4 | 3 | 242 | LEU |
| 4 | 4 | 242 | LEU |
| 4 | 5 | 242 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4 | 6 | 242 | LEU |
| 4 | 7 | 242 | LEU |
| 4 | 8 | 242 | LEU |
| 4 | 9 | 242 | LEU |
| 4 | V | 242 | LEU |
| 4 | W | 242 | LEU |
| 4 | X | 242 | LEU |
| 4 | Y | 242 | LEU |
| 4 | Z | 242 | LEU |
| 1 | A | 287 | ILE |
| 1 | J | 287 | ILE |
| 1 | M | 287 | ILE |

5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|-----------|-----------|-------------|----|
| 1 | A | 672/672 (100%) | 512 (76%) | 160 (24%) | 0 | 4 |
| 1 | D | 672/672 (100%) | 514 (76%) | 158 (24%) | 1 | 4 |
| 1 | G | 672/672 (100%) | 514 (76%) | 158 (24%) | 1 | 4 |
| 1 | J | 672/672 (100%) | 513 (76%) | 159 (24%) | 1 | 4 |
| 1 | M | 672/672 (100%) | 513 (76%) | 159 (24%) | 1 | 4 |
| 1 | P | 672/672 (100%) | 515 (77%) | 157 (23%) | 1 | 4 |
| 2 | B | 120/120 (100%) | 119 (99%) | 1 (1%) | 81 | 89 |
| 2 | E | 120/120 (100%) | 119 (99%) | 1 (1%) | 81 | 89 |
| 2 | H | 120/120 (100%) | 119 (99%) | 1 (1%) | 81 | 89 |
| 2 | K | 120/120 (100%) | 119 (99%) | 1 (1%) | 81 | 89 |
| 2 | N | 120/120 (100%) | 119 (99%) | 1 (1%) | 81 | 89 |
| 2 | Q | 120/120 (100%) | 119 (99%) | 1 (1%) | 81 | 89 |
| 3 | C | 117/117 (100%) | 112 (96%) | 5 (4%) | 29 | 53 |
| 3 | F | 117/117 (100%) | 112 (96%) | 5 (4%) | 29 | 53 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|------------------|------------|------------|-------------|----|
| 3 | I | 117/117 (100%) | 112 (96%) | 5 (4%) | 29 | 53 |
| 3 | L | 117/117 (100%) | 112 (96%) | 5 (4%) | 29 | 53 |
| 3 | O | 117/117 (100%) | 112 (96%) | 5 (4%) | 29 | 53 |
| 3 | R | 117/117 (100%) | 112 (96%) | 5 (4%) | 29 | 53 |
| 4 | 1 | 315/318 (99%) | 268 (85%) | 47 (15%) | 3 | 15 |
| 4 | 2 | 315/318 (99%) | 268 (85%) | 47 (15%) | 3 | 15 |
| 4 | 3 | 315/318 (99%) | 269 (85%) | 46 (15%) | 3 | 15 |
| 4 | 4 | 315/318 (99%) | 269 (85%) | 46 (15%) | 3 | 15 |
| 4 | 5 | 315/318 (99%) | 268 (85%) | 47 (15%) | 3 | 15 |
| 4 | 6 | 315/318 (99%) | 268 (85%) | 47 (15%) | 3 | 15 |
| 4 | 7 | 315/318 (99%) | 269 (85%) | 46 (15%) | 3 | 15 |
| 4 | 8 | 315/318 (99%) | 269 (85%) | 46 (15%) | 3 | 15 |
| 4 | 9 | 315/318 (99%) | 268 (85%) | 47 (15%) | 3 | 15 |
| 4 | V | 315/318 (99%) | 268 (85%) | 47 (15%) | 3 | 15 |
| 4 | W | 315/318 (99%) | 269 (85%) | 46 (15%) | 3 | 15 |
| 4 | X | 315/318 (99%) | 269 (85%) | 46 (15%) | 3 | 15 |
| 4 | Y | 315/318 (99%) | 268 (85%) | 47 (15%) | 3 | 15 |
| 4 | Z | 315/318 (99%) | 269 (85%) | 46 (15%) | 3 | 15 |
| All | All | 9864/9906 (100%) | 8226 (83%) | 1638 (17%) | 5 | 12 |

All (1638) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 4 | ASP |
| 1 | A | 7 | MET |
| 1 | A | 12 | GLU |
| 1 | A | 15 | PRO |
| 1 | A | 17 | LEU |
| 1 | A | 20 | SER |
| 1 | A | 22 | LYS |
| 1 | A | 36 | SER |
| 1 | A | 37 | SER |
| 1 | A | 46 | SER |
| 1 | A | 61 | THR |
| 1 | A | 69 | THR |
| 1 | A | 70 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 72 | VAL |
| 1 | A | 73 | LYS |
| 1 | A | 75 | ASP |
| 1 | A | 76 | GLN |
| 1 | A | 97 | LEU |
| 1 | A | 106 | LEU |
| 1 | A | 109 | ARG |
| 1 | A | 114 | MET |
| 1 | A | 117 | THR |
| 1 | A | 121 | LEU |
| 1 | A | 126 | VAL |
| 1 | A | 127 | ASN |
| 1 | A | 135 | TYR |
| 1 | A | 136 | ASN |
| 1 | A | 146 | LYS |
| 1 | A | 148 | ARG |
| 1 | A | 149 | GLN |
| 1 | A | 155 | ILE |
| 1 | A | 157 | SER |
| 1 | A | 158 | ILE |
| 1 | A | 159 | SER |
| 1 | A | 165 | PHE |
| 1 | A | 167 | LEU |
| 1 | A | 169 | ASP |
| 1 | A | 173 | GLN |
| 1 | A | 178 | THR |
| 1 | A | 185 | LYS |
| 1 | A | 186 | THR |
| 1 | A | 187 | VAL |
| 1 | A | 191 | ARG |
| 1 | A | 193 | ILE |
| 1 | A | 194 | GLN |
| 1 | A | 198 | THR |
| 1 | A | 199 | ILE |
| 1 | A | 218 | LEU |
| 1 | A | 219 | GLU |
| 1 | A | 221 | GLN |
| 1 | A | 223 | ILE |
| 1 | A | 227 | PRO |
| 1 | A | 229 | LEU |
| 1 | A | 244 | SER |
| 1 | A | 245 | ARG |

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Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 251 | ARG |
| 1 | A | 264 | ASP |
| 1 | A | 273 | SER |
| 1 | A | 274 | ARG |
| 1 | A | 278 | GLN |
| 1 | A | 282 | GLU |
| 1 | A | 287 | ILE |
| 1 | A | 290 | GLN |
| 1 | A | 294 | ASN |
| 1 | A | 298 | GLU |
| 1 | A | 300 | ILE |
| 1 | A | 325 | ILE |
| 1 | A | 331 | LEU |
| 1 | A | 336 | SER |
| 1 | A | 351 | ILE |
| 1 | A | 354 | LEU |
| 1 | A | 364 | LEU |
| 1 | A | 365 | LYS |
| 1 | A | 372 | GLU |
| 1 | A | 376 | GLU |
| 1 | A | 381 | GLU |
| 1 | A | 389 | LEU |
| 1 | A | 392 | LEU |
| 1 | A | 394 | SER |
| 1 | A | 399 | LYS |
| 1 | A | 405 | ARG |
| 1 | A | 410 | ASN |
| 1 | A | 439 | LEU |
| 1 | A | 447 | GLN |
| 1 | A | 448 | GLN |
| 1 | A | 449 | LEU |
| 1 | A | 453 | GLN |
| 1 | A | 455 | ARG |
| 1 | A | 457 | TYR |
| 1 | A | 462 | LEU |
| 1 | A | 471 | ASP |
| 1 | A | 474 | SER |
| 1 | A | 480 | ILE |
| 1 | A | 487 | LEU |
| 1 | A | 495 | MET |
| 1 | A | 499 | GLU |
| 1 | A | 506 | GLU |

Continued on next page...

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 513 | ILE |
| 1 | A | 518 | ASP |
| 1 | A | 524 | GLU |
| 1 | A | 532 | ILE |
| 1 | A | 534 | SER |
| 1 | A | 537 | GLU |
| 1 | A | 543 | PRO |
| 1 | A | 549 | SER |
| 1 | A | 561 | LYS |
| 1 | A | 562 | SER |
| 1 | A | 563 | ASN |
| 1 | A | 569 | LYS |
| 1 | A | 580 | SER |
| 1 | A | 593 | SER |
| 1 | A | 597 | GLU |
| 1 | A | 604 | ASN |
| 1 | A | 608 | ILE |
| 1 | A | 610 | LEU |
| 1 | A | 615 | SER |
| 1 | A | 621 | LEU |
| 1 | A | 625 | THR |
| 1 | A | 664 | LEU |
| 1 | A | 666 | SER |
| 1 | A | 673 | ARG |
| 1 | A | 675 | ILE |
| 1 | A | 676 | ILE |
| 1 | A | 686 | MET |
| 1 | A | 689 | GLU |
| 1 | A | 690 | LEU |
| 1 | A | 693 | HIS |
| 1 | A | 698 | ASN |
| 1 | A | 701 | LEU |
| 1 | A | 702 | GLU |
| 1 | A | 704 | ILE |
| 1 | A | 708 | ARG |
| 1 | A | 713 | SER |
| 1 | A | 714 | ARG |
| 1 | A | 716 | LEU |
| 1 | A | 719 | ASP |
| 1 | A | 722 | GLN |
| 1 | A | 723 | ARG |
| 1 | A | 727 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 728 | ASN |
| 1 | A | 745 | GLU |
| 1 | A | 752 | ASP |
| 1 | A | 753 | VAL |
| 1 | A | 754 | ASP |
| 1 | A | 762 | HIS |
| 1 | A | 774 | LEU |
| 1 | A | 785 | GLU |
| 1 | A | 787 | ILE |
| 1 | A | 793 | ARG |
| 1 | A | 799 | MET |
| 1 | A | 802 | GLU |
| 1 | A | 804 | ARG |
| 1 | A | 810 | ARG |
| 1 | A | 816 | ILE |
| 1 | A | 822 | SER |
| 1 | A | 832 | MET |
| 1 | A | 834 | LEU |
| 1 | A | 838 | ILE |
| 1 | A | 842 | LEU |
| 1 | A | 843 | LYS |
| 2 | B | 142 | PRO |
| 3 | C | 48 | LYS |
| 3 | C | 68 | PHE |
| 3 | C | 83 | THR |
| 3 | C | 95 | ASP |
| 3 | C | 96 | LYS |
| 1 | D | 4 | ASP |
| 1 | D | 7 | MET |
| 1 | D | 12 | GLU |
| 1 | D | 15 | PRO |
| 1 | D | 17 | LEU |
| 1 | D | 20 | SER |
| 1 | D | 22 | LYS |
| 1 | D | 36 | SER |
| 1 | D | 37 | SER |
| 1 | D | 46 | SER |
| 1 | D | 61 | THR |
| 1 | D | 69 | THR |
| 1 | D | 70 | LEU |
| 1 | D | 72 | VAL |
| 1 | D | 73 | LYS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | D | 75 | ASP |
| 1 | D | 76 | GLN |
| 1 | D | 97 | LEU |
| 1 | D | 106 | LEU |
| 1 | D | 109 | ARG |
| 1 | D | 114 | MET |
| 1 | D | 117 | THR |
| 1 | D | 121 | LEU |
| 1 | D | 126 | VAL |
| 1 | D | 127 | ASN |
| 1 | D | 135 | TYR |
| 1 | D | 136 | ASN |
| 1 | D | 146 | LYS |
| 1 | D | 149 | GLN |
| 1 | D | 155 | ILE |
| 1 | D | 157 | SER |
| 1 | D | 158 | ILE |
| 1 | D | 159 | SER |
| 1 | D | 165 | PHE |
| 1 | D | 167 | LEU |
| 1 | D | 169 | ASP |
| 1 | D | 173 | GLN |
| 1 | D | 178 | THR |
| 1 | D | 185 | LYS |
| 1 | D | 186 | THR |
| 1 | D | 187 | VAL |
| 1 | D | 191 | ARG |
| 1 | D | 193 | ILE |
| 1 | D | 194 | GLN |
| 1 | D | 198 | THR |
| 1 | D | 199 | ILE |
| 1 | D | 218 | LEU |
| 1 | D | 219 | GLU |
| 1 | D | 221 | GLN |
| 1 | D | 223 | ILE |
| 1 | D | 229 | LEU |
| 1 | D | 244 | SER |
| 1 | D | 245 | ARG |
| 1 | D | 251 | ARG |
| 1 | D | 264 | ASP |
| 1 | D | 273 | SER |
| 1 | D | 274 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | D | 278 | GLN |
| 1 | D | 282 | GLU |
| 1 | D | 287 | ILE |
| 1 | D | 290 | GLN |
| 1 | D | 294 | ASN |
| 1 | D | 298 | GLU |
| 1 | D | 300 | ILE |
| 1 | D | 325 | ILE |
| 1 | D | 331 | LEU |
| 1 | D | 336 | SER |
| 1 | D | 351 | ILE |
| 1 | D | 354 | LEU |
| 1 | D | 364 | LEU |
| 1 | D | 365 | LYS |
| 1 | D | 372 | GLU |
| 1 | D | 376 | GLU |
| 1 | D | 381 | GLU |
| 1 | D | 389 | LEU |
| 1 | D | 392 | LEU |
| 1 | D | 394 | SER |
| 1 | D | 399 | LYS |
| 1 | D | 405 | ARG |
| 1 | D | 410 | ASN |
| 1 | D | 439 | LEU |
| 1 | D | 447 | GLN |
| 1 | D | 448 | GLN |
| 1 | D | 449 | LEU |
| 1 | D | 453 | GLN |
| 1 | D | 455 | ARG |
| 1 | D | 457 | TYR |
| 1 | D | 462 | LEU |
| 1 | D | 471 | ASP |
| 1 | D | 474 | SER |
| 1 | D | 480 | ILE |
| 1 | D | 487 | LEU |
| 1 | D | 495 | MET |
| 1 | D | 499 | GLU |
| 1 | D | 506 | GLU |
| 1 | D | 513 | ILE |
| 1 | D | 518 | ASP |
| 1 | D | 524 | GLU |
| 1 | D | 532 | ILE |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | D | 534 | SER |
| 1 | D | 537 | GLU |
| 1 | D | 543 | PRO |
| 1 | D | 549 | SER |
| 1 | D | 561 | LYS |
| 1 | D | 562 | SER |
| 1 | D | 563 | ASN |
| 1 | D | 569 | LYS |
| 1 | D | 580 | SER |
| 1 | D | 593 | SER |
| 1 | D | 597 | GLU |
| 1 | D | 604 | ASN |
| 1 | D | 608 | ILE |
| 1 | D | 610 | LEU |
| 1 | D | 615 | SER |
| 1 | D | 621 | LEU |
| 1 | D | 625 | THR |
| 1 | D | 664 | LEU |
| 1 | D | 666 | SER |
| 1 | D | 673 | ARG |
| 1 | D | 675 | ILE |
| 1 | D | 676 | ILE |
| 1 | D | 686 | MET |
| 1 | D | 689 | GLU |
| 1 | D | 690 | LEU |
| 1 | D | 693 | HIS |
| 1 | D | 698 | ASN |
| 1 | D | 701 | LEU |
| 1 | D | 702 | GLU |
| 1 | D | 704 | ILE |
| 1 | D | 708 | ARG |
| 1 | D | 713 | SER |
| 1 | D | 714 | ARG |
| 1 | D | 716 | LEU |
| 1 | D | 719 | ASP |
| 1 | D | 722 | GLN |
| 1 | D | 723 | ARG |
| 1 | D | 727 | LEU |
| 1 | D | 728 | ASN |
| 1 | D | 745 | GLU |
| 1 | D | 752 | ASP |
| 1 | D | 753 | VAL |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | D | 754 | ASP |
| 1 | D | 762 | HIS |
| 1 | D | 774 | LEU |
| 1 | D | 785 | GLU |
| 1 | D | 787 | ILE |
| 1 | D | 793 | ARG |
| 1 | D | 799 | MET |
| 1 | D | 802 | GLU |
| 1 | D | 804 | ARG |
| 1 | D | 810 | ARG |
| 1 | D | 816 | ILE |
| 1 | D | 822 | SER |
| 1 | D | 832 | MET |
| 1 | D | 834 | LEU |
| 1 | D | 838 | ILE |
| 1 | D | 842 | LEU |
| 1 | D | 843 | LYS |
| 2 | E | 142 | PRO |
| 3 | F | 48 | LYS |
| 3 | F | 68 | PHE |
| 3 | F | 83 | THR |
| 3 | F | 95 | ASP |
| 3 | F | 96 | LYS |
| 1 | G | 4 | ASP |
| 1 | G | 7 | MET |
| 1 | G | 12 | GLU |
| 1 | G | 15 | PRO |
| 1 | G | 17 | LEU |
| 1 | G | 20 | SER |
| 1 | G | 22 | LYS |
| 1 | G | 36 | SER |
| 1 | G | 37 | SER |
| 1 | G | 46 | SER |
| 1 | G | 61 | THR |
| 1 | G | 69 | THR |
| 1 | G | 70 | LEU |
| 1 | G | 72 | VAL |
| 1 | G | 73 | LYS |
| 1 | G | 75 | ASP |
| 1 | G | 76 | GLN |
| 1 | G | 97 | LEU |
| 1 | G | 106 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | G | 109 | ARG |
| 1 | G | 114 | MET |
| 1 | G | 117 | THR |
| 1 | G | 121 | LEU |
| 1 | G | 126 | VAL |
| 1 | G | 127 | ASN |
| 1 | G | 135 | TYR |
| 1 | G | 136 | ASN |
| 1 | G | 146 | LYS |
| 1 | G | 149 | GLN |
| 1 | G | 155 | ILE |
| 1 | G | 157 | SER |
| 1 | G | 158 | ILE |
| 1 | G | 159 | SER |
| 1 | G | 165 | PHE |
| 1 | G | 167 | LEU |
| 1 | G | 169 | ASP |
| 1 | G | 173 | GLN |
| 1 | G | 178 | THR |
| 1 | G | 185 | LYS |
| 1 | G | 186 | THR |
| 1 | G | 187 | VAL |
| 1 | G | 189 | THR |
| 1 | G | 191 | ARG |
| 1 | G | 193 | ILE |
| 1 | G | 194 | GLN |
| 1 | G | 198 | THR |
| 1 | G | 199 | ILE |
| 1 | G | 218 | LEU |
| 1 | G | 219 | GLU |
| 1 | G | 221 | GLN |
| 1 | G | 223 | ILE |
| 1 | G | 229 | LEU |
| 1 | G | 243 | SER |
| 1 | G | 244 | SER |
| 1 | G | 245 | ARG |
| 1 | G | 251 | ARG |
| 1 | G | 264 | ASP |
| 1 | G | 273 | SER |
| 1 | G | 274 | ARG |
| 1 | G | 278 | GLN |
| 1 | G | 282 | GLU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | G | 287 | ILE |
| 1 | G | 290 | GLN |
| 1 | G | 294 | ASN |
| 1 | G | 298 | GLU |
| 1 | G | 300 | ILE |
| 1 | G | 325 | ILE |
| 1 | G | 331 | LEU |
| 1 | G | 336 | SER |
| 1 | G | 351 | ILE |
| 1 | G | 354 | LEU |
| 1 | G | 364 | LEU |
| 1 | G | 365 | LYS |
| 1 | G | 372 | GLU |
| 1 | G | 376 | GLU |
| 1 | G | 381 | GLU |
| 1 | G | 389 | LEU |
| 1 | G | 392 | LEU |
| 1 | G | 394 | SER |
| 1 | G | 399 | LYS |
| 1 | G | 405 | ARG |
| 1 | G | 410 | ASN |
| 1 | G | 439 | LEU |
| 1 | G | 447 | GLN |
| 1 | G | 448 | GLN |
| 1 | G | 449 | LEU |
| 1 | G | 453 | GLN |
| 1 | G | 455 | ARG |
| 1 | G | 457 | TYR |
| 1 | G | 462 | LEU |
| 1 | G | 471 | ASP |
| 1 | G | 474 | SER |
| 1 | G | 480 | ILE |
| 1 | G | 487 | LEU |
| 1 | G | 495 | MET |
| 1 | G | 506 | GLU |
| 1 | G | 513 | ILE |
| 1 | G | 518 | ASP |
| 1 | G | 524 | GLU |
| 1 | G | 532 | ILE |
| 1 | G | 534 | SER |
| 1 | G | 537 | GLU |
| 1 | G | 543 | PRO |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | G | 549 | SER |
| 1 | G | 561 | LYS |
| 1 | G | 562 | SER |
| 1 | G | 563 | ASN |
| 1 | G | 569 | LYS |
| 1 | G | 580 | SER |
| 1 | G | 593 | SER |
| 1 | G | 597 | GLU |
| 1 | G | 604 | ASN |
| 1 | G | 608 | ILE |
| 1 | G | 610 | LEU |
| 1 | G | 615 | SER |
| 1 | G | 621 | LEU |
| 1 | G | 625 | THR |
| 1 | G | 664 | LEU |
| 1 | G | 666 | SER |
| 1 | G | 673 | ARG |
| 1 | G | 675 | ILE |
| 1 | G | 676 | ILE |
| 1 | G | 686 | MET |
| 1 | G | 689 | GLU |
| 1 | G | 690 | LEU |
| 1 | G | 693 | HIS |
| 1 | G | 698 | ASN |
| 1 | G | 701 | LEU |
| 1 | G | 702 | GLU |
| 1 | G | 708 | ARG |
| 1 | G | 713 | SER |
| 1 | G | 714 | ARG |
| 1 | G | 716 | LEU |
| 1 | G | 719 | ASP |
| 1 | G | 722 | GLN |
| 1 | G | 723 | ARG |
| 1 | G | 727 | LEU |
| 1 | G | 728 | ASN |
| 1 | G | 745 | GLU |
| 1 | G | 752 | ASP |
| 1 | G | 753 | VAL |
| 1 | G | 754 | ASP |
| 1 | G | 762 | HIS |
| 1 | G | 774 | LEU |
| 1 | G | 785 | GLU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | G | 787 | ILE |
| 1 | G | 793 | ARG |
| 1 | G | 799 | MET |
| 1 | G | 802 | GLU |
| 1 | G | 804 | ARG |
| 1 | G | 810 | ARG |
| 1 | G | 816 | ILE |
| 1 | G | 822 | SER |
| 1 | G | 832 | MET |
| 1 | G | 834 | LEU |
| 1 | G | 838 | ILE |
| 1 | G | 842 | LEU |
| 1 | G | 843 | LYS |
| 2 | H | 142 | PRO |
| 3 | I | 48 | LYS |
| 3 | I | 68 | PHE |
| 3 | I | 83 | THR |
| 3 | I | 95 | ASP |
| 3 | I | 96 | LYS |
| 1 | J | 4 | ASP |
| 1 | J | 7 | MET |
| 1 | J | 12 | GLU |
| 1 | J | 15 | PRO |
| 1 | J | 17 | LEU |
| 1 | J | 20 | SER |
| 1 | J | 22 | LYS |
| 1 | J | 36 | SER |
| 1 | J | 37 | SER |
| 1 | J | 46 | SER |
| 1 | J | 61 | THR |
| 1 | J | 69 | THR |
| 1 | J | 70 | LEU |
| 1 | J | 72 | VAL |
| 1 | J | 73 | LYS |
| 1 | J | 75 | ASP |
| 1 | J | 76 | GLN |
| 1 | J | 97 | LEU |
| 1 | J | 106 | LEU |
| 1 | J | 109 | ARG |
| 1 | J | 114 | MET |
| 1 | J | 117 | THR |
| 1 | J | 121 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | J | 126 | VAL |
| 1 | J | 127 | ASN |
| 1 | J | 135 | TYR |
| 1 | J | 136 | ASN |
| 1 | J | 146 | LYS |
| 1 | J | 149 | GLN |
| 1 | J | 155 | ILE |
| 1 | J | 157 | SER |
| 1 | J | 158 | ILE |
| 1 | J | 159 | SER |
| 1 | J | 165 | PHE |
| 1 | J | 167 | LEU |
| 1 | J | 169 | ASP |
| 1 | J | 173 | GLN |
| 1 | J | 178 | THR |
| 1 | J | 185 | LYS |
| 1 | J | 186 | THR |
| 1 | J | 187 | VAL |
| 1 | J | 189 | THR |
| 1 | J | 191 | ARG |
| 1 | J | 193 | ILE |
| 1 | J | 194 | GLN |
| 1 | J | 198 | THR |
| 1 | J | 199 | ILE |
| 1 | J | 218 | LEU |
| 1 | J | 219 | GLU |
| 1 | J | 221 | GLN |
| 1 | J | 223 | ILE |
| 1 | J | 229 | LEU |
| 1 | J | 244 | SER |
| 1 | J | 245 | ARG |
| 1 | J | 251 | ARG |
| 1 | J | 264 | ASP |
| 1 | J | 273 | SER |
| 1 | J | 274 | ARG |
| 1 | J | 278 | GLN |
| 1 | J | 282 | GLU |
| 1 | J | 287 | ILE |
| 1 | J | 290 | GLN |
| 1 | J | 294 | ASN |
| 1 | J | 298 | GLU |
| 1 | J | 300 | ILE |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | J | 325 | ILE |
| 1 | J | 331 | LEU |
| 1 | J | 336 | SER |
| 1 | J | 351 | ILE |
| 1 | J | 354 | LEU |
| 1 | J | 364 | LEU |
| 1 | J | 365 | LYS |
| 1 | J | 372 | GLU |
| 1 | J | 376 | GLU |
| 1 | J | 381 | GLU |
| 1 | J | 389 | LEU |
| 1 | J | 392 | LEU |
| 1 | J | 394 | SER |
| 1 | J | 399 | LYS |
| 1 | J | 405 | ARG |
| 1 | J | 410 | ASN |
| 1 | J | 439 | LEU |
| 1 | J | 447 | GLN |
| 1 | J | 448 | GLN |
| 1 | J | 449 | LEU |
| 1 | J | 453 | GLN |
| 1 | J | 455 | ARG |
| 1 | J | 457 | TYR |
| 1 | J | 462 | LEU |
| 1 | J | 471 | ASP |
| 1 | J | 474 | SER |
| 1 | J | 480 | ILE |
| 1 | J | 487 | LEU |
| 1 | J | 495 | MET |
| 1 | J | 499 | GLU |
| 1 | J | 506 | GLU |
| 1 | J | 513 | ILE |
| 1 | J | 518 | ASP |
| 1 | J | 524 | GLU |
| 1 | J | 532 | ILE |
| 1 | J | 534 | SER |
| 1 | J | 537 | GLU |
| 1 | J | 543 | PRO |
| 1 | J | 549 | SER |
| 1 | J | 561 | LYS |
| 1 | J | 562 | SER |
| 1 | J | 563 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | J | 569 | LYS |
| 1 | J | 580 | SER |
| 1 | J | 593 | SER |
| 1 | J | 597 | GLU |
| 1 | J | 604 | ASN |
| 1 | J | 608 | ILE |
| 1 | J | 610 | LEU |
| 1 | J | 615 | SER |
| 1 | J | 621 | LEU |
| 1 | J | 625 | THR |
| 1 | J | 664 | LEU |
| 1 | J | 666 | SER |
| 1 | J | 673 | ARG |
| 1 | J | 675 | ILE |
| 1 | J | 676 | ILE |
| 1 | J | 686 | MET |
| 1 | J | 689 | GLU |
| 1 | J | 690 | LEU |
| 1 | J | 693 | HIS |
| 1 | J | 698 | ASN |
| 1 | J | 701 | LEU |
| 1 | J | 702 | GLU |
| 1 | J | 704 | ILE |
| 1 | J | 708 | ARG |
| 1 | J | 713 | SER |
| 1 | J | 714 | ARG |
| 1 | J | 716 | LEU |
| 1 | J | 719 | ASP |
| 1 | J | 722 | GLN |
| 1 | J | 723 | ARG |
| 1 | J | 727 | LEU |
| 1 | J | 728 | ASN |
| 1 | J | 745 | GLU |
| 1 | J | 752 | ASP |
| 1 | J | 753 | VAL |
| 1 | J | 754 | ASP |
| 1 | J | 762 | HIS |
| 1 | J | 774 | LEU |
| 1 | J | 785 | GLU |
| 1 | J | 787 | ILE |
| 1 | J | 793 | ARG |
| 1 | J | 799 | MET |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | J | 802 | GLU |
| 1 | J | 804 | ARG |
| 1 | J | 810 | ARG |
| 1 | J | 816 | ILE |
| 1 | J | 822 | SER |
| 1 | J | 832 | MET |
| 1 | J | 834 | LEU |
| 1 | J | 838 | ILE |
| 1 | J | 842 | LEU |
| 1 | J | 843 | LYS |
| 2 | K | 142 | PRO |
| 3 | L | 48 | LYS |
| 3 | L | 68 | PHE |
| 3 | L | 83 | THR |
| 3 | L | 95 | ASP |
| 3 | L | 96 | LYS |
| 1 | M | 4 | ASP |
| 1 | M | 7 | MET |
| 1 | M | 12 | GLU |
| 1 | M | 15 | PRO |
| 1 | M | 17 | LEU |
| 1 | M | 20 | SER |
| 1 | M | 22 | LYS |
| 1 | M | 36 | SER |
| 1 | M | 37 | SER |
| 1 | M | 46 | SER |
| 1 | M | 61 | THR |
| 1 | M | 69 | THR |
| 1 | M | 70 | LEU |
| 1 | M | 72 | VAL |
| 1 | M | 73 | LYS |
| 1 | M | 75 | ASP |
| 1 | M | 76 | GLN |
| 1 | M | 97 | LEU |
| 1 | M | 106 | LEU |
| 1 | M | 109 | ARG |
| 1 | M | 114 | MET |
| 1 | M | 117 | THR |
| 1 | M | 121 | LEU |
| 1 | M | 126 | VAL |
| 1 | M | 127 | ASN |
| 1 | M | 135 | TYR |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | M | 136 | ASN |
| 1 | M | 146 | LYS |
| 1 | M | 148 | ARG |
| 1 | M | 149 | GLN |
| 1 | M | 155 | ILE |
| 1 | M | 157 | SER |
| 1 | M | 158 | ILE |
| 1 | M | 159 | SER |
| 1 | M | 165 | PHE |
| 1 | M | 167 | LEU |
| 1 | M | 169 | ASP |
| 1 | M | 173 | GLN |
| 1 | M | 178 | THR |
| 1 | M | 185 | LYS |
| 1 | M | 186 | THR |
| 1 | M | 187 | VAL |
| 1 | M | 189 | THR |
| 1 | M | 191 | ARG |
| 1 | M | 193 | ILE |
| 1 | M | 194 | GLN |
| 1 | M | 198 | THR |
| 1 | M | 199 | ILE |
| 1 | M | 218 | LEU |
| 1 | M | 219 | GLU |
| 1 | M | 221 | GLN |
| 1 | M | 223 | ILE |
| 1 | M | 229 | LEU |
| 1 | M | 244 | SER |
| 1 | M | 245 | ARG |
| 1 | M | 251 | ARG |
| 1 | M | 264 | ASP |
| 1 | M | 273 | SER |
| 1 | M | 274 | ARG |
| 1 | M | 278 | GLN |
| 1 | M | 282 | GLU |
| 1 | M | 287 | ILE |
| 1 | M | 290 | GLN |
| 1 | M | 294 | ASN |
| 1 | M | 298 | GLU |
| 1 | M | 300 | ILE |
| 1 | M | 325 | ILE |
| 1 | M | 331 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | M | 336 | SER |
| 1 | M | 351 | ILE |
| 1 | M | 354 | LEU |
| 1 | M | 364 | LEU |
| 1 | M | 365 | LYS |
| 1 | M | 372 | GLU |
| 1 | M | 376 | GLU |
| 1 | M | 381 | GLU |
| 1 | M | 389 | LEU |
| 1 | M | 392 | LEU |
| 1 | M | 394 | SER |
| 1 | M | 399 | LYS |
| 1 | M | 405 | ARG |
| 1 | M | 410 | ASN |
| 1 | M | 439 | LEU |
| 1 | M | 447 | GLN |
| 1 | M | 448 | GLN |
| 1 | M | 449 | LEU |
| 1 | M | 453 | GLN |
| 1 | M | 455 | ARG |
| 1 | M | 457 | TYR |
| 1 | M | 462 | LEU |
| 1 | M | 471 | ASP |
| 1 | M | 474 | SER |
| 1 | M | 480 | ILE |
| 1 | M | 487 | LEU |
| 1 | M | 495 | MET |
| 1 | M | 499 | GLU |
| 1 | M | 506 | GLU |
| 1 | M | 513 | ILE |
| 1 | M | 518 | ASP |
| 1 | M | 524 | GLU |
| 1 | M | 532 | ILE |
| 1 | M | 534 | SER |
| 1 | M | 537 | GLU |
| 1 | M | 543 | PRO |
| 1 | M | 549 | SER |
| 1 | M | 561 | LYS |
| 1 | M | 562 | SER |
| 1 | M | 563 | ASN |
| 1 | M | 569 | LYS |
| 1 | M | 580 | SER |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | M | 593 | SER |
| 1 | M | 597 | GLU |
| 1 | M | 604 | ASN |
| 1 | M | 608 | ILE |
| 1 | M | 610 | LEU |
| 1 | M | 615 | SER |
| 1 | M | 621 | LEU |
| 1 | M | 625 | THR |
| 1 | M | 664 | LEU |
| 1 | M | 666 | SER |
| 1 | M | 673 | ARG |
| 1 | M | 675 | ILE |
| 1 | M | 676 | ILE |
| 1 | M | 686 | MET |
| 1 | M | 689 | GLU |
| 1 | M | 690 | LEU |
| 1 | M | 693 | HIS |
| 1 | M | 698 | ASN |
| 1 | M | 701 | LEU |
| 1 | M | 702 | GLU |
| 1 | M | 708 | ARG |
| 1 | M | 713 | SER |
| 1 | M | 714 | ARG |
| 1 | M | 716 | LEU |
| 1 | M | 719 | ASP |
| 1 | M | 722 | GLN |
| 1 | M | 723 | ARG |
| 1 | M | 727 | LEU |
| 1 | M | 728 | ASN |
| 1 | M | 745 | GLU |
| 1 | M | 752 | ASP |
| 1 | M | 753 | VAL |
| 1 | M | 754 | ASP |
| 1 | M | 762 | HIS |
| 1 | M | 774 | LEU |
| 1 | M | 785 | GLU |
| 1 | M | 787 | ILE |
| 1 | M | 793 | ARG |
| 1 | M | 799 | MET |
| 1 | M | 802 | GLU |
| 1 | M | 804 | ARG |
| 1 | M | 810 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | M | 816 | ILE |
| 1 | M | 822 | SER |
| 1 | M | 832 | MET |
| 1 | M | 834 | LEU |
| 1 | M | 838 | ILE |
| 1 | M | 842 | LEU |
| 1 | M | 843 | LYS |
| 2 | N | 142 | PRO |
| 3 | O | 48 | LYS |
| 3 | O | 68 | PHE |
| 3 | O | 83 | THR |
| 3 | O | 95 | ASP |
| 3 | O | 96 | LYS |
| 1 | P | 4 | ASP |
| 1 | P | 7 | MET |
| 1 | P | 12 | GLU |
| 1 | P | 15 | PRO |
| 1 | P | 17 | LEU |
| 1 | P | 20 | SER |
| 1 | P | 22 | LYS |
| 1 | P | 36 | SER |
| 1 | P | 37 | SER |
| 1 | P | 46 | SER |
| 1 | P | 61 | THR |
| 1 | P | 69 | THR |
| 1 | P | 70 | LEU |
| 1 | P | 72 | VAL |
| 1 | P | 73 | LYS |
| 1 | P | 75 | ASP |
| 1 | P | 76 | GLN |
| 1 | P | 97 | LEU |
| 1 | P | 106 | LEU |
| 1 | P | 109 | ARG |
| 1 | P | 114 | MET |
| 1 | P | 117 | THR |
| 1 | P | 121 | LEU |
| 1 | P | 126 | VAL |
| 1 | P | 127 | ASN |
| 1 | P | 135 | TYR |
| 1 | P | 136 | ASN |
| 1 | P | 146 | LYS |
| 1 | P | 149 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | P | 155 | ILE |
| 1 | P | 157 | SER |
| 1 | P | 158 | ILE |
| 1 | P | 159 | SER |
| 1 | P | 165 | PHE |
| 1 | P | 167 | LEU |
| 1 | P | 169 | ASP |
| 1 | P | 173 | GLN |
| 1 | P | 178 | THR |
| 1 | P | 185 | LYS |
| 1 | P | 186 | THR |
| 1 | P | 187 | VAL |
| 1 | P | 191 | ARG |
| 1 | P | 193 | ILE |
| 1 | P | 194 | GLN |
| 1 | P | 198 | THR |
| 1 | P | 199 | ILE |
| 1 | P | 218 | LEU |
| 1 | P | 219 | GLU |
| 1 | P | 221 | GLN |
| 1 | P | 223 | ILE |
| 1 | P | 229 | LEU |
| 1 | P | 244 | SER |
| 1 | P | 245 | ARG |
| 1 | P | 251 | ARG |
| 1 | P | 264 | ASP |
| 1 | P | 273 | SER |
| 1 | P | 274 | ARG |
| 1 | P | 278 | GLN |
| 1 | P | 282 | GLU |
| 1 | P | 287 | ILE |
| 1 | P | 290 | GLN |
| 1 | P | 294 | ASN |
| 1 | P | 298 | GLU |
| 1 | P | 300 | ILE |
| 1 | P | 325 | ILE |
| 1 | P | 331 | LEU |
| 1 | P | 336 | SER |
| 1 | P | 351 | ILE |
| 1 | P | 354 | LEU |
| 1 | P | 364 | LEU |
| 1 | P | 365 | LYS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | P | 372 | GLU |
| 1 | P | 376 | GLU |
| 1 | P | 381 | GLU |
| 1 | P | 389 | LEU |
| 1 | P | 392 | LEU |
| 1 | P | 394 | SER |
| 1 | P | 399 | LYS |
| 1 | P | 405 | ARG |
| 1 | P | 410 | ASN |
| 1 | P | 439 | LEU |
| 1 | P | 447 | GLN |
| 1 | P | 448 | GLN |
| 1 | P | 449 | LEU |
| 1 | P | 453 | GLN |
| 1 | P | 455 | ARG |
| 1 | P | 457 | TYR |
| 1 | P | 462 | LEU |
| 1 | P | 471 | ASP |
| 1 | P | 474 | SER |
| 1 | P | 480 | ILE |
| 1 | P | 487 | LEU |
| 1 | P | 495 | MET |
| 1 | P | 499 | GLU |
| 1 | P | 506 | GLU |
| 1 | P | 513 | ILE |
| 1 | P | 518 | ASP |
| 1 | P | 524 | GLU |
| 1 | P | 532 | ILE |
| 1 | P | 534 | SER |
| 1 | P | 537 | GLU |
| 1 | P | 543 | PRO |
| 1 | P | 549 | SER |
| 1 | P | 561 | LYS |
| 1 | P | 562 | SER |
| 1 | P | 563 | ASN |
| 1 | P | 569 | LYS |
| 1 | P | 580 | SER |
| 1 | P | 593 | SER |
| 1 | P | 597 | GLU |
| 1 | P | 604 | ASN |
| 1 | P | 608 | ILE |
| 1 | P | 610 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | P | 615 | SER |
| 1 | P | 621 | LEU |
| 1 | P | 625 | THR |
| 1 | P | 664 | LEU |
| 1 | P | 666 | SER |
| 1 | P | 673 | ARG |
| 1 | P | 675 | ILE |
| 1 | P | 676 | ILE |
| 1 | P | 686 | MET |
| 1 | P | 689 | GLU |
| 1 | P | 690 | LEU |
| 1 | P | 693 | HIS |
| 1 | P | 698 | ASN |
| 1 | P | 701 | LEU |
| 1 | P | 702 | GLU |
| 1 | P | 708 | ARG |
| 1 | P | 713 | SER |
| 1 | P | 714 | ARG |
| 1 | P | 716 | LEU |
| 1 | P | 719 | ASP |
| 1 | P | 722 | GLN |
| 1 | P | 723 | ARG |
| 1 | P | 727 | LEU |
| 1 | P | 728 | ASN |
| 1 | P | 745 | GLU |
| 1 | P | 752 | ASP |
| 1 | P | 753 | VAL |
| 1 | P | 754 | ASP |
| 1 | P | 762 | HIS |
| 1 | P | 774 | LEU |
| 1 | P | 785 | GLU |
| 1 | P | 787 | ILE |
| 1 | P | 793 | ARG |
| 1 | P | 799 | MET |
| 1 | P | 802 | GLU |
| 1 | P | 804 | ARG |
| 1 | P | 810 | ARG |
| 1 | P | 816 | ILE |
| 1 | P | 822 | SER |
| 1 | P | 832 | MET |
| 1 | P | 834 | LEU |
| 1 | P | 838 | ILE |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | P | 842 | LEU |
| 1 | P | 843 | LYS |
| 2 | Q | 142 | PRO |
| 3 | R | 48 | LYS |
| 3 | R | 68 | PHE |
| 3 | R | 83 | THR |
| 3 | R | 95 | ASP |
| 3 | R | 96 | LYS |
| 4 | 1 | 16 | LEU |
| 4 | 1 | 33 | SER |
| 4 | 1 | 34 | ILE |
| 4 | 1 | 37 | ARG |
| 4 | 1 | 66 | THR |
| 4 | 1 | 72 | GLU |
| 4 | 1 | 80 | ASP |
| 4 | 1 | 100 | GLU |
| 4 | 1 | 109 | PRO |
| 4 | 1 | 116 | ARG |
| 4 | 1 | 145 | SER |
| 4 | 1 | 153 | LEU |
| 4 | 1 | 159 | VAL |
| 4 | 1 | 180 | LEU |
| 4 | 1 | 191 | LYS |
| 4 | 1 | 196 | ARG |
| 4 | 1 | 199 | SER |
| 4 | 1 | 201 | VAL |
| 4 | 1 | 206 | ARG |
| 4 | 1 | 221 | LEU |
| 4 | 1 | 223 | PHE |
| 4 | 1 | 229 | THR |
| 4 | 1 | 239 | SER |
| 4 | 1 | 242 | LEU |
| 4 | 1 | 246 | GLN |
| 4 | 1 | 263 | GLN |
| 4 | 1 | 281 | SER |
| 4 | 1 | 283 | MET |
| 4 | 1 | 287 | ILE |
| 4 | 1 | 291 | LYS |
| 4 | 1 | 293 | LEU |
| 4 | 1 | 297 | ASN |
| 4 | 1 | 299 | MET |
| 4 | 1 | 312 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4 | 1 | 315 | LYS |
| 4 | 1 | 318 | THR |
| 4 | 1 | 320 | LEU |
| 4 | 1 | 327 | ILE |
| 4 | 1 | 334 | GLU |
| 4 | 1 | 349 | LEU |
| 4 | 1 | 350 | SER |
| 4 | 1 | 351 | THR |
| 4 | 1 | 354 | GLN |
| 4 | 1 | 359 | LYS |
| 4 | 1 | 360 | GLN |
| 4 | 1 | 361 | GLU |
| 4 | 1 | 368 | SER |
| 4 | 2 | 16 | LEU |
| 4 | 2 | 33 | SER |
| 4 | 2 | 34 | ILE |
| 4 | 2 | 37 | ARG |
| 4 | 2 | 66 | THR |
| 4 | 2 | 72 | GLU |
| 4 | 2 | 80 | ASP |
| 4 | 2 | 100 | GLU |
| 4 | 2 | 109 | PRO |
| 4 | 2 | 116 | ARG |
| 4 | 2 | 145 | SER |
| 4 | 2 | 153 | LEU |
| 4 | 2 | 159 | VAL |
| 4 | 2 | 180 | LEU |
| 4 | 2 | 191 | LYS |
| 4 | 2 | 196 | ARG |
| 4 | 2 | 199 | SER |
| 4 | 2 | 201 | VAL |
| 4 | 2 | 206 | ARG |
| 4 | 2 | 221 | LEU |
| 4 | 2 | 223 | PHE |
| 4 | 2 | 229 | THR |
| 4 | 2 | 239 | SER |
| 4 | 2 | 242 | LEU |
| 4 | 2 | 246 | GLN |
| 4 | 2 | 263 | GLN |
| 4 | 2 | 281 | SER |
| 4 | 2 | 283 | MET |
| 4 | 2 | 287 | ILE |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4 | 2 | 291 | LYS |
| 4 | 2 | 293 | LEU |
| 4 | 2 | 297 | ASN |
| 4 | 2 | 299 | MET |
| 4 | 2 | 312 | ARG |
| 4 | 2 | 315 | LYS |
| 4 | 2 | 318 | THR |
| 4 | 2 | 320 | LEU |
| 4 | 2 | 327 | ILE |
| 4 | 2 | 334 | GLU |
| 4 | 2 | 349 | LEU |
| 4 | 2 | 350 | SER |
| 4 | 2 | 351 | THR |
| 4 | 2 | 354 | GLN |
| 4 | 2 | 359 | LYS |
| 4 | 2 | 360 | GLN |
| 4 | 2 | 361 | GLU |
| 4 | 2 | 368 | SER |
| 4 | 3 | 33 | SER |
| 4 | 3 | 34 | ILE |
| 4 | 3 | 37 | ARG |
| 4 | 3 | 66 | THR |
| 4 | 3 | 72 | GLU |
| 4 | 3 | 80 | ASP |
| 4 | 3 | 100 | GLU |
| 4 | 3 | 109 | PRO |
| 4 | 3 | 116 | ARG |
| 4 | 3 | 145 | SER |
| 4 | 3 | 153 | LEU |
| 4 | 3 | 159 | VAL |
| 4 | 3 | 180 | LEU |
| 4 | 3 | 191 | LYS |
| 4 | 3 | 196 | ARG |
| 4 | 3 | 199 | SER |
| 4 | 3 | 201 | VAL |
| 4 | 3 | 206 | ARG |
| 4 | 3 | 221 | LEU |
| 4 | 3 | 223 | PHE |
| 4 | 3 | 229 | THR |
| 4 | 3 | 239 | SER |
| 4 | 3 | 242 | LEU |
| 4 | 3 | 246 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4 | 3 | 263 | GLN |
| 4 | 3 | 281 | SER |
| 4 | 3 | 283 | MET |
| 4 | 3 | 287 | ILE |
| 4 | 3 | 291 | LYS |
| 4 | 3 | 293 | LEU |
| 4 | 3 | 297 | ASN |
| 4 | 3 | 299 | MET |
| 4 | 3 | 312 | ARG |
| 4 | 3 | 315 | LYS |
| 4 | 3 | 318 | THR |
| 4 | 3 | 320 | LEU |
| 4 | 3 | 327 | ILE |
| 4 | 3 | 334 | GLU |
| 4 | 3 | 349 | LEU |
| 4 | 3 | 350 | SER |
| 4 | 3 | 351 | THR |
| 4 | 3 | 354 | GLN |
| 4 | 3 | 359 | LYS |
| 4 | 3 | 360 | GLN |
| 4 | 3 | 361 | GLU |
| 4 | 3 | 368 | SER |
| 4 | 4 | 33 | SER |
| 4 | 4 | 34 | ILE |
| 4 | 4 | 37 | ARG |
| 4 | 4 | 66 | THR |
| 4 | 4 | 72 | GLU |
| 4 | 4 | 80 | ASP |
| 4 | 4 | 100 | GLU |
| 4 | 4 | 109 | PRO |
| 4 | 4 | 116 | ARG |
| 4 | 4 | 145 | SER |
| 4 | 4 | 153 | LEU |
| 4 | 4 | 159 | VAL |
| 4 | 4 | 180 | LEU |
| 4 | 4 | 191 | LYS |
| 4 | 4 | 196 | ARG |
| 4 | 4 | 199 | SER |
| 4 | 4 | 201 | VAL |
| 4 | 4 | 206 | ARG |
| 4 | 4 | 221 | LEU |
| 4 | 4 | 223 | PHE |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4 | 4 | 229 | THR |
| 4 | 4 | 239 | SER |
| 4 | 4 | 242 | LEU |
| 4 | 4 | 246 | GLN |
| 4 | 4 | 263 | GLN |
| 4 | 4 | 281 | SER |
| 4 | 4 | 283 | MET |
| 4 | 4 | 287 | ILE |
| 4 | 4 | 291 | LYS |
| 4 | 4 | 293 | LEU |
| 4 | 4 | 297 | ASN |
| 4 | 4 | 299 | MET |
| 4 | 4 | 312 | ARG |
| 4 | 4 | 315 | LYS |
| 4 | 4 | 318 | THR |
| 4 | 4 | 320 | LEU |
| 4 | 4 | 327 | ILE |
| 4 | 4 | 334 | GLU |
| 4 | 4 | 349 | LEU |
| 4 | 4 | 350 | SER |
| 4 | 4 | 351 | THR |
| 4 | 4 | 354 | GLN |
| 4 | 4 | 359 | LYS |
| 4 | 4 | 360 | GLN |
| 4 | 4 | 361 | GLU |
| 4 | 4 | 368 | SER |
| 4 | 5 | 16 | LEU |
| 4 | 5 | 33 | SER |
| 4 | 5 | 34 | ILE |
| 4 | 5 | 37 | ARG |
| 4 | 5 | 66 | THR |
| 4 | 5 | 72 | GLU |
| 4 | 5 | 80 | ASP |
| 4 | 5 | 100 | GLU |
| 4 | 5 | 109 | PRO |
| 4 | 5 | 116 | ARG |
| 4 | 5 | 145 | SER |
| 4 | 5 | 153 | LEU |
| 4 | 5 | 159 | VAL |
| 4 | 5 | 180 | LEU |
| 4 | 5 | 191 | LYS |
| 4 | 5 | 196 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4 | 5 | 199 | SER |
| 4 | 5 | 201 | VAL |
| 4 | 5 | 206 | ARG |
| 4 | 5 | 221 | LEU |
| 4 | 5 | 223 | PHE |
| 4 | 5 | 229 | THR |
| 4 | 5 | 239 | SER |
| 4 | 5 | 242 | LEU |
| 4 | 5 | 246 | GLN |
| 4 | 5 | 263 | GLN |
| 4 | 5 | 281 | SER |
| 4 | 5 | 283 | MET |
| 4 | 5 | 287 | ILE |
| 4 | 5 | 291 | LYS |
| 4 | 5 | 293 | LEU |
| 4 | 5 | 297 | ASN |
| 4 | 5 | 299 | MET |
| 4 | 5 | 312 | ARG |
| 4 | 5 | 315 | LYS |
| 4 | 5 | 318 | THR |
| 4 | 5 | 320 | LEU |
| 4 | 5 | 327 | ILE |
| 4 | 5 | 334 | GLU |
| 4 | 5 | 349 | LEU |
| 4 | 5 | 350 | SER |
| 4 | 5 | 351 | THR |
| 4 | 5 | 354 | GLN |
| 4 | 5 | 359 | LYS |
| 4 | 5 | 360 | GLN |
| 4 | 5 | 361 | GLU |
| 4 | 5 | 368 | SER |
| 4 | 6 | 16 | LEU |
| 4 | 6 | 33 | SER |
| 4 | 6 | 34 | ILE |
| 4 | 6 | 37 | ARG |
| 4 | 6 | 66 | THR |
| 4 | 6 | 72 | GLU |
| 4 | 6 | 80 | ASP |
| 4 | 6 | 100 | GLU |
| 4 | 6 | 109 | PRO |
| 4 | 6 | 116 | ARG |
| 4 | 6 | 145 | SER |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4 | 6 | 153 | LEU |
| 4 | 6 | 159 | VAL |
| 4 | 6 | 180 | LEU |
| 4 | 6 | 191 | LYS |
| 4 | 6 | 196 | ARG |
| 4 | 6 | 199 | SER |
| 4 | 6 | 201 | VAL |
| 4 | 6 | 206 | ARG |
| 4 | 6 | 221 | LEU |
| 4 | 6 | 223 | PHE |
| 4 | 6 | 229 | THR |
| 4 | 6 | 239 | SER |
| 4 | 6 | 242 | LEU |
| 4 | 6 | 246 | GLN |
| 4 | 6 | 263 | GLN |
| 4 | 6 | 281 | SER |
| 4 | 6 | 283 | MET |
| 4 | 6 | 287 | ILE |
| 4 | 6 | 291 | LYS |
| 4 | 6 | 293 | LEU |
| 4 | 6 | 297 | ASN |
| 4 | 6 | 299 | MET |
| 4 | 6 | 312 | ARG |
| 4 | 6 | 315 | LYS |
| 4 | 6 | 318 | THR |
| 4 | 6 | 320 | LEU |
| 4 | 6 | 327 | ILE |
| 4 | 6 | 334 | GLU |
| 4 | 6 | 349 | LEU |
| 4 | 6 | 350 | SER |
| 4 | 6 | 351 | THR |
| 4 | 6 | 354 | GLN |
| 4 | 6 | 359 | LYS |
| 4 | 6 | 360 | GLN |
| 4 | 6 | 361 | GLU |
| 4 | 6 | 368 | SER |
| 4 | 7 | 33 | SER |
| 4 | 7 | 34 | ILE |
| 4 | 7 | 37 | ARG |
| 4 | 7 | 66 | THR |
| 4 | 7 | 72 | GLU |
| 4 | 7 | 80 | ASP |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4 | 7 | 100 | GLU |
| 4 | 7 | 109 | PRO |
| 4 | 7 | 116 | ARG |
| 4 | 7 | 145 | SER |
| 4 | 7 | 153 | LEU |
| 4 | 7 | 159 | VAL |
| 4 | 7 | 180 | LEU |
| 4 | 7 | 191 | LYS |
| 4 | 7 | 196 | ARG |
| 4 | 7 | 199 | SER |
| 4 | 7 | 201 | VAL |
| 4 | 7 | 206 | ARG |
| 4 | 7 | 221 | LEU |
| 4 | 7 | 223 | PHE |
| 4 | 7 | 229 | THR |
| 4 | 7 | 239 | SER |
| 4 | 7 | 242 | LEU |
| 4 | 7 | 246 | GLN |
| 4 | 7 | 263 | GLN |
| 4 | 7 | 281 | SER |
| 4 | 7 | 283 | MET |
| 4 | 7 | 287 | ILE |
| 4 | 7 | 291 | LYS |
| 4 | 7 | 293 | LEU |
| 4 | 7 | 297 | ASN |
| 4 | 7 | 299 | MET |
| 4 | 7 | 312 | ARG |
| 4 | 7 | 315 | LYS |
| 4 | 7 | 318 | THR |
| 4 | 7 | 320 | LEU |
| 4 | 7 | 327 | ILE |
| 4 | 7 | 334 | GLU |
| 4 | 7 | 349 | LEU |
| 4 | 7 | 350 | SER |
| 4 | 7 | 351 | THR |
| 4 | 7 | 354 | GLN |
| 4 | 7 | 359 | LYS |
| 4 | 7 | 360 | GLN |
| 4 | 7 | 361 | GLU |
| 4 | 7 | 368 | SER |
| 4 | 8 | 33 | SER |
| 4 | 8 | 34 | ILE |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4 | 8 | 37 | ARG |
| 4 | 8 | 66 | THR |
| 4 | 8 | 72 | GLU |
| 4 | 8 | 80 | ASP |
| 4 | 8 | 100 | GLU |
| 4 | 8 | 109 | PRO |
| 4 | 8 | 116 | ARG |
| 4 | 8 | 145 | SER |
| 4 | 8 | 153 | LEU |
| 4 | 8 | 159 | VAL |
| 4 | 8 | 180 | LEU |
| 4 | 8 | 191 | LYS |
| 4 | 8 | 196 | ARG |
| 4 | 8 | 199 | SER |
| 4 | 8 | 201 | VAL |
| 4 | 8 | 206 | ARG |
| 4 | 8 | 221 | LEU |
| 4 | 8 | 223 | PHE |
| 4 | 8 | 229 | THR |
| 4 | 8 | 239 | SER |
| 4 | 8 | 242 | LEU |
| 4 | 8 | 246 | GLN |
| 4 | 8 | 263 | GLN |
| 4 | 8 | 281 | SER |
| 4 | 8 | 283 | MET |
| 4 | 8 | 287 | ILE |
| 4 | 8 | 291 | LYS |
| 4 | 8 | 293 | LEU |
| 4 | 8 | 297 | ASN |
| 4 | 8 | 299 | MET |
| 4 | 8 | 312 | ARG |
| 4 | 8 | 315 | LYS |
| 4 | 8 | 318 | THR |
| 4 | 8 | 320 | LEU |
| 4 | 8 | 327 | ILE |
| 4 | 8 | 334 | GLU |
| 4 | 8 | 349 | LEU |
| 4 | 8 | 350 | SER |
| 4 | 8 | 351 | THR |
| 4 | 8 | 354 | GLN |
| 4 | 8 | 359 | LYS |
| 4 | 8 | 360 | GLN |

Continued on next page...

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4 | 8 | 361 | GLU |
| 4 | 8 | 368 | SER |
| 4 | 9 | 16 | LEU |
| 4 | 9 | 33 | SER |
| 4 | 9 | 34 | ILE |
| 4 | 9 | 37 | ARG |
| 4 | 9 | 66 | THR |
| 4 | 9 | 72 | GLU |
| 4 | 9 | 80 | ASP |
| 4 | 9 | 100 | GLU |
| 4 | 9 | 109 | PRO |
| 4 | 9 | 116 | ARG |
| 4 | 9 | 145 | SER |
| 4 | 9 | 153 | LEU |
| 4 | 9 | 159 | VAL |
| 4 | 9 | 180 | LEU |
| 4 | 9 | 191 | LYS |
| 4 | 9 | 196 | ARG |
| 4 | 9 | 199 | SER |
| 4 | 9 | 201 | VAL |
| 4 | 9 | 206 | ARG |
| 4 | 9 | 221 | LEU |
| 4 | 9 | 223 | PHE |
| 4 | 9 | 229 | THR |
| 4 | 9 | 239 | SER |
| 4 | 9 | 242 | LEU |
| 4 | 9 | 246 | GLN |
| 4 | 9 | 263 | GLN |
| 4 | 9 | 281 | SER |
| 4 | 9 | 283 | MET |
| 4 | 9 | 287 | ILE |
| 4 | 9 | 291 | LYS |
| 4 | 9 | 293 | LEU |
| 4 | 9 | 297 | ASN |
| 4 | 9 | 299 | MET |
| 4 | 9 | 312 | ARG |
| 4 | 9 | 315 | LYS |
| 4 | 9 | 318 | THR |
| 4 | 9 | 320 | LEU |
| 4 | 9 | 327 | ILE |
| 4 | 9 | 334 | GLU |
| 4 | 9 | 349 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4 | 9 | 350 | SER |
| 4 | 9 | 351 | THR |
| 4 | 9 | 354 | GLN |
| 4 | 9 | 359 | LYS |
| 4 | 9 | 360 | GLN |
| 4 | 9 | 361 | GLU |
| 4 | 9 | 368 | SER |
| 4 | V | 16 | LEU |
| 4 | V | 33 | SER |
| 4 | V | 34 | ILE |
| 4 | V | 37 | ARG |
| 4 | V | 66 | THR |
| 4 | V | 72 | GLU |
| 4 | V | 80 | ASP |
| 4 | V | 100 | GLU |
| 4 | V | 109 | PRO |
| 4 | V | 116 | ARG |
| 4 | V | 145 | SER |
| 4 | V | 153 | LEU |
| 4 | V | 159 | VAL |
| 4 | V | 180 | LEU |
| 4 | V | 191 | LYS |
| 4 | V | 196 | ARG |
| 4 | V | 199 | SER |
| 4 | V | 201 | VAL |
| 4 | V | 206 | ARG |
| 4 | V | 221 | LEU |
| 4 | V | 223 | PHE |
| 4 | V | 229 | THR |
| 4 | V | 239 | SER |
| 4 | V | 242 | LEU |
| 4 | V | 246 | GLN |
| 4 | V | 263 | GLN |
| 4 | V | 281 | SER |
| 4 | V | 283 | MET |
| 4 | V | 287 | ILE |
| 4 | V | 291 | LYS |
| 4 | V | 293 | LEU |
| 4 | V | 297 | ASN |
| 4 | V | 299 | MET |
| 4 | V | 312 | ARG |
| 4 | V | 315 | LYS |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4 | V | 318 | THR |
| 4 | V | 320 | LEU |
| 4 | V | 327 | ILE |
| 4 | V | 334 | GLU |
| 4 | V | 349 | LEU |
| 4 | V | 350 | SER |
| 4 | V | 351 | THR |
| 4 | V | 354 | GLN |
| 4 | V | 359 | LYS |
| 4 | V | 360 | GLN |
| 4 | V | 361 | GLU |
| 4 | V | 368 | SER |
| 4 | W | 33 | SER |
| 4 | W | 34 | ILE |
| 4 | W | 37 | ARG |
| 4 | W | 66 | THR |
| 4 | W | 72 | GLU |
| 4 | W | 80 | ASP |
| 4 | W | 100 | GLU |
| 4 | W | 109 | PRO |
| 4 | W | 116 | ARG |
| 4 | W | 145 | SER |
| 4 | W | 153 | LEU |
| 4 | W | 159 | VAL |
| 4 | W | 180 | LEU |
| 4 | W | 191 | LYS |
| 4 | W | 196 | ARG |
| 4 | W | 199 | SER |
| 4 | W | 201 | VAL |
| 4 | W | 206 | ARG |
| 4 | W | 221 | LEU |
| 4 | W | 223 | PHE |
| 4 | W | 229 | THR |
| 4 | W | 239 | SER |
| 4 | W | 242 | LEU |
| 4 | W | 246 | GLN |
| 4 | W | 263 | GLN |
| 4 | W | 281 | SER |
| 4 | W | 283 | MET |
| 4 | W | 287 | ILE |
| 4 | W | 291 | LYS |
| 4 | W | 293 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4 | W | 297 | ASN |
| 4 | W | 299 | MET |
| 4 | W | 312 | ARG |
| 4 | W | 315 | LYS |
| 4 | W | 318 | THR |
| 4 | W | 320 | LEU |
| 4 | W | 327 | ILE |
| 4 | W | 334 | GLU |
| 4 | W | 349 | LEU |
| 4 | W | 350 | SER |
| 4 | W | 351 | THR |
| 4 | W | 354 | GLN |
| 4 | W | 359 | LYS |
| 4 | W | 360 | GLN |
| 4 | W | 361 | GLU |
| 4 | W | 368 | SER |
| 4 | X | 33 | SER |
| 4 | X | 34 | ILE |
| 4 | X | 37 | ARG |
| 4 | X | 66 | THR |
| 4 | X | 72 | GLU |
| 4 | X | 80 | ASP |
| 4 | X | 100 | GLU |
| 4 | X | 109 | PRO |
| 4 | X | 116 | ARG |
| 4 | X | 145 | SER |
| 4 | X | 153 | LEU |
| 4 | X | 159 | VAL |
| 4 | X | 180 | LEU |
| 4 | X | 191 | LYS |
| 4 | X | 196 | ARG |
| 4 | X | 199 | SER |
| 4 | X | 201 | VAL |
| 4 | X | 206 | ARG |
| 4 | X | 221 | LEU |
| 4 | X | 223 | PHE |
| 4 | X | 229 | THR |
| 4 | X | 239 | SER |
| 4 | X | 242 | LEU |
| 4 | X | 246 | GLN |
| 4 | X | 263 | GLN |
| 4 | X | 281 | SER |

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Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4 | X | 283 | MET |
| 4 | X | 287 | ILE |
| 4 | X | 291 | LYS |
| 4 | X | 293 | LEU |
| 4 | X | 297 | ASN |
| 4 | X | 299 | MET |
| 4 | X | 312 | ARG |
| 4 | X | 315 | LYS |
| 4 | X | 318 | THR |
| 4 | X | 320 | LEU |
| 4 | X | 327 | ILE |
| 4 | X | 334 | GLU |
| 4 | X | 349 | LEU |
| 4 | X | 350 | SER |
| 4 | X | 351 | THR |
| 4 | X | 354 | GLN |
| 4 | X | 359 | LYS |
| 4 | X | 360 | GLN |
| 4 | X | 361 | GLU |
| 4 | X | 368 | SER |
| 4 | Y | 16 | LEU |
| 4 | Y | 33 | SER |
| 4 | Y | 34 | ILE |
| 4 | Y | 37 | ARG |
| 4 | Y | 66 | THR |
| 4 | Y | 72 | GLU |
| 4 | Y | 80 | ASP |
| 4 | Y | 100 | GLU |
| 4 | Y | 109 | PRO |
| 4 | Y | 116 | ARG |
| 4 | Y | 145 | SER |
| 4 | Y | 153 | LEU |
| 4 | Y | 159 | VAL |
| 4 | Y | 180 | LEU |
| 4 | Y | 191 | LYS |
| 4 | Y | 196 | ARG |
| 4 | Y | 199 | SER |
| 4 | Y | 201 | VAL |
| 4 | Y | 206 | ARG |
| 4 | Y | 221 | LEU |
| 4 | Y | 223 | PHE |
| 4 | Y | 229 | THR |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4 | Y | 239 | SER |
| 4 | Y | 242 | LEU |
| 4 | Y | 246 | GLN |
| 4 | Y | 263 | GLN |
| 4 | Y | 281 | SER |
| 4 | Y | 283 | MET |
| 4 | Y | 287 | ILE |
| 4 | Y | 291 | LYS |
| 4 | Y | 293 | LEU |
| 4 | Y | 297 | ASN |
| 4 | Y | 299 | MET |
| 4 | Y | 312 | ARG |
| 4 | Y | 315 | LYS |
| 4 | Y | 318 | THR |
| 4 | Y | 320 | LEU |
| 4 | Y | 327 | ILE |
| 4 | Y | 334 | GLU |
| 4 | Y | 349 | LEU |
| 4 | Y | 350 | SER |
| 4 | Y | 351 | THR |
| 4 | Y | 354 | GLN |
| 4 | Y | 359 | LYS |
| 4 | Y | 360 | GLN |
| 4 | Y | 361 | GLU |
| 4 | Y | 368 | SER |
| 4 | Z | 33 | SER |
| 4 | Z | 34 | ILE |
| 4 | Z | 37 | ARG |
| 4 | Z | 66 | THR |
| 4 | Z | 72 | GLU |
| 4 | Z | 80 | ASP |
| 4 | Z | 100 | GLU |
| 4 | Z | 109 | PRO |
| 4 | Z | 116 | ARG |
| 4 | Z | 145 | SER |
| 4 | Z | 153 | LEU |
| 4 | Z | 159 | VAL |
| 4 | Z | 180 | LEU |
| 4 | Z | 191 | LYS |
| 4 | Z | 196 | ARG |
| 4 | Z | 199 | SER |
| 4 | Z | 201 | VAL |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4 | Z | 206 | ARG |
| 4 | Z | 221 | LEU |
| 4 | Z | 223 | PHE |
| 4 | Z | 229 | THR |
| 4 | Z | 239 | SER |
| 4 | Z | 242 | LEU |
| 4 | Z | 246 | GLN |
| 4 | Z | 263 | GLN |
| 4 | Z | 281 | SER |
| 4 | Z | 283 | MET |
| 4 | Z | 287 | ILE |
| 4 | Z | 291 | LYS |
| 4 | Z | 293 | LEU |
| 4 | Z | 297 | ASN |
| 4 | Z | 299 | MET |
| 4 | Z | 312 | ARG |
| 4 | Z | 315 | LYS |
| 4 | Z | 318 | THR |
| 4 | Z | 320 | LEU |
| 4 | Z | 327 | ILE |
| 4 | Z | 334 | GLU |
| 4 | Z | 349 | LEU |
| 4 | Z | 350 | SER |
| 4 | Z | 351 | THR |
| 4 | Z | 354 | GLN |
| 4 | Z | 359 | LYS |
| 4 | Z | 360 | GLN |
| 4 | Z | 361 | GLU |
| 4 | Z | 368 | SER |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (231) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 28 | GLN |
| 1 | A | 29 | ASN |
| 1 | A | 127 | ASN |
| 1 | A | 164 | GLN |
| 1 | A | 188 | ASN |
| 1 | A | 194 | GLN |
| 1 | A | 221 | GLN |
| 1 | A | 253 | HIS |
| 1 | A | 290 | GLN |

Continued on next page...

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 368 | GLN |
| 1 | A | 424 | ASN |
| 1 | A | 447 | GLN |
| 1 | A | 453 | GLN |
| 1 | A | 481 | ASN |
| 1 | A | 484 | ASN |
| 1 | A | 563 | ASN |
| 1 | A | 564 | ASN |
| 1 | A | 578 | HIS |
| 1 | A | 612 | GLN |
| 1 | A | 656 | ASN |
| 1 | A | 670 | HIS |
| 1 | A | 757 | GLN |
| 1 | A | 762 | HIS |
| 1 | A | 791 | GLN |
| 2 | B | 159 | HIS |
| 3 | C | 52 | ASN |
| 1 | D | 29 | ASN |
| 1 | D | 127 | ASN |
| 1 | D | 149 | GLN |
| 1 | D | 164 | GLN |
| 1 | D | 188 | ASN |
| 1 | D | 194 | GLN |
| 1 | D | 221 | GLN |
| 1 | D | 253 | HIS |
| 1 | D | 290 | GLN |
| 1 | D | 368 | GLN |
| 1 | D | 424 | ASN |
| 1 | D | 447 | GLN |
| 1 | D | 453 | GLN |
| 1 | D | 481 | ASN |
| 1 | D | 484 | ASN |
| 1 | D | 563 | ASN |
| 1 | D | 564 | ASN |
| 1 | D | 578 | HIS |
| 1 | D | 612 | GLN |
| 1 | D | 656 | ASN |
| 1 | D | 670 | HIS |
| 1 | D | 698 | ASN |
| 1 | D | 757 | GLN |
| 1 | D | 762 | HIS |
| 3 | F | 40 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3 | F | 52 | ASN |
| 1 | G | 29 | ASN |
| 1 | G | 127 | ASN |
| 1 | G | 149 | GLN |
| 1 | G | 164 | GLN |
| 1 | G | 188 | ASN |
| 1 | G | 194 | GLN |
| 1 | G | 221 | GLN |
| 1 | G | 253 | HIS |
| 1 | G | 290 | GLN |
| 1 | G | 368 | GLN |
| 1 | G | 424 | ASN |
| 1 | G | 447 | GLN |
| 1 | G | 453 | GLN |
| 1 | G | 481 | ASN |
| 1 | G | 484 | ASN |
| 1 | G | 563 | ASN |
| 1 | G | 564 | ASN |
| 1 | G | 578 | HIS |
| 1 | G | 612 | GLN |
| 1 | G | 656 | ASN |
| 1 | G | 670 | HIS |
| 1 | G | 698 | ASN |
| 1 | G | 791 | GLN |
| 3 | I | 39 | GLN |
| 3 | I | 52 | ASN |
| 1 | J | 29 | ASN |
| 1 | J | 127 | ASN |
| 1 | J | 164 | GLN |
| 1 | J | 188 | ASN |
| 1 | J | 194 | GLN |
| 1 | J | 221 | GLN |
| 1 | J | 253 | HIS |
| 1 | J | 290 | GLN |
| 1 | J | 368 | GLN |
| 1 | J | 424 | ASN |
| 1 | J | 447 | GLN |
| 1 | J | 453 | GLN |
| 1 | J | 481 | ASN |
| 1 | J | 484 | ASN |
| 1 | J | 563 | ASN |
| 1 | J | 564 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | J | 578 | HIS |
| 1 | J | 612 | GLN |
| 1 | J | 656 | ASN |
| 1 | J | 670 | HIS |
| 1 | J | 698 | ASN |
| 1 | J | 722 | GLN |
| 1 | J | 762 | HIS |
| 1 | J | 791 | GLN |
| 2 | K | 159 | HIS |
| 3 | L | 39 | GLN |
| 3 | L | 40 | ASN |
| 3 | L | 52 | ASN |
| 1 | M | 29 | ASN |
| 1 | M | 127 | ASN |
| 1 | M | 149 | GLN |
| 1 | M | 164 | GLN |
| 1 | M | 188 | ASN |
| 1 | M | 194 | GLN |
| 1 | M | 221 | GLN |
| 1 | M | 253 | HIS |
| 1 | M | 290 | GLN |
| 1 | M | 368 | GLN |
| 1 | M | 424 | ASN |
| 1 | M | 453 | GLN |
| 1 | M | 481 | ASN |
| 1 | M | 484 | ASN |
| 1 | M | 563 | ASN |
| 1 | M | 564 | ASN |
| 1 | M | 578 | HIS |
| 1 | M | 612 | GLN |
| 1 | M | 656 | ASN |
| 1 | M | 670 | HIS |
| 1 | M | 757 | GLN |
| 1 | M | 762 | HIS |
| 2 | N | 159 | HIS |
| 3 | O | 39 | GLN |
| 3 | O | 52 | ASN |
| 1 | P | 127 | ASN |
| 1 | P | 164 | GLN |
| 1 | P | 188 | ASN |
| 1 | P | 194 | GLN |
| 1 | P | 221 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | P | 253 | HIS |
| 1 | P | 290 | GLN |
| 1 | P | 368 | GLN |
| 1 | P | 424 | ASN |
| 1 | P | 447 | GLN |
| 1 | P | 453 | GLN |
| 1 | P | 481 | ASN |
| 1 | P | 484 | ASN |
| 1 | P | 563 | ASN |
| 1 | P | 564 | ASN |
| 1 | P | 578 | HIS |
| 1 | P | 612 | GLN |
| 1 | P | 656 | ASN |
| 1 | P | 670 | HIS |
| 1 | P | 757 | GLN |
| 1 | P | 791 | GLN |
| 2 | Q | 159 | HIS |
| 3 | R | 39 | GLN |
| 3 | R | 52 | ASN |
| 4 | 1 | 41 | GLN |
| 4 | 1 | 92 | ASN |
| 4 | 1 | 137 | GLN |
| 4 | 1 | 252 | ASN |
| 4 | 1 | 263 | GLN |
| 4 | 2 | 92 | ASN |
| 4 | 2 | 137 | GLN |
| 4 | 2 | 252 | ASN |
| 4 | 2 | 263 | GLN |
| 4 | 2 | 354 | GLN |
| 4 | 3 | 49 | GLN |
| 4 | 3 | 92 | ASN |
| 4 | 3 | 137 | GLN |
| 4 | 3 | 252 | ASN |
| 4 | 3 | 263 | GLN |
| 4 | 3 | 354 | GLN |
| 4 | 4 | 41 | GLN |
| 4 | 4 | 92 | ASN |
| 4 | 4 | 137 | GLN |
| 4 | 4 | 252 | ASN |
| 4 | 4 | 263 | GLN |
| 4 | 4 | 354 | GLN |
| 4 | 5 | 41 | GLN |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4 | 5 | 92 | ASN |
| 4 | 5 | 137 | GLN |
| 4 | 5 | 252 | ASN |
| 4 | 5 | 263 | GLN |
| 4 | 5 | 354 | GLN |
| 4 | 6 | 41 | GLN |
| 4 | 6 | 92 | ASN |
| 4 | 6 | 137 | GLN |
| 4 | 6 | 252 | ASN |
| 4 | 6 | 263 | GLN |
| 4 | 6 | 354 | GLN |
| 4 | 7 | 41 | GLN |
| 4 | 7 | 92 | ASN |
| 4 | 7 | 137 | GLN |
| 4 | 7 | 252 | ASN |
| 4 | 7 | 263 | GLN |
| 4 | 7 | 354 | GLN |
| 4 | 8 | 41 | GLN |
| 4 | 8 | 92 | ASN |
| 4 | 8 | 137 | GLN |
| 4 | 8 | 252 | ASN |
| 4 | 8 | 263 | GLN |
| 4 | 9 | 41 | GLN |
| 4 | 9 | 92 | ASN |
| 4 | 9 | 137 | GLN |
| 4 | 9 | 252 | ASN |
| 4 | 9 | 263 | GLN |
| 4 | V | 41 | GLN |
| 4 | V | 92 | ASN |
| 4 | V | 137 | GLN |
| 4 | V | 252 | ASN |
| 4 | V | 263 | GLN |
| 4 | W | 41 | GLN |
| 4 | W | 92 | ASN |
| 4 | W | 137 | GLN |
| 4 | W | 252 | ASN |
| 4 | W | 263 | GLN |
| 4 | X | 41 | GLN |
| 4 | X | 92 | ASN |
| 4 | X | 137 | GLN |
| 4 | X | 252 | ASN |
| 4 | X | 263 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4 | X | 354 | GLN |
| 4 | Y | 41 | GLN |
| 4 | Y | 92 | ASN |
| 4 | Y | 137 | GLN |
| 4 | Y | 252 | ASN |
| 4 | Y | 263 | GLN |
| 4 | Y | 354 | GLN |
| 4 | Z | 41 | GLN |
| 4 | Z | 92 | ASN |
| 4 | Z | 137 | GLN |
| 4 | Z | 252 | ASN |
| 4 | Z | 263 | GLN |

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

270 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|-------------|-------------|------|-------------|
| | | | | | Counts | RMSZ | $\# Z > 2$ | Counts | RMSZ | $\# Z > 2$ |
| 1 | MLY | A | 348 | 1 | 9,10,11 | 0.85 | 0 | 6,11,13 | 0.48 | 0 |
| 1 | MLY | G | 49 | 1 | 9,10,11 | 1.07 | 1 (11%) | 6,11,13 | 0.73 | 0 |
| 1 | MLY | D | 130 | 1 | 9,10,11 | 0.79 | 0 | 6,11,13 | 0.74 | 0 |
| 1 | MLY | M | 385 | 1 | 9,10,11 | 1.03 | 1 (11%) | 6,11,13 | 0.44 | 0 |
| 1 | MLY | M | 190 | 1 | 9,10,11 | 1.24 | 1 (11%) | 6,11,13 | 0.52 | 0 |
| 1 | MLY | G | 833 | 1 | 9,10,11 | 1.16 | 1 (11%) | 6,11,13 | 0.32 | 0 |
| 1 | MLY | D | 353 | 1 | 9,10,11 | 0.86 | 0 | 6,11,13 | 0.79 | 0 |
| 1 | MLY | J | 35 | 1 | 9,10,11 | 0.71 | 0 | 6,11,13 | 0.38 | 0 |
| 1 | MLY | D | 553 | 4,1 | 9,10,11 | 0.69 | 0 | 6,11,13 | 0.55 | 0 |
| 1 | MLY | M | 107 | 1 | 9,10,11 | 0.49 | 0 | 6,11,13 | 0.35 | 0 |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 1 | MLY | J | 504 | 1 | 9,10,11 | 0.85 | 0 | 6,11,13 | 0.23 | 0 |
| 1 | MLY | D | 551 | 1 | 9,10,11 | 0.54 | 0 | 6,11,13 | 0.19 | 0 |
| 1 | MLY | D | 107 | 1 | 9,10,11 | 0.51 | 0 | 6,11,13 | 0.34 | 0 |
| 1 | MLY | M | 59 | 1 | 9,10,11 | 0.88 | 0 | 6,11,13 | 0.49 | 0 |
| 1 | MLY | A | 248 | 1 | 9,10,11 | 0.82 | 0 | 6,11,13 | 0.60 | 0 |
| 1 | MLY | D | 613 | 1 | 9,10,11 | 0.57 | 0 | 6,11,13 | 0.64 | 0 |
| 1 | MLY | J | 138 | 1 | 9,10,11 | 1.32 | 1 (11%) | 6,11,13 | 0.83 | 0 |
| 1 | MLY | G | 600 | 1 | 9,10,11 | 0.52 | 0 | 6,11,13 | 0.37 | 0 |
| 1 | MLY | P | 107 | 1 | 9,10,11 | 0.48 | 0 | 6,11,13 | 0.34 | 0 |
| 1 | MLY | P | 659 | 1 | 9,10,11 | 0.85 | 0 | 6,11,13 | 0.58 | 0 |
| 1 | MLY | J | 415 | 1 | 9,10,11 | 0.77 | 0 | 6,11,13 | 0.19 | 0 |
| 1 | MLY | M | 659 | 1 | 9,10,11 | 0.82 | 0 | 6,11,13 | 0.57 | 0 |
| 1 | MLY | J | 431 | 1 | 9,10,11 | 0.53 | 0 | 6,11,13 | 0.45 | 0 |
| 1 | MLY | J | 839 | 1 | 9,10,11 | 0.69 | 0 | 6,11,13 | 0.75 | 0 |
| 1 | MLY | D | 659 | 1 | 9,10,11 | 0.83 | 0 | 6,11,13 | 0.59 | 0 |
| 1 | MLY | A | 353 | 1 | 9,10,11 | 0.87 | 0 | 6,11,13 | 0.79 | 0 |
| 1 | MLY | G | 681 | 1 | 9,10,11 | 0.64 | 0 | 6,11,13 | 0.46 | 0 |
| 1 | MLY | P | 681 | 1 | 9,10,11 | 0.61 | 0 | 6,11,13 | 0.46 | 0 |
| 1 | MLY | P | 839 | 1 | 9,10,11 | 0.69 | 0 | 6,11,13 | 0.75 | 0 |
| 1 | MLY | J | 837 | 1 | 9,10,11 | 0.59 | 0 | 6,11,13 | 0.55 | 0 |
| 1 | MLY | A | 35 | 1 | 9,10,11 | 0.71 | 0 | 6,11,13 | 0.38 | 0 |
| 1 | MLY | A | 617 | 1 | 9,10,11 | 0.94 | 1 (11%) | 6,11,13 | 0.34 | 0 |
| 1 | MLY | G | 84 | 1 | 9,10,11 | 0.49 | 0 | 6,11,13 | 0.80 | 0 |
| 1 | MLY | J | 49 | 1 | 9,10,11 | 1.09 | 1 (11%) | 6,11,13 | 0.75 | 0 |
| 1 | MLY | D | 30 | 1 | 9,10,11 | 0.92 | 0 | 6,11,13 | 0.32 | 0 |
| 1 | MLY | A | 190 | 1 | 9,10,11 | 1.25 | 1 (11%) | 6,11,13 | 0.50 | 0 |
| 1 | MLY | A | 837 | 1 | 9,10,11 | 0.59 | 0 | 6,11,13 | 0.55 | 0 |
| 1 | MLY | A | 504 | 1 | 9,10,11 | 0.89 | 0 | 6,11,13 | 0.25 | 0 |
| 1 | MLY | D | 296 | 1 | 9,10,11 | 0.65 | 0 | 6,11,13 | 0.37 | 0 |
| 1 | MLY | J | 833 | 1 | 9,10,11 | 1.15 | 1 (11%) | 6,11,13 | 0.31 | 0 |
| 1 | MLY | P | 49 | 1 | 9,10,11 | 1.10 | 1 (11%) | 6,11,13 | 0.76 | 0 |
| 1 | MLY | G | 130 | 1 | 9,10,11 | 0.77 | 0 | 6,11,13 | 0.76 | 0 |
| 1 | MLY | M | 236 | 1 | 9,10,11 | 0.81 | 1 (11%) | 6,11,13 | 0.47 | 0 |
| 1 | MLY | G | 528 | 1 | 9,10,11 | 0.90 | 0 | 6,11,13 | 0.66 | 0 |
| 1 | MLY | P | 782 | 1 | 9,10,11 | 0.77 | 0 | 6,11,13 | 0.37 | 0 |
| 1 | MLY | D | 190 | 1 | 9,10,11 | 1.21 | 1 (11%) | 6,11,13 | 0.54 | 0 |
| 1 | MLY | M | 768 | 1 | 9,10,11 | 0.78 | 0 | 6,11,13 | 0.43 | 0 |
| 1 | MLY | G | 295 | 1 | 9,10,11 | 0.78 | 0 | 6,11,13 | 0.34 | 0 |
| 1 | MLY | G | 551 | 1 | 9,10,11 | 0.54 | 0 | 6,11,13 | 0.20 | 0 |
| 1 | MLY | A | 839 | 1 | 9,10,11 | 0.68 | 0 | 6,11,13 | 0.81 | 0 |
| 1 | MLY | P | 236 | 1 | 9,10,11 | 0.80 | 1 (11%) | 6,11,13 | 0.48 | 0 |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 1 | MLY | G | 107 | 1 | 9,10,11 | 0.48 | 0 | 6,11,13 | 0.35 | 0 |
| 1 | MLY | D | 782 | 1 | 9,10,11 | 0.78 | 0 | 6,11,13 | 0.34 | 0 |
| 1 | MLY | D | 598 | 1 | 9,10,11 | 0.88 | 1 (11%) | 6,11,13 | 0.43 | 0 |
| 1 | MLY | M | 87 | 1 | 9,10,11 | 1.21 | 1 (11%) | 6,11,13 | 0.44 | 0 |
| 1 | MLY | G | 367 | 1 | 9,10,11 | 0.65 | 0 | 6,11,13 | 0.38 | 0 |
| 1 | MLY | J | 681 | 1 | 9,10,11 | 0.60 | 0 | 6,11,13 | 0.46 | 0 |
| 1 | MLY | P | 35 | 1 | 9,10,11 | 0.71 | 0 | 6,11,13 | 0.38 | 0 |
| 1 | MLY | P | 385 | 1 | 9,10,11 | 1.00 | 1 (11%) | 6,11,13 | 0.44 | 0 |
| 1 | MLY | G | 617 | 1 | 9,10,11 | 0.95 | 1 (11%) | 6,11,13 | 0.35 | 0 |
| 1 | MLY | A | 49 | 1 | 9,10,11 | 1.03 | 1 (11%) | 6,11,13 | 0.73 | 0 |
| 1 | MLY | M | 348 | 1 | 9,10,11 | 0.81 | 0 | 6,11,13 | 0.47 | 0 |
| 1 | MLY | D | 63 | 1 | 9,10,11 | 0.90 | 0 | 6,11,13 | 0.45 | 0 |
| 1 | MLY | D | 248 | 1 | 9,10,11 | 0.84 | 0 | 6,11,13 | 0.62 | 0 |
| 1 | MLY | J | 63 | 1 | 9,10,11 | 0.88 | 0 | 6,11,13 | 0.42 | 0 |
| 1 | MLY | A | 436 | 1 | 9,10,11 | 1.03 | 1 (11%) | 6,11,13 | 0.47 | 0 |
| 1 | MLY | D | 385 | 1 | 9,10,11 | 0.98 | 1 (11%) | 6,11,13 | 0.45 | 0 |
| 1 | MLY | D | 764 | 1 | 9,10,11 | 0.85 | 0 | 6,11,13 | 0.37 | 0 |
| 1 | MLY | J | 84 | 1 | 9,10,11 | 0.49 | 0 | 6,11,13 | 0.81 | 0 |
| 1 | MLY | P | 55 | 1 | 9,10,11 | 0.72 | 0 | 6,11,13 | 0.78 | 0 |
| 1 | MLY | P | 837 | 1 | 9,10,11 | 0.59 | 0 | 6,11,13 | 0.55 | 0 |
| 1 | MLY | G | 369 | 1 | 9,10,11 | 0.71 | 0 | 6,11,13 | 0.46 | 0 |
| 1 | MLY | J | 436 | 1 | 9,10,11 | 1.06 | 1 (11%) | 6,11,13 | 0.50 | 0 |
| 1 | MLY | G | 486 | 1 | 9,10,11 | 0.65 | 0 | 6,11,13 | 0.39 | 0 |
| 1 | MLY | M | 55 | 1 | 9,10,11 | 0.72 | 0 | 6,11,13 | 0.77 | 0 |
| 1 | MLY | P | 59 | 1 | 9,10,11 | 0.86 | 0 | 6,11,13 | 0.50 | 0 |
| 1 | MLY | A | 659 | 1 | 9,10,11 | 0.85 | 0 | 6,11,13 | 0.59 | 0 |
| 1 | MLY | J | 782 | 1 | 9,10,11 | 0.79 | 0 | 6,11,13 | 0.37 | 0 |
| 1 | MLY | D | 55 | 1 | 9,10,11 | 0.72 | 0 | 6,11,13 | 0.79 | 0 |
| 1 | MLY | M | 486 | 1 | 9,10,11 | 0.64 | 0 | 6,11,13 | 0.38 | 0 |
| 1 | MLY | P | 63 | 1 | 9,10,11 | 0.88 | 0 | 6,11,13 | 0.42 | 0 |
| 1 | MLY | M | 764 | 1 | 9,10,11 | 0.83 | 0 | 6,11,13 | 0.37 | 0 |
| 1 | MLY | P | 138 | 1 | 9,10,11 | 1.30 | 1 (11%) | 6,11,13 | 0.82 | 0 |
| 1 | MLY | P | 367 | 1 | 9,10,11 | 0.61 | 0 | 6,11,13 | 0.37 | 0 |
| 1 | MLY | P | 436 | 1 | 9,10,11 | 1.05 | 1 (11%) | 6,11,13 | 0.50 | 0 |
| 1 | MLY | P | 296 | 1 | 9,10,11 | 0.64 | 0 | 6,11,13 | 0.36 | 0 |
| 1 | MLY | D | 295 | 1 | 9,10,11 | 0.77 | 0 | 6,11,13 | 0.34 | 0 |
| 1 | MLY | D | 486 | 1 | 9,10,11 | 0.65 | 0 | 6,11,13 | 0.40 | 0 |
| 1 | MLY | A | 296 | 1 | 9,10,11 | 0.65 | 0 | 6,11,13 | 0.37 | 0 |
| 1 | MLY | D | 348 | 1 | 9,10,11 | 0.80 | 0 | 6,11,13 | 0.47 | 0 |
| 1 | MLY | J | 130 | 1 | 9,10,11 | 0.76 | 0 | 6,11,13 | 0.74 | 0 |
| 1 | MLY | A | 431 | 1 | 9,10,11 | 0.51 | 0 | 6,11,13 | 0.44 | 0 |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 1 | MLY | G | 505 | 1 | 9,10,11 | 0.83 | 1 (11%) | 6,11,13 | 0.35 | 0 |
| 1 | MLY | D | 138 | 1 | 9,10,11 | 1.35 | 1 (11%) | 6,11,13 | 0.84 | 0 |
| 1 | MLY | G | 19 | 1 | 9,10,11 | 1.13 | 1 (11%) | 6,11,13 | 0.59 | 0 |
| 1 | MLY | P | 486 | 1 | 9,10,11 | 0.62 | 0 | 6,11,13 | 0.39 | 0 |
| 1 | MLY | P | 130 | 1 | 9,10,11 | 0.76 | 0 | 6,11,13 | 0.74 | 0 |
| 1 | MLY | A | 30 | 1 | 9,10,11 | 0.89 | 0 | 6,11,13 | 0.32 | 0 |
| 1 | MLY | D | 367 | 1 | 9,10,11 | 0.62 | 0 | 6,11,13 | 0.39 | 0 |
| 1 | MLY | G | 236 | 1 | 9,10,11 | 0.80 | 1 (11%) | 6,11,13 | 0.48 | 0 |
| 1 | MLY | J | 295 | 1 | 9,10,11 | 0.78 | 0 | 6,11,13 | 0.35 | 0 |
| 1 | MLY | J | 551 | 1 | 9,10,11 | 0.54 | 0 | 6,11,13 | 0.20 | 0 |
| 1 | MLY | D | 504 | 1 | 9,10,11 | 0.88 | 0 | 6,11,13 | 0.20 | 0 |
| 1 | MLY | J | 55 | 1 | 9,10,11 | 0.72 | 0 | 6,11,13 | 0.79 | 0 |
| 1 | MLY | M | 248 | 1 | 9,10,11 | 0.83 | 0 | 6,11,13 | 0.62 | 0 |
| 1 | MLY | M | 30 | 1 | 9,10,11 | 0.89 | 0 | 6,11,13 | 0.32 | 0 |
| 1 | MLY | D | 528 | 1 | 9,10,11 | 0.93 | 0 | 6,11,13 | 0.63 | 0 |
| 1 | MLY | G | 415 | 1 | 9,10,11 | 0.77 | 0 | 6,11,13 | 0.19 | 0 |
| 1 | MLY | P | 295 | 1 | 9,10,11 | 0.81 | 0 | 6,11,13 | 0.35 | 0 |
| 1 | MLY | A | 486 | 1 | 9,10,11 | 0.65 | 0 | 6,11,13 | 0.38 | 0 |
| 1 | MLY | J | 59 | 1 | 9,10,11 | 0.88 | 0 | 6,11,13 | 0.50 | 0 |
| 1 | MLY | D | 369 | 1 | 9,10,11 | 0.69 | 0 | 6,11,13 | 0.45 | 0 |
| 1 | MLY | G | 782 | 1 | 9,10,11 | 0.77 | 0 | 6,11,13 | 0.34 | 0 |
| 1 | MLY | J | 617 | 1 | 9,10,11 | 0.98 | 1 (11%) | 6,11,13 | 0.33 | 0 |
| 1 | MLY | G | 598 | 1 | 9,10,11 | 0.88 | 1 (11%) | 6,11,13 | 0.43 | 0 |
| 1 | MLY | M | 827 | 1 | 9,10,11 | 0.72 | 0 | 6,11,13 | 0.48 | 0 |
| 1 | MLY | M | 613 | 1 | 9,10,11 | 0.57 | 0 | 6,11,13 | 0.64 | 0 |
| 1 | MLY | G | 87 | 1 | 9,10,11 | 1.20 | 1 (11%) | 6,11,13 | 0.44 | 0 |
| 1 | MLY | J | 659 | 1 | 9,10,11 | 0.83 | 0 | 6,11,13 | 0.58 | 0 |
| 1 | MLY | G | 348 | 1 | 9,10,11 | 0.84 | 0 | 6,11,13 | 0.47 | 0 |
| 1 | MLY | P | 415 | 1 | 9,10,11 | 0.75 | 0 | 6,11,13 | 0.19 | 0 |
| 1 | MLY | G | 353 | 1 | 9,10,11 | 0.87 | 0 | 6,11,13 | 0.80 | 0 |
| 1 | MLY | G | 248 | 1 | 9,10,11 | 0.79 | 0 | 6,11,13 | 0.62 | 0 |
| 1 | MLY | G | 764 | 1 | 9,10,11 | 0.80 | 0 | 6,11,13 | 0.35 | 0 |
| 1 | MLY | G | 385 | 1 | 9,10,11 | 1.01 | 1 (11%) | 6,11,13 | 0.43 | 0 |
| 1 | MLY | G | 553 | 4,1 | 9,10,11 | 0.67 | 0 | 6,11,13 | 0.54 | 0 |
| 1 | MLY | P | 827 | 1 | 9,10,11 | 0.73 | 0 | 6,11,13 | 0.48 | 0 |
| 1 | MLY | A | 385 | 1 | 9,10,11 | 1.00 | 1 (11%) | 6,11,13 | 0.43 | 0 |
| 1 | MLY | G | 55 | 1 | 9,10,11 | 0.74 | 0 | 6,11,13 | 0.79 | 0 |
| 1 | MLY | G | 837 | 1 | 9,10,11 | 0.60 | 0 | 6,11,13 | 0.54 | 0 |
| 1 | MLY | M | 272 | 1 | 9,10,11 | 1.03 | 1 (11%) | 6,11,13 | 0.56 | 0 |
| 1 | MLY | M | 600 | 1 | 9,10,11 | 0.52 | 0 | 6,11,13 | 0.37 | 0 |
| 1 | MLY | M | 431 | 1 | 9,10,11 | 0.50 | 0 | 6,11,13 | 0.44 | 0 |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 1 | MLY | A | 681 | 1 | 9,10,11 | 0.58 | 0 | 6,11,13 | 0.45 | 0 |
| 1 | MLY | M | 528 | 1 | 9,10,11 | 0.89 | 0 | 6,11,13 | 0.65 | 0 |
| 1 | MLY | G | 59 | 1 | 9,10,11 | 0.84 | 0 | 6,11,13 | 0.51 | 0 |
| 1 | MLY | G | 659 | 1 | 9,10,11 | 0.85 | 0 | 6,11,13 | 0.58 | 0 |
| 1 | MLY | D | 272 | 1 | 9,10,11 | 0.94 | 1 (11%) | 6,11,13 | 0.56 | 0 |
| 1 | MLY | A | 107 | 1 | 9,10,11 | 0.47 | 0 | 6,11,13 | 0.35 | 0 |
| 1 | MLY | D | 600 | 1 | 9,10,11 | 0.52 | 0 | 6,11,13 | 0.37 | 0 |
| 1 | MLY | J | 19 | 1 | 9,10,11 | 1.21 | 1 (11%) | 6,11,13 | 0.57 | 0 |
| 1 | MLY | J | 600 | 1 | 9,10,11 | 0.52 | 0 | 6,11,13 | 0.35 | 0 |
| 1 | MLY | D | 833 | 1 | 9,10,11 | 1.14 | 2 (22%) | 6,11,13 | 0.32 | 0 |
| 1 | MLY | A | 613 | 1 | 9,10,11 | 0.57 | 0 | 6,11,13 | 0.63 | 0 |
| 1 | MLY | P | 248 | 1 | 9,10,11 | 0.84 | 0 | 6,11,13 | 0.61 | 0 |
| 1 | MLY | M | 681 | 1 | 9,10,11 | 0.60 | 0 | 6,11,13 | 0.46 | 0 |
| 1 | MLY | J | 236 | 1 | 9,10,11 | 0.80 | 1 (11%) | 6,11,13 | 0.47 | 0 |
| 1 | MLY | A | 63 | 1 | 9,10,11 | 0.91 | 0 | 6,11,13 | 0.42 | 0 |
| 1 | MLY | P | 505 | 1 | 9,10,11 | 0.92 | 1 (11%) | 6,11,13 | 0.34 | 0 |
| 1 | MLY | A | 84 | 1 | 9,10,11 | 0.48 | 0 | 6,11,13 | 0.78 | 0 |
| 1 | MLY | D | 681 | 1 | 9,10,11 | 0.60 | 0 | 6,11,13 | 0.46 | 0 |
| 1 | MLY | A | 833 | 1 | 9,10,11 | 1.15 | 1 (11%) | 6,11,13 | 0.31 | 0 |
| 1 | MLY | M | 49 | 1 | 9,10,11 | 1.06 | 1 (11%) | 6,11,13 | 0.74 | 0 |
| 1 | MLY | M | 553 | 1 | 9,10,11 | 0.66 | 0 | 6,11,13 | 0.55 | 0 |
| 1 | MLY | M | 436 | 1 | 9,10,11 | 1.07 | 1 (11%) | 6,11,13 | 0.48 | 0 |
| 1 | MLY | J | 598 | 1 | 9,10,11 | 0.87 | 1 (11%) | 6,11,13 | 0.43 | 0 |
| 1 | MLY | A | 369 | 1 | 9,10,11 | 0.72 | 0 | 6,11,13 | 0.45 | 0 |
| 1 | MLY | A | 130 | 1 | 9,10,11 | 0.80 | 0 | 6,11,13 | 0.75 | 0 |
| 1 | MLY | A | 272 | 1 | 9,10,11 | 1.00 | 1 (11%) | 6,11,13 | 0.56 | 0 |
| 1 | MLY | A | 600 | 1 | 9,10,11 | 0.51 | 0 | 6,11,13 | 0.39 | 0 |
| 1 | MLY | J | 553 | 1 | 9,10,11 | 0.67 | 0 | 6,11,13 | 0.54 | 0 |
| 1 | MLY | M | 369 | 1 | 9,10,11 | 0.70 | 0 | 6,11,13 | 0.47 | 0 |
| 1 | MLY | P | 348 | 1 | 9,10,11 | 0.80 | 0 | 6,11,13 | 0.47 | 0 |
| 1 | MLY | P | 553 | 1 | 9,10,11 | 0.67 | 0 | 6,11,13 | 0.53 | 0 |
| 1 | MLY | P | 551 | 1 | 9,10,11 | 0.53 | 0 | 6,11,13 | 0.20 | 0 |
| 1 | MLY | G | 190 | 1 | 9,10,11 | 1.22 | 1 (11%) | 6,11,13 | 0.52 | 0 |
| 1 | MLY | D | 49 | 1 | 9,10,11 | 1.09 | 1 (11%) | 6,11,13 | 0.75 | 0 |
| 1 | MLY | A | 551 | 1 | 9,10,11 | 0.53 | 0 | 6,11,13 | 0.19 | 0 |
| 1 | MLY | J | 385 | 1 | 9,10,11 | 1.00 | 1 (11%) | 6,11,13 | 0.44 | 0 |
| 1 | MLY | J | 248 | 1 | 9,10,11 | 0.84 | 0 | 6,11,13 | 0.62 | 0 |
| 1 | MLY | D | 436 | 1 | 9,10,11 | 1.09 | 1 (11%) | 6,11,13 | 0.50 | 0 |
| 1 | MLY | D | 84 | 1 | 9,10,11 | 0.49 | 0 | 6,11,13 | 0.80 | 0 |
| 1 | MLY | J | 107 | 1 | 9,10,11 | 0.47 | 0 | 6,11,13 | 0.34 | 0 |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 1 | MLY | A | 236 | 1 | 9,10,11 | 0.80 | 1 (11%) | 6,11,13 | 0.48 | 0 |
| 1 | MLY | A | 367 | 1 | 9,10,11 | 0.64 | 0 | 6,11,13 | 0.36 | 0 |
| 1 | MLY | P | 617 | 1 | 9,10,11 | 0.99 | 1 (11%) | 6,11,13 | 0.32 | 0 |
| 1 | MLY | J | 613 | 1 | 9,10,11 | 0.57 | 0 | 6,11,13 | 0.64 | 0 |
| 1 | MLY | M | 505 | 1 | 9,10,11 | 0.92 | 1 (11%) | 6,11,13 | 0.34 | 0 |
| 1 | MLY | J | 369 | 1 | 9,10,11 | 0.70 | 0 | 6,11,13 | 0.45 | 0 |
| 1 | MLY | D | 837 | 1 | 9,10,11 | 0.62 | 0 | 6,11,13 | 0.58 | 0 |
| 1 | MLY | G | 431 | 1 | 9,10,11 | 0.50 | 0 | 6,11,13 | 0.45 | 0 |
| 1 | MLY | D | 505 | 1 | 9,10,11 | 0.84 | 1 (11%) | 6,11,13 | 0.35 | 0 |
| 1 | MLY | J | 486 | 1 | 9,10,11 | 0.63 | 0 | 6,11,13 | 0.40 | 0 |
| 1 | MLY | M | 617 | 1 | 9,10,11 | 0.94 | 1 (11%) | 6,11,13 | 0.33 | 0 |
| 1 | MLY | D | 59 | 1 | 9,10,11 | 0.87 | 0 | 6,11,13 | 0.50 | 0 |
| 1 | MLY | D | 87 | 1 | 9,10,11 | 1.18 | 1 (11%) | 6,11,13 | 0.43 | 0 |
| 1 | MLY | M | 35 | 1 | 9,10,11 | 0.72 | 0 | 6,11,13 | 0.39 | 0 |
| 1 | MLY | P | 369 | 1 | 9,10,11 | 0.69 | 0 | 6,11,13 | 0.45 | 0 |
| 1 | MLY | D | 617 | 1 | 9,10,11 | 0.97 | 1 (11%) | 6,11,13 | 0.34 | 0 |
| 1 | MLY | G | 272 | 1 | 9,10,11 | 0.97 | 1 (11%) | 6,11,13 | 0.55 | 0 |
| 1 | MLY | M | 837 | 1 | 9,10,11 | 0.58 | 0 | 6,11,13 | 0.56 | 0 |
| 1 | MLY | D | 35 | 1 | 9,10,11 | 0.72 | 0 | 6,11,13 | 0.37 | 0 |
| 1 | MLY | A | 415 | 1 | 9,10,11 | 0.75 | 0 | 6,11,13 | 0.18 | 0 |
| 1 | MLY | A | 87 | 1 | 9,10,11 | 1.20 | 1 (11%) | 6,11,13 | 0.43 | 0 |
| 1 | MLY | J | 296 | 1 | 9,10,11 | 0.69 | 0 | 6,11,13 | 0.35 | 0 |
| 1 | MLY | J | 827 | 1 | 9,10,11 | 0.76 | 0 | 6,11,13 | 0.48 | 0 |
| 1 | MLY | J | 528 | 1 | 9,10,11 | 0.89 | 0 | 6,11,13 | 0.64 | 0 |
| 1 | MLY | A | 505 | 1 | 9,10,11 | 0.88 | 1 (11%) | 6,11,13 | 0.33 | 0 |
| 1 | MLY | J | 30 | 1 | 9,10,11 | 0.89 | 0 | 6,11,13 | 0.31 | 0 |
| 1 | MLY | P | 272 | 1 | 9,10,11 | 0.96 | 1 (11%) | 6,11,13 | 0.55 | 0 |
| 1 | MLY | P | 600 | 1 | 9,10,11 | 0.52 | 0 | 6,11,13 | 0.36 | 0 |
| 1 | MLY | J | 190 | 1 | 9,10,11 | 1.26 | 1 (11%) | 6,11,13 | 0.53 | 0 |
| 1 | MLY | A | 55 | 1 | 9,10,11 | 0.72 | 0 | 6,11,13 | 0.77 | 0 |
| 1 | MLY | P | 30 | 1 | 9,10,11 | 0.89 | 0 | 6,11,13 | 0.31 | 0 |
| 1 | MLY | P | 353 | 1 | 9,10,11 | 0.85 | 0 | 6,11,13 | 0.79 | 0 |
| 1 | MLY | D | 431 | 1 | 9,10,11 | 0.55 | 0 | 6,11,13 | 0.45 | 0 |
| 1 | MLY | A | 59 | 1 | 9,10,11 | 0.87 | 0 | 6,11,13 | 0.49 | 0 |
| 1 | MLY | D | 839 | 1 | 9,10,11 | 0.72 | 0 | 6,11,13 | 0.79 | 0 |
| 1 | MLY | M | 551 | 1 | 9,10,11 | 0.54 | 0 | 6,11,13 | 0.20 | 0 |
| 1 | MLY | A | 138 | 1 | 9,10,11 | 1.33 | 1 (11%) | 6,11,13 | 0.85 | 0 |
| 1 | MLY | P | 190 | 1 | 9,10,11 | 1.24 | 1 (11%) | 6,11,13 | 0.52 | 0 |
| 1 | MLY | P | 764 | 1 | 9,10,11 | 0.82 | 0 | 6,11,13 | 0.39 | 0 |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 1 | MLY | P | 833 | 1 | 9,10,11 | 1.16 | 1 (11%) | 6,11,13 | 0.31 | 0 |
| 1 | MLY | P | 431 | 1 | 9,10,11 | 0.53 | 0 | 6,11,13 | 0.44 | 0 |
| 1 | MLY | G | 768 | 1 | 9,10,11 | 0.75 | 0 | 6,11,13 | 0.42 | 0 |
| 1 | MLY | G | 827 | 1 | 9,10,11 | 0.69 | 0 | 6,11,13 | 0.49 | 0 |
| 1 | MLY | P | 598 | 1 | 9,10,11 | 0.89 | 1 (11%) | 6,11,13 | 0.42 | 0 |
| 1 | MLY | P | 19 | 1 | 9,10,11 | 1.20 | 1 (11%) | 6,11,13 | 0.55 | 0 |
| 1 | MLY | A | 598 | 1 | 9,10,11 | 0.90 | 1 (11%) | 6,11,13 | 0.45 | 0 |
| 1 | MLY | M | 598 | 1 | 9,10,11 | 0.89 | 1 (11%) | 6,11,13 | 0.44 | 0 |
| 1 | MLY | M | 833 | 1 | 9,10,11 | 1.20 | 1 (11%) | 6,11,13 | 0.30 | 0 |
| 1 | MLY | J | 367 | 1 | 9,10,11 | 0.62 | 0 | 6,11,13 | 0.37 | 0 |
| 1 | MLY | J | 272 | 1 | 9,10,11 | 1.01 | 1 (11%) | 6,11,13 | 0.54 | 0 |
| 1 | MLY | M | 353 | 1 | 9,10,11 | 0.88 | 0 | 6,11,13 | 0.79 | 0 |
| 1 | MLY | A | 764 | 1 | 9,10,11 | 0.86 | 0 | 6,11,13 | 0.35 | 0 |
| 1 | MLY | G | 63 | 1 | 9,10,11 | 0.89 | 0 | 6,11,13 | 0.43 | 0 |
| 1 | MLY | P | 768 | 1 | 9,10,11 | 0.74 | 0 | 6,11,13 | 0.40 | 0 |
| 1 | MLY | A | 768 | 1 | 9,10,11 | 0.77 | 0 | 6,11,13 | 0.41 | 0 |
| 1 | MLY | A | 553 | 4,1 | 9,10,11 | 0.68 | 0 | 6,11,13 | 0.55 | 0 |
| 1 | MLY | M | 130 | 1 | 9,10,11 | 0.77 | 0 | 6,11,13 | 0.74 | 0 |
| 1 | MLY | J | 353 | 1 | 9,10,11 | 0.86 | 0 | 6,11,13 | 0.79 | 0 |
| 1 | MLY | G | 35 | 1 | 9,10,11 | 0.72 | 0 | 6,11,13 | 0.39 | 0 |
| 1 | MLY | J | 764 | 1 | 9,10,11 | 0.81 | 0 | 6,11,13 | 0.37 | 0 |
| 1 | MLY | M | 296 | 1 | 9,10,11 | 0.67 | 0 | 6,11,13 | 0.36 | 0 |
| 1 | MLY | J | 348 | 1 | 9,10,11 | 0.81 | 0 | 6,11,13 | 0.47 | 0 |
| 1 | MLY | D | 415 | 1 | 9,10,11 | 0.78 | 0 | 6,11,13 | 0.19 | 0 |
| 1 | MLY | M | 839 | 1 | 9,10,11 | 0.71 | 0 | 6,11,13 | 0.77 | 0 |
| 1 | MLY | P | 87 | 1 | 9,10,11 | 1.20 | 1 (11%) | 6,11,13 | 0.42 | 0 |
| 1 | MLY | J | 505 | 1 | 9,10,11 | 0.92 | 1 (11%) | 6,11,13 | 0.35 | 0 |
| 1 | MLY | G | 504 | 1 | 9,10,11 | 0.90 | 0 | 6,11,13 | 0.23 | 0 |
| 1 | MLY | A | 295 | 1 | 9,10,11 | 0.79 | 0 | 6,11,13 | 0.33 | 0 |
| 1 | MLY | M | 295 | 1 | 9,10,11 | 0.77 | 0 | 6,11,13 | 0.35 | 0 |
| 1 | MLY | M | 19 | 1 | 9,10,11 | 1.15 | 1 (11%) | 6,11,13 | 0.58 | 0 |
| 1 | MLY | D | 827 | 1 | 9,10,11 | 0.67 | 0 | 6,11,13 | 0.48 | 0 |
| 1 | MLY | A | 19 | 1 | 9,10,11 | 1.10 | 1 (11%) | 6,11,13 | 0.57 | 0 |
| 1 | MLY | D | 768 | 1 | 9,10,11 | 0.76 | 0 | 6,11,13 | 0.40 | 0 |
| 1 | MLY | G | 138 | 1 | 9,10,11 | 1.37 | 1 (11%) | 6,11,13 | 0.85 | 0 |
| 1 | MLY | M | 367 | 1 | 9,10,11 | 0.61 | 0 | 6,11,13 | 0.37 | 0 |
| 1 | MLY | A | 782 | 1 | 9,10,11 | 0.80 | 0 | 6,11,13 | 0.35 | 0 |
| 1 | MLY | M | 63 | 1 | 9,10,11 | 0.91 | 0 | 6,11,13 | 0.43 | 0 |
| 1 | MLY | G | 436 | 1 | 9,10,11 | 1.03 | 1 (11%) | 6,11,13 | 0.47 | 0 |
| 1 | MLY | M | 138 | 1 | 9,10,11 | 1.34 | 1 (11%) | 6,11,13 | 0.84 | 0 |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 1 | MLY | M | 84 | 1 | 9,10,11 | 0.50 | 0 | 6,11,13 | 0.80 | 0 |
| 1 | MLY | G | 296 | 1 | 9,10,11 | 0.64 | 0 | 6,11,13 | 0.38 | 0 |
| 1 | MLY | P | 613 | 1 | 9,10,11 | 0.57 | 0 | 6,11,13 | 0.64 | 0 |
| 1 | MLY | P | 504 | 1 | 9,10,11 | 0.84 | 0 | 6,11,13 | 0.24 | 0 |
| 1 | MLY | A | 827 | 1 | 9,10,11 | 0.71 | 0 | 6,11,13 | 0.45 | 0 |
| 1 | MLY | G | 839 | 1 | 9,10,11 | 0.69 | 0 | 6,11,13 | 0.80 | 0 |
| 1 | MLY | J | 768 | 1 | 9,10,11 | 0.77 | 0 | 6,11,13 | 0.42 | 0 |
| 1 | MLY | M | 504 | 1 | 9,10,11 | 0.85 | 0 | 6,11,13 | 0.24 | 0 |
| 1 | MLY | G | 613 | 1 | 9,10,11 | 0.60 | 0 | 6,11,13 | 0.63 | 0 |
| 1 | MLY | M | 782 | 1 | 9,10,11 | 0.79 | 0 | 6,11,13 | 0.36 | 0 |
| 1 | MLY | P | 528 | 1 | 9,10,11 | 0.88 | 0 | 6,11,13 | 0.65 | 0 |
| 1 | MLY | A | 528 | 1 | 9,10,11 | 0.88 | 0 | 6,11,13 | 0.67 | 0 |
| 1 | MLY | D | 19 | 1 | 9,10,11 | 1.21 | 1 (11%) | 6,11,13 | 0.56 | 0 |
| 1 | MLY | G | 30 | 1 | 9,10,11 | 0.88 | 0 | 6,11,13 | 0.31 | 0 |
| 1 | MLY | P | 84 | 1 | 9,10,11 | 0.50 | 0 | 6,11,13 | 0.80 | 0 |
| 1 | MLY | D | 236 | 1 | 9,10,11 | 0.80 | 1 (11%) | 6,11,13 | 0.48 | 0 |
| 1 | MLY | M | 415 | 1 | 9,10,11 | 0.79 | 0 | 6,11,13 | 0.18 | 0 |
| 1 | MLY | J | 87 | 1 | 9,10,11 | 1.21 | 1 (11%) | 6,11,13 | 0.42 | 0 |

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|----------|-------|
| 1 | MLY | A | 348 | 1 | - | 5/8/9/11 | - |
| 1 | MLY | G | 49 | 1 | - | 3/8/9/11 | - |
| 1 | MLY | D | 130 | 1 | - | 5/8/9/11 | - |
| 1 | MLY | M | 385 | 1 | - | 2/8/9/11 | - |
| 1 | MLY | M | 190 | 1 | - | 5/8/9/11 | - |
| 1 | MLY | G | 833 | 1 | - | 6/8/9/11 | - |
| 1 | MLY | D | 353 | 1 | - | 4/8/9/11 | - |
| 1 | MLY | J | 35 | 1 | - | 3/8/9/11 | - |
| 1 | MLY | D | 553 | 4,1 | - | 5/8/9/11 | - |
| 1 | MLY | M | 107 | 1 | - | 2/8/9/11 | - |
| 1 | MLY | J | 504 | 1 | - | 4/8/9/11 | - |
| 1 | MLY | D | 551 | 1 | - | 3/8/9/11 | - |
| 1 | MLY | D | 107 | 1 | - | 2/8/9/11 | - |
| 1 | MLY | M | 59 | 1 | - | 3/8/9/11 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|----------|-------|
| 1 | MLY | A | 248 | 1 | - | 6/8/9/11 | - |
| 1 | MLY | D | 613 | 1 | - | 4/8/9/11 | - |
| 1 | MLY | J | 138 | 1 | - | 4/8/9/11 | - |
| 1 | MLY | G | 600 | 1 | - | 3/8/9/11 | - |
| 1 | MLY | P | 107 | 1 | - | 2/8/9/11 | - |
| 1 | MLY | P | 659 | 1 | - | 3/8/9/11 | - |
| 1 | MLY | J | 415 | 1 | - | 3/8/9/11 | - |
| 1 | MLY | M | 659 | 1 | - | 3/8/9/11 | - |
| 1 | MLY | J | 431 | 1 | - | 4/8/9/11 | - |
| 1 | MLY | J | 839 | 1 | - | 3/8/9/11 | - |
| 1 | MLY | D | 659 | 1 | - | 3/8/9/11 | - |
| 1 | MLY | A | 353 | 1 | - | 4/8/9/11 | - |
| 1 | MLY | G | 681 | 1 | - | 4/8/9/11 | - |
| 1 | MLY | P | 681 | 1 | - | 4/8/9/11 | - |
| 1 | MLY | P | 839 | 1 | - | 3/8/9/11 | - |
| 1 | MLY | J | 837 | 1 | - | 5/8/9/11 | - |
| 1 | MLY | A | 35 | 1 | - | 3/8/9/11 | - |
| 1 | MLY | A | 617 | 1 | - | 1/8/9/11 | - |
| 1 | MLY | G | 84 | 1 | - | 4/8/9/11 | - |
| 1 | MLY | J | 49 | 1 | - | 3/8/9/11 | - |
| 1 | MLY | D | 30 | 1 | - | 2/8/9/11 | - |
| 1 | MLY | A | 190 | 1 | - | 5/8/9/11 | - |
| 1 | MLY | A | 837 | 1 | - | 5/8/9/11 | - |
| 1 | MLY | A | 504 | 1 | - | 4/8/9/11 | - |
| 1 | MLY | D | 296 | 1 | - | 4/8/9/11 | - |
| 1 | MLY | J | 833 | 1 | - | 6/8/9/11 | - |
| 1 | MLY | P | 49 | 1 | - | 3/8/9/11 | - |
| 1 | MLY | G | 130 | 1 | - | 5/8/9/11 | - |
| 1 | MLY | M | 236 | 1 | - | 3/8/9/11 | - |
| 1 | MLY | G | 528 | 1 | - | 4/8/9/11 | - |
| 1 | MLY | P | 782 | 1 | - | 6/8/9/11 | - |
| 1 | MLY | D | 190 | 1 | - | 5/8/9/11 | - |
| 1 | MLY | M | 768 | 1 | - | 4/8/9/11 | - |
| 1 | MLY | G | 295 | 1 | - | 2/8/9/11 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|----------|-------|
| 1 | MLY | G | 551 | 1 | - | 3/8/9/11 | - |
| 1 | MLY | A | 839 | 1 | - | 3/8/9/11 | - |
| 1 | MLY | P | 236 | 1 | - | 3/8/9/11 | - |
| 1 | MLY | G | 107 | 1 | - | 2/8/9/11 | - |
| 1 | MLY | D | 782 | 1 | - | 6/8/9/11 | - |
| 1 | MLY | D | 598 | 1 | - | 5/8/9/11 | - |
| 1 | MLY | M | 87 | 1 | - | 2/8/9/11 | - |
| 1 | MLY | G | 367 | 1 | - | 2/8/9/11 | - |
| 1 | MLY | J | 681 | 1 | - | 4/8/9/11 | - |
| 1 | MLY | P | 35 | 1 | - | 3/8/9/11 | - |
| 1 | MLY | P | 385 | 1 | - | 2/8/9/11 | - |
| 1 | MLY | G | 617 | 1 | - | 1/8/9/11 | - |
| 1 | MLY | A | 49 | 1 | - | 3/8/9/11 | - |
| 1 | MLY | M | 348 | 1 | - | 5/8/9/11 | - |
| 1 | MLY | D | 63 | 1 | - | 4/8/9/11 | - |
| 1 | MLY | D | 248 | 1 | - | 6/8/9/11 | - |
| 1 | MLY | J | 63 | 1 | - | 4/8/9/11 | - |
| 1 | MLY | A | 436 | 1 | - | 4/8/9/11 | - |
| 1 | MLY | D | 385 | 1 | - | 2/8/9/11 | - |
| 1 | MLY | D | 764 | 1 | - | 2/8/9/11 | - |
| 1 | MLY | J | 84 | 1 | - | 4/8/9/11 | - |
| 1 | MLY | P | 55 | 1 | - | 6/8/9/11 | - |
| 1 | MLY | P | 837 | 1 | - | 5/8/9/11 | - |
| 1 | MLY | G | 369 | 1 | - | 2/8/9/11 | - |
| 1 | MLY | J | 436 | 1 | - | 4/8/9/11 | - |
| 1 | MLY | G | 486 | 1 | - | 2/8/9/11 | - |
| 1 | MLY | M | 55 | 1 | - | 6/8/9/11 | - |
| 1 | MLY | P | 59 | 1 | - | 3/8/9/11 | - |
| 1 | MLY | A | 659 | 1 | - | 3/8/9/11 | - |
| 1 | MLY | J | 782 | 1 | - | 6/8/9/11 | - |
| 1 | MLY | D | 55 | 1 | - | 6/8/9/11 | - |
| 1 | MLY | M | 486 | 1 | - | 2/8/9/11 | - |
| 1 | MLY | P | 63 | 1 | - | 4/8/9/11 | - |
| 1 | MLY | M | 764 | 1 | - | 2/8/9/11 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|----------|-------|
| 1 | MLY | P | 138 | 1 | - | 4/8/9/11 | - |
| 1 | MLY | P | 367 | 1 | - | 2/8/9/11 | - |
| 1 | MLY | P | 436 | 1 | - | 4/8/9/11 | - |
| 1 | MLY | P | 296 | 1 | - | 4/8/9/11 | - |
| 1 | MLY | D | 295 | 1 | - | 2/8/9/11 | - |
| 1 | MLY | D | 486 | 1 | - | 2/8/9/11 | - |
| 1 | MLY | A | 296 | 1 | - | 4/8/9/11 | - |
| 1 | MLY | D | 348 | 1 | - | 5/8/9/11 | - |
| 1 | MLY | J | 130 | 1 | - | 5/8/9/11 | - |
| 1 | MLY | A | 431 | 1 | - | 4/8/9/11 | - |
| 1 | MLY | G | 505 | 1 | - | 5/8/9/11 | - |
| 1 | MLY | D | 138 | 1 | - | 4/8/9/11 | - |
| 1 | MLY | G | 19 | 1 | - | 4/8/9/11 | - |
| 1 | MLY | P | 486 | 1 | - | 2/8/9/11 | - |
| 1 | MLY | P | 130 | 1 | - | 5/8/9/11 | - |
| 1 | MLY | A | 30 | 1 | - | 2/8/9/11 | - |
| 1 | MLY | D | 367 | 1 | - | 2/8/9/11 | - |
| 1 | MLY | G | 236 | 1 | - | 3/8/9/11 | - |
| 1 | MLY | J | 295 | 1 | - | 2/8/9/11 | - |
| 1 | MLY | J | 551 | 1 | - | 3/8/9/11 | - |
| 1 | MLY | D | 504 | 1 | - | 4/8/9/11 | - |
| 1 | MLY | J | 55 | 1 | - | 6/8/9/11 | - |
| 1 | MLY | M | 248 | 1 | - | 6/8/9/11 | - |
| 1 | MLY | M | 30 | 1 | - | 2/8/9/11 | - |
| 1 | MLY | D | 528 | 1 | - | 4/8/9/11 | - |
| 1 | MLY | G | 415 | 1 | - | 3/8/9/11 | - |
| 1 | MLY | P | 295 | 1 | - | 2/8/9/11 | - |
| 1 | MLY | A | 486 | 1 | - | 2/8/9/11 | - |
| 1 | MLY | J | 59 | 1 | - | 3/8/9/11 | - |
| 1 | MLY | D | 369 | 1 | - | 2/8/9/11 | - |
| 1 | MLY | G | 782 | 1 | - | 6/8/9/11 | - |
| 1 | MLY | J | 617 | 1 | - | 1/8/9/11 | - |
| 1 | MLY | G | 598 | 1 | - | 5/8/9/11 | - |
| 1 | MLY | M | 827 | 1 | - | 0/8/9/11 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|----------|-------|
| 1 | MLY | M | 613 | 1 | - | 4/8/9/11 | - |
| 1 | MLY | G | 87 | 1 | - | 2/8/9/11 | - |
| 1 | MLY | J | 659 | 1 | - | 3/8/9/11 | - |
| 1 | MLY | G | 348 | 1 | - | 5/8/9/11 | - |
| 1 | MLY | P | 415 | 1 | - | 3/8/9/11 | - |
| 1 | MLY | G | 353 | 1 | - | 4/8/9/11 | - |
| 1 | MLY | G | 248 | 1 | - | 6/8/9/11 | - |
| 1 | MLY | G | 764 | 1 | - | 2/8/9/11 | - |
| 1 | MLY | G | 385 | 1 | - | 2/8/9/11 | - |
| 1 | MLY | G | 553 | 4,1 | - | 4/8/9/11 | - |
| 1 | MLY | P | 827 | 1 | - | 0/8/9/11 | - |
| 1 | MLY | A | 385 | 1 | - | 2/8/9/11 | - |
| 1 | MLY | G | 55 | 1 | - | 6/8/9/11 | - |
| 1 | MLY | G | 837 | 1 | - | 5/8/9/11 | - |
| 1 | MLY | M | 272 | 1 | - | 3/8/9/11 | - |
| 1 | MLY | M | 600 | 1 | - | 3/8/9/11 | - |
| 1 | MLY | M | 431 | 1 | - | 4/8/9/11 | - |
| 1 | MLY | A | 681 | 1 | - | 4/8/9/11 | - |
| 1 | MLY | M | 528 | 1 | - | 4/8/9/11 | - |
| 1 | MLY | G | 59 | 1 | - | 3/8/9/11 | - |
| 1 | MLY | G | 659 | 1 | - | 3/8/9/11 | - |
| 1 | MLY | D | 272 | 1 | - | 3/8/9/11 | - |
| 1 | MLY | A | 107 | 1 | - | 2/8/9/11 | - |
| 1 | MLY | D | 600 | 1 | - | 3/8/9/11 | - |
| 1 | MLY | J | 19 | 1 | - | 4/8/9/11 | - |
| 1 | MLY | J | 600 | 1 | - | 3/8/9/11 | - |
| 1 | MLY | D | 833 | 1 | - | 6/8/9/11 | - |
| 1 | MLY | A | 613 | 1 | - | 4/8/9/11 | - |
| 1 | MLY | P | 248 | 1 | - | 6/8/9/11 | - |
| 1 | MLY | M | 681 | 1 | - | 4/8/9/11 | - |
| 1 | MLY | J | 236 | 1 | - | 3/8/9/11 | - |
| 1 | MLY | A | 63 | 1 | - | 4/8/9/11 | - |
| 1 | MLY | P | 505 | 1 | - | 5/8/9/11 | - |
| 1 | MLY | A | 84 | 1 | - | 4/8/9/11 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|----------|-------|
| 1 | MLY | D | 681 | 1 | - | 4/8/9/11 | - |
| 1 | MLY | A | 833 | 1 | - | 6/8/9/11 | - |
| 1 | MLY | M | 49 | 1 | - | 3/8/9/11 | - |
| 1 | MLY | M | 553 | 1 | - | 4/8/9/11 | - |
| 1 | MLY | M | 436 | 1 | - | 4/8/9/11 | - |
| 1 | MLY | J | 598 | 1 | - | 5/8/9/11 | - |
| 1 | MLY | A | 369 | 1 | - | 2/8/9/11 | - |
| 1 | MLY | A | 130 | 1 | - | 5/8/9/11 | - |
| 1 | MLY | A | 272 | 1 | - | 3/8/9/11 | - |
| 1 | MLY | A | 600 | 1 | - | 3/8/9/11 | - |
| 1 | MLY | J | 553 | 1 | - | 4/8/9/11 | - |
| 1 | MLY | M | 369 | 1 | - | 2/8/9/11 | - |
| 1 | MLY | P | 348 | 1 | - | 5/8/9/11 | - |
| 1 | MLY | P | 553 | 1 | - | 4/8/9/11 | - |
| 1 | MLY | P | 551 | 1 | - | 3/8/9/11 | - |
| 1 | MLY | G | 190 | 1 | - | 5/8/9/11 | - |
| 1 | MLY | D | 49 | 1 | - | 3/8/9/11 | - |
| 1 | MLY | A | 551 | 1 | - | 3/8/9/11 | - |
| 1 | MLY | J | 385 | 1 | - | 2/8/9/11 | - |
| 1 | MLY | J | 248 | 1 | - | 6/8/9/11 | - |
| 1 | MLY | D | 436 | 1 | - | 4/8/9/11 | - |
| 1 | MLY | D | 84 | 1 | - | 4/8/9/11 | - |
| 1 | MLY | J | 107 | 1 | - | 2/8/9/11 | - |
| 1 | MLY | A | 236 | 1 | - | 3/8/9/11 | - |
| 1 | MLY | A | 367 | 1 | - | 2/8/9/11 | - |
| 1 | MLY | P | 617 | 1 | - | 1/8/9/11 | - |
| 1 | MLY | J | 613 | 1 | - | 4/8/9/11 | - |
| 1 | MLY | M | 505 | 1 | - | 5/8/9/11 | - |
| 1 | MLY | J | 369 | 1 | - | 2/8/9/11 | - |
| 1 | MLY | D | 837 | 1 | - | 5/8/9/11 | - |
| 1 | MLY | G | 431 | 1 | - | 4/8/9/11 | - |
| 1 | MLY | D | 505 | 1 | - | 5/8/9/11 | - |
| 1 | MLY | J | 486 | 1 | - | 2/8/9/11 | - |
| 1 | MLY | M | 617 | 1 | - | 1/8/9/11 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|----------|-------|
| 1 | MLY | D | 59 | 1 | - | 3/8/9/11 | - |
| 1 | MLY | D | 87 | 1 | - | 2/8/9/11 | - |
| 1 | MLY | M | 35 | 1 | - | 3/8/9/11 | - |
| 1 | MLY | P | 369 | 1 | - | 2/8/9/11 | - |
| 1 | MLY | D | 617 | 1 | - | 1/8/9/11 | - |
| 1 | MLY | G | 272 | 1 | - | 3/8/9/11 | - |
| 1 | MLY | M | 837 | 1 | - | 5/8/9/11 | - |
| 1 | MLY | D | 35 | 1 | - | 3/8/9/11 | - |
| 1 | MLY | A | 415 | 1 | - | 3/8/9/11 | - |
| 1 | MLY | A | 87 | 1 | - | 2/8/9/11 | - |
| 1 | MLY | J | 296 | 1 | - | 4/8/9/11 | - |
| 1 | MLY | J | 827 | 1 | - | 0/8/9/11 | - |
| 1 | MLY | J | 528 | 1 | - | 5/8/9/11 | - |
| 1 | MLY | A | 505 | 1 | - | 5/8/9/11 | - |
| 1 | MLY | J | 30 | 1 | - | 2/8/9/11 | - |
| 1 | MLY | P | 272 | 1 | - | 3/8/9/11 | - |
| 1 | MLY | P | 600 | 1 | - | 3/8/9/11 | - |
| 1 | MLY | J | 190 | 1 | - | 5/8/9/11 | - |
| 1 | MLY | A | 55 | 1 | - | 6/8/9/11 | - |
| 1 | MLY | P | 30 | 1 | - | 2/8/9/11 | - |
| 1 | MLY | P | 353 | 1 | - | 4/8/9/11 | - |
| 1 | MLY | D | 431 | 1 | - | 4/8/9/11 | - |
| 1 | MLY | A | 59 | 1 | - | 3/8/9/11 | - |
| 1 | MLY | D | 839 | 1 | - | 3/8/9/11 | - |
| 1 | MLY | M | 551 | 1 | - | 3/8/9/11 | - |
| 1 | MLY | A | 138 | 1 | - | 4/8/9/11 | - |
| 1 | MLY | P | 190 | 1 | - | 5/8/9/11 | - |
| 1 | MLY | P | 764 | 1 | - | 2/8/9/11 | - |
| 1 | MLY | P | 833 | 1 | - | 6/8/9/11 | - |
| 1 | MLY | P | 431 | 1 | - | 4/8/9/11 | - |
| 1 | MLY | G | 768 | 1 | - | 4/8/9/11 | - |
| 1 | MLY | G | 827 | 1 | - | 0/8/9/11 | - |
| 1 | MLY | P | 598 | 1 | - | 5/8/9/11 | - |
| 1 | MLY | P | 19 | 1 | - | 4/8/9/11 | - |
| 1 | MLY | A | 598 | 1 | - | 5/8/9/11 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|----------|-------|
| 1 | MLY | M | 598 | 1 | - | 5/8/9/11 | - |
| 1 | MLY | M | 833 | 1 | - | 6/8/9/11 | - |
| 1 | MLY | J | 367 | 1 | - | 2/8/9/11 | - |
| 1 | MLY | J | 272 | 1 | - | 3/8/9/11 | - |
| 1 | MLY | M | 353 | 1 | - | 4/8/9/11 | - |
| 1 | MLY | A | 764 | 1 | - | 2/8/9/11 | - |
| 1 | MLY | G | 63 | 1 | - | 4/8/9/11 | - |
| 1 | MLY | P | 768 | 1 | - | 4/8/9/11 | - |
| 1 | MLY | A | 768 | 1 | - | 4/8/9/11 | - |
| 1 | MLY | A | 553 | 4,1 | - | 4/8/9/11 | - |
| 1 | MLY | M | 130 | 1 | - | 5/8/9/11 | - |
| 1 | MLY | J | 353 | 1 | - | 4/8/9/11 | - |
| 1 | MLY | G | 35 | 1 | - | 3/8/9/11 | - |
| 1 | MLY | J | 764 | 1 | - | 2/8/9/11 | - |
| 1 | MLY | M | 296 | 1 | - | 4/8/9/11 | - |
| 1 | MLY | J | 348 | 1 | - | 5/8/9/11 | - |
| 1 | MLY | D | 415 | 1 | - | 3/8/9/11 | - |
| 1 | MLY | M | 839 | 1 | - | 3/8/9/11 | - |
| 1 | MLY | P | 87 | 1 | - | 2/8/9/11 | - |
| 1 | MLY | J | 505 | 1 | - | 5/8/9/11 | - |
| 1 | MLY | G | 504 | 1 | - | 4/8/9/11 | - |
| 1 | MLY | A | 295 | 1 | - | 2/8/9/11 | - |
| 1 | MLY | M | 295 | 1 | - | 2/8/9/11 | - |
| 1 | MLY | M | 19 | 1 | - | 4/8/9/11 | - |
| 1 | MLY | D | 827 | 1 | - | 0/8/9/11 | - |
| 1 | MLY | A | 19 | 1 | - | 4/8/9/11 | - |
| 1 | MLY | D | 768 | 1 | - | 4/8/9/11 | - |
| 1 | MLY | G | 138 | 1 | - | 4/8/9/11 | - |
| 1 | MLY | M | 367 | 1 | - | 2/8/9/11 | - |
| 1 | MLY | A | 782 | 1 | - | 6/8/9/11 | - |
| 1 | MLY | M | 63 | 1 | - | 4/8/9/11 | - |
| 1 | MLY | G | 436 | 1 | - | 4/8/9/11 | - |
| 1 | MLY | M | 138 | 1 | - | 4/8/9/11 | - |
| 1 | MLY | M | 84 | 1 | - | 4/8/9/11 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|----------|-------|
| 1 | MLY | G | 296 | 1 | - | 4/8/9/11 | - |
| 1 | MLY | P | 613 | 1 | - | 4/8/9/11 | - |
| 1 | MLY | P | 504 | 1 | - | 4/8/9/11 | - |
| 1 | MLY | A | 827 | 1 | - | 0/8/9/11 | - |
| 1 | MLY | G | 839 | 1 | - | 3/8/9/11 | - |
| 1 | MLY | J | 768 | 1 | - | 4/8/9/11 | - |
| 1 | MLY | M | 504 | 1 | - | 4/8/9/11 | - |
| 1 | MLY | G | 613 | 1 | - | 4/8/9/11 | - |
| 1 | MLY | M | 782 | 1 | - | 6/8/9/11 | - |
| 1 | MLY | P | 528 | 1 | - | 5/8/9/11 | - |
| 1 | MLY | A | 528 | 1 | - | 5/8/9/11 | - |
| 1 | MLY | D | 19 | 1 | - | 4/8/9/11 | - |
| 1 | MLY | G | 30 | 1 | - | 2/8/9/11 | - |
| 1 | MLY | P | 84 | 1 | - | 4/8/9/11 | - |
| 1 | MLY | D | 236 | 1 | - | 3/8/9/11 | - |
| 1 | MLY | M | 415 | 1 | - | 3/8/9/11 | - |
| 1 | MLY | J | 87 | 1 | - | 2/8/9/11 | - |

All (79) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1 | G | 138 | MLY | CB-CA | -3.76 | 1.48 | 1.53 |
| 1 | D | 138 | MLY | CB-CA | -3.71 | 1.48 | 1.53 |
| 1 | M | 138 | MLY | CB-CA | -3.66 | 1.48 | 1.53 |
| 1 | A | 138 | MLY | CB-CA | -3.64 | 1.48 | 1.53 |
| 1 | J | 138 | MLY | CB-CA | -3.59 | 1.48 | 1.53 |
| 1 | P | 138 | MLY | CB-CA | -3.51 | 1.48 | 1.53 |
| 1 | J | 19 | MLY | CB-CA | -3.25 | 1.49 | 1.53 |
| 1 | D | 19 | MLY | CB-CA | -3.24 | 1.49 | 1.53 |
| 1 | P | 19 | MLY | CB-CA | -3.22 | 1.49 | 1.53 |
| 1 | G | 87 | MLY | CB-CA | -3.10 | 1.49 | 1.53 |
| 1 | J | 87 | MLY | CB-CA | -3.08 | 1.49 | 1.53 |
| 1 | M | 87 | MLY | CB-CA | -3.07 | 1.49 | 1.53 |
| 1 | A | 87 | MLY | CB-CA | -3.05 | 1.49 | 1.53 |
| 1 | P | 87 | MLY | CB-CA | -3.05 | 1.49 | 1.53 |
| 1 | M | 19 | MLY | CB-CA | -3.05 | 1.49 | 1.53 |
| 1 | D | 87 | MLY | CB-CA | -3.02 | 1.49 | 1.53 |
| 1 | D | 436 | MLY | CB-CA | -3.02 | 1.49 | 1.53 |
| 1 | G | 19 | MLY | CB-CA | -2.98 | 1.49 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1 | M | 436 | MLY | CB-CA | -2.96 | 1.49 | 1.53 |
| 1 | A | 19 | MLY | CB-CA | -2.90 | 1.49 | 1.53 |
| 1 | J | 436 | MLY | CB-CA | -2.90 | 1.49 | 1.53 |
| 1 | P | 436 | MLY | CB-CA | -2.89 | 1.49 | 1.53 |
| 1 | P | 49 | MLY | CB-CA | -2.89 | 1.49 | 1.53 |
| 1 | J | 49 | MLY | CB-CA | -2.85 | 1.49 | 1.53 |
| 1 | G | 436 | MLY | CB-CA | -2.84 | 1.49 | 1.53 |
| 1 | M | 272 | MLY | CB-CA | -2.83 | 1.49 | 1.53 |
| 1 | D | 49 | MLY | CB-CA | -2.80 | 1.49 | 1.53 |
| 1 | A | 436 | MLY | CB-CA | -2.80 | 1.49 | 1.53 |
| 1 | G | 49 | MLY | CB-CA | -2.77 | 1.49 | 1.53 |
| 1 | J | 272 | MLY | CB-CA | -2.76 | 1.49 | 1.53 |
| 1 | M | 49 | MLY | CB-CA | -2.74 | 1.49 | 1.53 |
| 1 | A | 272 | MLY | CB-CA | -2.70 | 1.50 | 1.53 |
| 1 | A | 49 | MLY | CB-CA | -2.66 | 1.50 | 1.53 |
| 1 | P | 272 | MLY | CB-CA | -2.64 | 1.50 | 1.53 |
| 1 | G | 272 | MLY | CB-CA | -2.64 | 1.50 | 1.53 |
| 1 | J | 190 | MLY | CB-CA | -2.56 | 1.50 | 1.53 |
| 1 | M | 833 | MLY | CB-CA | -2.54 | 1.50 | 1.53 |
| 1 | M | 190 | MLY | CB-CA | -2.54 | 1.50 | 1.53 |
| 1 | M | 385 | MLY | CB-CA | -2.53 | 1.50 | 1.53 |
| 1 | D | 272 | MLY | CB-CA | -2.52 | 1.50 | 1.53 |
| 1 | A | 190 | MLY | CB-CA | -2.51 | 1.50 | 1.53 |
| 1 | P | 190 | MLY | CB-CA | -2.51 | 1.50 | 1.53 |
| 1 | G | 190 | MLY | CB-CA | -2.47 | 1.50 | 1.53 |
| 1 | G | 385 | MLY | CB-CA | -2.47 | 1.50 | 1.53 |
| 1 | A | 385 | MLY | CB-CA | -2.45 | 1.50 | 1.53 |
| 1 | J | 385 | MLY | CB-CA | -2.44 | 1.50 | 1.53 |
| 1 | P | 385 | MLY | CB-CA | -2.41 | 1.50 | 1.53 |
| 1 | D | 190 | MLY | CB-CA | -2.34 | 1.50 | 1.53 |
| 1 | P | 617 | MLY | CB-CA | -2.33 | 1.50 | 1.53 |
| 1 | P | 833 | MLY | CB-CA | -2.33 | 1.50 | 1.53 |
| 1 | D | 385 | MLY | CB-CA | -2.33 | 1.50 | 1.53 |
| 1 | J | 833 | MLY | CB-CA | -2.32 | 1.50 | 1.53 |
| 1 | A | 833 | MLY | CB-CA | -2.30 | 1.50 | 1.53 |
| 1 | J | 505 | MLY | CB-CA | -2.29 | 1.50 | 1.53 |
| 1 | G | 833 | MLY | CB-CA | -2.29 | 1.50 | 1.53 |
| 1 | J | 617 | MLY | CB-CA | -2.29 | 1.50 | 1.53 |
| 1 | D | 617 | MLY | CB-CA | -2.28 | 1.50 | 1.53 |
| 1 | P | 505 | MLY | CB-CA | -2.27 | 1.50 | 1.53 |
| 1 | A | 598 | MLY | CB-CA | -2.27 | 1.50 | 1.53 |
| 1 | M | 505 | MLY | CB-CA | -2.27 | 1.50 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1 | M | 598 | MLY | CB-CA | -2.25 | 1.50 | 1.53 |
| 1 | P | 598 | MLY | CB-CA | -2.21 | 1.50 | 1.53 |
| 1 | G | 598 | MLY | CB-CA | -2.18 | 1.50 | 1.53 |
| 1 | A | 505 | MLY | CB-CA | -2.17 | 1.50 | 1.53 |
| 1 | J | 598 | MLY | CB-CA | -2.17 | 1.50 | 1.53 |
| 1 | D | 598 | MLY | CB-CA | -2.17 | 1.50 | 1.53 |
| 1 | M | 236 | MLY | CA-N | -2.16 | 1.41 | 1.48 |
| 1 | A | 236 | MLY | CA-N | -2.16 | 1.41 | 1.48 |
| 1 | M | 617 | MLY | CB-CA | -2.14 | 1.50 | 1.53 |
| 1 | D | 833 | MLY | CB-CA | -2.14 | 1.50 | 1.53 |
| 1 | G | 236 | MLY | CA-N | -2.13 | 1.41 | 1.48 |
| 1 | G | 617 | MLY | CB-CA | -2.13 | 1.50 | 1.53 |
| 1 | D | 236 | MLY | CA-N | -2.13 | 1.41 | 1.48 |
| 1 | P | 236 | MLY | CA-N | -2.12 | 1.41 | 1.48 |
| 1 | J | 236 | MLY | CA-N | -2.12 | 1.41 | 1.48 |
| 1 | A | 617 | MLY | CB-CA | -2.12 | 1.50 | 1.53 |
| 1 | D | 505 | MLY | CB-CA | -2.06 | 1.50 | 1.53 |
| 1 | D | 833 | MLY | CA-N | -2.02 | 1.42 | 1.48 |
| 1 | G | 505 | MLY | CB-CA | -2.01 | 1.50 | 1.53 |

There are no bond angle outliers.

There are no chirality outliers.

All (958) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|------------|
| 1 | A | 19 | MLY | C-CA-CB-CG |
| 1 | A | 49 | MLY | N-CA-CB-CG |
| 1 | A | 49 | MLY | C-CA-CB-CG |
| 1 | A | 55 | MLY | N-CA-CB-CG |
| 1 | A | 55 | MLY | C-CA-CB-CG |
| 1 | A | 84 | MLY | C-CA-CB-CG |
| 1 | A | 130 | MLY | C-CA-CB-CG |
| 1 | A | 248 | MLY | N-CA-CB-CG |
| 1 | A | 248 | MLY | C-CA-CB-CG |
| 1 | A | 348 | MLY | N-CA-CB-CG |
| 1 | A | 436 | MLY | C-CA-CB-CG |
| 1 | A | 486 | MLY | C-CA-CB-CG |
| 1 | A | 505 | MLY | N-CA-CB-CG |
| 1 | A | 505 | MLY | C-CA-CB-CG |
| 1 | A | 528 | MLY | C-CA-CB-CG |
| 1 | A | 551 | MLY | C-CA-CB-CG |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|------------|
| 1 | A | 553 | MLY | C-CA-CB-CG |
| 1 | A | 598 | MLY | N-CA-CB-CG |
| 1 | A | 598 | MLY | C-CA-CB-CG |
| 1 | A | 613 | MLY | N-CA-CB-CG |
| 1 | A | 613 | MLY | C-CA-CB-CG |
| 1 | A | 681 | MLY | C-CA-CB-CG |
| 1 | A | 782 | MLY | C-CA-CB-CG |
| 1 | A | 782 | MLY | O-C-CA-CB |
| 1 | D | 19 | MLY | C-CA-CB-CG |
| 1 | D | 49 | MLY | N-CA-CB-CG |
| 1 | D | 49 | MLY | C-CA-CB-CG |
| 1 | D | 55 | MLY | N-CA-CB-CG |
| 1 | D | 55 | MLY | C-CA-CB-CG |
| 1 | D | 84 | MLY | C-CA-CB-CG |
| 1 | D | 130 | MLY | C-CA-CB-CG |
| 1 | D | 248 | MLY | N-CA-CB-CG |
| 1 | D | 248 | MLY | C-CA-CB-CG |
| 1 | D | 436 | MLY | C-CA-CB-CG |
| 1 | D | 486 | MLY | C-CA-CB-CG |
| 1 | D | 505 | MLY | N-CA-CB-CG |
| 1 | D | 505 | MLY | C-CA-CB-CG |
| 1 | D | 528 | MLY | C-CA-CB-CG |
| 1 | D | 551 | MLY | C-CA-CB-CG |
| 1 | D | 553 | MLY | C-CA-CB-CG |
| 1 | D | 553 | MLY | O-C-CA-CB |
| 1 | D | 598 | MLY | N-CA-CB-CG |
| 1 | D | 598 | MLY | C-CA-CB-CG |
| 1 | D | 613 | MLY | N-CA-CB-CG |
| 1 | D | 613 | MLY | C-CA-CB-CG |
| 1 | D | 681 | MLY | C-CA-CB-CG |
| 1 | D | 782 | MLY | C-CA-CB-CG |
| 1 | D | 782 | MLY | O-C-CA-CB |
| 1 | G | 19 | MLY | C-CA-CB-CG |
| 1 | G | 49 | MLY | N-CA-CB-CG |
| 1 | G | 49 | MLY | C-CA-CB-CG |
| 1 | G | 55 | MLY | N-CA-CB-CG |
| 1 | G | 55 | MLY | C-CA-CB-CG |
| 1 | G | 84 | MLY | C-CA-CB-CG |
| 1 | G | 130 | MLY | C-CA-CB-CG |
| 1 | G | 248 | MLY | N-CA-CB-CG |
| 1 | G | 248 | MLY | C-CA-CB-CG |
| 1 | G | 348 | MLY | N-CA-CB-CG |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|------------|
| 1 | G | 436 | MLY | C-CA-CB-CG |
| 1 | G | 486 | MLY | C-CA-CB-CG |
| 1 | G | 505 | MLY | N-CA-CB-CG |
| 1 | G | 505 | MLY | C-CA-CB-CG |
| 1 | G | 528 | MLY | C-CA-CB-CG |
| 1 | G | 551 | MLY | C-CA-CB-CG |
| 1 | G | 553 | MLY | C-CA-CB-CG |
| 1 | G | 598 | MLY | N-CA-CB-CG |
| 1 | G | 598 | MLY | C-CA-CB-CG |
| 1 | G | 613 | MLY | N-CA-CB-CG |
| 1 | G | 613 | MLY | C-CA-CB-CG |
| 1 | G | 681 | MLY | C-CA-CB-CG |
| 1 | G | 782 | MLY | C-CA-CB-CG |
| 1 | G | 782 | MLY | O-C-CA-CB |
| 1 | J | 19 | MLY | C-CA-CB-CG |
| 1 | J | 49 | MLY | N-CA-CB-CG |
| 1 | J | 49 | MLY | C-CA-CB-CG |
| 1 | J | 55 | MLY | N-CA-CB-CG |
| 1 | J | 55 | MLY | C-CA-CB-CG |
| 1 | J | 84 | MLY | C-CA-CB-CG |
| 1 | J | 130 | MLY | C-CA-CB-CG |
| 1 | J | 248 | MLY | N-CA-CB-CG |
| 1 | J | 248 | MLY | C-CA-CB-CG |
| 1 | J | 348 | MLY | N-CA-CB-CG |
| 1 | J | 436 | MLY | C-CA-CB-CG |
| 1 | J | 486 | MLY | C-CA-CB-CG |
| 1 | J | 505 | MLY | N-CA-CB-CG |
| 1 | J | 505 | MLY | C-CA-CB-CG |
| 1 | J | 528 | MLY | C-CA-CB-CG |
| 1 | J | 551 | MLY | C-CA-CB-CG |
| 1 | J | 553 | MLY | C-CA-CB-CG |
| 1 | J | 598 | MLY | N-CA-CB-CG |
| 1 | J | 598 | MLY | C-CA-CB-CG |
| 1 | J | 613 | MLY | N-CA-CB-CG |
| 1 | J | 613 | MLY | C-CA-CB-CG |
| 1 | J | 681 | MLY | C-CA-CB-CG |
| 1 | J | 782 | MLY | C-CA-CB-CG |
| 1 | J | 782 | MLY | O-C-CA-CB |
| 1 | M | 19 | MLY | C-CA-CB-CG |
| 1 | M | 49 | MLY | N-CA-CB-CG |
| 1 | M | 49 | MLY | C-CA-CB-CG |
| 1 | M | 55 | MLY | N-CA-CB-CG |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|------------|
| 1 | M | 55 | MLY | C-CA-CB-CG |
| 1 | M | 84 | MLY | C-CA-CB-CG |
| 1 | M | 130 | MLY | C-CA-CB-CG |
| 1 | M | 248 | MLY | N-CA-CB-CG |
| 1 | M | 248 | MLY | C-CA-CB-CG |
| 1 | M | 348 | MLY | N-CA-CB-CG |
| 1 | M | 436 | MLY | C-CA-CB-CG |
| 1 | M | 486 | MLY | C-CA-CB-CG |
| 1 | M | 505 | MLY | N-CA-CB-CG |
| 1 | M | 505 | MLY | C-CA-CB-CG |
| 1 | M | 528 | MLY | C-CA-CB-CG |
| 1 | M | 551 | MLY | C-CA-CB-CG |
| 1 | M | 553 | MLY | C-CA-CB-CG |
| 1 | M | 598 | MLY | N-CA-CB-CG |
| 1 | M | 598 | MLY | C-CA-CB-CG |
| 1 | M | 613 | MLY | N-CA-CB-CG |
| 1 | M | 613 | MLY | C-CA-CB-CG |
| 1 | M | 681 | MLY | C-CA-CB-CG |
| 1 | M | 782 | MLY | C-CA-CB-CG |
| 1 | M | 782 | MLY | O-C-CA-CB |
| 1 | P | 19 | MLY | C-CA-CB-CG |
| 1 | P | 49 | MLY | N-CA-CB-CG |
| 1 | P | 49 | MLY | C-CA-CB-CG |
| 1 | P | 55 | MLY | N-CA-CB-CG |
| 1 | P | 55 | MLY | C-CA-CB-CG |
| 1 | P | 84 | MLY | C-CA-CB-CG |
| 1 | P | 130 | MLY | C-CA-CB-CG |
| 1 | P | 248 | MLY | N-CA-CB-CG |
| 1 | P | 248 | MLY | C-CA-CB-CG |
| 1 | P | 348 | MLY | N-CA-CB-CG |
| 1 | P | 436 | MLY | C-CA-CB-CG |
| 1 | P | 486 | MLY | C-CA-CB-CG |
| 1 | P | 505 | MLY | N-CA-CB-CG |
| 1 | P | 505 | MLY | C-CA-CB-CG |
| 1 | P | 528 | MLY | C-CA-CB-CG |
| 1 | P | 551 | MLY | C-CA-CB-CG |
| 1 | P | 553 | MLY | C-CA-CB-CG |
| 1 | P | 598 | MLY | N-CA-CB-CG |
| 1 | P | 598 | MLY | C-CA-CB-CG |
| 1 | P | 613 | MLY | N-CA-CB-CG |
| 1 | P | 613 | MLY | C-CA-CB-CG |
| 1 | P | 681 | MLY | C-CA-CB-CG |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|--------------|
| 1 | P | 782 | MLY | C-CA-CB-CG |
| 1 | P | 782 | MLY | O-C-CA-CB |
| 1 | A | 84 | MLY | CD-CE-NZ-CH1 |
| 1 | D | 84 | MLY | CD-CE-NZ-CH1 |
| 1 | G | 84 | MLY | CD-CE-NZ-CH1 |
| 1 | J | 84 | MLY | CD-CE-NZ-CH1 |
| 1 | M | 84 | MLY | CD-CE-NZ-CH1 |
| 1 | P | 84 | MLY | CD-CE-NZ-CH1 |
| 1 | A | 59 | MLY | CD-CE-NZ-CH1 |
| 1 | A | 59 | MLY | CD-CE-NZ-CH2 |
| 1 | A | 63 | MLY | CD-CE-NZ-CH1 |
| 1 | A | 84 | MLY | CD-CE-NZ-CH2 |
| 1 | A | 130 | MLY | CD-CE-NZ-CH1 |
| 1 | A | 130 | MLY | CD-CE-NZ-CH2 |
| 1 | A | 138 | MLY | CD-CE-NZ-CH1 |
| 1 | A | 138 | MLY | CD-CE-NZ-CH2 |
| 1 | A | 190 | MLY | CD-CE-NZ-CH1 |
| 1 | A | 190 | MLY | CD-CE-NZ-CH2 |
| 1 | A | 248 | MLY | CD-CE-NZ-CH1 |
| 1 | A | 272 | MLY | CD-CE-NZ-CH1 |
| 1 | A | 296 | MLY | CD-CE-NZ-CH1 |
| 1 | A | 296 | MLY | CD-CE-NZ-CH2 |
| 1 | A | 353 | MLY | CD-CE-NZ-CH1 |
| 1 | A | 353 | MLY | CD-CE-NZ-CH2 |
| 1 | A | 367 | MLY | CD-CE-NZ-CH2 |
| 1 | A | 385 | MLY | CD-CE-NZ-CH1 |
| 1 | A | 385 | MLY | CD-CE-NZ-CH2 |
| 1 | A | 431 | MLY | CD-CE-NZ-CH2 |
| 1 | A | 505 | MLY | CD-CE-NZ-CH2 |
| 1 | A | 528 | MLY | CD-CE-NZ-CH1 |
| 1 | A | 528 | MLY | CD-CE-NZ-CH2 |
| 1 | A | 553 | MLY | CD-CE-NZ-CH2 |
| 1 | A | 600 | MLY | CD-CE-NZ-CH2 |
| 1 | A | 764 | MLY | CD-CE-NZ-CH1 |
| 1 | A | 764 | MLY | CD-CE-NZ-CH2 |
| 1 | A | 768 | MLY | CD-CE-NZ-CH1 |
| 1 | A | 782 | MLY | CD-CE-NZ-CH1 |
| 1 | A | 782 | MLY | CD-CE-NZ-CH2 |
| 1 | A | 833 | MLY | CD-CE-NZ-CH1 |
| 1 | A | 833 | MLY | CD-CE-NZ-CH2 |
| 1 | A | 837 | MLY | CD-CE-NZ-CH1 |
| 1 | A | 837 | MLY | CD-CE-NZ-CH2 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|--------------|
| 1 | A | 839 | MLY | CD-CE-NZ-CH2 |
| 1 | D | 55 | MLY | CD-CE-NZ-CH2 |
| 1 | D | 59 | MLY | CD-CE-NZ-CH1 |
| 1 | D | 59 | MLY | CD-CE-NZ-CH2 |
| 1 | D | 63 | MLY | CD-CE-NZ-CH1 |
| 1 | D | 84 | MLY | CD-CE-NZ-CH2 |
| 1 | D | 130 | MLY | CD-CE-NZ-CH1 |
| 1 | D | 130 | MLY | CD-CE-NZ-CH2 |
| 1 | D | 138 | MLY | CD-CE-NZ-CH1 |
| 1 | D | 138 | MLY | CD-CE-NZ-CH2 |
| 1 | D | 190 | MLY | CD-CE-NZ-CH2 |
| 1 | D | 248 | MLY | CD-CE-NZ-CH1 |
| 1 | D | 272 | MLY | CD-CE-NZ-CH1 |
| 1 | D | 296 | MLY | CD-CE-NZ-CH1 |
| 1 | D | 296 | MLY | CD-CE-NZ-CH2 |
| 1 | D | 353 | MLY | CD-CE-NZ-CH1 |
| 1 | D | 353 | MLY | CD-CE-NZ-CH2 |
| 1 | D | 367 | MLY | CD-CE-NZ-CH2 |
| 1 | D | 385 | MLY | CD-CE-NZ-CH1 |
| 1 | D | 385 | MLY | CD-CE-NZ-CH2 |
| 1 | D | 431 | MLY | CD-CE-NZ-CH2 |
| 1 | D | 505 | MLY | CD-CE-NZ-CH2 |
| 1 | D | 528 | MLY | CD-CE-NZ-CH1 |
| 1 | D | 528 | MLY | CD-CE-NZ-CH2 |
| 1 | D | 553 | MLY | CD-CE-NZ-CH2 |
| 1 | D | 600 | MLY | CD-CE-NZ-CH2 |
| 1 | D | 764 | MLY | CD-CE-NZ-CH1 |
| 1 | D | 764 | MLY | CD-CE-NZ-CH2 |
| 1 | D | 768 | MLY | CD-CE-NZ-CH1 |
| 1 | D | 782 | MLY | CD-CE-NZ-CH1 |
| 1 | D | 782 | MLY | CD-CE-NZ-CH2 |
| 1 | D | 833 | MLY | CD-CE-NZ-CH1 |
| 1 | D | 833 | MLY | CD-CE-NZ-CH2 |
| 1 | D | 837 | MLY | CD-CE-NZ-CH1 |
| 1 | D | 837 | MLY | CD-CE-NZ-CH2 |
| 1 | D | 839 | MLY | CD-CE-NZ-CH2 |
| 1 | G | 59 | MLY | CD-CE-NZ-CH1 |
| 1 | G | 59 | MLY | CD-CE-NZ-CH2 |
| 1 | G | 63 | MLY | CD-CE-NZ-CH1 |
| 1 | G | 84 | MLY | CD-CE-NZ-CH2 |
| 1 | G | 130 | MLY | CD-CE-NZ-CH1 |
| 1 | G | 130 | MLY | CD-CE-NZ-CH2 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|--------------|
| 1 | G | 138 | MLY | CD-CE-NZ-CH1 |
| 1 | G | 138 | MLY | CD-CE-NZ-CH2 |
| 1 | G | 190 | MLY | CD-CE-NZ-CH2 |
| 1 | G | 248 | MLY | CD-CE-NZ-CH1 |
| 1 | G | 272 | MLY | CD-CE-NZ-CH1 |
| 1 | G | 296 | MLY | CD-CE-NZ-CH1 |
| 1 | G | 296 | MLY | CD-CE-NZ-CH2 |
| 1 | G | 353 | MLY | CD-CE-NZ-CH1 |
| 1 | G | 353 | MLY | CD-CE-NZ-CH2 |
| 1 | G | 385 | MLY | CD-CE-NZ-CH1 |
| 1 | G | 385 | MLY | CD-CE-NZ-CH2 |
| 1 | G | 431 | MLY | CD-CE-NZ-CH2 |
| 1 | G | 505 | MLY | CD-CE-NZ-CH2 |
| 1 | G | 528 | MLY | CD-CE-NZ-CH1 |
| 1 | G | 528 | MLY | CD-CE-NZ-CH2 |
| 1 | G | 553 | MLY | CD-CE-NZ-CH2 |
| 1 | G | 600 | MLY | CD-CE-NZ-CH2 |
| 1 | G | 764 | MLY | CD-CE-NZ-CH1 |
| 1 | G | 764 | MLY | CD-CE-NZ-CH2 |
| 1 | G | 768 | MLY | CD-CE-NZ-CH1 |
| 1 | G | 782 | MLY | CD-CE-NZ-CH1 |
| 1 | G | 782 | MLY | CD-CE-NZ-CH2 |
| 1 | G | 833 | MLY | CD-CE-NZ-CH1 |
| 1 | G | 833 | MLY | CD-CE-NZ-CH2 |
| 1 | G | 837 | MLY | CD-CE-NZ-CH1 |
| 1 | G | 837 | MLY | CD-CE-NZ-CH2 |
| 1 | G | 839 | MLY | CD-CE-NZ-CH2 |
| 1 | J | 55 | MLY | CD-CE-NZ-CH2 |
| 1 | J | 59 | MLY | CD-CE-NZ-CH1 |
| 1 | J | 59 | MLY | CD-CE-NZ-CH2 |
| 1 | J | 63 | MLY | CD-CE-NZ-CH1 |
| 1 | J | 84 | MLY | CD-CE-NZ-CH2 |
| 1 | J | 130 | MLY | CD-CE-NZ-CH1 |
| 1 | J | 130 | MLY | CD-CE-NZ-CH2 |
| 1 | J | 138 | MLY | CD-CE-NZ-CH1 |
| 1 | J | 138 | MLY | CD-CE-NZ-CH2 |
| 1 | J | 190 | MLY | CD-CE-NZ-CH2 |
| 1 | J | 248 | MLY | CD-CE-NZ-CH1 |
| 1 | J | 272 | MLY | CD-CE-NZ-CH1 |
| 1 | J | 296 | MLY | CD-CE-NZ-CH1 |
| 1 | J | 296 | MLY | CD-CE-NZ-CH2 |
| 1 | J | 353 | MLY | CD-CE-NZ-CH1 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|--------------|
| 1 | J | 353 | MLY | CD-CE-NZ-CH2 |
| 1 | J | 367 | MLY | CD-CE-NZ-CH2 |
| 1 | J | 385 | MLY | CD-CE-NZ-CH1 |
| 1 | J | 385 | MLY | CD-CE-NZ-CH2 |
| 1 | J | 431 | MLY | CD-CE-NZ-CH2 |
| 1 | J | 505 | MLY | CD-CE-NZ-CH2 |
| 1 | J | 528 | MLY | CD-CE-NZ-CH1 |
| 1 | J | 528 | MLY | CD-CE-NZ-CH2 |
| 1 | J | 553 | MLY | CD-CE-NZ-CH2 |
| 1 | J | 600 | MLY | CD-CE-NZ-CH2 |
| 1 | J | 764 | MLY | CD-CE-NZ-CH1 |
| 1 | J | 764 | MLY | CD-CE-NZ-CH2 |
| 1 | J | 768 | MLY | CD-CE-NZ-CH1 |
| 1 | J | 782 | MLY | CD-CE-NZ-CH1 |
| 1 | J | 782 | MLY | CD-CE-NZ-CH2 |
| 1 | J | 833 | MLY | CD-CE-NZ-CH1 |
| 1 | J | 833 | MLY | CD-CE-NZ-CH2 |
| 1 | J | 837 | MLY | CD-CE-NZ-CH1 |
| 1 | J | 837 | MLY | CD-CE-NZ-CH2 |
| 1 | J | 839 | MLY | CD-CE-NZ-CH2 |
| 1 | M | 59 | MLY | CD-CE-NZ-CH1 |
| 1 | M | 59 | MLY | CD-CE-NZ-CH2 |
| 1 | M | 63 | MLY | CD-CE-NZ-CH1 |
| 1 | M | 84 | MLY | CD-CE-NZ-CH2 |
| 1 | M | 130 | MLY | CD-CE-NZ-CH1 |
| 1 | M | 130 | MLY | CD-CE-NZ-CH2 |
| 1 | M | 138 | MLY | CD-CE-NZ-CH1 |
| 1 | M | 138 | MLY | CD-CE-NZ-CH2 |
| 1 | M | 190 | MLY | CD-CE-NZ-CH2 |
| 1 | M | 248 | MLY | CD-CE-NZ-CH1 |
| 1 | M | 272 | MLY | CD-CE-NZ-CH1 |
| 1 | M | 296 | MLY | CD-CE-NZ-CH1 |
| 1 | M | 296 | MLY | CD-CE-NZ-CH2 |
| 1 | M | 353 | MLY | CD-CE-NZ-CH1 |
| 1 | M | 353 | MLY | CD-CE-NZ-CH2 |
| 1 | M | 367 | MLY | CD-CE-NZ-CH2 |
| 1 | M | 385 | MLY | CD-CE-NZ-CH1 |
| 1 | M | 385 | MLY | CD-CE-NZ-CH2 |
| 1 | M | 431 | MLY | CD-CE-NZ-CH2 |
| 1 | M | 505 | MLY | CD-CE-NZ-CH2 |
| 1 | M | 528 | MLY | CD-CE-NZ-CH1 |
| 1 | M | 528 | MLY | CD-CE-NZ-CH2 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|--------------|
| 1 | M | 553 | MLY | CD-CE-NZ-CH2 |
| 1 | M | 600 | MLY | CD-CE-NZ-CH2 |
| 1 | M | 764 | MLY | CD-CE-NZ-CH1 |
| 1 | M | 764 | MLY | CD-CE-NZ-CH2 |
| 1 | M | 768 | MLY | CD-CE-NZ-CH1 |
| 1 | M | 782 | MLY | CD-CE-NZ-CH1 |
| 1 | M | 782 | MLY | CD-CE-NZ-CH2 |
| 1 | M | 833 | MLY | CD-CE-NZ-CH1 |
| 1 | M | 833 | MLY | CD-CE-NZ-CH2 |
| 1 | M | 837 | MLY | CD-CE-NZ-CH1 |
| 1 | M | 837 | MLY | CD-CE-NZ-CH2 |
| 1 | M | 839 | MLY | CD-CE-NZ-CH2 |
| 1 | P | 55 | MLY | CD-CE-NZ-CH2 |
| 1 | P | 59 | MLY | CD-CE-NZ-CH1 |
| 1 | P | 59 | MLY | CD-CE-NZ-CH2 |
| 1 | P | 63 | MLY | CD-CE-NZ-CH1 |
| 1 | P | 84 | MLY | CD-CE-NZ-CH2 |
| 1 | P | 130 | MLY | CD-CE-NZ-CH1 |
| 1 | P | 130 | MLY | CD-CE-NZ-CH2 |
| 1 | P | 138 | MLY | CD-CE-NZ-CH1 |
| 1 | P | 138 | MLY | CD-CE-NZ-CH2 |
| 1 | P | 190 | MLY | CD-CE-NZ-CH2 |
| 1 | P | 248 | MLY | CD-CE-NZ-CH1 |
| 1 | P | 272 | MLY | CD-CE-NZ-CH1 |
| 1 | P | 296 | MLY | CD-CE-NZ-CH1 |
| 1 | P | 296 | MLY | CD-CE-NZ-CH2 |
| 1 | P | 353 | MLY | CD-CE-NZ-CH1 |
| 1 | P | 353 | MLY | CD-CE-NZ-CH2 |
| 1 | P | 367 | MLY | CD-CE-NZ-CH2 |
| 1 | P | 385 | MLY | CD-CE-NZ-CH1 |
| 1 | P | 385 | MLY | CD-CE-NZ-CH2 |
| 1 | P | 431 | MLY | CD-CE-NZ-CH2 |
| 1 | P | 505 | MLY | CD-CE-NZ-CH2 |
| 1 | P | 528 | MLY | CD-CE-NZ-CH1 |
| 1 | P | 528 | MLY | CD-CE-NZ-CH2 |
| 1 | P | 553 | MLY | CD-CE-NZ-CH2 |
| 1 | P | 600 | MLY | CD-CE-NZ-CH2 |
| 1 | P | 764 | MLY | CD-CE-NZ-CH1 |
| 1 | P | 764 | MLY | CD-CE-NZ-CH2 |
| 1 | P | 768 | MLY | CD-CE-NZ-CH1 |
| 1 | P | 782 | MLY | CD-CE-NZ-CH1 |
| 1 | P | 782 | MLY | CD-CE-NZ-CH2 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|--------------|
| 1 | P | 833 | MLY | CD-CE-NZ-CH1 |
| 1 | P | 833 | MLY | CD-CE-NZ-CH2 |
| 1 | P | 837 | MLY | CD-CE-NZ-CH1 |
| 1 | P | 837 | MLY | CD-CE-NZ-CH2 |
| 1 | P | 839 | MLY | CD-CE-NZ-CH2 |
| 1 | A | 659 | MLY | CG-CD-CE-NZ |
| 1 | G | 659 | MLY | CG-CD-CE-NZ |
| 1 | J | 659 | MLY | CG-CD-CE-NZ |
| 1 | M | 659 | MLY | CG-CD-CE-NZ |
| 1 | P | 659 | MLY | CG-CD-CE-NZ |
| 1 | A | 35 | MLY | CG-CD-CE-NZ |
| 1 | A | 87 | MLY | CG-CD-CE-NZ |
| 1 | D | 35 | MLY | CG-CD-CE-NZ |
| 1 | D | 87 | MLY | CG-CD-CE-NZ |
| 1 | D | 659 | MLY | CG-CD-CE-NZ |
| 1 | G | 35 | MLY | CG-CD-CE-NZ |
| 1 | G | 87 | MLY | CG-CD-CE-NZ |
| 1 | J | 87 | MLY | CG-CD-CE-NZ |
| 1 | M | 87 | MLY | CG-CD-CE-NZ |
| 1 | P | 87 | MLY | CG-CD-CE-NZ |
| 1 | J | 35 | MLY | CG-CD-CE-NZ |
| 1 | M | 35 | MLY | CG-CD-CE-NZ |
| 1 | P | 35 | MLY | CG-CD-CE-NZ |
| 1 | A | 295 | MLY | CG-CD-CE-NZ |
| 1 | D | 295 | MLY | CG-CD-CE-NZ |
| 1 | G | 295 | MLY | CG-CD-CE-NZ |
| 1 | J | 295 | MLY | CG-CD-CE-NZ |
| 1 | M | 295 | MLY | CG-CD-CE-NZ |
| 1 | P | 295 | MLY | CG-CD-CE-NZ |
| 1 | A | 138 | MLY | CG-CD-CE-NZ |
| 1 | A | 782 | MLY | CG-CD-CE-NZ |
| 1 | D | 782 | MLY | CG-CD-CE-NZ |
| 1 | G | 782 | MLY | CG-CD-CE-NZ |
| 1 | J | 782 | MLY | CG-CD-CE-NZ |
| 1 | M | 782 | MLY | CG-CD-CE-NZ |
| 1 | P | 138 | MLY | CG-CD-CE-NZ |
| 1 | P | 782 | MLY | CG-CD-CE-NZ |
| 1 | D | 138 | MLY | CG-CD-CE-NZ |
| 1 | J | 138 | MLY | CG-CD-CE-NZ |
| 1 | M | 138 | MLY | CG-CD-CE-NZ |
| 1 | G | 138 | MLY | CG-CD-CE-NZ |
| 1 | A | 55 | MLY | CD-CE-NZ-CH2 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|--------------|
| 1 | A | 248 | MLY | CD-CE-NZ-CH2 |
| 1 | A | 272 | MLY | CD-CE-NZ-CH2 |
| 1 | A | 348 | MLY | CD-CE-NZ-CH1 |
| 1 | A | 348 | MLY | CD-CE-NZ-CH2 |
| 1 | A | 367 | MLY | CD-CE-NZ-CH1 |
| 1 | A | 431 | MLY | CD-CE-NZ-CH1 |
| 1 | A | 504 | MLY | CD-CE-NZ-CH1 |
| 1 | A | 504 | MLY | CD-CE-NZ-CH2 |
| 1 | A | 505 | MLY | CD-CE-NZ-CH1 |
| 1 | A | 600 | MLY | CD-CE-NZ-CH1 |
| 1 | A | 659 | MLY | CD-CE-NZ-CH2 |
| 1 | D | 190 | MLY | CD-CE-NZ-CH1 |
| 1 | D | 248 | MLY | CD-CE-NZ-CH2 |
| 1 | D | 272 | MLY | CD-CE-NZ-CH2 |
| 1 | D | 348 | MLY | CD-CE-NZ-CH1 |
| 1 | D | 348 | MLY | CD-CE-NZ-CH2 |
| 1 | D | 367 | MLY | CD-CE-NZ-CH1 |
| 1 | D | 431 | MLY | CD-CE-NZ-CH1 |
| 1 | D | 504 | MLY | CD-CE-NZ-CH1 |
| 1 | D | 504 | MLY | CD-CE-NZ-CH2 |
| 1 | D | 505 | MLY | CD-CE-NZ-CH1 |
| 1 | D | 600 | MLY | CD-CE-NZ-CH1 |
| 1 | D | 659 | MLY | CD-CE-NZ-CH2 |
| 1 | G | 55 | MLY | CD-CE-NZ-CH2 |
| 1 | G | 190 | MLY | CD-CE-NZ-CH1 |
| 1 | G | 248 | MLY | CD-CE-NZ-CH2 |
| 1 | G | 272 | MLY | CD-CE-NZ-CH2 |
| 1 | G | 348 | MLY | CD-CE-NZ-CH1 |
| 1 | G | 348 | MLY | CD-CE-NZ-CH2 |
| 1 | G | 367 | MLY | CD-CE-NZ-CH1 |
| 1 | G | 367 | MLY | CD-CE-NZ-CH2 |
| 1 | G | 431 | MLY | CD-CE-NZ-CH1 |
| 1 | G | 504 | MLY | CD-CE-NZ-CH1 |
| 1 | G | 504 | MLY | CD-CE-NZ-CH2 |
| 1 | G | 505 | MLY | CD-CE-NZ-CH1 |
| 1 | G | 600 | MLY | CD-CE-NZ-CH1 |
| 1 | G | 659 | MLY | CD-CE-NZ-CH2 |
| 1 | J | 190 | MLY | CD-CE-NZ-CH1 |
| 1 | J | 248 | MLY | CD-CE-NZ-CH2 |
| 1 | J | 348 | MLY | CD-CE-NZ-CH1 |
| 1 | J | 348 | MLY | CD-CE-NZ-CH2 |
| 1 | J | 367 | MLY | CD-CE-NZ-CH1 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|--------------|
| 1 | J | 431 | MLY | CD-CE-NZ-CH1 |
| 1 | J | 504 | MLY | CD-CE-NZ-CH1 |
| 1 | J | 504 | MLY | CD-CE-NZ-CH2 |
| 1 | J | 505 | MLY | CD-CE-NZ-CH1 |
| 1 | J | 600 | MLY | CD-CE-NZ-CH1 |
| 1 | J | 659 | MLY | CD-CE-NZ-CH2 |
| 1 | M | 55 | MLY | CD-CE-NZ-CH2 |
| 1 | M | 190 | MLY | CD-CE-NZ-CH1 |
| 1 | M | 248 | MLY | CD-CE-NZ-CH2 |
| 1 | M | 348 | MLY | CD-CE-NZ-CH1 |
| 1 | M | 348 | MLY | CD-CE-NZ-CH2 |
| 1 | M | 367 | MLY | CD-CE-NZ-CH1 |
| 1 | M | 431 | MLY | CD-CE-NZ-CH1 |
| 1 | M | 504 | MLY | CD-CE-NZ-CH1 |
| 1 | M | 504 | MLY | CD-CE-NZ-CH2 |
| 1 | M | 505 | MLY | CD-CE-NZ-CH1 |
| 1 | M | 600 | MLY | CD-CE-NZ-CH1 |
| 1 | M | 659 | MLY | CD-CE-NZ-CH2 |
| 1 | P | 190 | MLY | CD-CE-NZ-CH1 |
| 1 | P | 248 | MLY | CD-CE-NZ-CH2 |
| 1 | P | 348 | MLY | CD-CE-NZ-CH1 |
| 1 | P | 348 | MLY | CD-CE-NZ-CH2 |
| 1 | P | 367 | MLY | CD-CE-NZ-CH1 |
| 1 | P | 431 | MLY | CD-CE-NZ-CH1 |
| 1 | P | 504 | MLY | CD-CE-NZ-CH1 |
| 1 | P | 504 | MLY | CD-CE-NZ-CH2 |
| 1 | P | 505 | MLY | CD-CE-NZ-CH1 |
| 1 | P | 600 | MLY | CD-CE-NZ-CH1 |
| 1 | P | 659 | MLY | CD-CE-NZ-CH2 |
| 1 | A | 130 | MLY | CG-CD-CE-NZ |
| 1 | A | 84 | MLY | CG-CD-CE-NZ |
| 1 | D | 130 | MLY | CG-CD-CE-NZ |
| 1 | G | 84 | MLY | CG-CD-CE-NZ |
| 1 | G | 130 | MLY | CG-CD-CE-NZ |
| 1 | J | 84 | MLY | CG-CD-CE-NZ |
| 1 | J | 130 | MLY | CG-CD-CE-NZ |
| 1 | M | 84 | MLY | CG-CD-CE-NZ |
| 1 | M | 130 | MLY | CG-CD-CE-NZ |
| 1 | P | 84 | MLY | CG-CD-CE-NZ |
| 1 | P | 130 | MLY | CG-CD-CE-NZ |
| 1 | A | 504 | MLY | CG-CD-CE-NZ |
| 1 | G | 504 | MLY | CG-CD-CE-NZ |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|--------------|
| 1 | M | 504 | MLY | CG-CD-CE-NZ |
| 1 | A | 681 | MLY | CG-CD-CE-NZ |
| 1 | D | 84 | MLY | CG-CD-CE-NZ |
| 1 | D | 504 | MLY | CG-CD-CE-NZ |
| 1 | D | 681 | MLY | CG-CD-CE-NZ |
| 1 | G | 681 | MLY | CG-CD-CE-NZ |
| 1 | J | 681 | MLY | CG-CD-CE-NZ |
| 1 | P | 681 | MLY | CG-CD-CE-NZ |
| 1 | A | 295 | MLY | CA-CB-CG-CD |
| 1 | D | 295 | MLY | CA-CB-CG-CD |
| 1 | G | 295 | MLY | CA-CB-CG-CD |
| 1 | J | 295 | MLY | CA-CB-CG-CD |
| 1 | M | 295 | MLY | CA-CB-CG-CD |
| 1 | P | 295 | MLY | CA-CB-CG-CD |
| 1 | J | 504 | MLY | CG-CD-CE-NZ |
| 1 | M | 681 | MLY | CG-CD-CE-NZ |
| 1 | P | 504 | MLY | CG-CD-CE-NZ |
| 1 | A | 107 | MLY | CD-CE-NZ-CH1 |
| 1 | A | 369 | MLY | CD-CE-NZ-CH2 |
| 1 | A | 768 | MLY | CD-CE-NZ-CH2 |
| 1 | D | 107 | MLY | CD-CE-NZ-CH1 |
| 1 | D | 369 | MLY | CD-CE-NZ-CH2 |
| 1 | D | 768 | MLY | CD-CE-NZ-CH2 |
| 1 | G | 107 | MLY | CD-CE-NZ-CH1 |
| 1 | G | 369 | MLY | CD-CE-NZ-CH2 |
| 1 | G | 768 | MLY | CD-CE-NZ-CH2 |
| 1 | J | 107 | MLY | CD-CE-NZ-CH1 |
| 1 | J | 369 | MLY | CD-CE-NZ-CH2 |
| 1 | J | 768 | MLY | CD-CE-NZ-CH2 |
| 1 | M | 107 | MLY | CD-CE-NZ-CH1 |
| 1 | M | 369 | MLY | CD-CE-NZ-CH2 |
| 1 | M | 768 | MLY | CD-CE-NZ-CH2 |
| 1 | P | 107 | MLY | CD-CE-NZ-CH1 |
| 1 | P | 369 | MLY | CD-CE-NZ-CH2 |
| 1 | P | 768 | MLY | CD-CE-NZ-CH2 |
| 1 | A | 598 | MLY | CG-CD-CE-NZ |
| 1 | G | 598 | MLY | CG-CD-CE-NZ |
| 1 | J | 598 | MLY | CG-CD-CE-NZ |
| 1 | M | 598 | MLY | CG-CD-CE-NZ |
| 1 | P | 598 | MLY | CG-CD-CE-NZ |
| 1 | D | 598 | MLY | CG-CD-CE-NZ |
| 1 | A | 504 | MLY | CA-CB-CG-CD |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|--------------|
| 1 | A | 768 | MLY | CA-CB-CG-CD |
| 1 | D | 504 | MLY | CA-CB-CG-CD |
| 1 | D | 768 | MLY | CA-CB-CG-CD |
| 1 | G | 504 | MLY | CA-CB-CG-CD |
| 1 | G | 768 | MLY | CA-CB-CG-CD |
| 1 | J | 504 | MLY | CA-CB-CG-CD |
| 1 | J | 768 | MLY | CA-CB-CG-CD |
| 1 | M | 504 | MLY | CA-CB-CG-CD |
| 1 | M | 768 | MLY | CA-CB-CG-CD |
| 1 | P | 504 | MLY | CA-CB-CG-CD |
| 1 | P | 768 | MLY | CA-CB-CG-CD |
| 1 | A | 63 | MLY | CD-CE-NZ-CH2 |
| 1 | A | 87 | MLY | CD-CE-NZ-CH1 |
| 1 | A | 415 | MLY | CD-CE-NZ-CH1 |
| 1 | A | 415 | MLY | CD-CE-NZ-CH2 |
| 1 | A | 553 | MLY | CD-CE-NZ-CH1 |
| 1 | A | 659 | MLY | CD-CE-NZ-CH1 |
| 1 | D | 55 | MLY | CD-CE-NZ-CH1 |
| 1 | D | 63 | MLY | CD-CE-NZ-CH2 |
| 1 | D | 87 | MLY | CD-CE-NZ-CH1 |
| 1 | D | 415 | MLY | CD-CE-NZ-CH1 |
| 1 | D | 415 | MLY | CD-CE-NZ-CH2 |
| 1 | D | 553 | MLY | CD-CE-NZ-CH1 |
| 1 | D | 659 | MLY | CD-CE-NZ-CH1 |
| 1 | G | 55 | MLY | CD-CE-NZ-CH1 |
| 1 | G | 63 | MLY | CD-CE-NZ-CH2 |
| 1 | G | 415 | MLY | CD-CE-NZ-CH1 |
| 1 | G | 415 | MLY | CD-CE-NZ-CH2 |
| 1 | G | 553 | MLY | CD-CE-NZ-CH1 |
| 1 | G | 659 | MLY | CD-CE-NZ-CH1 |
| 1 | J | 55 | MLY | CD-CE-NZ-CH1 |
| 1 | J | 63 | MLY | CD-CE-NZ-CH2 |
| 1 | J | 87 | MLY | CD-CE-NZ-CH1 |
| 1 | J | 272 | MLY | CD-CE-NZ-CH2 |
| 1 | J | 415 | MLY | CD-CE-NZ-CH1 |
| 1 | J | 415 | MLY | CD-CE-NZ-CH2 |
| 1 | J | 553 | MLY | CD-CE-NZ-CH1 |
| 1 | J | 659 | MLY | CD-CE-NZ-CH1 |
| 1 | M | 63 | MLY | CD-CE-NZ-CH2 |
| 1 | M | 87 | MLY | CD-CE-NZ-CH1 |
| 1 | M | 272 | MLY | CD-CE-NZ-CH2 |
| 1 | M | 415 | MLY | CD-CE-NZ-CH1 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|--------------|
| 1 | M | 415 | MLY | CD-CE-NZ-CH2 |
| 1 | M | 553 | MLY | CD-CE-NZ-CH1 |
| 1 | M | 659 | MLY | CD-CE-NZ-CH1 |
| 1 | P | 55 | MLY | CD-CE-NZ-CH1 |
| 1 | P | 63 | MLY | CD-CE-NZ-CH2 |
| 1 | P | 87 | MLY | CD-CE-NZ-CH1 |
| 1 | P | 272 | MLY | CD-CE-NZ-CH2 |
| 1 | P | 415 | MLY | CD-CE-NZ-CH1 |
| 1 | P | 415 | MLY | CD-CE-NZ-CH2 |
| 1 | P | 553 | MLY | CD-CE-NZ-CH1 |
| 1 | P | 659 | MLY | CD-CE-NZ-CH1 |
| 1 | A | 415 | MLY | CA-CB-CG-CD |
| 1 | G | 415 | MLY | CA-CB-CG-CD |
| 1 | M | 415 | MLY | CA-CB-CG-CD |
| 1 | A | 19 | MLY | CD-CE-NZ-CH2 |
| 1 | A | 55 | MLY | CD-CE-NZ-CH1 |
| 1 | D | 19 | MLY | CD-CE-NZ-CH2 |
| 1 | G | 19 | MLY | CD-CE-NZ-CH2 |
| 1 | G | 87 | MLY | CD-CE-NZ-CH1 |
| 1 | J | 19 | MLY | CD-CE-NZ-CH2 |
| 1 | M | 19 | MLY | CD-CE-NZ-CH2 |
| 1 | M | 55 | MLY | CD-CE-NZ-CH1 |
| 1 | P | 19 | MLY | CD-CE-NZ-CH2 |
| 1 | D | 551 | MLY | CG-CD-CE-NZ |
| 1 | G | 551 | MLY | CG-CD-CE-NZ |
| 1 | J | 551 | MLY | CG-CD-CE-NZ |
| 1 | M | 551 | MLY | CG-CD-CE-NZ |
| 1 | P | 551 | MLY | CG-CD-CE-NZ |
| 1 | A | 551 | MLY | CG-CD-CE-NZ |
| 1 | D | 415 | MLY | CA-CB-CG-CD |
| 1 | J | 415 | MLY | CA-CB-CG-CD |
| 1 | P | 415 | MLY | CA-CB-CG-CD |
| 1 | A | 272 | MLY | CE-CD-CG-CB |
| 1 | D | 272 | MLY | CE-CD-CG-CB |
| 1 | G | 272 | MLY | CE-CD-CG-CB |
| 1 | J | 272 | MLY | CE-CD-CG-CB |
| 1 | M | 272 | MLY | CE-CD-CG-CB |
| 1 | P | 272 | MLY | CE-CD-CG-CB |
| 1 | A | 30 | MLY | CE-CD-CG-CB |
| 1 | A | 296 | MLY | CE-CD-CG-CB |
| 1 | D | 30 | MLY | CE-CD-CG-CB |
| 1 | D | 296 | MLY | CE-CD-CG-CB |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|--------------|
| 1 | G | 296 | MLY | CE-CD-CG-CB |
| 1 | J | 30 | MLY | CE-CD-CG-CB |
| 1 | J | 296 | MLY | CE-CD-CG-CB |
| 1 | M | 296 | MLY | CE-CD-CG-CB |
| 1 | P | 30 | MLY | CE-CD-CG-CB |
| 1 | P | 296 | MLY | CE-CD-CG-CB |
| 1 | A | 505 | MLY | CE-CD-CG-CB |
| 1 | D | 505 | MLY | CE-CD-CG-CB |
| 1 | G | 505 | MLY | CE-CD-CG-CB |
| 1 | J | 505 | MLY | CE-CD-CG-CB |
| 1 | M | 505 | MLY | CE-CD-CG-CB |
| 1 | P | 505 | MLY | CE-CD-CG-CB |
| 1 | A | 839 | MLY | CD-CE-NZ-CH1 |
| 1 | D | 839 | MLY | CD-CE-NZ-CH1 |
| 1 | G | 839 | MLY | CD-CE-NZ-CH1 |
| 1 | J | 107 | MLY | CD-CE-NZ-CH2 |
| 1 | J | 839 | MLY | CD-CE-NZ-CH1 |
| 1 | M | 107 | MLY | CD-CE-NZ-CH2 |
| 1 | M | 839 | MLY | CD-CE-NZ-CH1 |
| 1 | P | 107 | MLY | CD-CE-NZ-CH2 |
| 1 | P | 839 | MLY | CD-CE-NZ-CH1 |
| 1 | A | 681 | MLY | CE-CD-CG-CB |
| 1 | D | 681 | MLY | CE-CD-CG-CB |
| 1 | G | 30 | MLY | CE-CD-CG-CB |
| 1 | G | 681 | MLY | CE-CD-CG-CB |
| 1 | J | 681 | MLY | CE-CD-CG-CB |
| 1 | M | 30 | MLY | CE-CD-CG-CB |
| 1 | P | 681 | MLY | CE-CD-CG-CB |
| 1 | D | 49 | MLY | CE-CD-CG-CB |
| 1 | G | 49 | MLY | CE-CD-CG-CB |
| 1 | J | 49 | MLY | CE-CD-CG-CB |
| 1 | M | 681 | MLY | CE-CD-CG-CB |
| 1 | A | 49 | MLY | CE-CD-CG-CB |
| 1 | M | 49 | MLY | CE-CD-CG-CB |
| 1 | P | 49 | MLY | CE-CD-CG-CB |
| 1 | J | 353 | MLY | CE-CD-CG-CB |
| 1 | M | 353 | MLY | CE-CD-CG-CB |
| 1 | D | 353 | MLY | CE-CD-CG-CB |
| 1 | P | 353 | MLY | CE-CD-CG-CB |
| 1 | D | 768 | MLY | CE-CD-CG-CB |
| 1 | G | 353 | MLY | CE-CD-CG-CB |
| 1 | A | 190 | MLY | CE-CD-CG-CB |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|--------------|
| 1 | A | 353 | MLY | CE-CD-CG-CB |
| 1 | A | 768 | MLY | CE-CD-CG-CB |
| 1 | G | 190 | MLY | CE-CD-CG-CB |
| 1 | G | 768 | MLY | CE-CD-CG-CB |
| 1 | J | 190 | MLY | CE-CD-CG-CB |
| 1 | J | 768 | MLY | CE-CD-CG-CB |
| 1 | M | 190 | MLY | CE-CD-CG-CB |
| 1 | M | 768 | MLY | CE-CD-CG-CB |
| 1 | P | 768 | MLY | CE-CD-CG-CB |
| 1 | D | 190 | MLY | CE-CD-CG-CB |
| 1 | P | 190 | MLY | CE-CD-CG-CB |
| 1 | A | 782 | MLY | CE-CD-CG-CB |
| 1 | D | 782 | MLY | CE-CD-CG-CB |
| 1 | G | 782 | MLY | CE-CD-CG-CB |
| 1 | A | 369 | MLY | CE-CD-CG-CB |
| 1 | G | 369 | MLY | CE-CD-CG-CB |
| 1 | J | 369 | MLY | CE-CD-CG-CB |
| 1 | J | 782 | MLY | CE-CD-CG-CB |
| 1 | M | 369 | MLY | CE-CD-CG-CB |
| 1 | P | 369 | MLY | CE-CD-CG-CB |
| 1 | D | 369 | MLY | CE-CD-CG-CB |
| 1 | M | 782 | MLY | CE-CD-CG-CB |
| 1 | P | 782 | MLY | CE-CD-CG-CB |
| 1 | A | 107 | MLY | CD-CE-NZ-CH2 |
| 1 | A | 236 | MLY | CD-CE-NZ-CH1 |
| 1 | D | 107 | MLY | CD-CE-NZ-CH2 |
| 1 | D | 236 | MLY | CD-CE-NZ-CH1 |
| 1 | G | 107 | MLY | CD-CE-NZ-CH2 |
| 1 | G | 236 | MLY | CD-CE-NZ-CH1 |
| 1 | J | 236 | MLY | CD-CE-NZ-CH1 |
| 1 | M | 236 | MLY | CD-CE-NZ-CH1 |
| 1 | P | 236 | MLY | CD-CE-NZ-CH1 |
| 1 | D | 190 | MLY | CG-CD-CE-NZ |
| 1 | A | 436 | MLY | CA-CB-CG-CD |
| 1 | A | 837 | MLY | CA-CB-CG-CD |
| 1 | D | 436 | MLY | CA-CB-CG-CD |
| 1 | D | 837 | MLY | CA-CB-CG-CD |
| 1 | G | 436 | MLY | CA-CB-CG-CD |
| 1 | G | 837 | MLY | CA-CB-CG-CD |
| 1 | J | 436 | MLY | CA-CB-CG-CD |
| 1 | J | 837 | MLY | CA-CB-CG-CD |
| 1 | M | 436 | MLY | CA-CB-CG-CD |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-------------|
| 1 | M | 837 | MLY | CA-CB-CG-CD |
| 1 | P | 436 | MLY | CA-CB-CG-CD |
| 1 | P | 837 | MLY | CA-CB-CG-CD |
| 1 | J | 190 | MLY | CG-CD-CE-NZ |
| 1 | M | 190 | MLY | CG-CD-CE-NZ |
| 1 | P | 190 | MLY | CG-CD-CE-NZ |
| 1 | G | 190 | MLY | CG-CD-CE-NZ |
| 1 | A | 190 | MLY | CG-CD-CE-NZ |
| 1 | J | 833 | MLY | CE-CD-CG-CB |
| 1 | P | 833 | MLY | CE-CD-CG-CB |
| 1 | D | 833 | MLY | CE-CD-CG-CB |
| 1 | G | 833 | MLY | CE-CD-CG-CB |
| 1 | M | 833 | MLY | CE-CD-CG-CB |
| 1 | A | 431 | MLY | CA-CB-CG-CD |
| 1 | D | 236 | MLY | CA-CB-CG-CD |
| 1 | D | 431 | MLY | CA-CB-CG-CD |
| 1 | G | 431 | MLY | CA-CB-CG-CD |
| 1 | J | 236 | MLY | CA-CB-CG-CD |
| 1 | J | 431 | MLY | CA-CB-CG-CD |
| 1 | M | 236 | MLY | CA-CB-CG-CD |
| 1 | M | 431 | MLY | CA-CB-CG-CD |
| 1 | M | 833 | MLY | CA-CB-CG-CD |
| 1 | P | 431 | MLY | CA-CB-CG-CD |
| 1 | A | 833 | MLY | CE-CD-CG-CB |
| 1 | M | 55 | MLY | CG-CD-CE-NZ |
| 1 | A | 55 | MLY | CG-CD-CE-NZ |
| 1 | D | 55 | MLY | CG-CD-CE-NZ |
| 1 | G | 55 | MLY | CG-CD-CE-NZ |
| 1 | G | 617 | MLY | CE-CD-CG-CB |
| 1 | M | 617 | MLY | CE-CD-CG-CB |
| 1 | A | 617 | MLY | CE-CD-CG-CB |
| 1 | D | 617 | MLY | CE-CD-CG-CB |
| 1 | J | 617 | MLY | CE-CD-CG-CB |
| 1 | P | 617 | MLY | CE-CD-CG-CB |
| 1 | A | 236 | MLY | CA-CB-CG-CD |
| 1 | A | 833 | MLY | CA-CB-CG-CD |
| 1 | D | 833 | MLY | CA-CB-CG-CD |
| 1 | G | 236 | MLY | CA-CB-CG-CD |
| 1 | G | 833 | MLY | CA-CB-CG-CD |
| 1 | J | 833 | MLY | CA-CB-CG-CD |
| 1 | P | 236 | MLY | CA-CB-CG-CD |
| 1 | P | 833 | MLY | CA-CB-CG-CD |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-------------|
| 1 | A | 348 | MLY | C-CA-CB-CG |
| 1 | D | 348 | MLY | C-CA-CB-CG |
| 1 | G | 348 | MLY | C-CA-CB-CG |
| 1 | J | 348 | MLY | C-CA-CB-CG |
| 1 | M | 348 | MLY | C-CA-CB-CG |
| 1 | P | 348 | MLY | C-CA-CB-CG |
| 1 | A | 551 | MLY | CE-CD-CG-CB |
| 1 | D | 551 | MLY | CE-CD-CG-CB |
| 1 | J | 55 | MLY | CG-CD-CE-NZ |
| 1 | J | 551 | MLY | CE-CD-CG-CB |
| 1 | P | 55 | MLY | CG-CD-CE-NZ |
| 1 | G | 551 | MLY | CE-CD-CG-CB |
| 1 | M | 551 | MLY | CE-CD-CG-CB |
| 1 | P | 551 | MLY | CE-CD-CG-CB |
| 1 | M | 59 | MLY | CE-CD-CG-CB |
| 1 | A | 55 | MLY | CE-CD-CG-CB |
| 1 | A | 59 | MLY | CE-CD-CG-CB |
| 1 | A | 553 | MLY | CE-CD-CG-CB |
| 1 | D | 59 | MLY | CE-CD-CG-CB |
| 1 | D | 553 | MLY | CE-CD-CG-CB |
| 1 | G | 55 | MLY | CE-CD-CG-CB |
| 1 | G | 59 | MLY | CE-CD-CG-CB |
| 1 | G | 553 | MLY | CE-CD-CG-CB |
| 1 | J | 55 | MLY | CE-CD-CG-CB |
| 1 | J | 59 | MLY | CE-CD-CG-CB |
| 1 | P | 55 | MLY | CE-CD-CG-CB |
| 1 | P | 59 | MLY | CE-CD-CG-CB |
| 1 | P | 553 | MLY | CE-CD-CG-CB |
| 1 | D | 55 | MLY | CE-CD-CG-CB |
| 1 | M | 55 | MLY | CE-CD-CG-CB |
| 1 | M | 553 | MLY | CE-CD-CG-CB |
| 1 | J | 553 | MLY | CE-CD-CG-CB |
| 1 | A | 431 | MLY | CE-CD-CG-CB |
| 1 | J | 431 | MLY | CE-CD-CG-CB |
| 1 | M | 431 | MLY | CE-CD-CG-CB |
| 1 | P | 431 | MLY | CE-CD-CG-CB |
| 1 | G | 248 | MLY | CE-CD-CG-CB |
| 1 | G | 431 | MLY | CE-CD-CG-CB |
| 1 | A | 248 | MLY | CE-CD-CG-CB |
| 1 | D | 35 | MLY | CE-CD-CG-CB |
| 1 | D | 431 | MLY | CE-CD-CG-CB |
| 1 | P | 248 | MLY | CE-CD-CG-CB |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-------------|
| 1 | J | 138 | MLY | CA-CB-CG-CD |
| 1 | M | 138 | MLY | CA-CB-CG-CD |
| 1 | D | 248 | MLY | CE-CD-CG-CB |
| 1 | J | 248 | MLY | CE-CD-CG-CB |
| 1 | M | 248 | MLY | CE-CD-CG-CB |
| 1 | A | 35 | MLY | CE-CD-CG-CB |
| 1 | G | 35 | MLY | CE-CD-CG-CB |
| 1 | J | 35 | MLY | CE-CD-CG-CB |
| 1 | M | 35 | MLY | CE-CD-CG-CB |
| 1 | P | 35 | MLY | CE-CD-CG-CB |
| 1 | D | 528 | MLY | CG-CD-CE-NZ |
| 1 | G | 528 | MLY | CG-CD-CE-NZ |
| 1 | A | 528 | MLY | CG-CD-CE-NZ |
| 1 | J | 528 | MLY | CG-CD-CE-NZ |
| 1 | M | 528 | MLY | CG-CD-CE-NZ |
| 1 | P | 528 | MLY | CG-CD-CE-NZ |
| 1 | A | 138 | MLY | CA-CB-CG-CD |
| 1 | A | 296 | MLY | CA-CB-CG-CD |
| 1 | D | 138 | MLY | CA-CB-CG-CD |
| 1 | G | 138 | MLY | CA-CB-CG-CD |
| 1 | G | 296 | MLY | CA-CB-CG-CD |
| 1 | J | 296 | MLY | CA-CB-CG-CD |
| 1 | M | 296 | MLY | CA-CB-CG-CD |
| 1 | P | 138 | MLY | CA-CB-CG-CD |
| 1 | P | 296 | MLY | CA-CB-CG-CD |
| 1 | A | 248 | MLY | CG-CD-CE-NZ |
| 1 | G | 248 | MLY | CG-CD-CE-NZ |
| 1 | J | 248 | MLY | CG-CD-CE-NZ |
| 1 | M | 248 | MLY | CG-CD-CE-NZ |
| 1 | P | 248 | MLY | CG-CD-CE-NZ |
| 1 | D | 248 | MLY | CG-CD-CE-NZ |
| 1 | D | 296 | MLY | CA-CB-CG-CD |
| 1 | A | 436 | MLY | CE-CD-CG-CB |
| 1 | D | 600 | MLY | CE-CD-CG-CB |
| 1 | P | 436 | MLY | CE-CD-CG-CB |
| 1 | A | 598 | MLY | CE-CD-CG-CB |
| 1 | A | 600 | MLY | CE-CD-CG-CB |
| 1 | D | 436 | MLY | CE-CD-CG-CB |
| 1 | D | 598 | MLY | CE-CD-CG-CB |
| 1 | G | 436 | MLY | CE-CD-CG-CB |
| 1 | G | 598 | MLY | CE-CD-CG-CB |
| 1 | G | 600 | MLY | CE-CD-CG-CB |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|--------------|
| 1 | J | 436 | MLY | CE-CD-CG-CB |
| 1 | J | 600 | MLY | CE-CD-CG-CB |
| 1 | M | 436 | MLY | CE-CD-CG-CB |
| 1 | M | 598 | MLY | CE-CD-CG-CB |
| 1 | M | 600 | MLY | CE-CD-CG-CB |
| 1 | P | 598 | MLY | CE-CD-CG-CB |
| 1 | P | 600 | MLY | CE-CD-CG-CB |
| 1 | J | 598 | MLY | CE-CD-CG-CB |
| 1 | A | 486 | MLY | CE-CD-CG-CB |
| 1 | G | 486 | MLY | CE-CD-CG-CB |
| 1 | M | 486 | MLY | CE-CD-CG-CB |
| 1 | D | 486 | MLY | CE-CD-CG-CB |
| 1 | J | 486 | MLY | CE-CD-CG-CB |
| 1 | P | 486 | MLY | CE-CD-CG-CB |
| 1 | G | 839 | MLY | CE-CD-CG-CB |
| 1 | J | 839 | MLY | CE-CD-CG-CB |
| 1 | M | 839 | MLY | CE-CD-CG-CB |
| 1 | A | 839 | MLY | CE-CD-CG-CB |
| 1 | P | 839 | MLY | CE-CD-CG-CB |
| 1 | D | 839 | MLY | CE-CD-CG-CB |
| 1 | A | 236 | MLY | CD-CE-NZ-CH2 |
| 1 | D | 236 | MLY | CD-CE-NZ-CH2 |
| 1 | G | 236 | MLY | CD-CE-NZ-CH2 |
| 1 | J | 236 | MLY | CD-CE-NZ-CH2 |
| 1 | M | 236 | MLY | CD-CE-NZ-CH2 |
| 1 | P | 236 | MLY | CD-CE-NZ-CH2 |
| 1 | A | 35 | MLY | N-CA-CB-CG |
| 1 | A | 63 | MLY | N-CA-CB-CG |
| 1 | A | 130 | MLY | N-CA-CB-CG |
| 1 | A | 436 | MLY | N-CA-CB-CG |
| 1 | A | 681 | MLY | N-CA-CB-CG |
| 1 | A | 833 | MLY | N-CA-CB-CG |
| 1 | A | 837 | MLY | N-CA-CB-CG |
| 1 | D | 35 | MLY | N-CA-CB-CG |
| 1 | D | 63 | MLY | N-CA-CB-CG |
| 1 | D | 130 | MLY | N-CA-CB-CG |
| 1 | D | 348 | MLY | N-CA-CB-CG |
| 1 | D | 436 | MLY | N-CA-CB-CG |
| 1 | D | 681 | MLY | N-CA-CB-CG |
| 1 | D | 833 | MLY | N-CA-CB-CG |
| 1 | D | 837 | MLY | N-CA-CB-CG |
| 1 | G | 35 | MLY | N-CA-CB-CG |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-------------|
| 1 | G | 63 | MLY | N-CA-CB-CG |
| 1 | G | 130 | MLY | N-CA-CB-CG |
| 1 | G | 436 | MLY | N-CA-CB-CG |
| 1 | G | 681 | MLY | N-CA-CB-CG |
| 1 | G | 833 | MLY | N-CA-CB-CG |
| 1 | G | 837 | MLY | N-CA-CB-CG |
| 1 | J | 35 | MLY | N-CA-CB-CG |
| 1 | J | 63 | MLY | N-CA-CB-CG |
| 1 | J | 130 | MLY | N-CA-CB-CG |
| 1 | J | 436 | MLY | N-CA-CB-CG |
| 1 | J | 681 | MLY | N-CA-CB-CG |
| 1 | J | 833 | MLY | N-CA-CB-CG |
| 1 | J | 837 | MLY | N-CA-CB-CG |
| 1 | M | 35 | MLY | N-CA-CB-CG |
| 1 | M | 63 | MLY | N-CA-CB-CG |
| 1 | M | 130 | MLY | N-CA-CB-CG |
| 1 | M | 436 | MLY | N-CA-CB-CG |
| 1 | M | 681 | MLY | N-CA-CB-CG |
| 1 | M | 833 | MLY | N-CA-CB-CG |
| 1 | M | 837 | MLY | N-CA-CB-CG |
| 1 | P | 35 | MLY | N-CA-CB-CG |
| 1 | P | 63 | MLY | N-CA-CB-CG |
| 1 | P | 130 | MLY | N-CA-CB-CG |
| 1 | P | 436 | MLY | N-CA-CB-CG |
| 1 | P | 681 | MLY | N-CA-CB-CG |
| 1 | P | 833 | MLY | N-CA-CB-CG |
| 1 | P | 837 | MLY | N-CA-CB-CG |
| 1 | M | 19 | MLY | CA-CB-CG-CD |
| 1 | D | 833 | MLY | C-CA-CB-CG |
| 1 | J | 833 | MLY | C-CA-CB-CG |
| 1 | M | 833 | MLY | C-CA-CB-CG |
| 1 | P | 833 | MLY | C-CA-CB-CG |
| 1 | A | 19 | MLY | CA-CB-CG-CD |
| 1 | D | 19 | MLY | CA-CB-CG-CD |
| 1 | G | 19 | MLY | CA-CB-CG-CD |
| 1 | J | 19 | MLY | CA-CB-CG-CD |
| 1 | P | 19 | MLY | CA-CB-CG-CD |
| 1 | P | 837 | MLY | CE-CD-CG-CB |
| 1 | A | 19 | MLY | CE-CD-CG-CB |
| 1 | D | 837 | MLY | CE-CD-CG-CB |
| 1 | G | 837 | MLY | CE-CD-CG-CB |
| 1 | M | 837 | MLY | CE-CD-CG-CB |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|--------------|
| 1 | J | 837 | MLY | CE-CD-CG-CB |
| 1 | A | 837 | MLY | CE-CD-CG-CB |
| 1 | D | 19 | MLY | CE-CD-CG-CB |
| 1 | J | 19 | MLY | CE-CD-CG-CB |
| 1 | P | 19 | MLY | CE-CD-CG-CB |
| 1 | G | 19 | MLY | CE-CD-CG-CB |
| 1 | M | 19 | MLY | CE-CD-CG-CB |
| 1 | G | 613 | MLY | CE-CD-CG-CB |
| 1 | J | 613 | MLY | CE-CD-CG-CB |
| 1 | M | 613 | MLY | CE-CD-CG-CB |
| 1 | P | 613 | MLY | CE-CD-CG-CB |
| 1 | A | 613 | MLY | CE-CD-CG-CB |
| 1 | D | 613 | MLY | CE-CD-CG-CB |
| 1 | A | 598 | MLY | CD-CE-NZ-CH2 |
| 1 | D | 598 | MLY | CD-CE-NZ-CH2 |
| 1 | G | 598 | MLY | CD-CE-NZ-CH2 |
| 1 | J | 598 | MLY | CD-CE-NZ-CH2 |
| 1 | M | 598 | MLY | CD-CE-NZ-CH2 |
| 1 | P | 598 | MLY | CD-CE-NZ-CH2 |
| 1 | A | 63 | MLY | C-CA-CB-CG |
| 1 | A | 353 | MLY | C-CA-CB-CG |
| 1 | A | 833 | MLY | C-CA-CB-CG |
| 1 | D | 63 | MLY | C-CA-CB-CG |
| 1 | D | 353 | MLY | C-CA-CB-CG |
| 1 | G | 63 | MLY | C-CA-CB-CG |
| 1 | G | 353 | MLY | C-CA-CB-CG |
| 1 | G | 833 | MLY | C-CA-CB-CG |
| 1 | J | 63 | MLY | C-CA-CB-CG |
| 1 | J | 353 | MLY | C-CA-CB-CG |
| 1 | M | 63 | MLY | C-CA-CB-CG |
| 1 | M | 353 | MLY | C-CA-CB-CG |
| 1 | P | 63 | MLY | C-CA-CB-CG |
| 1 | P | 353 | MLY | C-CA-CB-CG |
| 1 | A | 30 | MLY | CA-CB-CG-CD |
| 1 | D | 30 | MLY | CA-CB-CG-CD |
| 1 | G | 30 | MLY | CA-CB-CG-CD |
| 1 | J | 30 | MLY | CA-CB-CG-CD |
| 1 | M | 30 | MLY | CA-CB-CG-CD |
| 1 | P | 30 | MLY | CA-CB-CG-CD |
| 1 | M | 348 | MLY | CE-CD-CG-CB |
| 1 | P | 348 | MLY | CE-CD-CG-CB |
| 1 | J | 348 | MLY | CE-CD-CG-CB |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-------------|
| 1 | A | 348 | MLY | CE-CD-CG-CB |
| 1 | D | 348 | MLY | CE-CD-CG-CB |
| 1 | G | 348 | MLY | CE-CD-CG-CB |
| 1 | A | 613 | MLY | CA-CB-CG-CD |
| 1 | J | 613 | MLY | CA-CB-CG-CD |
| 1 | M | 613 | MLY | CA-CB-CG-CD |
| 1 | P | 613 | MLY | CA-CB-CG-CD |
| 1 | D | 613 | MLY | CA-CB-CG-CD |
| 1 | A | 190 | MLY | CA-CB-CG-CD |
| 1 | A | 528 | MLY | CA-CB-CG-CD |
| 1 | D | 190 | MLY | CA-CB-CG-CD |
| 1 | G | 190 | MLY | CA-CB-CG-CD |
| 1 | G | 613 | MLY | CA-CB-CG-CD |
| 1 | J | 190 | MLY | CA-CB-CG-CD |
| 1 | J | 528 | MLY | CA-CB-CG-CD |
| 1 | M | 190 | MLY | CA-CB-CG-CD |
| 1 | P | 190 | MLY | CA-CB-CG-CD |
| 1 | P | 528 | MLY | CA-CB-CG-CD |

There are no ring outliers.

180 monomers are involved in 650 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 1 | A | 348 | MLY | 6 | 0 |
| 1 | G | 49 | MLY | 3 | 0 |
| 1 | M | 190 | MLY | 2 | 0 |
| 1 | D | 553 | MLY | 16 | 0 |
| 1 | M | 107 | MLY | 2 | 0 |
| 1 | D | 551 | MLY | 2 | 0 |
| 1 | D | 107 | MLY | 3 | 0 |
| 1 | M | 59 | MLY | 2 | 0 |
| 1 | A | 248 | MLY | 2 | 0 |
| 1 | J | 138 | MLY | 1 | 0 |
| 1 | G | 600 | MLY | 1 | 0 |
| 1 | P | 107 | MLY | 2 | 0 |
| 1 | P | 659 | MLY | 2 | 0 |
| 1 | J | 415 | MLY | 1 | 0 |
| 1 | M | 659 | MLY | 2 | 0 |
| 1 | J | 839 | MLY | 9 | 0 |
| 1 | D | 659 | MLY | 2 | 0 |
| 1 | P | 839 | MLY | 8 | 0 |
| 1 | J | 837 | MLY | 1 | 0 |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 1 | A | 617 | MLY | 1 | 0 |
| 1 | G | 84 | MLY | 28 | 0 |
| 1 | J | 49 | MLY | 2 | 0 |
| 1 | D | 30 | MLY | 1 | 0 |
| 1 | A | 190 | MLY | 2 | 0 |
| 1 | A | 837 | MLY | 11 | 0 |
| 1 | D | 296 | MLY | 3 | 0 |
| 1 | P | 49 | MLY | 3 | 0 |
| 1 | G | 528 | MLY | 2 | 0 |
| 1 | P | 782 | MLY | 3 | 0 |
| 1 | D | 190 | MLY | 2 | 0 |
| 1 | M | 768 | MLY | 2 | 0 |
| 1 | G | 295 | MLY | 6 | 0 |
| 1 | A | 839 | MLY | 8 | 0 |
| 1 | G | 107 | MLY | 3 | 0 |
| 1 | D | 782 | MLY | 52 | 0 |
| 1 | D | 598 | MLY | 1 | 0 |
| 1 | M | 87 | MLY | 2 | 0 |
| 1 | P | 35 | MLY | 1 | 0 |
| 1 | G | 617 | MLY | 1 | 0 |
| 1 | A | 49 | MLY | 3 | 0 |
| 1 | M | 348 | MLY | 5 | 0 |
| 1 | D | 63 | MLY | 4 | 0 |
| 1 | D | 248 | MLY | 2 | 0 |
| 1 | J | 63 | MLY | 4 | 0 |
| 1 | A | 436 | MLY | 2 | 0 |
| 1 | D | 764 | MLY | 8 | 0 |
| 1 | J | 84 | MLY | 18 | 0 |
| 1 | P | 55 | MLY | 1 | 0 |
| 1 | P | 837 | MLY | 1 | 0 |
| 1 | J | 436 | MLY | 2 | 0 |
| 1 | G | 486 | MLY | 3 | 0 |
| 1 | M | 55 | MLY | 1 | 0 |
| 1 | P | 59 | MLY | 2 | 0 |
| 1 | A | 659 | MLY | 2 | 0 |
| 1 | J | 782 | MLY | 1 | 0 |
| 1 | D | 55 | MLY | 1 | 0 |
| 1 | M | 486 | MLY | 3 | 0 |
| 1 | P | 63 | MLY | 4 | 0 |
| 1 | M | 764 | MLY | 1 | 0 |
| 1 | P | 138 | MLY | 1 | 0 |
| 1 | P | 436 | MLY | 2 | 0 |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 1 | P | 296 | MLY | 2 | 0 |
| 1 | D | 295 | MLY | 6 | 0 |
| 1 | D | 486 | MLY | 3 | 0 |
| 1 | A | 296 | MLY | 3 | 0 |
| 1 | D | 348 | MLY | 6 | 0 |
| 1 | G | 505 | MLY | 19 | 0 |
| 1 | D | 138 | MLY | 1 | 0 |
| 1 | P | 486 | MLY | 3 | 0 |
| 1 | A | 30 | MLY | 1 | 0 |
| 1 | J | 295 | MLY | 5 | 0 |
| 1 | J | 55 | MLY | 1 | 0 |
| 1 | M | 248 | MLY | 2 | 0 |
| 1 | M | 30 | MLY | 1 | 0 |
| 1 | D | 528 | MLY | 3 | 0 |
| 1 | G | 415 | MLY | 1 | 0 |
| 1 | P | 295 | MLY | 6 | 0 |
| 1 | A | 486 | MLY | 3 | 0 |
| 1 | J | 59 | MLY | 3 | 0 |
| 1 | D | 369 | MLY | 1 | 0 |
| 1 | G | 782 | MLY | 1 | 0 |
| 1 | J | 617 | MLY | 1 | 0 |
| 1 | G | 598 | MLY | 1 | 0 |
| 1 | G | 87 | MLY | 2 | 0 |
| 1 | J | 659 | MLY | 2 | 0 |
| 1 | G | 348 | MLY | 5 | 0 |
| 1 | P | 415 | MLY | 1 | 0 |
| 1 | G | 248 | MLY | 2 | 0 |
| 1 | G | 764 | MLY | 18 | 0 |
| 1 | G | 553 | MLY | 26 | 0 |
| 1 | G | 55 | MLY | 1 | 0 |
| 1 | G | 837 | MLY | 1 | 0 |
| 1 | M | 272 | MLY | 1 | 0 |
| 1 | M | 600 | MLY | 1 | 0 |
| 1 | M | 528 | MLY | 3 | 0 |
| 1 | G | 59 | MLY | 2 | 0 |
| 1 | G | 659 | MLY | 2 | 0 |
| 1 | D | 272 | MLY | 1 | 0 |
| 1 | A | 107 | MLY | 3 | 0 |
| 1 | D | 600 | MLY | 1 | 0 |
| 1 | J | 600 | MLY | 1 | 0 |
| 1 | P | 248 | MLY | 2 | 0 |
| 1 | A | 63 | MLY | 3 | 0 |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 1 | P | 505 | MLY | 2 | 0 |
| 1 | A | 833 | MLY | 1 | 0 |
| 1 | M | 49 | MLY | 4 | 0 |
| 1 | M | 553 | MLY | 3 | 0 |
| 1 | M | 436 | MLY | 2 | 0 |
| 1 | J | 598 | MLY | 1 | 0 |
| 1 | A | 272 | MLY | 1 | 0 |
| 1 | A | 600 | MLY | 1 | 0 |
| 1 | J | 553 | MLY | 12 | 0 |
| 1 | P | 348 | MLY | 4 | 0 |
| 1 | P | 553 | MLY | 3 | 0 |
| 1 | G | 190 | MLY | 2 | 0 |
| 1 | D | 49 | MLY | 3 | 0 |
| 1 | A | 551 | MLY | 2 | 0 |
| 1 | J | 248 | MLY | 2 | 0 |
| 1 | D | 436 | MLY | 2 | 0 |
| 1 | J | 107 | MLY | 3 | 0 |
| 1 | P | 617 | MLY | 1 | 0 |
| 1 | J | 369 | MLY | 1 | 0 |
| 1 | D | 837 | MLY | 1 | 0 |
| 1 | J | 486 | MLY | 3 | 0 |
| 1 | M | 617 | MLY | 1 | 0 |
| 1 | D | 59 | MLY | 3 | 0 |
| 1 | D | 87 | MLY | 2 | 0 |
| 1 | M | 35 | MLY | 3 | 0 |
| 1 | D | 617 | MLY | 1 | 0 |
| 1 | G | 272 | MLY | 1 | 0 |
| 1 | M | 837 | MLY | 1 | 0 |
| 1 | A | 415 | MLY | 1 | 0 |
| 1 | A | 87 | MLY | 3 | 0 |
| 1 | J | 296 | MLY | 3 | 0 |
| 1 | J | 528 | MLY | 3 | 0 |
| 1 | A | 505 | MLY | 19 | 0 |
| 1 | J | 30 | MLY | 1 | 0 |
| 1 | P | 272 | MLY | 1 | 0 |
| 1 | P | 600 | MLY | 1 | 0 |
| 1 | J | 190 | MLY | 2 | 0 |
| 1 | A | 55 | MLY | 1 | 0 |
| 1 | P | 30 | MLY | 1 | 0 |
| 1 | A | 59 | MLY | 3 | 0 |
| 1 | D | 839 | MLY | 4 | 0 |
| 1 | A | 138 | MLY | 1 | 0 |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 1 | P | 190 | MLY | 2 | 0 |
| 1 | P | 764 | MLY | 3 | 0 |
| 1 | G | 768 | MLY | 2 | 0 |
| 1 | P | 598 | MLY | 1 | 0 |
| 1 | A | 598 | MLY | 1 | 0 |
| 1 | M | 598 | MLY | 1 | 0 |
| 1 | J | 272 | MLY | 1 | 0 |
| 1 | A | 764 | MLY | 10 | 0 |
| 1 | G | 63 | MLY | 3 | 0 |
| 1 | A | 768 | MLY | 6 | 0 |
| 1 | A | 553 | MLY | 18 | 0 |
| 1 | J | 764 | MLY | 1 | 0 |
| 1 | M | 296 | MLY | 3 | 0 |
| 1 | J | 348 | MLY | 6 | 0 |
| 1 | D | 415 | MLY | 1 | 0 |
| 1 | M | 839 | MLY | 7 | 0 |
| 1 | P | 87 | MLY | 3 | 0 |
| 1 | J | 505 | MLY | 9 | 0 |
| 1 | A | 295 | MLY | 6 | 0 |
| 1 | M | 295 | MLY | 6 | 0 |
| 1 | G | 138 | MLY | 1 | 0 |
| 1 | A | 782 | MLY | 6 | 0 |
| 1 | M | 63 | MLY | 4 | 0 |
| 1 | G | 436 | MLY | 2 | 0 |
| 1 | M | 138 | MLY | 1 | 0 |
| 1 | G | 296 | MLY | 3 | 0 |
| 1 | A | 827 | MLY | 1 | 0 |
| 1 | G | 839 | MLY | 4 | 0 |
| 1 | J | 768 | MLY | 1 | 0 |
| 1 | M | 782 | MLY | 4 | 0 |
| 1 | P | 528 | MLY | 3 | 0 |
| 1 | A | 528 | MLY | 3 | 0 |
| 1 | G | 30 | MLY | 1 | 0 |
| 1 | M | 415 | MLY | 1 | 0 |
| 1 | J | 87 | MLY | 3 | 0 |

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

| Mol | Chain | Number of breaks |
|-----|-------|------------------|
| 1 | M | 7 |
| 1 | P | 6 |
| 1 | D | 4 |
| 1 | A | 4 |
| 1 | J | 3 |
| 1 | G | 3 |
| 3 | C | 1 |
| 3 | F | 1 |
| 3 | I | 1 |
| 3 | L | 1 |
| 3 | O | 1 |
| 3 | R | 1 |
| 2 | H | 1 |
| 2 | B | 1 |
| 2 | E | 1 |
| 2 | K | 1 |
| 2 | N | 1 |
| 2 | Q | 1 |

All chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1 | J | 769:ALA | C | 770:GLY | N | 5.57 |
| 1 | D | 769:ALA | C | 770:GLY | N | 4.88 |
| 1 | G | 769:ALA | C | 770:GLY | N | 4.51 |
| 1 | D | 709:LYS | C | 710:GLY | N | 3.44 |
| 1 | M | 786:ILE | C | 787:ILE | N | 2.71 |
| 1 | A | 709:LYS | C | 710:GLY | N | 2.67 |
| 1 | C | 4:LYS | C | 5:ALA | N | 2.61 |
| 1 | F | 4:LYS | C | 5:ALA | N | 2.61 |

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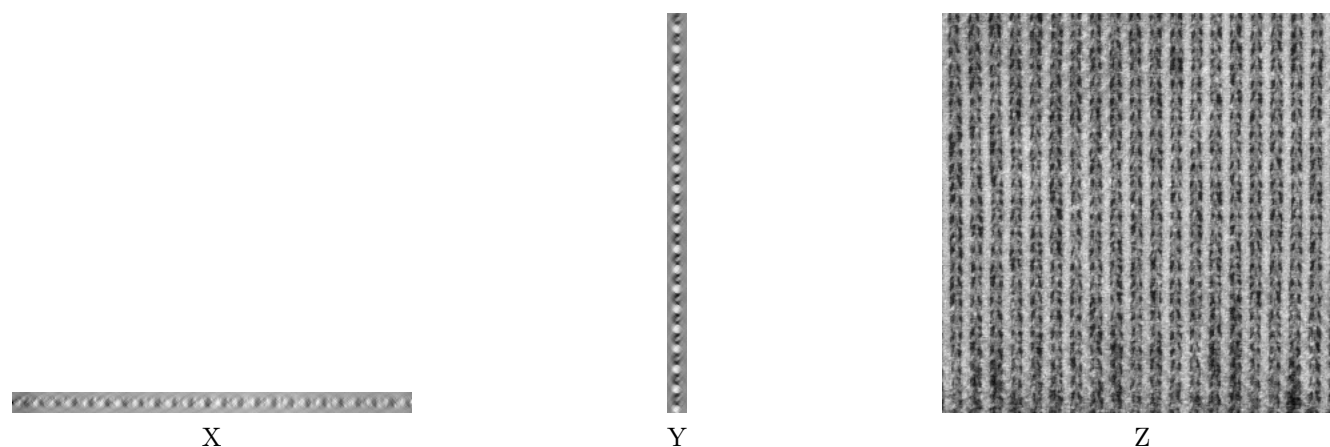
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| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1 | I | 4:LYS | C | 5:ALA | N | 2.61 |
| 1 | L | 4:LYS | C | 5:ALA | N | 2.61 |
| 1 | O | 4:LYS | C | 5:ALA | N | 2.61 |
| 1 | R | 4:LYS | C | 5:ALA | N | 2.61 |
| 1 | A | 769:ALA | C | 770:GLY | N | 2.45 |
| 1 | M | 769:ALA | C | 770:GLY | N | 2.33 |
| 1 | P | 786:ILE | C | 787:ILE | N | 2.28 |
| 1 | P | 709:LYS | C | 710:GLY | N | 2.24 |
| 1 | P | 769:ALA | C | 770:GLY | N | 2.09 |
| 1 | M | 785:GLU | C | 786:ILE | N | 2.05 |
| 1 | M | 709:LYS | C | 710:GLY | N | 1.99 |
| 1 | M | 806:MET | C | 807:VAL | N | 1.99 |
| 1 | P | 806:MET | C | 807:VAL | N | 1.78 |
| 1 | H | 140:PHE | C | 141:PRO | N | 1.10 |
| 1 | B | 140:PHE | C | 141:PRO | N | 1.09 |
| 1 | E | 140:PHE | C | 141:PRO | N | 1.09 |
| 1 | K | 140:PHE | C | 141:PRO | N | 1.09 |
| 1 | N | 140:PHE | C | 141:PRO | N | 1.09 |
| 1 | Q | 140:PHE | C | 141:PRO | N | 1.09 |
| 1 | A | 637:LYS | C | 638:GLY | N | 1.06 |
| 1 | D | 637:LYS | C | 638:GLY | N | 1.06 |
| 1 | G | 637:LYS | C | 638:GLY | N | 1.06 |
| 1 | J | 637:LYS | C | 638:GLY | N | 1.06 |
| 1 | M | 637:LYS | C | 638:GLY | N | 1.06 |
| 1 | P | 637:LYS | C | 638:GLY | N | 1.06 |
| 1 | A | 649:VAL | C | 650:SER | N | 1.03 |
| 1 | D | 649:VAL | C | 650:SER | N | 1.03 |
| 1 | G | 649:VAL | C | 650:SER | N | 1.03 |
| 1 | J | 649:VAL | C | 650:SER | N | 1.03 |
| 1 | M | 649:VAL | C | 650:SER | N | 1.03 |
| 1 | P | 649:VAL | C | 650:SER | N | 1.03 |

6 Tomogram visualisation [i](#)

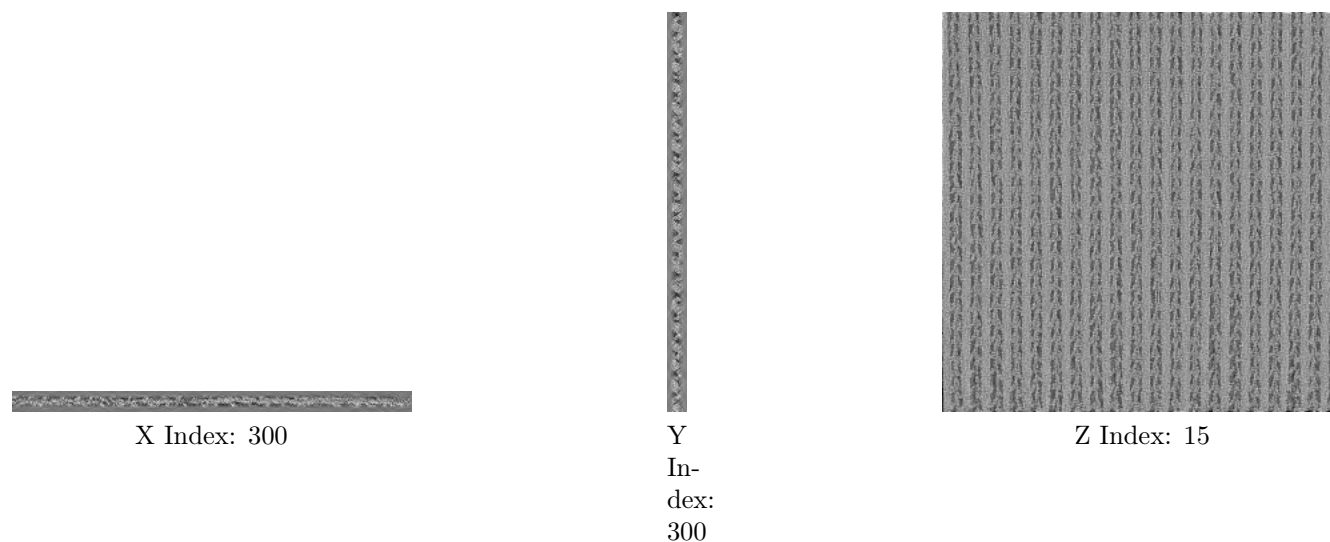
This section contains visualisations of the EMDB entry EMD-1001. These allow visual inspection of the internal detail of the tomogram and identification of artifacts.

6.1 Orthogonal projections [i](#)



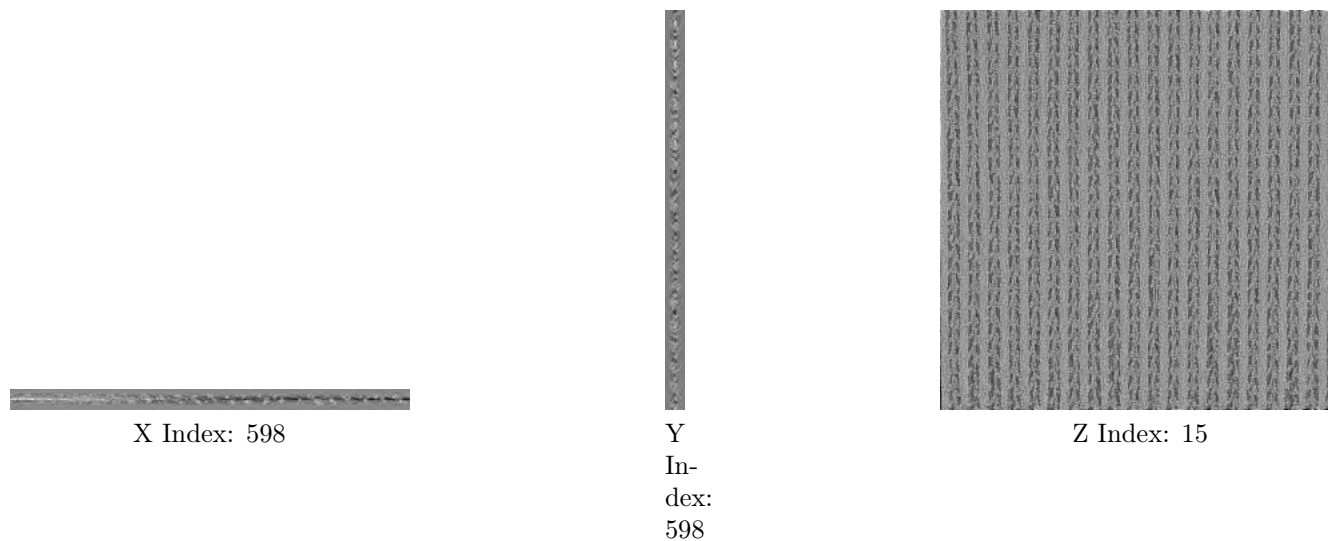
The images above show the tomogram projected in three orthogonal directions.

6.2 Central slices [i](#)



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

6.3 Largest variance slices [i](#)



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

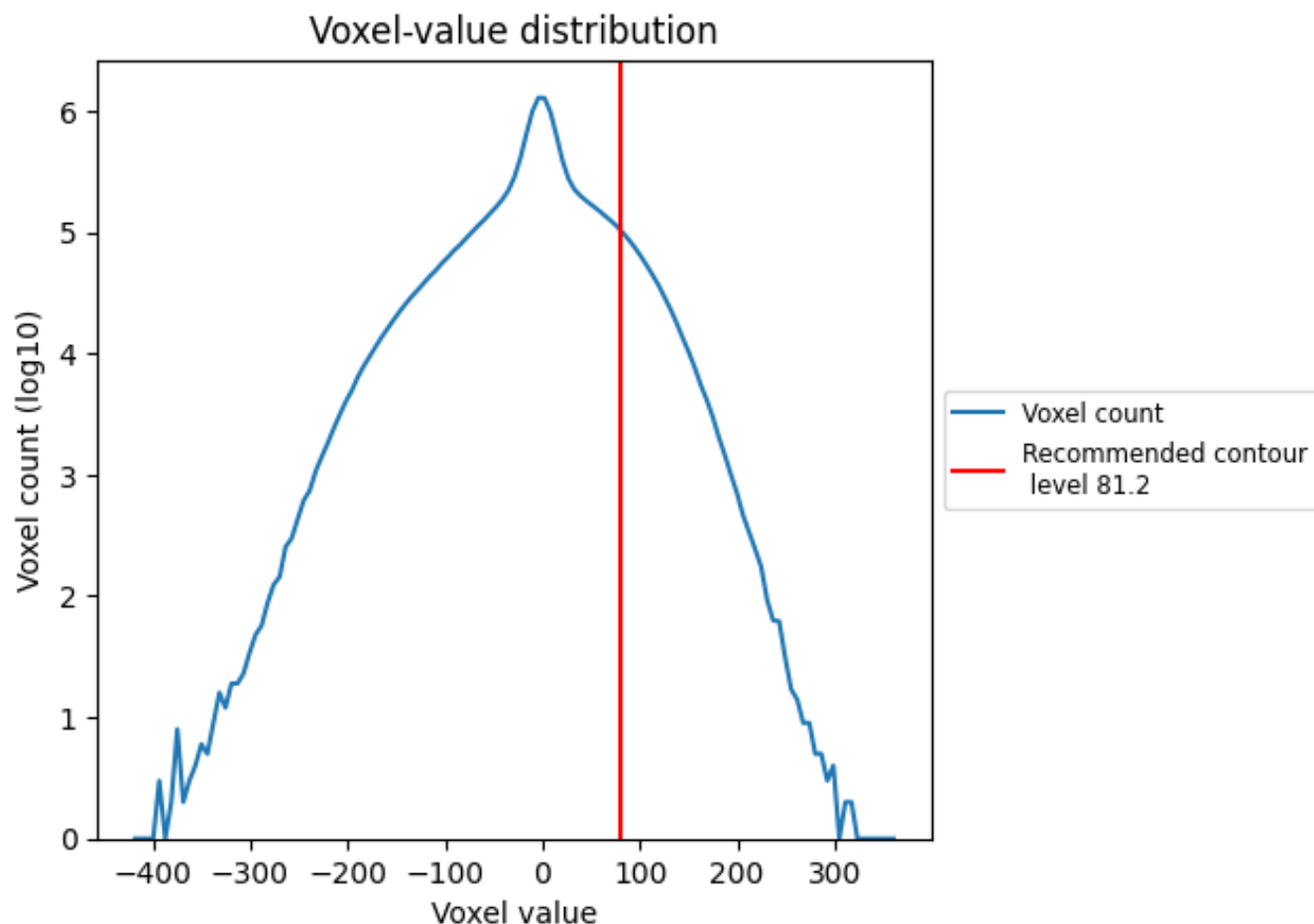
6.4 Mask visualisation [i](#)

This section was not generated.

7 Tomogram analysis [i](#)

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

7.1 Voxel-value distribution [i](#)



The voxel-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic.

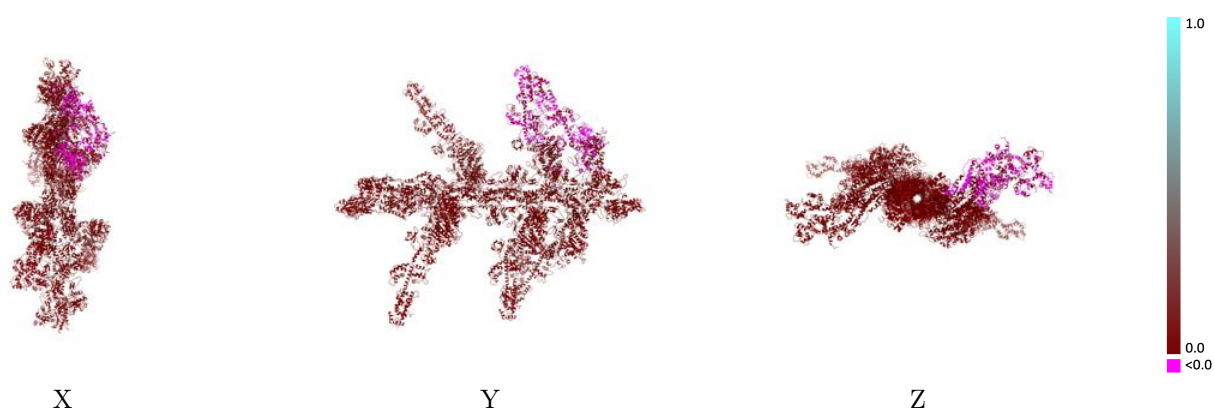
8 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-1001 and PDB model 1O1A. Per-residue inclusion information can be found in section 3 on page 7.

8.1 Map-model overlay [i](#)

This section was not generated.

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

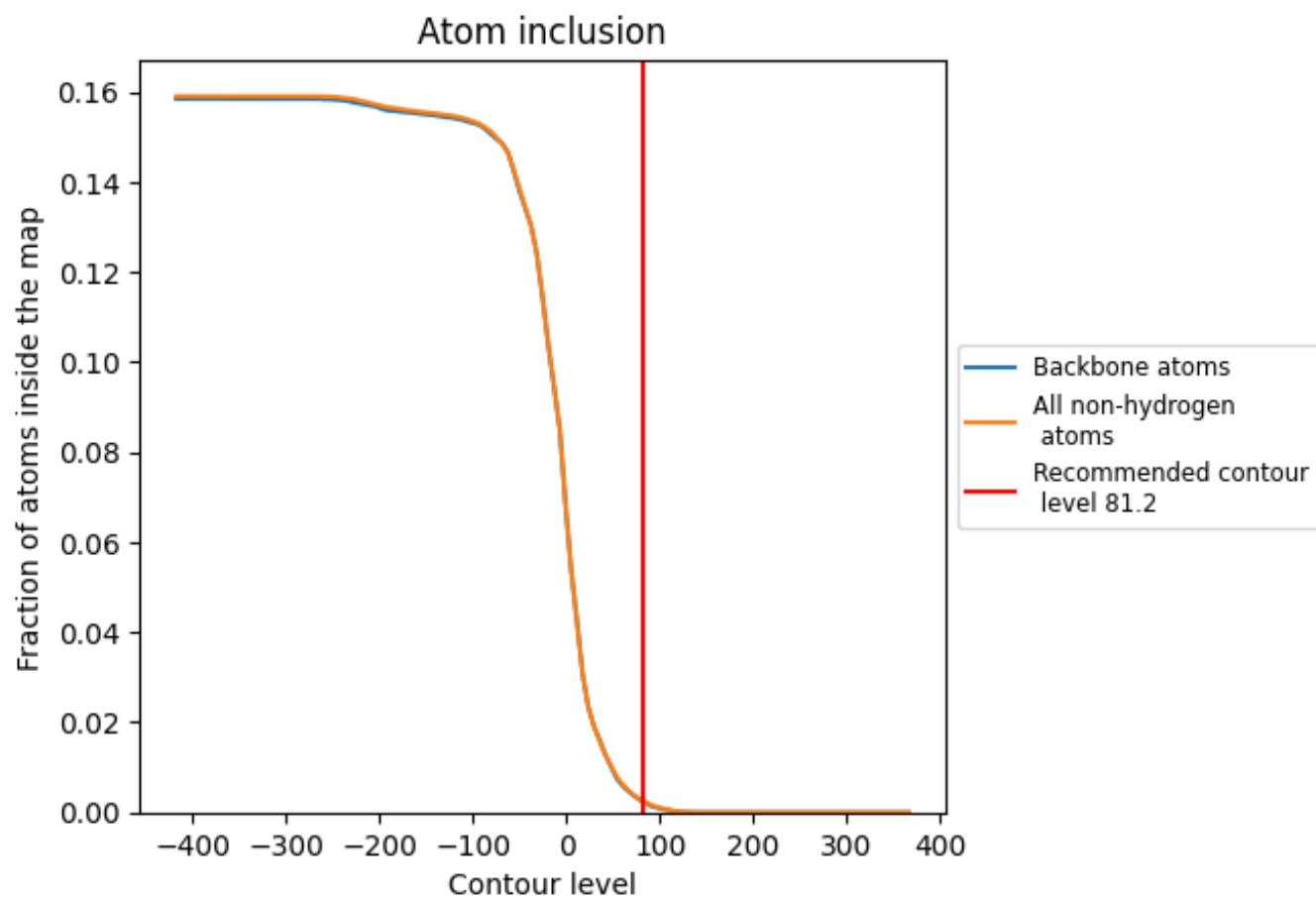


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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

This section was not generated.



































































8.4 Atom inclusion [i](#)



At the recommended contour level, 0% of all backbone atoms, 0% of all non-hydrogen atoms, are inside the map.

8.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (81.2) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion | Q-score |
|-------|--|---|
| All |  0.0026 |  -0.0010 |
| 1 |  0.0014 |  0.0000 |
| 2 |  0.0000 |  0.0000 |
| 3 |  0.0000 |  0.0000 |
| 4 |  0.0000 |  0.0000 |
| 5 |  0.0000 |  0.0000 |
| 6 |  0.0000 |  0.0000 |
| 7 |  0.0000 |  0.0000 |
| 8 |  0.0000 |  -0.0010 |
| 9 |  0.0000 |  0.0000 |
| A |  0.0000 |  -0.0140 |
| B |  0.0000 |  -0.0020 |
| C |  0.0000 |  0.0160 |
| D |  0.0000 |  0.0000 |
| E |  0.0000 |  0.0000 |
| F |  0.0000 |  0.0000 |
| G |  0.0000 |  -0.0010 |
| H |  0.0000 |  -0.0080 |
| I |  0.0700 |  0.0010 |
| J |  0.0000 |  0.0000 |
| K |  0.0000 |  0.0000 |
| L |  0.0000 |  0.0000 |
| M |  0.0000 |  0.0000 |
| N |  0.0000 |  0.0000 |
| O |  0.0000 |  0.0000 |
| P |  0.0000 |  0.0000 |
| Q |  0.0000 |  0.0000 |
| R |  0.0000 |  0.0000 |
| V |  0.0000 |  0.0010 |
| W |  0.0000 |  0.0000 |
| X |  0.0000 |  -0.0000 |
| Y |  0.0551 |  0.0000 |
| Z |  0.0000 |  0.0000 |

