



Full wwPDB EM Validation Report ⓘ

Jun 25, 2025 – 11:59 PM JST

PDB ID : 6AHF / pdb_00006ahf
EMDB ID : EMD-9625
Title : CryoEM Reconstruction of Hsp104 N728A Hexamer
Authors : Zhang, X.; Zhang, L.; Zhang, S.
Deposited on : 2018-08-17
Resolution : 6.78 Å(reported)

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

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

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.dev118
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0rc1
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.44

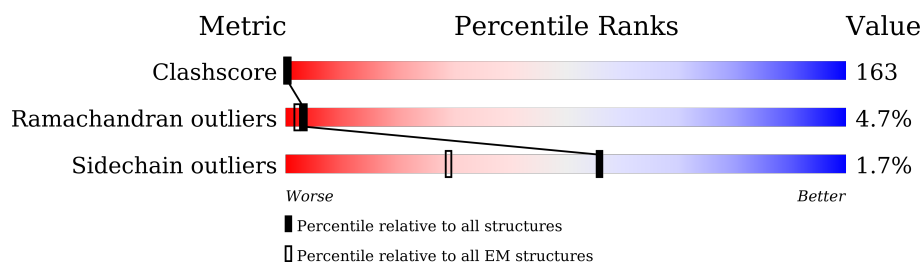
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 6.78 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 | 210492 | 15764 |
| Ramachandran outliers | 207382 | 16835 |
| Sidechain outliers | 206894 | 16415 |

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 | 908 | |
| 1 | B | 908 | |
| 1 | C | 908 | |
| 1 | D | 908 | |
| 1 | E | 908 | |
| 1 | F | 908 | |

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 criteria:

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 2 | AGS | C | 1001 | - | - | X | - |
| 2 | AGS | D | 1001 | - | - | X | - |
| 2 | AGS | E | 1001 | - | - | X | - |
| 2 | AGS | E | 1002 | - | - | X | - |
| 2 | AGS | F | 1001 | - | - | X | - |
| 2 | AGS | F | 1002 | - | - | X | - |

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 32108 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.

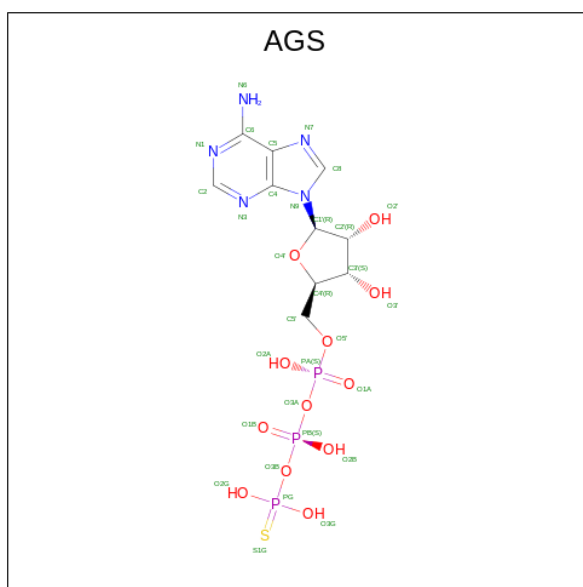
- Molecule 1 is a protein called Heat shock protein 104.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
| 1 | A | 577 | Total | C | N | O | S | 0 | 0 |
| | | | 4456 | 2803 | 773 | 862 | 18 | | |
| 1 | B | 737 | Total | C | N | O | S | 0 | 0 |
| | | | 5142 | 3152 | 948 | 1024 | 18 | | |
| 1 | C | 865 | Total | C | N | O | S | 0 | 0 |
| | | | 6162 | 3769 | 1133 | 1241 | 19 | | |
| 1 | D | 865 | Total | C | N | O | S | 0 | 0 |
| | | | 6170 | 3778 | 1133 | 1240 | 19 | | |
| 1 | E | 705 | Total | C | N | O | S | 0 | 0 |
| | | | 5512 | 3443 | 973 | 1078 | 18 | | |
| 1 | F | 574 | Total | C | N | O | S | 0 | 0 |
| | | | 4480 | 2821 | 783 | 858 | 18 | | |

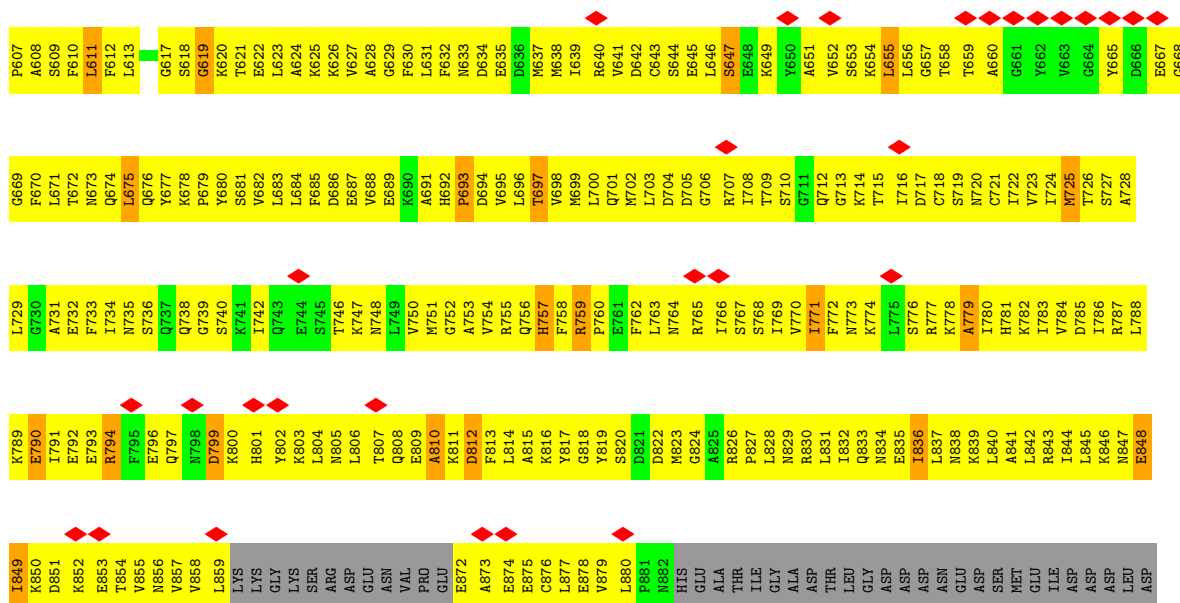
There are 6 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|---------------------|------------|
| A | 728 | ALA | ASN | engineered mutation | UNP P31539 |
| B | 728 | ALA | ASN | engineered mutation | UNP P31539 |
| C | 728 | ALA | ASN | engineered mutation | UNP P31539 |
| D | 728 | ALA | ASN | engineered mutation | UNP P31539 |
| E | 728 | ALA | ASN | engineered mutation | UNP P31539 |
| F | 728 | ALA | ASN | engineered mutation | UNP P31539 |

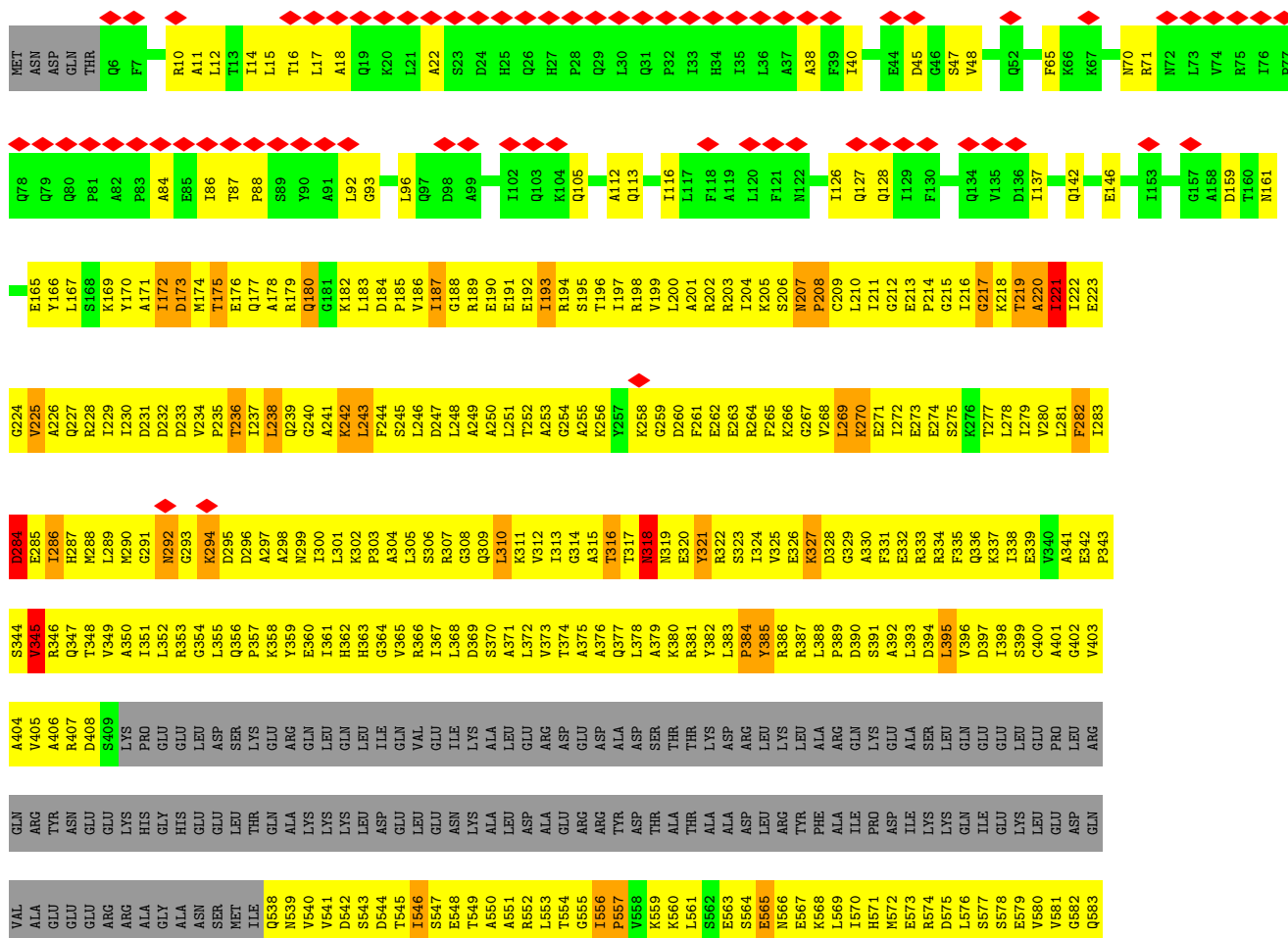
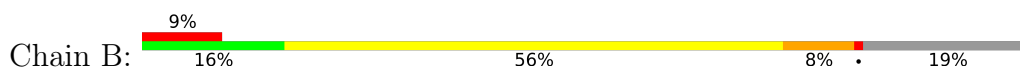
- Molecule 2 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (CCD ID: AGS) (formula: C₁₀H₁₆N₅O₁₂P₃S).

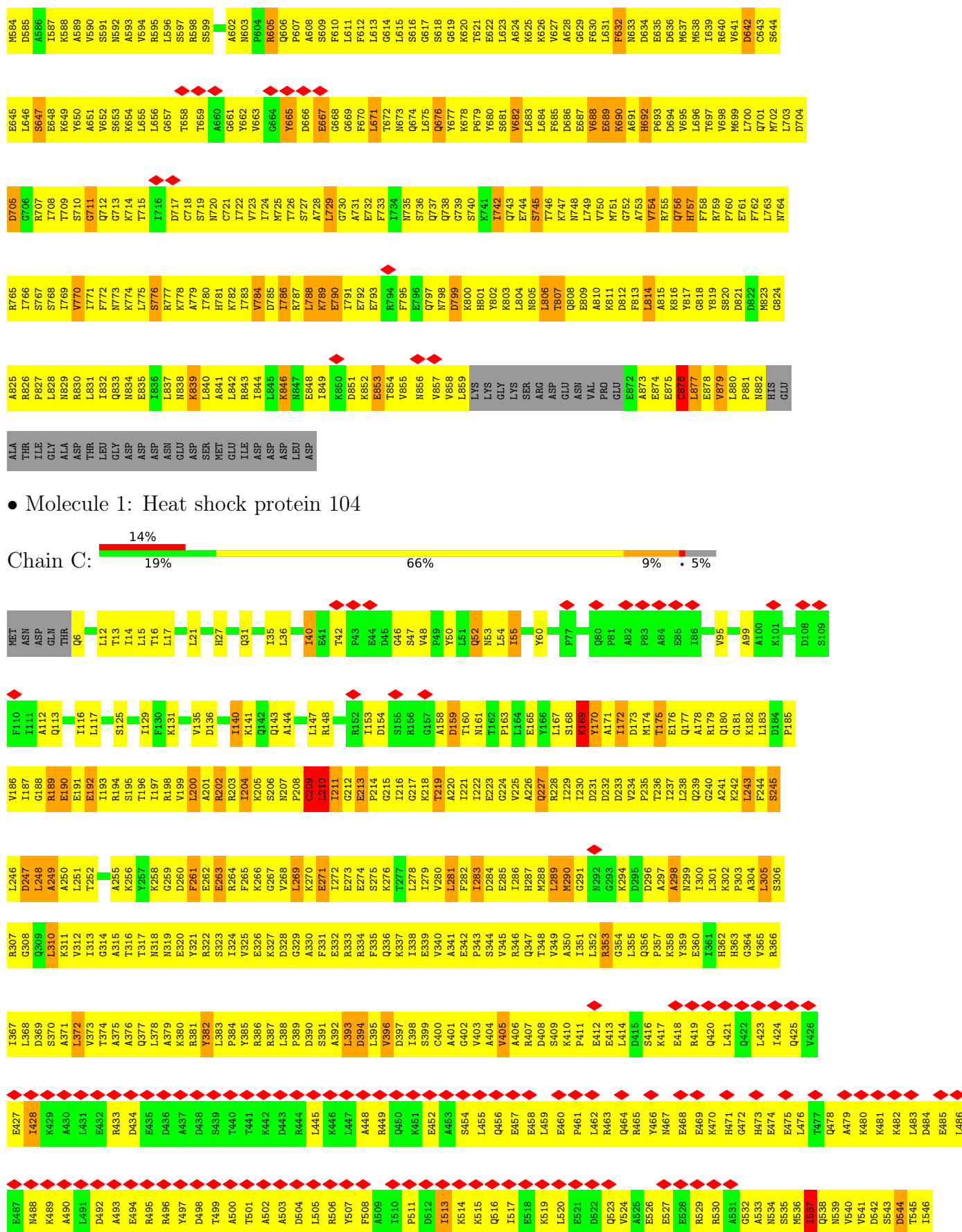


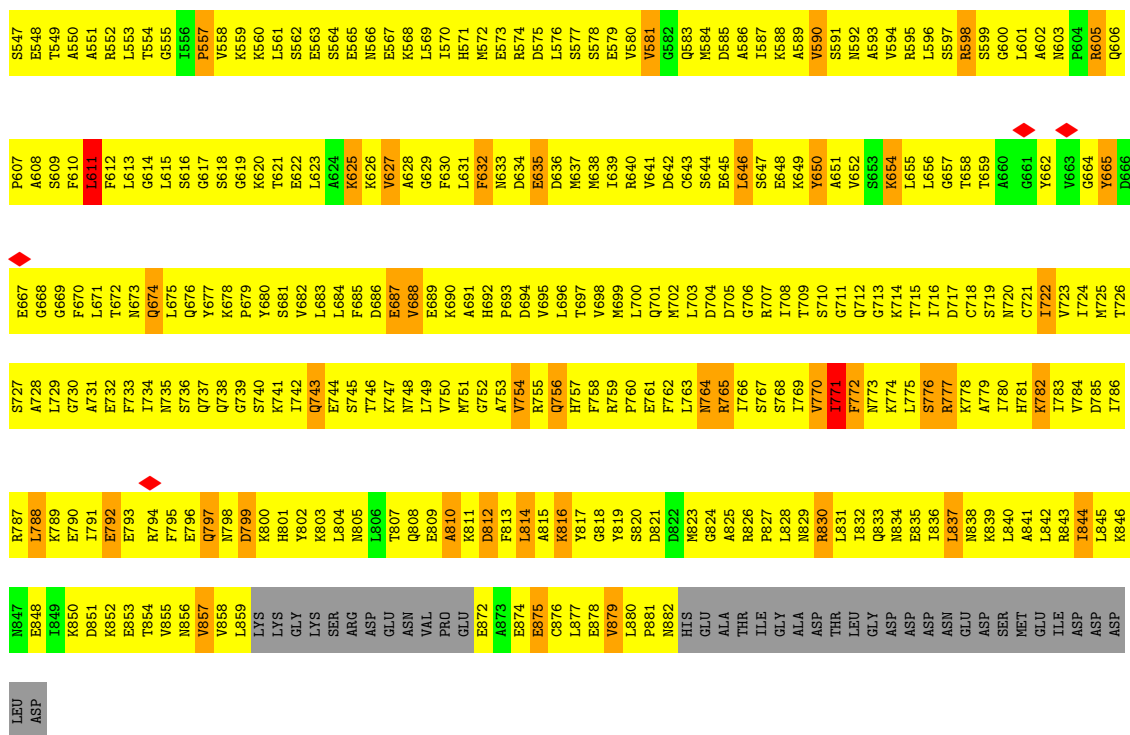
| Mol | Chain | Residues | Atoms | | | | | AltConf | |
|-----|-------|----------|-------------|---------|--------|---------|--------|---------|---|
| 2 | C | 1 | Total 31 | C 10 | N 5 | O 12 | P 3 | S 1 | 0 |
| 2 | D | 1 | Total 31 | C 10 | N 5 | O 12 | P 3 | S 1 | 0 |
| 2 | E | 1 | Total 31 | C 10 | N 5 | O 12 | P 3 | S 1 | 0 |
| 2 | E | 1 | Total 31 | C 10 | N 5 | O 12 | P 3 | S 1 | 0 |
| 2 | F | 1 | Total 31 | C 10 | N 5 | O 12 | P 3 | S 1 | 0 |
| 2 | F | 1 | Total 31 | C 10 | N 5 | O 12 | P 3 | S 1 | 0 |



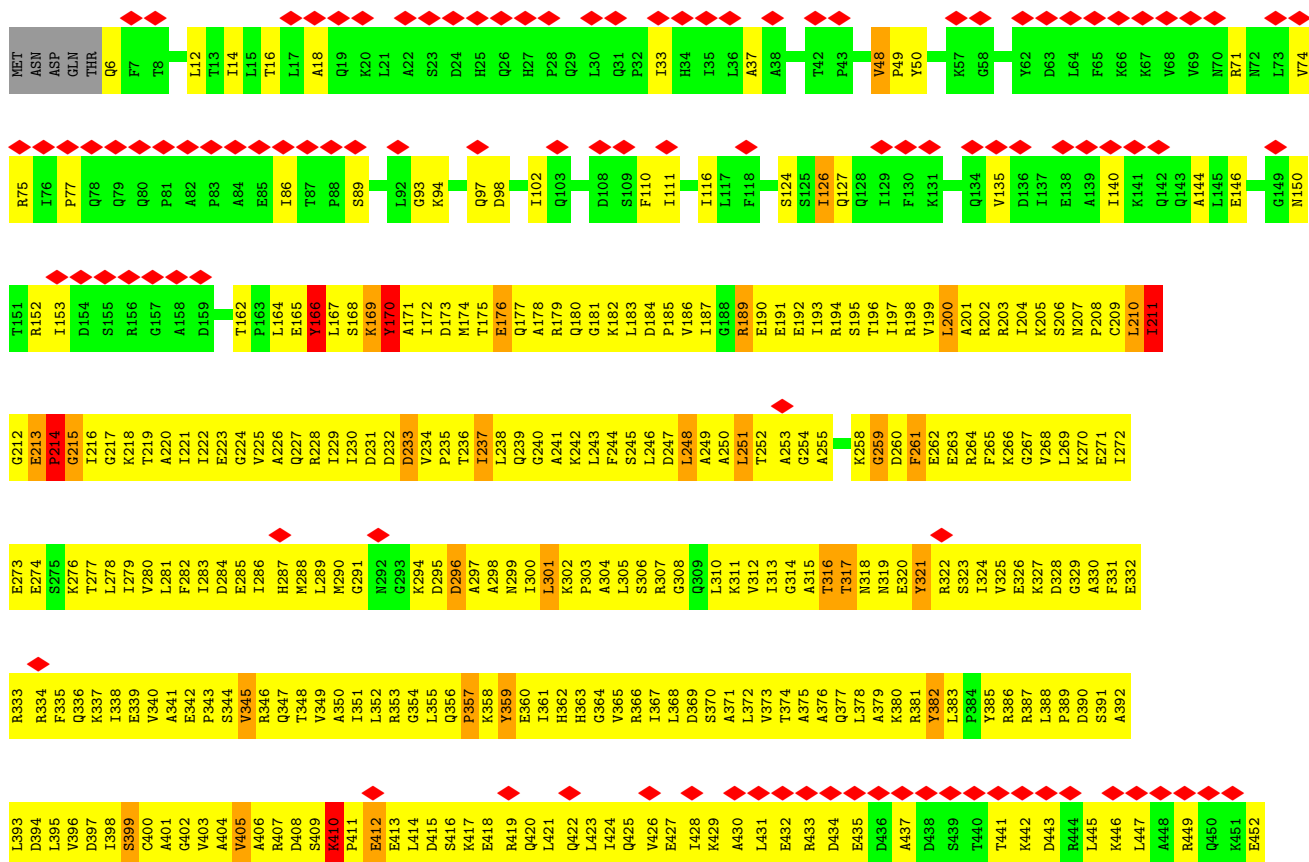
• Molecule 1: Heat shock protein 104

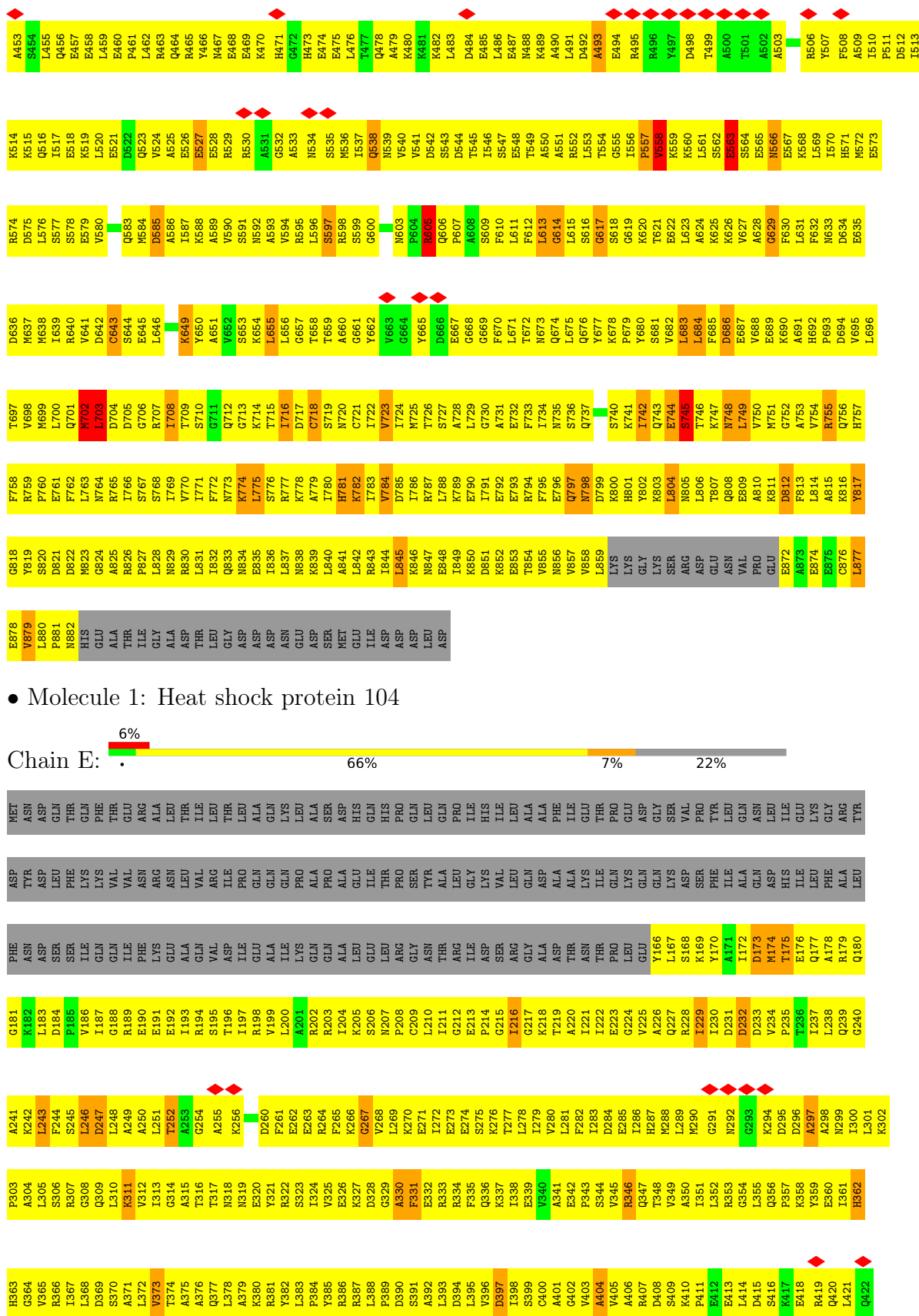


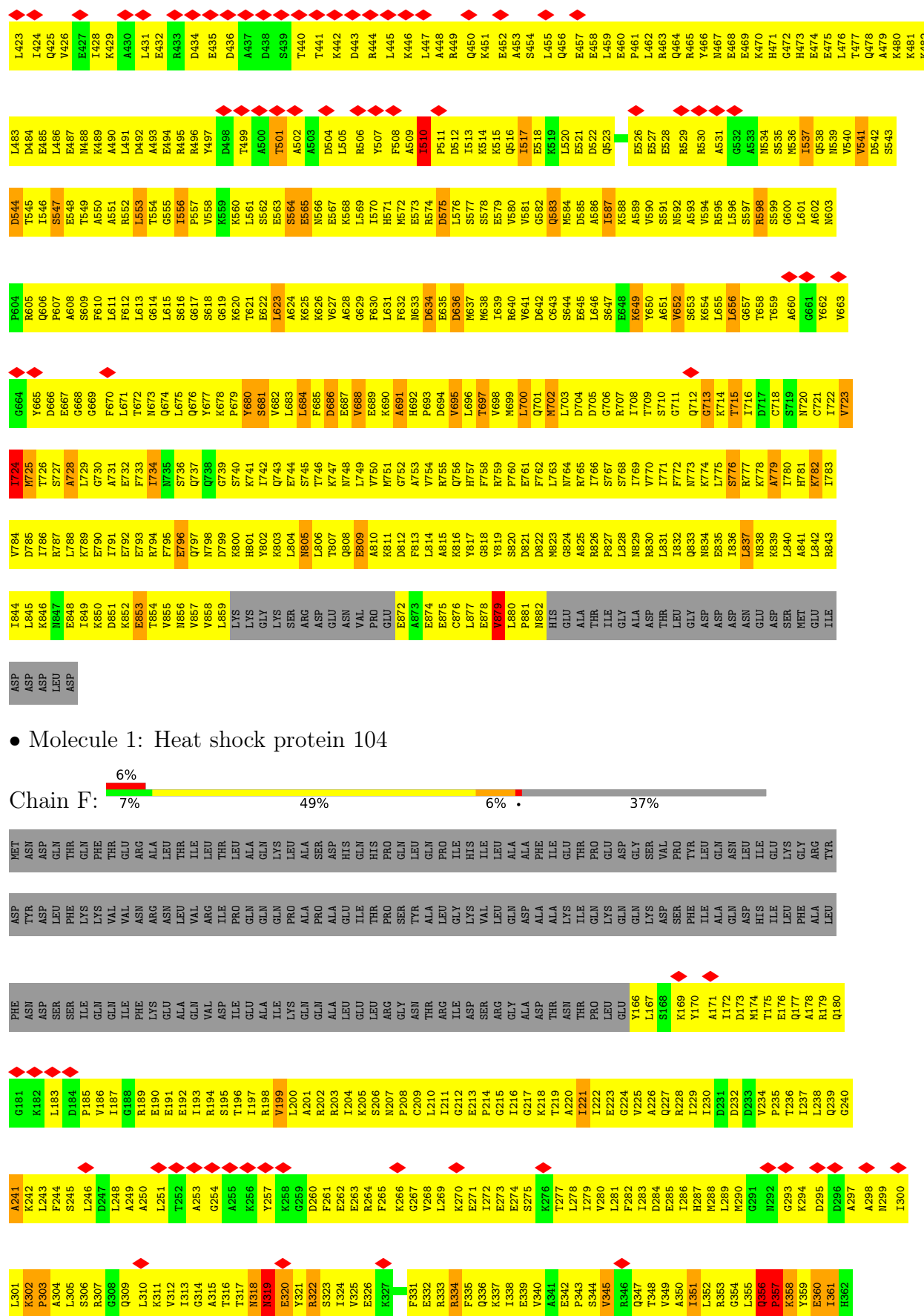




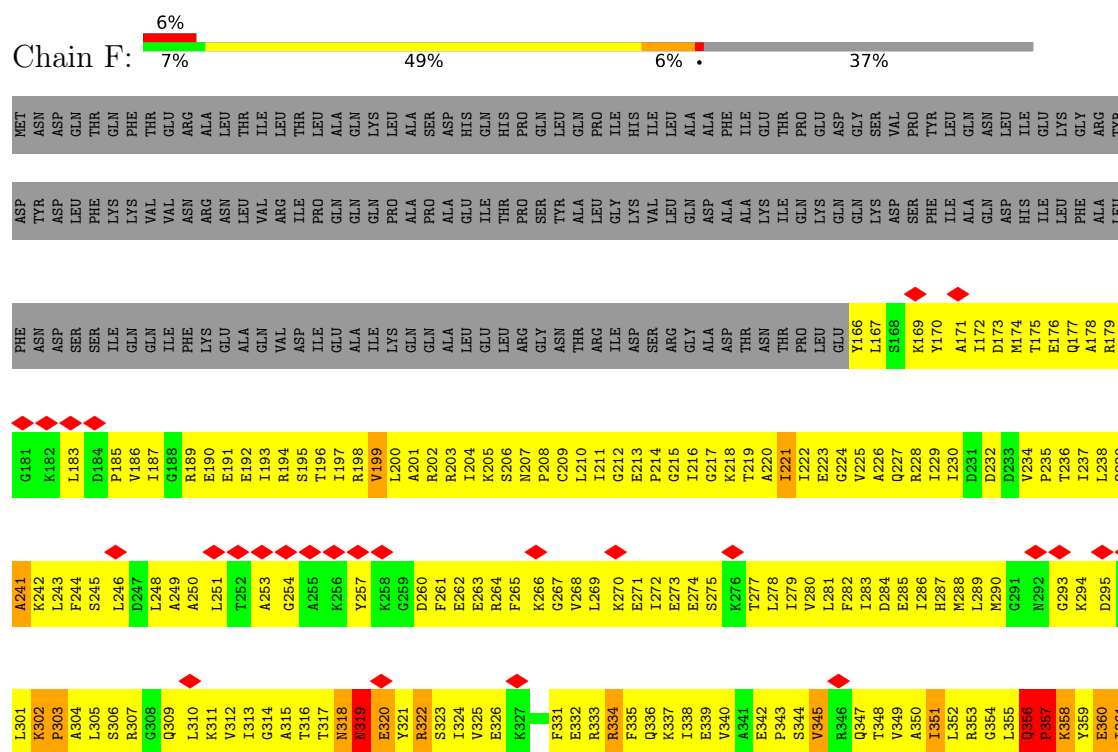
• Molecule 1: Heat shock protein 104







• Molecule 1: Heat shock protein 104



| | | | | | | | | | |
|--------------------------|------|------|------|------|------|------|------|-----|------|
| ASP ASP LEU ASP | L845 | D785 | M725 | Y665 | P604 | D544 | ASP | ILE | H563 |
| | R846 | T786 | T726 | G666 | R605 | T545 | GLU | GLN | G364 |
| | N847 | R787 | S727 | E667 | Q606 | T546 | LEU | VAL | V365 |
| | E848 | L788 | A728 | G668 | P607 | S547 | GLU | GLU | R366 |
| ASP | L849 | K789 | L729 | G669 | A608 | E548 | ASN | ILE | I367 |
| | R850 | E790 | G730 | F670 | S609 | T549 | LYS | LYS | L368 |
| | D851 | I791 | A731 | L671 | F610 | A550 | ALA | ALA | D369 |
| | K852 | E792 | E732 | T672 | L611 | A551 | LEU | LEU | S370 |
| ASP | E853 | E793 | F733 | N673 | F612 | R552 | ASP | GLU | A371 |
| | T854 | R794 | L734 | Q674 | G614 | L553 | ALA | ARG | L372 |
| | R855 | F795 | N735 | Q674 | G614 | T554 | GLU | ASP | V373 |
| | N856 | E796 | S736 | L675 | L615 | G555 | ARG | GLU | T374 |
| LYS | R857 | Q797 | Q737 | Q676 | S616 | T556 | ARG | ASP | A375 |
| | V858 | N798 | G738 | G677 | G617 | P557 | TYR | ALA | A376 |
| | L859 | D799 | G739 | P679 | S618 | V558 | ASP | ASP | Q377 |
| | K800 | R801 | S740 | G680 | G619 | K559 | THR | SER | L378 |
| LYS | H802 | K803 | K741 | Y680 | K620 | K560 | ALA | THR | A379 |
| | G804 | I742 | S812 | S682 | T621 | L561 | THR | THR | K380 |
| | L805 | Q743 | L683 | E684 | E622 | S562 | ALA | LYS | R381 |
| | SER | E744 | L683 | L623 | E563 | E563 | ALA | ASP | Y382 |
| ARG | N805 | S745 | F685 | G686 | K625 | S564 | ASP | ARG | L383 |
| | L806 | T746 | D687 | E687 | K626 | E565 | LEU | LEU | |
| | GLU | T807 | K747 | E688 | G628 | N566 | ARG | LYS | |
| | ASN | Q808 | M748 | V688 | A624 | E567 | PHE | ALA | |
| VAL | E809 | L749 | G689 | G629 | A628 | E567 | THR | ALA | R387 |
| | A810 | K811 | M751 | K690 | G629 | L569 | ALA | ARG | L388 |
| | D812 | G752 | G52 | A691 | F630 | I570 | ILE | GLN | D389 |
| | R813 | F813 | A753 | H692 | F632 | M572 | PRO | LYS | S391 |
| E874 | L814 | R754 | D694 | N633 | N633 | E573 | ILE | ALA | A392 |
| | A815 | R755 | D694 | D634 | D634 | R574 | LYS | SER | D394 |
| | R816 | K816 | Q756 | E635 | E635 | D575 | LYS | LEU | L395 |
| | L877 | X817 | H757 | L696 | D636 | R576 | GLN | GLN | V396 |
| E878 | G818 | F758 | T697 | T697 | M637 | L576 | ILE | GLU | D397 |
| | R819 | R759 | V698 | M638 | G638 | S577 | GLU | GLU | I398 |
| | L880 | S820 | P760 | M699 | I639 | S578 | LYS | LEU | S399 |
| | P881 | D821 | E761 | L700 | R640 | E579 | LEU | GLU | C400 |
| HIS | N882 | D822 | E762 | Q701 | V641 | V580 | GLU | PRO | A401 |
| | M823 | L763 | M702 | M702 | D642 | G582 | ASP | LEU | G402 |
| | G824 | R765 | L703 | C643 | C643 | G582 | GLN | ARG | V403 |
| | ALA | A825 | M764 | D704 | S644 | M584 | VAL | GLN | A404 |
| THR | R826 | R826 | I766 | D705 | E845 | M584 | ALA | TYR | V405 |
| | P827 | S767 | T767 | G706 | L646 | D585 | GLU | ARG | A406 |
| | GLY | L828 | R768 | R707 | S647 | A586 | GLU | ASN | R407 |
| | ALA | N829 | I769 | I708 | E648 | T587 | GLU | GLU | D408 |
| ASP | R830 | E830 | I769 | T709 | K649 | K588 | ARG | GLU | S409 |
| | L831 | L831 | V770 | S710 | Y650 | A589 | ARG | LYS | LYS |
| | LEU | R832 | I771 | G711 | V690 | S591 | ALA | HIS | PRO |
| | GLY | Q833 | N772 | Q712 | A651 | S591 | GLY | GLY | GLU |
| ASP | N834 | N834 | N773 | G713 | S653 | N592 | ALA | HIS | GLU |
| | ASP | E835 | K774 | G713 | V652 | N592 | ASN | GLU | LEU |
| | ASP | E836 | L775 | K714 | K654 | A593 | GLU | GLU | ASP |
| | ASN | R836 | S776 | T715 | L655 | R595 | SER | GLU | ASP |
| GLU | L837 | R777 | T776 | I716 | L656 | L596 | MET | LEU | SER |
| | N838 | K778 | R777 | I716 | L656 | L596 | ILE | THR | LYS |
| | ASP | R839 | K778 | D717 | G657 | S597 | GLN | GLN | GLU |
| | SER | L840 | A779 | T718 | T658 | R598 | ALA | ALA | ARG |
| MET | A841 | I780 | I780 | G719 | G661 | S599 | VAL | LYS | GLN |
| | L842 | H781 | H781 | N720 | G661 | G600 | VAL | LYS | LEU |
| | R843 | K782 | C721 | C721 | V662 | D542 | | LYS | GLN |
| | ILE | L844 | I783 | I722 | V663 | A602 | S543 | LYS | LEU |
| ASP | | | I724 | G664 | G664 | N603 | | | |

4 Experimental information

| Property | Value | Source |
|--------------------------------------|---|-----------|
| EM reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, Not provided | |
| Number of particles used | 69537 | Depositor |
| Resolution determination method | FSC 0.143 CUT-OFF | Depositor |
| CTF correction method | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope | FEI TITAN KRIOS | Depositor |
| Voltage (kV) | 300 | Depositor |
| Electron dose ($e^-/\text{\AA}^2$) | 50 | Depositor |
| Minimum defocus (nm) | Not provided | |
| Maximum defocus (nm) | Not provided | |
| Magnification | Not provided | |
| Image detector | GATAN K2 SUMMIT (4k x 4k) | Depositor |
| Maximum map value | 0.506 | Depositor |
| Minimum map value | -0.223 | Depositor |
| Average map value | 0.000 | Depositor |
| Map value standard deviation | 0.024 | Depositor |
| Recommended contour level | 0.08 | Depositor |
| Map size (Å) | 285.12003, 285.12003, 285.12003 | wwPDB |
| Map dimensions | 108, 108, 108 | wwPDB |
| Map angles (°) | 90.0, 90.0, 90.0 | wwPDB |
| Pixel spacing (Å) | 2.6400003, 2.6400003, 2.6400003 | Depositor |

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|----------------|-------------|-----------------|
| | | RMSZ | $\# Z > 5$ | RMSZ | $\# Z > 5$ |
| 1 | A | 0.62 | 0/4509 | 0.96 | 5/6077 (0.1%) |
| 1 | B | 0.74 | 0/5196 | 1.06 | 10/6932 (0.1%) |
| 1 | C | 0.83 | 1/6223 (0.0%) | 1.12 | 20/8312 (0.2%) |
| 1 | D | 1.14 | 7/6233 (0.1%) | 1.16 | 29/8325 (0.3%) |
| 1 | E | 0.82 | 0/5573 | 1.11 | 12/7501 (0.2%) |
| 1 | F | 0.66 | 0/4535 | 0.96 | 6/6103 (0.1%) |
| All | All | 0.84 | 8/32269 (0.0%) | 1.07 | 82/43250 (0.2%) |

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 | 0 | 30 |
| 1 | B | 0 | 43 |
| 1 | C | 0 | 28 |
| 1 | D | 0 | 41 |
| 1 | E | 0 | 22 |
| 1 | F | 0 | 20 |
| All | All | 0 | 184 |

All (8) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1 | D | 321 | TYR | CD2-CE2 | 31.75 | 2.33 | 1.38 |
| 1 | D | 321 | TYR | CD1-CE1 | 29.93 | 2.28 | 1.38 |
| 1 | D | 321 | TYR | CE2-CZ | 21.61 | 1.90 | 1.38 |
| 1 | D | 321 | TYR | CE1-CZ | 21.51 | 1.89 | 1.38 |
| 1 | D | 321 | TYR | CG-CD1 | 18.66 | 1.78 | 1.39 |
| 1 | D | 321 | TYR | CG-CD2 | 18.45 | 1.78 | 1.39 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|--------|-------------|----------|
| 1 | D | 745 | SER | CA-C | -10.07 | 1.38 | 1.52 |
| 1 | C | 772 | PHE | CA-C | -5.62 | 1.48 | 1.53 |

All (82) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|--------|-------------|----------|
| 1 | D | 213 | GLU | CA-C-N | 15.01 | 135.99 | 119.93 |
| 1 | D | 213 | GLU | C-N-CA | 15.01 | 135.99 | 119.93 |
| 1 | E | 510 | ILE | CA-C-N | -14.58 | 101.61 | 119.84 |
| 1 | E | 510 | ILE | C-N-CA | -14.58 | 101.61 | 119.84 |
| 1 | C | 772 | PHE | CB-CA-C | -11.05 | 103.81 | 116.63 |
| 1 | A | 249 | ALA | N-CA-C | -9.65 | 101.05 | 112.92 |
| 1 | D | 775 | LEU | N-CA-C | 8.83 | 124.36 | 113.50 |
| 1 | D | 215 | GLY | N-CA-C | 7.77 | 124.35 | 114.25 |
| 1 | D | 214 | PRO | N-CA-C | 7.74 | 123.87 | 111.26 |
| 1 | F | 609 | SER | N-CA-C | 7.73 | 122.86 | 107.62 |
| 1 | D | 528 | GLU | N-CA-C | -7.41 | 94.99 | 107.80 |
| 1 | D | 744 | GLU | CA-C-N | 7.17 | 134.32 | 120.99 |
| 1 | D | 744 | GLU | C-N-CA | 7.17 | 134.32 | 120.99 |
| 1 | C | 771 | ILE | N-CA-CB | -7.14 | 104.36 | 112.21 |
| 1 | A | 291 | GLY | N-CA-C | -6.93 | 96.75 | 113.18 |
| 1 | D | 614 | GLY | N-CA-C | 6.84 | 121.00 | 112.79 |
| 1 | D | 605 | ARG | CA-C-N | -6.77 | 110.30 | 122.28 |
| 1 | D | 605 | ARG | C-N-CA | -6.77 | 110.30 | 122.28 |
| 1 | B | 776 | SER | CB-CA-C | -6.74 | 107.78 | 115.79 |
| 1 | D | 563 | GLU | N-CA-C | 6.73 | 118.84 | 109.15 |
| 1 | C | 269 | LEU | N-CA-C | -6.59 | 102.98 | 111.02 |
| 1 | D | 613 | LEU | CA-CB-CG | -6.59 | 93.25 | 116.30 |
| 1 | E | 553 | LEU | CA-CB-CG | -6.57 | 93.32 | 116.30 |
| 1 | A | 260 | ASP | N-CA-C | -6.50 | 100.96 | 111.04 |
| 1 | D | 382 | TYR | CA-CB-CG | -6.50 | 102.20 | 113.90 |
| 1 | C | 290 | MET | CB-CA-C | -6.33 | 108.62 | 117.23 |
| 1 | D | 200 | LEU | CA-CB-CG | -6.07 | 95.07 | 116.30 |
| 1 | C | 271 | GLU | N-CA-C | -6.06 | 103.63 | 111.02 |
| 1 | E | 267 | GLY | N-CA-C | -5.97 | 105.58 | 112.50 |
| 1 | C | 598 | ARG | CA-CB-CG | -5.94 | 102.22 | 114.10 |
| 1 | D | 782 | LYS | CA-CB-CG | -5.89 | 102.32 | 114.10 |
| 1 | C | 646 | LEU | CA-CB-CG | -5.86 | 95.79 | 116.30 |
| 1 | D | 170 | TYR | CA-CB-CG | 5.81 | 124.36 | 113.90 |
| 1 | E | 598 | ARG | CA-CB-CG | -5.78 | 102.54 | 114.10 |
| 1 | A | 206 | SER | N-CA-C | 5.75 | 118.01 | 108.13 |
| 1 | C | 665 | TYR | CA-CB-CG | -5.73 | 103.59 | 113.90 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 1 | D | 166 | TYR | CA-CB-CG | 5.72 | 124.20 | 113.90 |
| 1 | B | 814 | LEU | CA-CB-CG | -5.71 | 96.31 | 116.30 |
| 1 | F | 318 | ASN | CA-C-N | 5.67 | 132.37 | 121.54 |
| 1 | F | 318 | ASN | C-N-CA | 5.67 | 132.37 | 121.54 |
| 1 | F | 610 | PHE | N-CA-C | 5.67 | 119.00 | 111.30 |
| 1 | D | 176 | GLU | CA-CB-CG | -5.64 | 102.82 | 114.10 |
| 1 | C | 393 | LEU | N-CA-C | -5.63 | 104.36 | 111.11 |
| 1 | B | 310 | LEU | CA-CB-CG | -5.59 | 96.75 | 116.30 |
| 1 | E | 702 | MET | CA-C-N | -5.58 | 111.20 | 120.68 |
| 1 | E | 702 | MET | C-N-CA | -5.58 | 111.20 | 120.68 |
| 1 | B | 284 | ASP | N-CA-C | 5.55 | 122.63 | 110.80 |
| 1 | D | 782 | LYS | CG-CD-CE | -5.54 | 98.55 | 111.30 |
| 1 | B | 221 | ILE | CA-C-N | 5.52 | 127.72 | 120.60 |
| 1 | B | 221 | ILE | C-N-CA | 5.52 | 127.72 | 120.60 |
| 1 | C | 210 | LEU | CA-CB-CG | 5.52 | 135.61 | 116.30 |
| 1 | C | 382 | TYR | CA-CB-CG | -5.51 | 103.98 | 113.90 |
| 1 | E | 796 | GLU | CB-CA-C | -5.50 | 100.90 | 113.33 |
| 1 | C | 200 | LEU | CA-CB-CG | -5.44 | 97.25 | 116.30 |
| 1 | D | 166 | TYR | CA-C-N | -5.43 | 111.87 | 121.81 |
| 1 | D | 166 | TYR | C-N-CA | -5.43 | 111.87 | 121.81 |
| 1 | B | 207 | ASN | N-CA-CB | -5.42 | 100.71 | 110.37 |
| 1 | C | 305 | LEU | CA-CB-CG | -5.41 | 97.37 | 116.30 |
| 1 | C | 654 | LYS | CB-CG-CD | 5.41 | 123.73 | 111.30 |
| 1 | C | 830 | ARG | CA-C-N | -5.37 | 113.33 | 120.63 |
| 1 | C | 830 | ARG | C-N-CA | -5.37 | 113.33 | 120.63 |
| 1 | B | 705 | ASP | CB-CA-C | -5.36 | 110.37 | 116.54 |
| 1 | D | 316 | THR | CA-C-O | -5.35 | 113.51 | 120.25 |
| 1 | E | 600 | GLY | N-CA-C | -5.35 | 100.51 | 113.18 |
| 1 | D | 629 | GLY | CA-C-N | -5.34 | 111.33 | 121.54 |
| 1 | D | 629 | GLY | C-N-CA | -5.34 | 111.33 | 121.54 |
| 1 | D | 211 | ILE | CA-C-N | 5.32 | 131.84 | 121.41 |
| 1 | D | 211 | ILE | C-N-CA | 5.32 | 131.84 | 121.41 |
| 1 | C | 289 | LEU | CA-CB-CG | -5.29 | 97.78 | 116.30 |
| 1 | E | 547 | SER | N-CA-C | -5.28 | 104.58 | 111.02 |
| 1 | C | 654 | LYS | CG-CD-CE | -5.26 | 99.21 | 111.30 |
| 1 | F | 758 | PHE | CA-C-N | 5.26 | 134.62 | 121.80 |
| 1 | F | 758 | PHE | C-N-CA | 5.26 | 134.62 | 121.80 |
| 1 | D | 702 | MET | CA-CB-CG | -5.23 | 103.63 | 114.10 |
| 1 | D | 817 | TYR | CA-CB-CG | -5.23 | 104.49 | 113.90 |
| 1 | C | 654 | LYS | CA-CB-CG | -5.21 | 103.67 | 114.10 |
| 1 | B | 692 | HIS | N-CA-C | 5.14 | 119.85 | 108.64 |
| 1 | E | 713 | GLY | N-CA-C | -5.10 | 101.09 | 113.18 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 1 | C | 189 | ARG | CG-CD-NE | -5.09 | 100.81 | 112.00 |
| 1 | B | 225 | VAL | N-CA-C | -5.08 | 105.37 | 110.30 |
| 1 | A | 378 | LEU | CA-CB-CG | -5.07 | 98.57 | 116.30 |
| 1 | E | 724 | ILE | N-CA-C | -5.02 | 98.91 | 109.34 |

There are no chirality outliers.

All (184) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|---------|
| 1 | A | 200 | LEU | Peptide |
| 1 | A | 206 | SER | Peptide |
| 1 | A | 210 | LEU | Peptide |
| 1 | A | 224 | GLY | Peptide |
| 1 | A | 231 | ASP | Peptide |
| 1 | A | 234 | VAL | Peptide |
| 1 | A | 244 | PHE | Peptide |
| 1 | A | 248 | LEU | Peptide |
| 1 | A | 249 | ALA | Peptide |
| 1 | A | 260 | ASP | Peptide |
| 1 | A | 290 | MET | Peptide |
| 1 | A | 291 | GLY | Peptide |
| 1 | A | 334 | ARG | Peptide |
| 1 | A | 339 | GLU | Peptide |
| 1 | A | 356 | GLN | Peptide |
| 1 | A | 558 | VAL | Peptide |
| 1 | A | 560 | LYS | Peptide |
| 1 | A | 561 | LEU | Peptide |
| 1 | A | 569 | LEU | Peptide |
| 1 | A | 606 | GLN | Peptide |
| 1 | A | 611 | LEU | Peptide |
| 1 | A | 619 | GLY | Peptide |
| 1 | A | 679 | PRO | Peptide |
| 1 | A | 725 | MET | Peptide |
| 1 | A | 757 | HIS | Peptide |
| 1 | A | 771 | ILE | Peptide |
| 1 | A | 779 | ALA | Peptide |
| 1 | A | 810 | ALA | Peptide |
| 1 | A | 812 | ASP | Peptide |
| 1 | A | 848 | GLU | Peptide |
| 1 | B | 105 | GLN | Peptide |
| 1 | B | 126 | ILE | Peptide |
| 1 | B | 127 | GLN | Peptide |

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| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|---------|
| 1 | B | 128 | GLN | Peptide |
| 1 | B | 180 | GLN | Peptide |
| 1 | B | 217 | GLY | Peptide |
| 1 | B | 219 | THR | Peptide |
| 1 | B | 236 | THR | Peptide |
| 1 | B | 242 | LYS | Peptide |
| 1 | B | 270 | LYS | Peptide |
| 1 | B | 282 | PHE | Peptide |
| 1 | B | 284 | ASP | Peptide |
| 1 | B | 294 | LYS | Peptide |
| 1 | B | 318 | ASN | Peptide |
| 1 | B | 327 | LYS | Peptide |
| 1 | B | 345 | VAL | Peptide |
| 1 | B | 385 | TYR | Peptide |
| 1 | B | 45 | ASP | Peptide |
| 1 | B | 557 | PRO | Peptide |
| 1 | B | 565 | GLU | Peptide |
| 1 | B | 578 | SER | Peptide |
| 1 | B | 605 | ARG | Peptide |
| 1 | B | 642 | ASP | Peptide |
| 1 | B | 647 | SER | Peptide |
| 1 | B | 665 | TYR | Peptide |
| 1 | B | 679 | PRO | Peptide |
| 1 | B | 682 | VAL | Peptide |
| 1 | B | 688 | VAL | Peptide |
| 1 | B | 689 | GLU | Peptide |
| 1 | B | 690 | LYS | Peptide |
| 1 | B | 711 | GLY | Peptide |
| 1 | B | 729 | LEU | Peptide |
| 1 | B | 757 | HIS | Peptide |
| 1 | B | 770 | VAL | Peptide |
| 1 | B | 789 | LYS | Peptide |
| 1 | B | 806 | LEU | Peptide |
| 1 | B | 807 | THR | Peptide |
| 1 | B | 839 | LYS | Peptide |
| 1 | B | 846 | LYS | Peptide |
| 1 | B | 853 | GLU | Peptide |
| 1 | B | 874 | GLU | Peptide |
| 1 | B | 876 | CYS | Peptide |
| 1 | B | 877 | LEU | Peptide |
| 1 | C | 202 | ARG | Peptide |
| 1 | C | 209 | CYS | Peptide |

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| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|---------|
| 1 | C | 243 | LEU | Peptide |
| 1 | C | 245 | SER | Peptide |
| 1 | C | 247 | ASP | Peptide |
| 1 | C | 248 | LEU | Peptide |
| 1 | C | 249 | ALA | Peptide |
| 1 | C | 298 | ALA | Peptide |
| 1 | C | 310 | LEU | Peptide |
| 1 | C | 353 | ARG | Peptide |
| 1 | C | 369 | ASP | Peptide |
| 1 | C | 537 | ILE | Peptide |
| 1 | C | 557 | PRO | Peptide |
| 1 | C | 600 | GLY | Peptide |
| 1 | C | 605 | ARG | Peptide |
| 1 | C | 611 | LEU | Peptide |
| 1 | C | 625 | LYS | Peptide |
| 1 | C | 632 | PHE | Peptide |
| 1 | C | 635 | GLU | Peptide |
| 1 | C | 650 | TYR | Peptide |
| 1 | C | 651 | ALA | Peptide |
| 1 | C | 722 | ILE | Peptide |
| 1 | C | 743 | GLN | Peptide |
| 1 | C | 765 | ARG | Peptide |
| 1 | C | 771 | ILE | Peptide |
| 1 | C | 776 | SER | Peptide |
| 1 | C | 782 | LYS | Peptide |
| 1 | C | 799 | ASP | Peptide |
| 1 | D | 127 | GLN | Peptide |
| 1 | D | 166 | TYR | Peptide |
| 1 | D | 169 | LYS | Peptide |
| 1 | D | 189 | ARG | Peptide |
| 1 | D | 210 | LEU | Peptide |
| 1 | D | 214 | PRO | Peptide |
| 1 | D | 233 | ASP | Peptide |
| 1 | D | 248 | LEU | Peptide |
| 1 | D | 251 | LEU | Peptide |
| 1 | D | 259 | GLY | Peptide |
| 1 | D | 296 | ASP | Peptide |
| 1 | D | 357 | PRO | Peptide |
| 1 | D | 359 | TYR | Peptide |
| 1 | D | 410 | LYS | Peptide |
| 1 | D | 412 | GLU | Peptide |
| 1 | D | 493 | ALA | Peptide |

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| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|---------|
| 1 | D | 527 | GLU | Peptide |
| 1 | D | 538 | GLN | Peptide |
| 1 | D | 557 | PRO | Peptide |
| 1 | D | 558 | VAL | Peptide |
| 1 | D | 563 | GLU | Peptide |
| 1 | D | 605 | ARG | Peptide |
| 1 | D | 617 | GLY | Peptide |
| 1 | D | 649 | LYS | Peptide |
| 1 | D | 655 | LEU | Peptide |
| 1 | D | 683 | LEU | Peptide |
| 1 | D | 684 | LEU | Peptide |
| 1 | D | 686 | ASP | Peptide |
| 1 | D | 702 | MET | Peptide |
| 1 | D | 703 | LEU | Peptide |
| 1 | D | 708 | ILE | Peptide |
| 1 | D | 716 | ILE | Peptide |
| 1 | D | 718 | CYS | Peptide |
| 1 | D | 723 | VAL | Peptide |
| 1 | D | 74 | VAL | Peptide |
| 1 | D | 745 | SER | Peptide |
| 1 | D | 75 | ARG | Peptide |
| 1 | D | 774 | LYS | Peptide |
| 1 | D | 798 | ASN | Peptide |
| 1 | D | 804 | LEU | Peptide |
| 1 | D | 877 | LEU | Peptide |
| 1 | E | 173 | ASP | Peptide |
| 1 | E | 232 | ASP | Peptide |
| 1 | E | 243 | LEU | Peptide |
| 1 | E | 246 | LEU | Peptide |
| 1 | E | 247 | ASP | Peptide |
| 1 | E | 311 | LYS | Peptide |
| 1 | E | 510 | ILE | Peptide |
| 1 | E | 541 | VAL | Peptide |
| 1 | E | 564 | SER | Peptide |
| 1 | E | 565 | GLU | Peptide |
| 1 | E | 634 | ASP | Peptide |
| 1 | E | 670 | PHE | Peptide |
| 1 | E | 680 | TYR | Peptide |
| 1 | E | 681 | SER | Peptide |
| 1 | E | 684 | LEU | Peptide |
| 1 | E | 686 | ASP | Peptide |
| 1 | E | 691 | ALA | Peptide |

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| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|---------|
| 1 | E | 715 | THR | Peptide |
| 1 | E | 728 | ALA | Peptide |
| 1 | E | 776 | SER | Peptide |
| 1 | E | 782 | LYS | Peptide |
| 1 | E | 879 | VAL | Peptide |
| 1 | F | 199 | VAL | Peptide |
| 1 | F | 241 | ALA | Peptide |
| 1 | F | 302 | LYS | Peptide |
| 1 | F | 334 | ARG | Peptide |
| 1 | F | 369 | ASP | Peptide |
| 1 | F | 373 | VAL | Peptide |
| 1 | F | 544 | ASP | Peptide |
| 1 | F | 555 | GLY | Peptide |
| 1 | F | 561 | LEU | Peptide |
| 1 | F | 565 | GLU | Peptide |
| 1 | F | 603 | ASN | Peptide |
| 1 | F | 609 | SER | Peptide |
| 1 | F | 717 | ASP | Peptide |
| 1 | F | 748 | ASN | Peptide |
| 1 | F | 767 | SER | Peptide |
| 1 | F | 778 | LYS | Peptide |
| 1 | F | 802 | TYR | Peptide |
| 1 | F | 817 | TYR | Peptide |
| 1 | F | 826 | ARG | Peptide |
| 1 | F | 848 | GLU | Peptide |

5.2 Too-close contacts

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | A | 4456 | 0 | 4540 | 1223 | 0 |
| 1 | B | 5142 | 0 | 4785 | 1688 | 0 |
| 1 | C | 6162 | 0 | 5790 | 2042 | 0 |
| 1 | D | 6170 | 0 | 5790 | 2074 | 0 |
| 1 | E | 5512 | 0 | 5602 | 2016 | 0 |
| 1 | F | 4480 | 0 | 4597 | 1446 | 0 |
| 2 | C | 31 | 0 | 12 | 29 | 0 |
| 2 | D | 31 | 0 | 12 | 38 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 2 | E | 62 | 0 | 24 | 65 | 0 |
| 2 | F | 62 | 0 | 24 | 38 | 0 |
| All | All | 32108 | 0 | 31176 | 10300 | 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 163.

All (10300) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:700:LEU:HD23 | 1:F:703:LEU:CD2 | 1.21 | 1.66 |
| 1:C:169:LYS:CE | 1:C:264:ARG:HD2 | 1.23 | 1.62 |
| 1:D:321:TYR:CD1 | 1:D:321:TYR:CG | 1.78 | 1.62 |
| 1:F:331:PHE:HA | 1:F:334:ARG:CG | 1.24 | 1.62 |
| 1:C:169:LYS:HE3 | 1:C:264:ARG:CB | 1.21 | 1.60 |
| 1:D:321:TYR:CG | 1:D:321:TYR:CD2 | 1.78 | 1.60 |
| 1:F:286:ILE:CD1 | 1:F:322:ARG:CD | 1.78 | 1.56 |
| 1:C:169:LYS:CG | 1:C:264:ARG:CD | 1.85 | 1.53 |
| 1:F:704:ASP:CB | 1:F:765:ARG:CZ | 1.83 | 1.52 |
| 1:F:322:ARG:NH2 | 1:F:325:VAL:CG2 | 1.68 | 1.51 |
| 1:C:169:LYS:HE3 | 1:C:264:ARG:CG | 1.36 | 1.50 |
| 1:F:286:ILE:HD11 | 1:F:322:ARG:CG | 1.39 | 1.50 |
| 1:C:168:SER:CA | 1:C:264:ARG:HH21 | 1.22 | 1.49 |
| 1:F:700:LEU:CD2 | 1:F:703:LEU:HD22 | 1.03 | 1.49 |
| 1:F:704:ASP:HB2 | 1:F:765:ARG:CZ | 1.00 | 1.48 |
| 1:F:286:ILE:HD12 | 1:F:322:ARG:CD | 1.34 | 1.48 |
| 1:C:169:LYS:CE | 1:C:264:ARG:CD | 1.77 | 1.44 |
| 1:F:331:PHE:CE1 | 1:F:335:PHE:N | 1.86 | 1.44 |
| 1:F:363:HIS:CE1 | 1:F:397:ASP:HA | 1.53 | 1.43 |
| 1:F:286:ILE:HD12 | 1:F:322:ARG:NE | 1.30 | 1.42 |
| 1:C:168:SER:HA | 1:C:264:ARG:NH2 | 1.21 | 1.41 |
| 1:F:286:ILE:CD1 | 1:F:322:ARG:HD3 | 1.43 | 1.39 |
| 1:F:704:ASP:HA | 1:F:765:ARG:CD | 1.52 | 1.37 |
| 1:C:169:LYS:HD3 | 1:C:264:ARG:NE | 1.05 | 1.36 |
| 1:D:317:THR:HG23 | 1:D:321:TYR:CE1 | 1.61 | 1.36 |
| 1:C:168:SER:HB2 | 1:C:271:GLU:OE1 | 1.25 | 1.35 |
| 1:F:322:ARG:NH2 | 1:F:325:VAL:HG23 | 1.03 | 1.35 |
| 1:C:170:TYR:OH | 1:C:250:ALA:N | 1.63 | 1.31 |
| 1:D:326:GLU:OE2 | 1:D:327:LYS:NZ | 1.60 | 1.30 |
| 1:C:169:LYS:CE | 1:C:264:ARG:CG | 2.02 | 1.27 |
| 1:C:515:LYS:NZ | 1:D:435:GLU:OE2 | 1.69 | 1.26 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:169:LYS:HD3 | 1:C:264:ARG:CG | 1.63 | 1.26 |
| 1:F:704:ASP:CG | 1:F:765:ARG:NE | 1.92 | 1.25 |
| 1:C:169:LYS:CE | 1:C:264:ARG:CB | 2.14 | 1.25 |
| 1:F:700:LEU:CG | 1:F:703:LEU:CD2 | 2.12 | 1.24 |
| 1:D:556:ILE:O | 1:D:560:LYS:NZ | 1.68 | 1.24 |
| 1:F:331:PHE:CE1 | 1:F:334:ARG:C | 2.16 | 1.23 |
| 1:F:704:ASP:CB | 1:F:765:ARG:NE | 2.00 | 1.23 |
| 1:B:785:ASP:O | 1:B:789:LYS:NZ | 1.71 | 1.21 |
| 1:C:169:LYS:CG | 1:C:264:ARG:HD2 | 1.60 | 1.21 |
| 1:C:169:LYS:CE | 1:C:264:ARG:HB2 | 1.69 | 1.21 |
| 1:F:356:GLN:HB3 | 1:F:357:PRO:CD | 1.70 | 1.21 |
| 1:F:357:PRO:O | 1:F:361:ILE:HB | 1.40 | 1.21 |
| 1:C:170:TYR:CE1 | 1:C:249:ALA:HA | 1.75 | 1.21 |
| 1:D:321:TYR:CD1 | 1:D:321:TYR:CE1 | 2.28 | 1.20 |
| 1:D:843:ARG:HD3 | 1:D:846:LYS:HZ1 | 1.07 | 1.19 |
| 1:F:700:LEU:CG | 1:F:703:LEU:HD22 | 1.69 | 1.19 |
| 1:D:317:THR:N | 1:D:321:TYR:CD1 | 2.11 | 1.19 |
| 1:F:331:PHE:CA | 1:F:334:ARG:CG | 2.20 | 1.18 |
| 1:F:704:ASP:HB2 | 1:F:765:ARG:NH2 | 1.59 | 1.18 |
| 1:D:556:ILE:O | 1:D:559:LYS:NZ | 1.77 | 1.17 |
| 1:D:317:THR:CG2 | 1:D:321:TYR:CE1 | 2.25 | 1.17 |
| 1:F:331:PHE:CA | 1:F:334:ARG:HG2 | 1.74 | 1.17 |
| 1:F:704:ASP:HB2 | 1:F:765:ARG:NH1 | 1.59 | 1.17 |
| 1:C:169:LYS:CG | 1:C:264:ARG:HD3 | 1.60 | 1.16 |
| 1:D:191:GLU:OE2 | 1:D:194:ARG:NH1 | 1.76 | 1.16 |
| 1:D:218:LYS:NZ | 2:D:1001:AGS:O3B | 1.79 | 1.16 |
| 1:E:618:SER:OG | 1:E:620:LYS:NZ | 1.77 | 1.16 |
| 1:C:168:SER:HA | 1:C:264:ARG:CZ | 1.77 | 1.15 |
| 1:B:353:ARG:HH11 | 1:B:373:VAL:HG23 | 0.98 | 1.15 |
| 1:C:169:LYS:H | 1:C:264:ARG:CZ | 1.59 | 1.15 |
| 1:F:363:HIS:CE1 | 1:F:397:ASP:OD1 | 2.00 | 1.15 |
| 1:F:605:ARG:HH12 | 1:F:705:ASP:HB3 | 1.02 | 1.14 |
| 1:F:699:MET:SD | 1:F:702:MET:SD | 2.45 | 1.14 |
| 1:F:700:LEU:CD2 | 1:F:703:LEU:CD2 | 1.89 | 1.14 |
| 1:C:170:TYR:OH | 1:C:249:ALA:HB1 | 1.46 | 1.14 |
| 1:E:360:GLU:OE2 | 1:E:365:VAL:N | 1.78 | 1.14 |
| 1:F:702:MET:HB2 | 1:F:708:ILE:HG13 | 1.23 | 1.14 |
| 1:C:170:TYR:CZ | 1:C:250:ALA:N | 2.09 | 1.14 |
| 1:E:602:ALA:O | 1:F:794:ARG:NH1 | 1.80 | 1.14 |
| 1:D:791:ILE:O | 1:D:794:ARG:NH1 | 1.79 | 1.14 |
| 1:D:323:SER:O | 1:D:327:LYS:NZ | 1.81 | 1.13 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:548:GLU:HB3 | 1:E:552:ARG:HH12 | 0.99 | 1.13 |
| 1:F:787:ARG:NH2 | 1:F:790:GLU:OE2 | 1.81 | 1.13 |
| 1:B:645:GLU:HA | 1:B:691:ALA:HB3 | 1.26 | 1.13 |
| 1:B:743:GLN:NE2 | 1:C:872:GLU:OE2 | 1.82 | 1.13 |
| 1:F:616:SER:HB2 | 1:F:620:LYS:HD3 | 1.30 | 1.12 |
| 1:F:286:ILE:CD1 | 1:F:322:ARG:NE | 2.01 | 1.12 |
| 1:C:169:LYS:CD | 1:C:264:ARG:NE | 1.76 | 1.12 |
| 1:C:205:LYS:HZ2 | 1:C:334:ARG:N | 1.46 | 1.12 |
| 1:F:699:MET:O | 1:F:703:LEU:HG | 1.49 | 1.12 |
| 1:C:654:LYS:HG3 | 1:C:655:LEU:H | 0.95 | 1.11 |
| 1:A:332:GLU:OE2 | 1:A:334:ARG:NH1 | 1.83 | 1.11 |
| 1:C:360:GLU:OE2 | 1:C:365:VAL:N | 1.79 | 1.11 |
| 1:F:704:ASP:OD1 | 1:F:765:ARG:NE | 1.78 | 1.11 |
| 1:C:170:TYR:CZ | 1:C:249:ALA:CA | 2.31 | 1.11 |
| 1:C:650:TYR:OH | 1:C:654:LYS:NZ | 1.84 | 1.11 |
| 1:D:714:LYS:NZ | 1:D:715:THR:O | 1.84 | 1.11 |
| 1:F:331:PHE:HA | 1:F:334:ARG:HG3 | 1.30 | 1.11 |
| 1:C:169:LYS:HD2 | 1:C:264:ARG:HD2 | 1.11 | 1.11 |
| 1:B:843:ARG:NH1 | 1:B:848:GLU:OE2 | 1.84 | 1.10 |
| 1:C:652:VAL:O | 1:C:654:LYS:NZ | 1.82 | 1.10 |
| 1:C:168:SER:CA | 1:C:271:GLU:OE2 | 2.00 | 1.10 |
| 1:A:644:SER:HB3 | 1:A:687:GLU:HB2 | 1.32 | 1.10 |
| 1:E:617:GLY:N | 2:E:1002:AGS:O1B | 1.84 | 1.10 |
| 1:E:794:ARG:HH12 | 1:E:796:GLU:C | 1.59 | 1.10 |
| 1:E:794:ARG:NH1 | 1:E:796:GLU:O | 1.83 | 1.10 |
| 1:C:168:SER:HB2 | 1:C:271:GLU:CD | 1.74 | 1.09 |
| 1:C:700:LEU:HA | 1:C:703:LEU:HB2 | 1.33 | 1.09 |
| 1:A:229:ILE:HA | 1:A:233:ASP:HB2 | 1.32 | 1.09 |
| 1:E:703:LEU:O | 1:E:707:ARG:NH1 | 1.84 | 1.09 |
| 1:C:597:SER:O | 1:C:598:ARG:NH1 | 1.83 | 1.09 |
| 1:F:285:GLU:HB2 | 1:F:288:MET:H | 1.16 | 1.09 |
| 1:F:656:LEU:HD13 | 1:F:711:GLY:HA3 | 1.35 | 1.09 |
| 1:C:168:SER:HA | 1:C:271:GLU:OE2 | 1.48 | 1.08 |
| 1:E:650:TYR:HB2 | 1:E:654:LYS:HG2 | 1.35 | 1.08 |
| 1:F:363:HIS:CE1 | 1:F:397:ASP:CA | 2.35 | 1.08 |
| 1:A:778:LYS:O | 1:A:782:LYS:NZ | 1.86 | 1.08 |
| 1:F:715:THR:O | 1:F:717:ASP:N | 1.85 | 1.08 |
| 1:D:530:ARG:NH1 | 1:D:539:ASN:H | 1.49 | 1.08 |
| 1:B:781:HIS:O | 1:B:811:LYS:NZ | 1.87 | 1.08 |
| 1:F:700:LEU:CG | 1:F:703:LEU:HD21 | 1.83 | 1.08 |
| 1:F:702:MET:HB3 | 1:F:708:ILE:HG23 | 1.36 | 1.08 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:800:LYS:HG3 | 1:D:801:HIS:H | 1.13 | 1.07 |
| 1:E:748:ASN:HA | 1:E:751:MET:HG2 | 1.34 | 1.07 |
| 1:B:189:ARG:NH1 | 1:B:341:ALA:O | 1.86 | 1.07 |
| 1:C:170:TYR:CZ | 1:C:249:ALA:HA | 1.89 | 1.07 |
| 1:F:701:GLN:OE1 | 1:F:709:THR:OG1 | 1.73 | 1.07 |
| 1:E:570:ILE:HA | 1:E:595:ARG:HH12 | 1.06 | 1.07 |
| 1:D:785:ASP:OD1 | 1:D:789:LYS:N | 1.88 | 1.07 |
| 1:B:829:ASN:HA | 1:B:832:ILE:HB | 1.29 | 1.06 |
| 1:E:214:PRO:C | 1:E:218:LYS:HZ1 | 1.62 | 1.06 |
| 1:C:205:LYS:NZ | 1:C:334:ARG:H | 1.53 | 1.06 |
| 1:F:785:ASP:HB3 | 1:F:789:LYS:HZ1 | 1.07 | 1.06 |
| 1:F:356:GLN:HE21 | 1:F:367:ILE:HG21 | 1.19 | 1.06 |
| 1:E:169:LYS:NZ | 1:E:264:ARG:O | 1.88 | 1.06 |
| 1:B:761:GLU:O | 1:B:765:ARG:NH1 | 1.88 | 1.05 |
| 1:A:316:THR:HG21 | 1:A:322:ARG:HH11 | 1.18 | 1.05 |
| 1:C:642:ASP:HB2 | 1:C:645:GLU:HG2 | 1.35 | 1.05 |
| 1:D:683:LEU:HB3 | 1:D:723:VAL:HG22 | 1.36 | 1.05 |
| 1:B:633:ASN:ND2 | 1:B:636:ASP:OD2 | 1.90 | 1.05 |
| 1:B:698:VAL:HA | 1:B:701:GLN:HB2 | 1.34 | 1.05 |
| 1:B:764:ASN:O | 1:C:830:ARG:NH1 | 1.88 | 1.05 |
| 1:D:618:SER:O | 1:D:826:ARG:NH1 | 1.89 | 1.05 |
| 1:C:637:MET:O | 1:C:678:LYS:NZ | 1.88 | 1.05 |
| 1:D:609:SER:HA | 1:D:724:ILE:HG13 | 1.39 | 1.05 |
| 1:D:806:LEU:O | 1:D:811:LYS:NZ | 1.89 | 1.05 |
| 1:E:215:GLY:O | 1:E:218:LYS:NZ | 1.88 | 1.05 |
| 1:A:210:LEU:HD22 | 1:A:339:GLU:HA | 1.39 | 1.05 |
| 1:D:205:LYS:NZ | 1:D:332:GLU:OE2 | 1.89 | 1.05 |
| 1:D:617:GLY:O | 1:D:826:ARG:NH1 | 1.89 | 1.05 |
| 1:D:857:VAL:HG12 | 1:D:859:LEU:H | 1.20 | 1.05 |
| 1:B:282:PHE:HB3 | 1:B:313:ILE:H | 1.22 | 1.04 |
| 1:C:195:SER:HA | 1:C:198:ARG:HE | 1.18 | 1.04 |
| 1:A:610:PHE:H | 1:A:724:ILE:HG12 | 1.18 | 1.04 |
| 1:C:686:ASP:HB3 | 1:C:690:LYS:HZ1 | 1.21 | 1.04 |
| 1:E:276:LYS:NZ | 1:E:279:ILE:O | 1.90 | 1.04 |
| 1:F:286:ILE:HD11 | 1:F:322:ARG:CD | 1.59 | 1.04 |
| 1:C:712:GLN:O | 1:C:714:LYS:NZ | 1.90 | 1.04 |
| 1:B:189:ARG:HH12 | 1:B:341:ALA:C | 1.65 | 1.04 |
| 1:B:244:PHE:H | 1:B:281:LEU:HB3 | 1.18 | 1.04 |
| 1:C:260:ASP:HA | 1:C:263:GLU:HG2 | 1.34 | 1.04 |
| 1:F:699:MET:O | 1:F:703:LEU:CG | 2.04 | 1.04 |
| 1:B:548:GLU:HG2 | 1:B:560:LYS:HZ3 | 1.20 | 1.03 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:316:THR:C | 1:D:321:TYR:CD2 | 2.33 | 1.03 |
| 1:D:617:GLY:H | 1:D:620:LYS:HE3 | 1.19 | 1.03 |
| 1:F:331:PHE:HA | 1:F:334:ARG:CD | 1.88 | 1.03 |
| 1:F:331:PHE:CE1 | 1:F:334:ARG:O | 2.09 | 1.03 |
| 1:E:734:ILE:O | 1:E:774:LYS:NZ | 1.90 | 1.03 |
| 1:F:625:LYS:NZ | 1:F:635:GLU:O | 1.91 | 1.03 |
| 1:F:779:ALA:O | 1:F:782:LYS:NZ | 1.90 | 1.03 |
| 1:D:748:ASN:O | 1:D:752:GLY:N | 1.91 | 1.03 |
| 1:D:302:LYS:O | 1:D:306:SER:N | 1.90 | 1.03 |
| 1:E:332:GLU:HA | 1:E:335:PHE:HB2 | 1.39 | 1.03 |
| 1:E:803:LYS:NZ | 1:E:853:GLU:O | 1.91 | 1.03 |
| 1:D:585:ASP:OD1 | 1:D:588:LYS:NZ | 1.90 | 1.03 |
| 1:E:228:ARG:NH1 | 1:E:228:ARG:O | 1.92 | 1.03 |
| 1:E:480:LYS:NZ | 1:E:521:GLU:OE1 | 1.90 | 1.03 |
| 1:F:802:TYR:HA | 1:F:852:LYS:HA | 1.38 | 1.03 |
| 1:C:223:GLU:N | 1:C:223:GLU:OE1 | 1.92 | 1.02 |
| 1:F:356:GLN:NE2 | 1:F:372:LEU:HD21 | 1.73 | 1.02 |
| 1:C:169:LYS:HD2 | 1:C:264:ARG:NH1 | 1.74 | 1.02 |
| 1:D:365:VAL:HG21 | 1:D:403:VAL:HG11 | 1.41 | 1.02 |
| 1:D:843:ARG:HH12 | 1:D:881:PRO:C | 1.67 | 1.02 |
| 1:E:639:ILE:HG21 | 1:E:683:LEU:HD12 | 1.37 | 1.02 |
| 1:E:651:ALA:HA | 1:E:656:LEU:HB2 | 1.41 | 1.02 |
| 1:E:857:VAL:HA | 1:E:878:GLU:HA | 1.41 | 1.02 |
| 1:F:704:ASP:HA | 1:F:765:ARG:HD2 | 1.03 | 1.02 |
| 1:A:380:LYS:NZ | 1:A:381:ARG:HA | 1.75 | 1.02 |
| 1:C:169:LYS:CD | 1:C:264:ARG:CG | 2.16 | 1.02 |
| 1:C:213:GLU:OE2 | 1:C:387:ARG:NH2 | 1.92 | 1.02 |
| 1:F:322:ARG:NH2 | 1:F:325:VAL:HG22 | 1.71 | 1.02 |
| 1:F:357:PRO:O | 1:F:361:ILE:CB | 2.07 | 1.02 |
| 1:F:704:ASP:CG | 1:F:765:ARG:HE | 1.59 | 1.02 |
| 1:D:783:ILE:HA | 1:D:786:ILE:HD12 | 1.40 | 1.01 |
| 1:F:331:PHE:HA | 1:F:334:ARG:HG2 | 1.03 | 1.01 |
| 1:D:755:ARG:HG3 | 1:D:756:GLN:H | 1.25 | 1.01 |
| 1:E:737:GLN:O | 1:E:774:LYS:NZ | 1.93 | 1.01 |
| 1:F:363:HIS:HE1 | 1:F:397:ASP:HA | 1.22 | 1.01 |
| 1:B:559:LYS:NZ | 1:B:629:GLY:O | 1.93 | 1.01 |
| 1:F:356:GLN:CD | 1:F:372:LEU:HD21 | 1.86 | 1.01 |
| 1:F:375:ALA:HA | 1:F:378:LEU:HB2 | 1.43 | 1.01 |
| 1:E:174:MET:HG3 | 1:E:177:GLN:HB2 | 1.42 | 1.01 |
| 1:F:363:HIS:NE2 | 1:F:397:ASP:HA | 1.73 | 1.01 |
| 1:C:169:LYS:CD | 1:C:264:ARG:HD3 | 1.52 | 1.00 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:170:TYR:CE2 | 1:C:250:ALA:N | 2.28 | 1.00 |
| 1:D:530:ARG:HH12 | 1:D:537:ILE:C | 1.69 | 1.00 |
| 1:E:429:LYS:NZ | 1:E:432:GLU:OE1 | 1.94 | 1.00 |
| 1:F:704:ASP:CA | 1:F:765:ARG:HD2 | 1.90 | 1.00 |
| 1:B:263:GLU:HA | 1:B:266:LYS:NZ | 1.77 | 1.00 |
| 1:C:708:ILE:HG22 | 1:C:709:THR:H | 1.26 | 1.00 |
| 1:F:286:ILE:HD11 | 1:F:322:ARG:HG3 | 1.42 | 1.00 |
| 1:B:803:LYS:NZ | 1:B:804:LEU:O | 1.93 | 1.00 |
| 1:F:744:GLU:HA | 1:F:747:LYS:HZ3 | 1.25 | 1.00 |
| 1:D:273:GLU:HG3 | 1:D:274:GLU:HG3 | 1.43 | 1.00 |
| 1:E:214:PRO:O | 1:E:387:ARG:NH1 | 1.93 | 1.00 |
| 1:F:356:GLN:NE2 | 1:F:367:ILE:HD13 | 1.76 | 1.00 |
| 1:C:807:THR:OG1 | 1:C:809:GLU:OE2 | 1.79 | 1.00 |
| 1:C:216:ILE:H | 1:C:218:LYS:HZ2 | 1.00 | 1.00 |
| 1:C:236:THR:HA | 1:C:239:GLN:HB2 | 1.44 | 1.00 |
| 1:C:606:GLN:NE2 | 1:C:703:LEU:O | 1.94 | 1.00 |
| 1:D:708:ILE:H | 1:D:716:ILE:H | 1.01 | 1.00 |
| 1:F:605:ARG:HH12 | 1:F:705:ASP:CB | 1.75 | 1.00 |
| 1:F:704:ASP:CA | 1:F:765:ARG:CD | 2.40 | 1.00 |
| 1:C:169:LYS:CD | 1:C:264:ARG:CZ | 2.39 | 1.00 |
| 1:C:366:ARG:NH2 | 1:C:537:ILE:O | 1.95 | 1.00 |
| 1:D:733:PHE:HZ | 1:D:749:LEU:HB3 | 1.25 | 0.99 |
| 1:C:168:SER:CB | 1:C:271:GLU:OE1 | 2.10 | 0.99 |
| 1:E:206:SER:O | 1:E:311:LYS:NZ | 1.95 | 0.99 |
| 1:F:331:PHE:CD1 | 1:F:334:ARG:C | 2.40 | 0.99 |
| 1:E:460:GLU:HA | 1:E:463:ARG:NH1 | 1.78 | 0.99 |
| 1:B:639:ILE:HB | 1:B:683:LEU:HA | 1.42 | 0.99 |
| 1:D:842:LEU:O | 1:D:846:LYS:NZ | 1.95 | 0.99 |
| 1:E:302:LYS:HZ3 | 1:E:334:ARG:HD3 | 1.24 | 0.99 |
| 1:C:407:ARG:HD3 | 1:C:538:GLN:HA | 1.41 | 0.99 |
| 1:F:707:ARG:HG3 | 1:F:715:THR:HG21 | 1.41 | 0.98 |
| 1:A:167:LEU:HA | 1:A:271:GLU:OE2 | 1.63 | 0.98 |
| 1:C:210:LEU:HB2 | 1:C:338:ILE:H | 1.25 | 0.98 |
| 1:D:681:SER:H | 1:D:721:CYS:HA | 1.27 | 0.98 |
| 1:C:169:LYS:HE3 | 1:C:264:ARG:HB2 | 1.01 | 0.98 |
| 1:E:807:THR:C | 1:E:811:LYS:HZ3 | 1.71 | 0.98 |
| 1:F:331:PHE:CD1 | 1:F:335:PHE:N | 2.31 | 0.98 |
| 1:B:806:LEU:HA | 1:B:810:ALA:HB3 | 1.44 | 0.98 |
| 1:D:203:ARG:HH12 | 1:E:363:HIS:CG | 1.81 | 0.98 |
| 1:D:548:GLU:HA | 1:D:551:ALA:HB3 | 1.45 | 0.98 |
| 1:F:167:LEU:H | 1:F:169:LYS:NZ | 1.61 | 0.98 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:700:LEU:HA | 1:B:703:LEU:HB2 | 1.43 | 0.98 |
| 1:D:636:ASP:O | 1:D:678:LYS:NZ | 1.96 | 0.98 |
| 1:F:610:PHE:HA | 1:F:768:SER:HB3 | 1.45 | 0.98 |
| 1:A:205:LYS:H | 1:A:334:ARG:HD2 | 1.27 | 0.98 |
| 1:A:818:GLY:HA3 | 1:A:828:LEU:HD13 | 1.44 | 0.98 |
| 1:D:414:LEU:O | 1:D:418:GLU:N | 1.94 | 0.97 |
| 1:F:241:ALA:HA | 1:F:279:ILE:HB | 1.45 | 0.97 |
| 1:F:322:ARG:CZ | 1:F:325:VAL:HG23 | 1.94 | 0.97 |
| 1:D:804:LEU:HD12 | 1:D:855:VAL:H | 1.30 | 0.97 |
| 1:A:776:SER:O | 1:A:780:ILE:N | 1.98 | 0.97 |
| 1:F:356:GLN:OE1 | 1:F:372:LEU:HD21 | 1.65 | 0.97 |
| 1:D:189:ARG:HH12 | 1:D:341:ALA:HB3 | 1.27 | 0.97 |
| 1:E:270:LYS:HZ3 | 1:E:274:GLU:HA | 1.26 | 0.97 |
| 1:C:169:LYS:HG2 | 1:C:264:ARG:HD3 | 1.46 | 0.97 |
| 1:C:264:ARG:NH2 | 1:C:271:GLU:OE2 | 1.98 | 0.97 |
| 1:F:699:MET:C | 1:F:703:LEU:HG | 1.88 | 0.97 |
| 1:B:208:PRO:HD2 | 1:B:313:ILE:HA | 1.41 | 0.97 |
| 1:B:563:GLU:OE1 | 1:B:568:LYS:NZ | 1.97 | 0.97 |
| 1:F:286:ILE:CD1 | 1:F:322:ARG:CG | 2.26 | 0.97 |
| 1:F:319:ASN:HA | 1:F:323:SER:OG | 1.64 | 0.97 |
| 1:F:700:LEU:HG | 1:F:703:LEU:HD21 | 1.45 | 0.97 |
| 1:A:872:GLU:HG2 | 1:F:200:LEU:HB2 | 1.46 | 0.97 |
| 1:D:223:GLU:HA | 1:D:226:ALA:HB3 | 1.46 | 0.97 |
| 1:C:618:SER:O | 1:C:826:ARG:NH1 | 1.97 | 0.97 |
| 1:E:592:ASN:O | 1:E:596:LEU:N | 1.98 | 0.97 |
| 1:F:607:PRO:HG3 | 1:F:703:LEU:O | 1.65 | 0.97 |
| 1:A:705:ASP:OD2 | 1:A:707:ARG:NH2 | 1.98 | 0.96 |
| 1:D:847:ASN:OD1 | 1:D:850:LYS:NZ | 1.98 | 0.96 |
| 1:C:282:PHE:HA | 1:C:312:VAL:HG23 | 1.43 | 0.96 |
| 1:C:397:ASP:O | 1:C:401:ALA:N | 1.97 | 0.96 |
| 1:E:645:GLU:OE1 | 1:E:649:LYS:NZ | 1.99 | 0.96 |
| 1:B:286:ILE:O | 1:B:290:MET:N | 1.97 | 0.96 |
| 1:C:654:LYS:HG3 | 1:C:655:LEU:N | 1.76 | 0.96 |
| 1:D:622:GLU:OE2 | 1:D:787:ARG:NH2 | 1.96 | 0.96 |
| 1:F:167:LEU:H | 1:F:169:LYS:HZ3 | 0.99 | 0.96 |
| 1:C:216:ILE:H | 1:C:218:LYS:NZ | 1.63 | 0.96 |
| 1:D:316:THR:O | 1:D:321:TYR:CE2 | 2.18 | 0.96 |
| 1:D:843:ARG:NH1 | 1:D:881:PRO:O | 1.97 | 0.96 |
| 1:E:610:PHE:H | 1:E:724:ILE:HA | 1.30 | 0.96 |
| 1:F:286:ILE:CG1 | 1:F:322:ARG:HD3 | 1.94 | 0.96 |
| 1:F:294:LYS:HE2 | 1:F:325:VAL:HG12 | 1.47 | 0.96 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:307:ARG:H | 1:A:310:LEU:HD12 | 1.29 | 0.96 |
| 1:D:407:ARG:HA | 1:D:411:PRO:HA | 1.47 | 0.96 |
| 1:E:193:ILE:O | 1:E:197:ILE:N | 1.97 | 0.96 |
| 1:F:702:MET:SD | 1:F:708:ILE:CG2 | 2.54 | 0.96 |
| 1:A:786:ILE:HD13 | 1:A:789:LYS:HZ1 | 1.31 | 0.96 |
| 1:B:203:ARG:NH1 | 1:C:362:HIS:HB2 | 1.80 | 0.96 |
| 1:F:286:ILE:HD11 | 1:F:322:ARG:HG2 | 1.43 | 0.96 |
| 1:B:205:LYS:HE3 | 1:B:334:ARG:HA | 1.45 | 0.96 |
| 1:D:812:ASP:O | 1:D:816:LYS:N | 1.98 | 0.96 |
| 1:B:620:LYS:NZ | 1:B:826:ARG:NH1 | 2.14 | 0.96 |
| 1:F:678:LYS:NZ | 1:F:679:PRO:O | 1.98 | 0.96 |
| 1:D:744:GLU:HB2 | 1:D:746:THR:HG23 | 1.47 | 0.95 |
| 1:A:174:MET:SD | 1:A:177:GLN:NE2 | 2.39 | 0.95 |
| 1:B:685:PHE:HD1 | 1:B:725:MET:HB3 | 1.26 | 0.95 |
| 1:B:831:LEU:HD12 | 1:B:834:ASN:HB2 | 1.48 | 0.95 |
| 1:C:787:ARG:NH1 | 1:C:826:ARG:HH21 | 1.64 | 0.95 |
| 2:E:1002:AGS:O1B | 2:E:1002:AGS:O2G | 1.77 | 0.95 |
| 1:C:405:VAL:O | 1:C:409:SER:OG | 1.84 | 0.95 |
| 1:C:485:GLU:HA | 1:C:488:ASN:HB3 | 1.48 | 0.95 |
| 1:D:570:ILE:HA | 1:D:595:ARG:HH12 | 1.30 | 0.95 |
| 1:E:186:VAL:HG21 | 1:E:220:ALA:HB1 | 1.46 | 0.95 |
| 1:E:248:LEU:O | 1:E:252:THR:N | 1.99 | 0.95 |
| 1:C:395:LEU:O | 1:C:399:SER:N | 1.99 | 0.95 |
| 1:C:799:ASP:O | 1:C:850:LYS:NZ | 1.98 | 0.95 |
| 1:E:576:LEU:HA | 1:E:579:GLU:HG2 | 1.46 | 0.95 |
| 1:F:202:ARG:HH12 | 1:F:208:PRO:HD3 | 1.32 | 0.95 |
| 1:A:707:ARG:HA | 1:A:717:ASP:HA | 1.49 | 0.95 |
| 1:E:284:ASP:O | 1:E:287:HIS:ND1 | 1.99 | 0.95 |
| 1:B:839:LYS:HZ3 | 1:B:877:LEU:HA | 1.32 | 0.94 |
| 1:C:622:GLU:OE2 | 1:C:787:ARG:NH2 | 2.00 | 0.94 |
| 1:E:207:ASN:OD1 | 1:E:311:LYS:NZ | 1.99 | 0.94 |
| 1:E:226:ALA:HA | 1:E:229:ILE:HD12 | 1.50 | 0.94 |
| 1:F:356:GLN:HE22 | 1:F:372:LEU:HD21 | 1.31 | 0.94 |
| 1:B:843:ARG:HA | 1:B:846:LYS:HB2 | 1.49 | 0.94 |
| 1:D:203:ARG:HD2 | 1:E:362:HIS:HB3 | 1.46 | 0.94 |
| 1:C:785:ASP:OD1 | 1:C:786:ILE:N | 1.98 | 0.94 |
| 1:F:751:MET:HE3 | 1:F:755:ARG:HD3 | 1.48 | 0.94 |
| 1:D:572:MET:O | 1:D:576:LEU:N | 2.00 | 0.94 |
| 1:E:569:LEU:HA | 1:E:630:PHE:HZ | 1.33 | 0.94 |
| 1:C:170:TYR:CE1 | 1:C:249:ALA:CA | 2.48 | 0.94 |
| 1:C:392:ALA:O | 1:C:396:VAL:N | 1.99 | 0.94 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:701:GLN:H | 1:D:701:GLN:CD | 1.73 | 0.94 |
| 1:B:211:ILE:HD13 | 1:B:321:TYR:HB2 | 1.45 | 0.94 |
| 1:B:331:PHE:O | 1:B:334:ARG:N | 2.00 | 0.94 |
| 1:C:158:ALA:O | 1:C:159:ASP:O | 1.85 | 0.94 |
| 1:F:556:ILE:HG12 | 1:F:559:LYS:HZ3 | 1.33 | 0.94 |
| 1:A:608:ALA:HB1 | 1:A:767:SER:HB3 | 1.48 | 0.94 |
| 1:C:226:ALA:O | 1:C:230:ILE:N | 1.99 | 0.94 |
| 1:D:354:GLY:O | 1:D:358:LYS:NZ | 1.98 | 0.94 |
| 1:E:186:VAL:HA | 2:E:1001:AGS:C6 | 1.96 | 0.94 |
| 1:E:216:ILE:HG22 | 1:E:218:LYS:HZ2 | 1.32 | 0.94 |
| 1:F:356:GLN:HB3 | 1:F:357:PRO:HD3 | 1.48 | 0.94 |
| 1:F:591:SER:O | 1:F:595:ARG:NH1 | 2.00 | 0.94 |
| 1:F:702:MET:SD | 1:F:708:ILE:HG21 | 2.08 | 0.94 |
| 1:B:357:PRO:O | 1:B:361:ILE:N | 2.01 | 0.94 |
| 1:A:176:GLU:HA | 1:A:179:ARG:HB3 | 1.49 | 0.94 |
| 1:A:205:LYS:HZ3 | 1:B:397:ASP:HB3 | 1.31 | 0.93 |
| 1:C:169:LYS:HD2 | 1:C:264:ARG:CZ | 1.98 | 0.93 |
| 1:F:794:ARG:NH1 | 1:F:795:PHE:HE1 | 1.66 | 0.93 |
| 1:A:380:LYS:HZ1 | 1:A:381:ARG:HA | 1.32 | 0.93 |
| 1:C:403:VAL:O | 1:C:407:ARG:N | 2.00 | 0.93 |
| 1:D:802:TYR:CE2 | 1:D:804:LEU:HB2 | 2.04 | 0.93 |
| 1:E:366:ARG:NH1 | 1:E:539:ASN:OD1 | 2.00 | 0.93 |
| 1:F:670:PHE:O | 1:F:674:GLN:N | 2.01 | 0.93 |
| 1:C:14:ILE:CA | 1:C:160:THR:H | 1.82 | 0.93 |
| 1:C:169:LYS:N | 1:C:264:ARG:CZ | 2.31 | 0.93 |
| 1:E:570:ILE:CA | 1:E:595:ARG:HH12 | 1.81 | 0.93 |
| 1:B:569:LEU:O | 1:B:595:ARG:NH2 | 2.00 | 0.93 |
| 1:B:820:SER:HB3 | 1:B:824:GLY:H | 1.33 | 0.93 |
| 1:D:843:ARG:HD3 | 1:D:846:LYS:NZ | 1.82 | 0.93 |
| 1:F:794:ARG:HH11 | 1:F:795:PHE:HE1 | 1.09 | 0.93 |
| 1:A:177:GLN:HB2 | 1:A:182:LYS:HZ1 | 1.33 | 0.93 |
| 1:C:733:PHE:HZ | 1:C:749:LEU:HB2 | 1.33 | 0.93 |
| 1:D:285:GLU:HB3 | 1:D:287:HIS:HB3 | 1.47 | 0.93 |
| 1:E:570:ILE:HA | 1:E:595:ARG:NH1 | 1.83 | 0.93 |
| 1:B:214:PRO:HA | 1:B:218:LYS:HB3 | 1.47 | 0.93 |
| 1:C:785:ASP:O | 1:C:789:LYS:N | 2.02 | 0.93 |
| 1:E:330:ALA:HA | 1:E:333:ARG:HB2 | 1.49 | 0.93 |
| 1:E:659:THR:HG23 | 1:E:711:GLY:HA2 | 1.48 | 0.93 |
| 1:F:194:ARG:N | 1:F:228:ARG:HH12 | 1.65 | 0.93 |
| 1:E:378:LEU:HA | 1:E:381:ARG:HB3 | 1.48 | 0.93 |
| 1:E:839:LYS:O | 1:E:843:ARG:N | 2.02 | 0.93 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:677:TYR:HB2 | 1:B:678:LYS:HZ3 | 1.32 | 0.93 |
| 1:D:488:ASN:HA | 1:D:491:LEU:HB3 | 1.51 | 0.93 |
| 1:D:567:GLU:OE2 | 1:D:571:HIS:NE2 | 2.01 | 0.93 |
| 1:D:811:LYS:H | 1:D:811:LYS:HD2 | 1.34 | 0.93 |
| 1:F:195:SER:O | 1:F:202:ARG:NH2 | 2.01 | 0.93 |
| 1:F:564:SER:H | 1:F:568:LYS:HD2 | 1.31 | 0.93 |
| 1:D:247:ASP:OD2 | 1:D:284:ASP:N | 2.00 | 0.92 |
| 1:D:682:VAL:HG22 | 1:D:722:ILE:HB | 1.50 | 0.92 |
| 1:E:628:ALA:O | 1:E:632:PHE:N | 2.02 | 0.92 |
| 1:B:614:GLY:HA3 | 1:B:772:PHE:HB3 | 1.52 | 0.92 |
| 1:C:173:ASP:OD2 | 1:C:176:GLU:HG3 | 1.70 | 0.92 |
| 1:C:302:LYS:O | 1:C:306:SER:N | 2.01 | 0.92 |
| 1:E:247:ASP:HB3 | 1:E:250:ALA:H | 1.32 | 0.92 |
| 1:F:576:LEU:HD22 | 1:F:627:VAL:HG12 | 1.52 | 0.92 |
| 1:B:353:ARG:NH1 | 1:B:373:VAL:HG23 | 1.84 | 0.92 |
| 1:C:800:LYS:HD3 | 1:C:850:LYS:HD2 | 1.48 | 0.92 |
| 1:D:779:ALA:O | 1:D:782:LYS:NZ | 2.01 | 0.92 |
| 1:F:656:LEU:HD13 | 1:F:711:GLY:CA | 2.00 | 0.92 |
| 1:A:830:ARG:HH22 | 1:F:275:SER:H | 1.16 | 0.92 |
| 1:E:548:GLU:HB3 | 1:E:552:ARG:NH1 | 1.84 | 0.92 |
| 1:E:712:GLN:H | 1:E:714:LYS:NZ | 1.66 | 0.92 |
| 1:F:349:VAL:HA | 1:F:352:LEU:HB3 | 1.51 | 0.92 |
| 1:C:344:SER:N | 1:C:347:GLN:OE1 | 2.02 | 0.92 |
| 1:A:277:THR:O | 1:A:309:GLN:NE2 | 2.02 | 0.92 |
| 1:B:646:LEU:N | 1:B:692:HIS:H | 1.67 | 0.92 |
| 1:C:169:LYS:HG2 | 1:C:264:ARG:CD | 1.99 | 0.92 |
| 1:C:465:ARG:HH12 | 1:C:529:ARG:HD2 | 1.31 | 0.92 |
| 1:E:646:LEU:H | 1:E:649:LYS:HD2 | 1.34 | 0.92 |
| 1:A:375:ALA:O | 1:A:379:ALA:N | 2.02 | 0.92 |
| 1:B:251:LEU:H | 1:B:264:ARG:NH1 | 1.67 | 0.92 |
| 1:B:760:PRO:O | 1:B:764:ASN:N | 2.03 | 0.92 |
| 1:B:785:ASP:OD1 | 1:B:811:LYS:NZ | 2.03 | 0.92 |
| 1:C:843:ARG:NH1 | 1:C:848:GLU:OE1 | 2.03 | 0.92 |
| 1:E:173:ASP:O | 1:E:175:THR:N | 2.02 | 0.92 |
| 1:C:557:PRO:O | 1:C:560:LYS:N | 2.00 | 0.92 |
| 1:C:558:VAL:HA | 1:C:561:LEU:HG | 1.50 | 0.92 |
| 1:A:777:ARG:HA | 1:A:780:ILE:HG12 | 1.50 | 0.92 |
| 1:D:790:GLU:O | 1:D:794:ARG:NH2 | 2.03 | 0.92 |
| 1:D:799:ASP:H | 1:D:801:HIS:CD2 | 1.87 | 0.92 |
| 1:D:857:VAL:HG11 | 1:D:878:GLU:HA | 1.52 | 0.92 |
| 1:F:349:VAL:O | 1:F:353:ARG:N | 2.03 | 0.92 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:A:696:LEU:HA | 1:A:699:MET:HB3 | 1.50 | 0.91 |
| 1:B:548:GLU:N | 1:B:560:LYS:HZ2 | 1.68 | 0.91 |
| 1:B:620:LYS:HG3 | 1:B:621:THR:H | 1.34 | 0.91 |
| 1:E:378:LEU:O | 1:E:382:TYR:N | 2.02 | 0.91 |
| 1:B:188:GLY:N | 1:B:190:GLU:OE2 | 2.01 | 0.91 |
| 1:B:646:LEU:H | 1:B:691:ALA:H | 1.17 | 0.91 |
| 1:D:202:ARG:HH12 | 1:D:205:LYS:HG2 | 1.35 | 0.91 |
| 1:D:587:ILE:O | 1:D:591:SER:N | 2.04 | 0.91 |
| 1:D:605:ARG:NH1 | 1:D:717:ASP:OD1 | 2.01 | 0.91 |
| 1:D:299:ASN:OD1 | 1:D:300:ILE:N | 2.03 | 0.91 |
| 1:D:413:GLU:OE2 | 1:D:539:ASN:ND2 | 2.02 | 0.91 |
| 1:C:616:SER:HA | 1:C:620:LYS:HD3 | 1.51 | 0.91 |
| 1:E:637:MET:HA | 1:E:678:LYS:NZ | 1.86 | 0.91 |
| 1:F:737:GLN:HG2 | 1:F:742:ILE:HD11 | 1.52 | 0.91 |
| 1:A:546:ILE:O | 1:A:550:ALA:N | 2.02 | 0.91 |
| 1:C:169:LYS:N | 1:C:264:ARG:NE | 2.19 | 0.91 |
| 1:D:800:LYS:HG3 | 1:D:801:HIS:N | 1.84 | 0.91 |
| 1:E:760:PRO:HA | 1:E:763:LEU:HB2 | 1.53 | 0.91 |
| 1:D:432:GLU:HA | 1:D:445:LEU:HD22 | 1.51 | 0.91 |
| 1:D:840:LEU:O | 1:D:844:ILE:N | 2.03 | 0.91 |
| 1:E:712:GLN:H | 1:E:714:LYS:HZ2 | 1.01 | 0.91 |
| 1:B:842:LEU:O | 1:B:846:LYS:N | 2.03 | 0.91 |
| 1:D:223:GLU:O | 1:D:227:GLN:N | 2.04 | 0.91 |
| 1:D:570:ILE:HA | 1:D:595:ARG:NH1 | 1.85 | 0.91 |
| 1:D:697:THR:O | 1:D:701:GLN:NE2 | 2.03 | 0.91 |
| 2:D:1001:AGS:H5'2 | 2:D:1001:AGS:H8 | 1.51 | 0.91 |
| 1:B:192:GLU:OE1 | 1:B:192:GLU:N | 2.02 | 0.91 |
| 1:B:202:ARG:NH1 | 1:B:205:LYS:HB2 | 1.86 | 0.91 |
| 1:C:172:ILE:H | 1:C:244:PHE:HB3 | 1.33 | 0.91 |
| 1:B:377:GLN:O | 1:B:381:ARG:N | 2.04 | 0.91 |
| 1:C:169:LYS:HD3 | 1:C:264:ARG:CZ | 1.97 | 0.91 |
| 1:C:588:LYS:O | 1:C:592:ASN:N | 2.04 | 0.91 |
| 1:C:857:VAL:HA | 1:C:880:LEU:HB3 | 1.52 | 0.91 |
| 1:F:331:PHE:CZ | 1:F:334:ARG:O | 2.24 | 0.91 |
| 1:F:702:MET:CB | 1:F:708:ILE:HG13 | 2.00 | 0.91 |
| 1:B:590:VAL:O | 1:B:594:VAL:N | 2.04 | 0.91 |
| 1:D:251:LEU:O | 1:D:254:GLY:N | 2.03 | 0.91 |
| 1:E:407:ARG:NH1 | 1:E:538:GLN:OE1 | 2.04 | 0.91 |
| 1:F:879:VAL:HG12 | 1:F:880:LEU:H | 1.34 | 0.91 |
| 1:D:625:LYS:O | 1:D:629:GLY:N | 2.03 | 0.90 |
| 1:F:584:MET:HB3 | 1:F:588:LYS:NZ | 1.86 | 0.90 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:170:TYR:CZ | 1:C:249:ALA:C | 2.47 | 0.90 |
| 1:C:831:LEU:O | 1:C:834:ASN:N | 2.04 | 0.90 |
| 1:E:189:ARG:NE | 1:E:192:GLU:OE2 | 2.03 | 0.90 |
| 1:F:699:MET:O | 1:F:703:LEU:CD1 | 2.04 | 0.90 |
| 1:C:170:TYR:HH | 1:C:250:ALA:H | 1.11 | 0.90 |
| 1:C:835:GLU:HA | 1:C:838:ASN:HD21 | 1.35 | 0.90 |
| 1:D:262:GLU:HB2 | 1:D:298:ALA:HB2 | 1.53 | 0.90 |
| 1:B:565:GLU:N | 1:B:568:LYS:HZ1 | 1.70 | 0.90 |
| 1:C:342:GLU:OE2 | 1:C:388:LEU:N | 2.05 | 0.90 |
| 1:C:799:ASP:C | 1:C:850:LYS:HZ1 | 1.79 | 0.90 |
| 1:D:302:LYS:NZ | 1:D:306:SER:HA | 1.84 | 0.90 |
| 1:D:672:THR:HA | 1:D:675:LEU:HG | 1.52 | 0.90 |
| 1:E:845:LEU:N | 1:E:848:GLU:OE2 | 2.05 | 0.90 |
| 1:B:210:LEU:HD21 | 1:B:337:LYS:HZ3 | 1.35 | 0.90 |
| 1:C:248:LEU:HG | 1:C:251:LEU:HD21 | 1.52 | 0.90 |
| 1:C:480:LYS:O | 1:C:484:ASP:N | 2.03 | 0.90 |
| 1:C:605:ARG:NH2 | 1:C:606:GLN:OE1 | 2.04 | 0.90 |
| 1:D:556:ILE:HG22 | 1:D:559:LYS:HZ1 | 1.36 | 0.90 |
| 1:A:621:THR:O | 1:A:625:LYS:N | 2.03 | 0.90 |
| 1:C:617:GLY:H | 1:C:620:LYS:HE3 | 1.33 | 0.90 |
| 1:E:290:MET:N | 1:E:295:ASP:OD2 | 2.05 | 0.90 |
| 1:E:712:GLN:N | 1:E:714:LYS:HZ2 | 1.68 | 0.90 |
| 1:F:172:ILE:HG12 | 1:F:245:SER:H | 1.35 | 0.90 |
| 1:F:356:GLN:HB3 | 1:F:357:PRO:HD2 | 1.50 | 0.90 |
| 1:F:640:ARG:HH11 | 1:F:686:ASP:CG | 1.80 | 0.90 |
| 1:C:189:ARG:HH22 | 1:C:342:GLU:HA | 1.35 | 0.90 |
| 1:D:243:LEU:HD21 | 1:D:282:PHE:HB2 | 1.54 | 0.90 |
| 1:F:357:PRO:O | 1:F:361:ILE:HG13 | 1.72 | 0.90 |
| 1:F:605:ARG:NH1 | 1:F:705:ASP:HB3 | 1.85 | 0.90 |
| 1:B:349:VAL:O | 1:B:353:ARG:N | 2.03 | 0.90 |
| 1:B:544:ASP:O | 1:B:548:GLU:N | 2.04 | 0.90 |
| 1:D:357:PRO:O | 1:D:361:ILE:N | 2.03 | 0.90 |
| 1:E:192:GLU:O | 1:E:196:THR:N | 2.05 | 0.90 |
| 1:E:622:GLU:O | 1:E:626:LYS:N | 2.05 | 0.90 |
| 1:F:299:ASN:HB3 | 1:F:302:LYS:HE3 | 1.53 | 0.90 |
| 1:A:695:VAL:O | 1:A:699:MET:N | 2.05 | 0.90 |
| 1:C:407:ARG:NH2 | 1:C:536:MET:O | 2.04 | 0.90 |
| 1:C:796:GLU:N | 1:C:802:TYR:OH | 2.04 | 0.90 |
| 1:D:359:TYR:O | 1:D:363:HIS:N | 2.03 | 0.90 |
| 1:D:634:ASP:OD2 | 1:D:637:MET:N | 2.05 | 0.90 |
| 1:F:260:ASP:O | 1:F:264:ARG:N | 2.05 | 0.90 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:702:MET:CB | 1:F:708:ILE:HG23 | 2.01 | 0.90 |
| 1:A:356:GLN:HB2 | 1:A:360:GLU:HB2 | 1.51 | 0.90 |
| 1:B:803:LYS:HZ1 | 1:B:854:THR:HG23 | 1.37 | 0.90 |
| 1:C:640:ARG:HA | 1:C:684:LEU:HB3 | 1.51 | 0.90 |
| 1:D:669:GLY:HA2 | 1:D:672:THR:HB | 1.51 | 0.90 |
| 1:D:736:SER:OG | 1:D:774:LYS:NZ | 2.03 | 0.90 |
| 1:D:789:LYS:NZ | 1:D:793:GLU:OE2 | 2.05 | 0.90 |
| 1:F:556:ILE:HG12 | 1:F:559:LYS:NZ | 1.86 | 0.90 |
| 1:A:613:LEU:HD21 | 1:A:726:THR:HB | 1.53 | 0.89 |
| 1:B:353:ARG:HH12 | 1:B:372:LEU:HB2 | 1.38 | 0.89 |
| 1:B:620:LYS:HZ2 | 1:B:826:ARG:NH1 | 1.70 | 0.89 |
| 1:B:559:LYS:HZ2 | 1:B:630:PHE:C | 1.81 | 0.89 |
| 1:C:579:GLU:HB2 | 1:C:626:LYS:NZ | 1.87 | 0.89 |
| 1:D:258:LYS:NZ | 1:D:262:GLU:HB3 | 1.87 | 0.89 |
| 1:D:271:GLU:HG2 | 1:D:276:LYS:NZ | 1.87 | 0.89 |
| 1:C:814:LEU:O | 1:C:818:GLY:N | 2.05 | 0.89 |
| 1:D:536:MET:O | 1:D:538:GLN:NE2 | 2.05 | 0.89 |
| 1:E:396:VAL:O | 1:E:399:SER:OG | 1.91 | 0.89 |
| 1:E:700:LEU:O | 1:E:704:ASP:N | 2.05 | 0.89 |
| 1:A:217:GLY:O | 1:A:221:ILE:N | 2.05 | 0.89 |
| 1:B:783:ILE:HA | 1:B:786:ILE:HD12 | 1.55 | 0.89 |
| 1:D:791:ILE:C | 1:D:794:ARG:HH12 | 1.79 | 0.89 |
| 1:D:804:LEU:H | 1:D:854:THR:HG23 | 1.37 | 0.89 |
| 1:B:842:LEU:HB3 | 1:B:846:LYS:HZ3 | 1.34 | 0.89 |
| 1:C:189:ARG:O | 1:C:193:ILE:N | 2.05 | 0.89 |
| 1:C:542:ASP:O | 1:C:546:ILE:N | 2.05 | 0.89 |
| 1:E:471:HIS:O | 1:E:475:GLU:N | 2.05 | 0.89 |
| 1:F:703:LEU:HD12 | 1:F:703:LEU:H | 1.36 | 0.89 |
| 1:C:174:MET:HG2 | 1:C:242:LYS:NZ | 1.88 | 0.89 |
| 1:E:205:LYS:HB2 | 1:E:336:GLN:HE22 | 1.35 | 0.89 |
| 1:E:296:ASP:HA | 1:E:299:ASN:HB3 | 1.55 | 0.89 |
| 1:E:709:THR:H | 1:E:716:ILE:H | 1.17 | 0.89 |
| 1:A:796:GLU:HG2 | 1:A:799:ASP:HB2 | 1.54 | 0.89 |
| 1:D:661:GLY:H | 1:D:665:TYR:HE1 | 1.20 | 0.89 |
| 1:E:837:LEU:O | 1:E:840:LEU:N | 2.05 | 0.89 |
| 1:F:657:GLY:HA3 | 1:F:667:GLU:HB2 | 1.54 | 0.89 |
| 1:F:687:GLU:HA | 1:F:727:SER:HA | 1.53 | 0.89 |
| 1:F:783:ILE:HA | 1:F:786:ILE:HD12 | 1.51 | 0.89 |
| 1:A:302:LYS:HE3 | 1:A:310:LEU:HD22 | 1.54 | 0.89 |
| 1:B:736:SER:OG | 1:B:774:LYS:NZ | 2.04 | 0.89 |
| 1:F:695:VAL:O | 1:F:699:MET:N | 2.06 | 0.89 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:260:ASP:O | 1:A:264:ARG:N | 2.04 | 0.89 |
| 1:C:674:GLN:O | 1:C:678:LYS:N | 2.06 | 0.89 |
| 1:D:575:ASP:O | 1:D:578:SER:N | 2.05 | 0.89 |
| 1:E:798:ASN:HA | 1:E:801:HIS:HB2 | 1.53 | 0.89 |
| 1:F:363:HIS:NE2 | 1:F:396:VAL:O | 2.04 | 0.89 |
| 1:F:585:ASP:O | 1:F:589:ALA:N | 2.06 | 0.89 |
| 1:F:704:ASP:CG | 1:F:765:ARG:CZ | 2.40 | 0.89 |
| 1:C:592:ASN:OD1 | 1:C:595:ARG:NH1 | 2.06 | 0.88 |
| 1:E:464:GLN:O | 1:E:468:GLU:N | 2.06 | 0.88 |
| 1:F:843:ARG:HH21 | 1:F:849:ILE:HG21 | 1.38 | 0.88 |
| 1:A:640:ARG:HG3 | 1:A:684:LEU:HD11 | 1.54 | 0.88 |
| 1:C:843:ARG:NH1 | 1:C:848:GLU:HB2 | 1.87 | 0.88 |
| 1:D:414:LEU:HA | 1:D:417:LYS:HB3 | 1.56 | 0.88 |
| 1:A:790:GLU:O | 1:A:794:ARG:NH1 | 2.05 | 0.88 |
| 1:B:400:CYS:O | 1:B:404:ALA:N | 2.05 | 0.88 |
| 1:B:698:VAL:O | 1:B:702:MET:N | 2.07 | 0.88 |
| 1:D:376:ALA:O | 1:D:380:LYS:N | 2.05 | 0.88 |
| 1:A:250:ALA:HA | 1:A:264:ARG:NH1 | 1.88 | 0.88 |
| 1:A:264:ARG:O | 1:A:268:VAL:N | 2.06 | 0.88 |
| 1:B:685:PHE:CD1 | 1:B:725:MET:HB3 | 2.08 | 0.88 |
| 1:C:784:VAL:HG23 | 1:C:785:ASP:H | 1.38 | 0.88 |
| 1:F:286:ILE:CD1 | 1:F:322:ARG:HE | 1.79 | 0.88 |
| 1:C:174:MET:HE2 | 1:C:244:PHE:HA | 1.54 | 0.88 |
| 1:C:593:ALA:O | 1:C:597:SER:N | 2.05 | 0.88 |
| 1:A:209:CYS:SG | 1:A:210:LEU:N | 2.47 | 0.88 |
| 1:B:192:GLU:O | 1:B:195:SER:OG | 1.91 | 0.88 |
| 1:C:174:MET:HG2 | 1:C:242:LYS:HZ3 | 1.36 | 0.88 |
| 1:E:410:LYS:HE3 | 1:E:463:ARG:HB2 | 1.56 | 0.88 |
| 1:E:743:GLN:O | 1:E:747:LYS:NZ | 2.05 | 0.88 |
| 1:A:640:ARG:HA | 1:A:684:LEU:HG | 1.55 | 0.88 |
| 1:B:209:CYS:HB3 | 1:B:315:ALA:HB2 | 1.55 | 0.88 |
| 1:F:375:ALA:O | 1:F:379:ALA:N | 2.06 | 0.88 |
| 1:F:605:ARG:CG | 1:F:707:ARG:H | 1.85 | 0.88 |
| 1:F:829:ASN:OD1 | 1:F:830:ARG:N | 2.06 | 0.88 |
| 1:A:669:GLY:O | 1:A:673:ASN:N | 2.07 | 0.88 |
| 1:B:306:SER:OG | 1:B:307:ARG:NH1 | 2.06 | 0.88 |
| 1:B:360:GLU:O | 1:B:364:GLY:N | 2.07 | 0.88 |
| 1:C:14:ILE:CA | 1:C:160:THR:N | 2.36 | 0.88 |
| 1:C:595:ARG:O | 1:C:599:SER:N | 2.06 | 0.88 |
| 1:E:529:ARG:HG3 | 1:E:530:ARG:H | 1.39 | 0.88 |
| 1:E:806:LEU:HB2 | 1:E:810:ALA:HB2 | 1.54 | 0.88 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:549:THR:HG22 | 1:B:552:ARG:NH1 | 1.88 | 0.88 |
| 1:E:349:VAL:O | 1:E:353:ARG:N | 2.06 | 0.88 |
| 1:E:569:LEU:HG | 1:E:595:ARG:NH1 | 1.89 | 0.88 |
| 1:E:754:VAL:HA | 1:E:757:HIS:CD2 | 2.09 | 0.88 |
| 1:A:174:MET:HA | 1:A:177:GLN:HE21 | 1.38 | 0.88 |
| 1:B:620:LYS:NZ | 1:B:826:ARG:HH12 | 1.72 | 0.88 |
| 1:D:834:ASN:O | 1:D:838:ASN:N | 2.07 | 0.88 |
| 1:E:203:ARG:HD3 | 1:F:359:TYR:CE1 | 2.08 | 0.88 |
| 1:F:357:PRO:O | 1:F:361:ILE:CG1 | 2.21 | 0.88 |
| 1:A:221:ILE:O | 1:A:225:VAL:N | 2.06 | 0.87 |
| 1:C:622:GLU:H | 1:C:826:ARG:HH12 | 1.21 | 0.87 |
| 1:D:166:TYR:O | 1:D:170:TYR:N | 2.05 | 0.87 |
| 1:D:285:GLU:HB2 | 1:D:288:MET:HG2 | 1.56 | 0.87 |
| 1:E:301:LEU:HA | 1:E:304:ALA:HB3 | 1.55 | 0.87 |
| 1:E:456:GLN:OE1 | 1:E:463:ARG:NH2 | 2.06 | 0.87 |
| 1:F:356:GLN:OE1 | 1:F:372:LEU:CD2 | 2.22 | 0.87 |
| 1:A:206:SER:H | 1:A:334:ARG:HB3 | 1.37 | 0.87 |
| 1:B:611:LEU:HD23 | 1:B:766:ILE:HG21 | 1.56 | 0.87 |
| 1:B:823:MET:HB3 | 1:B:827:PRO:HG2 | 1.54 | 0.87 |
| 1:C:301:LEU:HB2 | 1:C:305:LEU:HD12 | 1.56 | 0.87 |
| 1:C:650:TYR:OH | 1:C:652:VAL:O | 1.91 | 0.87 |
| 1:C:682:VAL:HG23 | 1:C:723:VAL:HA | 1.54 | 0.87 |
| 1:C:697:THR:O | 1:C:701:GLN:N | 2.06 | 0.87 |
| 1:C:790:GLU:O | 1:C:794:ARG:N | 2.06 | 0.87 |
| 1:B:825:ALA:O | 1:B:829:ASN:N | 2.07 | 0.87 |
| 1:B:829:ASN:O | 1:B:833:GLN:N | 2.08 | 0.87 |
| 1:C:614:GLY:HA2 | 1:C:728:ALA:HA | 1.55 | 0.87 |
| 1:C:671:LEU:O | 1:C:675:LEU:N | 2.06 | 0.87 |
| 1:E:609:SER:HA | 1:E:724:ILE:HD13 | 1.56 | 0.87 |
| 1:B:353:ARG:HH11 | 1:B:373:VAL:CG2 | 1.87 | 0.87 |
| 1:B:644:SER:OG | 1:B:645:GLU:OE2 | 1.93 | 0.87 |
| 1:B:693:PRO:O | 1:B:696:LEU:N | 2.07 | 0.87 |
| 1:C:170:TYR:OH | 1:C:249:ALA:CB | 2.22 | 0.87 |
| 1:C:185:PRO:HD2 | 1:C:358:LYS:HE2 | 1.57 | 0.87 |
| 1:C:577:SER:HA | 1:C:581:VAL:H | 1.39 | 0.87 |
| 1:E:777:ARG:O | 1:E:781:HIS:N | 2.08 | 0.87 |
| 1:A:547:SER:O | 1:A:551:ALA:N | 2.07 | 0.87 |
| 1:B:171:ALA:HA | 1:B:246:LEU:HD21 | 1.57 | 0.87 |
| 1:C:267:GLY:O | 1:C:271:GLU:N | 2.07 | 0.87 |
| 1:D:227:GLN:NE2 | 1:D:231:ASP:OD1 | 2.07 | 0.87 |
| 1:D:246:LEU:HD21 | 1:D:250:ALA:H | 1.38 | 0.87 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:248:LEU:HD22 | 1:B:253:ALA:HA | 1.54 | 0.87 |
| 1:D:258:LYS:NZ | 1:D:261:PHE:HD2 | 1.72 | 0.87 |
| 1:D:470:LYS:O | 1:D:474:GLU:N | 2.06 | 0.87 |
| 1:E:833:GLN:OE1 | 1:E:833:GLN:N | 2.06 | 0.87 |
| 2:E:1001:AGS:O1A | 2:E:1001:AGS:O1B | 1.87 | 0.87 |
| 1:A:832:ILE:HA | 1:A:835:GLU:OE2 | 1.74 | 0.87 |
| 1:C:471:HIS:HA | 1:C:474:GLU:HB3 | 1.55 | 0.87 |
| 1:E:410:LYS:O | 1:E:414:LEU:N | 2.06 | 0.87 |
| 1:F:303:PRO:O | 1:F:307:ARG:N | 2.06 | 0.87 |
| 1:F:605:ARG:HG2 | 1:F:706:GLY:HA3 | 1.57 | 0.87 |
| 1:B:764:ASN:OD1 | 1:C:830:ARG:NH1 | 2.08 | 0.87 |
| 1:D:258:LYS:HZ3 | 1:D:261:PHE:HD2 | 0.88 | 0.87 |
| 1:D:574:ARG:O | 1:D:577:SER:OG | 1.92 | 0.87 |
| 1:D:814:LEU:O | 1:D:818:GLY:N | 2.08 | 0.87 |
| 1:E:573:GLU:O | 1:E:577:SER:N | 2.07 | 0.87 |
| 1:E:627:VAL:O | 1:E:631:LEU:N | 2.08 | 0.87 |
| 1:E:688:VAL:HG13 | 1:E:690:LYS:H | 1.39 | 0.87 |
| 1:E:763:LEU:HA | 1:E:766:ILE:HD12 | 1.56 | 0.87 |
| 1:C:210:LEU:CB | 1:C:338:ILE:H | 1.87 | 0.86 |
| 1:C:214:PRO:O | 1:C:387:ARG:NE | 2.09 | 0.86 |
| 1:C:812:ASP:O | 1:C:816:LYS:N | 2.08 | 0.86 |
| 1:A:543:SER:HA | 1:A:547:SER:HB3 | 1.55 | 0.86 |
| 1:B:167:LEU:HD22 | 1:B:271:GLU:HA | 1.55 | 0.86 |
| 1:D:469:GLU:O | 1:D:473:HIS:N | 2.08 | 0.86 |
| 1:F:796:GLU:HG3 | 1:F:799:ASP:H | 1.39 | 0.86 |
| 1:A:646:LEU:HD12 | 1:A:692:HIS:H | 1.40 | 0.86 |
| 1:A:698:VAL:O | 1:A:702:MET:N | 2.08 | 0.86 |
| 1:A:372:LEU:HA | 1:A:542:ASP:HB3 | 1.56 | 0.86 |
| 1:C:628:ALA:O | 1:C:633:ASN:ND2 | 2.09 | 0.86 |
| 1:D:389:PRO:O | 1:D:393:LEU:N | 2.08 | 0.86 |
| 1:D:650:TYR:HD2 | 1:D:654:LYS:HB3 | 1.37 | 0.86 |
| 1:E:620:LYS:HZ3 | 2:E:1002:AGS:PA | 1.97 | 0.86 |
| 1:F:286:ILE:HD12 | 1:F:322:ARG:HD3 | 1.13 | 0.86 |
| 1:F:395:LEU:HA | 1:F:398:ILE:HB | 1.57 | 0.86 |
| 1:B:579:GLU:OE2 | 1:B:626:LYS:HE2 | 1.76 | 0.86 |
| 1:B:622:GLU:H | 1:B:826:ARG:NH2 | 1.73 | 0.86 |
| 1:B:750:VAL:O | 1:B:754:VAL:N | 2.08 | 0.86 |
| 1:C:170:TYR:CZ | 1:C:249:ALA:HB1 | 2.09 | 0.86 |
| 1:C:190:GLU:O | 1:C:194:ARG:N | 2.08 | 0.86 |
| 1:C:783:ILE:HG22 | 1:C:787:ARG:HG2 | 1.56 | 0.86 |
| 1:D:833:GLN:O | 1:D:837:LEU:N | 2.08 | 0.86 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:704:ASP:HA | 1:E:765:ARG:NH1 | 1.91 | 0.86 |
| 1:F:363:HIS:CE1 | 1:F:400:CYS:HG | 1.93 | 0.86 |
| 1:A:218:LYS:HG3 | 1:A:219:THR:H | 1.40 | 0.86 |
| 1:A:804:LEU:N | 1:A:853:GLU:O | 2.08 | 0.86 |
| 1:F:556:ILE:HG13 | 1:F:559:LYS:H | 1.41 | 0.86 |
| 1:F:699:MET:O | 1:F:703:LEU:HD12 | 1.76 | 0.86 |
| 1:B:287:HIS:O | 1:B:291:GLY:N | 2.07 | 0.86 |
| 1:B:654:LYS:HD3 | 1:B:692:HIS:HB3 | 1.57 | 0.86 |
| 1:E:621:THR:N | 2:E:1002:AGS:O1A | 2.08 | 0.86 |
| 1:F:179:ARG:NH1 | 1:F:179:ARG:O | 2.08 | 0.86 |
| 1:F:322:ARG:NH2 | 1:F:322:ARG:O | 2.08 | 0.86 |
| 1:B:193:ILE:O | 1:B:197:ILE:N | 2.09 | 0.86 |
| 1:D:377:GLN:N | 1:D:377:GLN:OE1 | 2.08 | 0.86 |
| 1:E:808:GLN:N | 1:E:811:LYS:HZ3 | 1.72 | 0.86 |
| 1:F:316:THR:HG21 | 1:F:322:ARG:HG2 | 1.55 | 0.86 |
| 1:F:605:ARG:NH1 | 1:F:706:GLY:H | 1.74 | 0.86 |
| 1:E:364:GLY:O | 1:E:407:ARG:NH1 | 2.09 | 0.86 |
| 1:F:744:GLU:HG3 | 1:F:747:LYS:HB2 | 1.58 | 0.86 |
| 1:A:572:MET:HB2 | 1:A:630:PHE:HE1 | 1.40 | 0.86 |
| 1:B:322:ARG:O | 1:B:326:GLU:N | 2.08 | 0.86 |
| 1:C:167:LEU:O | 1:C:264:ARG:NH2 | 2.08 | 0.86 |
| 1:C:465:ARG:NH1 | 1:C:529:ARG:NH1 | 2.24 | 0.85 |
| 1:D:225:VAL:O | 1:D:229:ILE:N | 2.09 | 0.85 |
| 1:D:755:ARG:NH1 | 1:D:756:GLN:HB3 | 1.90 | 0.85 |
| 1:E:550:ALA:O | 1:E:554:THR:N | 2.08 | 0.85 |
| 1:E:558:VAL:O | 1:E:562:SER:N | 2.08 | 0.85 |
| 1:E:754:VAL:HA | 1:E:757:HIS:HD2 | 1.39 | 0.85 |
| 1:F:307:ARG:NH1 | 1:F:333:ARG:HH12 | 1.73 | 0.85 |
| 1:A:200:LEU:HD12 | 1:A:201:ALA:HA | 1.58 | 0.85 |
| 1:A:248:LEU:HB2 | 1:A:251:LEU:HD13 | 1.57 | 0.85 |
| 1:A:779:ALA:O | 1:A:782:LYS:NZ | 2.08 | 0.85 |
| 1:B:265:PHE:O | 1:B:269:LEU:N | 2.08 | 0.85 |
| 1:B:842:LEU:HB3 | 1:B:846:LYS:NZ | 1.91 | 0.85 |
| 1:C:243:LEU:HD21 | 1:C:282:PHE:HB3 | 1.56 | 0.85 |
| 1:C:875:GLU:HG2 | 1:C:876:CYS:H | 1.41 | 0.85 |
| 1:D:242:LYS:O | 1:D:280:VAL:N | 2.09 | 0.85 |
| 1:D:744:GLU:C | 1:D:747:LYS:HZ3 | 1.84 | 0.85 |
| 1:E:401:ALA:O | 1:E:404:ALA:N | 2.10 | 0.85 |
| 1:E:812:ASP:O | 1:E:816:LYS:N | 2.09 | 0.85 |
| 1:C:782:LYS:O | 1:C:811:LYS:NZ | 2.09 | 0.85 |
| 1:E:270:LYS:NZ | 1:E:274:GLU:HA | 1.91 | 0.85 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:460:GLU:HA | 1:E:463:ARG:HH12 | 1.41 | 0.85 |
| 1:E:673:ASN:O | 1:E:676:GLN:NE2 | 2.09 | 0.85 |
| 1:F:613:LEU:HD13 | 1:F:770:VAL:H | 1.40 | 0.85 |
| 1:A:174:MET:HG2 | 1:A:245:SER:HB2 | 1.58 | 0.85 |
| 1:C:620:LYS:NZ | 1:C:621:THR:OG1 | 2.08 | 0.85 |
| 1:D:202:ARG:HH22 | 1:D:205:LYS:HB3 | 1.41 | 0.85 |
| 1:D:558:VAL:HA | 1:D:561:LEU:HB2 | 1.59 | 0.85 |
| 1:E:301:LEU:O | 1:E:305:LEU:N | 2.07 | 0.85 |
| 1:E:460:GLU:OE1 | 1:E:463:ARG:NH1 | 2.07 | 0.85 |
| 1:E:709:THR:N | 1:E:716:ILE:H | 1.74 | 0.85 |
| 1:F:605:ARG:HG2 | 1:F:706:GLY:CA | 2.06 | 0.85 |
| 1:A:285:GLU:HB3 | 1:A:288:MET:HG2 | 1.58 | 0.85 |
| 1:B:174:MET:HB3 | 1:B:243:LEU:HD12 | 1.59 | 0.85 |
| 1:B:242:LYS:HZ3 | 1:B:277:THR:HG21 | 1.42 | 0.85 |
| 1:B:589:ALA:O | 1:B:593:ALA:N | 2.09 | 0.85 |
| 1:B:786:ILE:O | 1:B:789:LYS:NZ | 2.08 | 0.85 |
| 1:C:355:LEU:O | 1:C:359:TYR:N | 2.09 | 0.85 |
| 1:D:828:LEU:O | 1:D:832:ILE:N | 2.09 | 0.85 |
| 1:E:205:LYS:NZ | 1:E:333:ARG:O | 2.09 | 0.85 |
| 1:E:754:VAL:O | 1:E:757:HIS:N | 2.07 | 0.85 |
| 1:F:213:GLU:OE1 | 1:F:387:ARG:NH2 | 2.09 | 0.85 |
| 1:B:596:LEU:HD13 | 1:C:837:LEU:HB2 | 1.57 | 0.85 |
| 1:B:744:GLU:O | 1:B:748:ASN:N | 2.10 | 0.85 |
| 1:C:223:GLU:O | 1:C:227:GLN:N | 2.10 | 0.85 |
| 1:C:242:LYS:NZ | 1:C:243:LEU:O | 2.09 | 0.85 |
| 1:D:569:LEU:O | 1:D:572:MET:N | 2.09 | 0.85 |
| 1:E:482:LYS:HE2 | 1:E:486:LEU:HD11 | 1.59 | 0.85 |
| 1:A:781:HIS:CE1 | 1:A:782:LYS:HZ2 | 1.94 | 0.85 |
| 1:B:564:SER:C | 1:B:568:LYS:HZ1 | 1.83 | 0.85 |
| 1:B:620:LYS:HG2 | 1:B:826:ARG:HH12 | 1.42 | 0.85 |
| 1:B:651:ALA:H | 1:B:692:HIS:CE1 | 1.94 | 0.85 |
| 1:C:192:GLU:OE1 | 1:C:192:GLU:N | 2.09 | 0.85 |
| 1:D:483:LEU:O | 1:D:487:GLU:N | 2.08 | 0.85 |
| 1:D:797:GLN:HE21 | 1:D:800:LYS:HZ1 | 1.24 | 0.85 |
| 1:F:702:MET:HB3 | 1:F:708:ILE:CG2 | 2.07 | 0.85 |
| 1:F:754:VAL:HA | 1:F:757:HIS:HB2 | 1.55 | 0.85 |
| 1:A:673:ASN:O | 1:A:677:TYR:N | 2.10 | 0.85 |
| 1:A:780:ILE:HA | 1:A:783:ILE:HB | 1.59 | 0.85 |
| 1:C:170:TYR:CZ | 1:C:249:ALA:CB | 2.59 | 0.85 |
| 1:C:190:GLU:HG2 | 1:C:191:GLU:H | 1.40 | 0.85 |
| 1:C:190:GLU:N | 1:C:190:GLU:OE1 | 2.10 | 0.85 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:678:LYS:HE2 | 1:C:681:SER:HB2 | 1.59 | 0.85 |
| 1:D:234:VAL:HG11 | 1:D:238:LEU:HB2 | 1.56 | 0.85 |
| 1:B:547:SER:O | 1:B:551:ALA:N | 2.10 | 0.85 |
| 1:C:738:GLN:NE2 | 1:C:746:THR:OG1 | 2.10 | 0.85 |
| 1:D:193:ILE:O | 1:D:197:ILE:N | 2.10 | 0.85 |
| 1:D:828:LEU:HD23 | 1:D:831:LEU:HD12 | 1.59 | 0.85 |
| 1:E:230:ILE:HG22 | 1:E:495:ARG:HH21 | 1.41 | 0.85 |
| 1:E:596:LEU:HD22 | 1:F:837:LEU:HG | 1.59 | 0.85 |
| 1:E:620:LYS:N | 2:E:1002:AGS:O1A | 2.10 | 0.85 |
| 1:F:381:ARG:NH1 | 1:F:565:GLU:OE2 | 2.09 | 0.85 |
| 1:C:168:SER:N | 1:C:264:ARG:HH21 | 1.73 | 0.84 |
| 1:C:269:LEU:O | 1:C:273:GLU:N | 2.10 | 0.84 |
| 1:E:612:PHE:HA | 1:E:771:ILE:HA | 1.59 | 0.84 |
| 1:F:202:ARG:NH1 | 1:F:208:PRO:HD3 | 1.92 | 0.84 |
| 1:F:353:ARG:O | 1:F:357:PRO:HD2 | 1.77 | 0.84 |
| 1:F:356:GLN:HE21 | 1:F:367:ILE:CG2 | 1.90 | 0.84 |
| 1:C:112:ALA:O | 1:C:116:ILE:N | 2.08 | 0.84 |
| 1:E:486:LEU:O | 1:E:490:ALA:N | 2.10 | 0.84 |
| 1:F:391:SER:O | 1:F:395:LEU:N | 2.09 | 0.84 |
| 1:A:248:LEU:HD22 | 1:A:251:LEU:HB2 | 1.57 | 0.84 |
| 1:A:302:LYS:NZ | 1:A:310:LEU:O | 2.09 | 0.84 |
| 1:C:842:LEU:HD11 | 1:C:881:PRO:HB3 | 1.58 | 0.84 |
| 1:D:316:THR:C | 1:D:321:TYR:CG | 2.55 | 0.84 |
| 1:D:586:ALA:O | 1:D:590:VAL:N | 2.10 | 0.84 |
| 1:E:459:LEU:HA | 1:E:462:LEU:HB3 | 1.59 | 0.84 |
| 1:C:170:TYR:CE1 | 1:C:249:ALA:CB | 2.60 | 0.84 |
| 1:C:349:VAL:O | 1:C:353:ARG:N | 2.11 | 0.84 |
| 1:C:785:ASP:OD1 | 1:C:786:ILE:HD12 | 1.77 | 0.84 |
| 1:F:193:ILE:O | 1:F:197:ILE:N | 2.10 | 0.84 |
| 1:A:395:LEU:HD11 | 1:A:549:THR:HG22 | 1.59 | 0.84 |
| 1:D:766:ILE:O | 1:E:830:ARG:NH2 | 2.10 | 0.84 |
| 1:D:767:SER:HA | 1:E:830:ARG:NH1 | 1.93 | 0.84 |
| 1:A:248:LEU:HD13 | 1:A:251:LEU:N | 1.93 | 0.84 |
| 1:B:194:ARG:HA | 1:B:197:ILE:HD12 | 1.59 | 0.84 |
| 1:B:372:LEU:HA | 1:B:375:ALA:HB3 | 1.59 | 0.84 |
| 1:B:539:ASN:OD1 | 1:B:540:VAL:N | 2.10 | 0.84 |
| 1:B:585:ASP:HA | 1:B:588:LYS:HD3 | 1.59 | 0.84 |
| 1:D:173:ASP:OD2 | 1:D:175:THR:HB | 1.78 | 0.84 |
| 1:D:333:ARG:NH1 | 2:E:1001:AGS:O3G | 2.09 | 0.84 |
| 1:D:349:VAL:O | 1:D:353:ARG:N | 2.10 | 0.84 |
| 1:D:788:LEU:HA | 1:D:791:ILE:HG12 | 1.56 | 0.84 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:202:ARG:HH12 | 1:F:208:PRO:CD | 1.91 | 0.84 |
| 1:F:700:LEU:HD23 | 1:F:703:LEU:HD23 | 1.54 | 0.84 |
| 1:F:804:LEU:C | 1:F:854:THR:HA | 2.02 | 0.84 |
| 1:A:856:ASN:O | 1:A:879:VAL:N | 2.08 | 0.84 |
| 1:C:189:ARG:NH1 | 1:C:341:ALA:H | 1.74 | 0.84 |
| 1:D:213:GLU:HG2 | 1:D:387:ARG:NH1 | 1.92 | 0.84 |
| 1:D:810:ALA:O | 1:D:814:LEU:N | 2.10 | 0.84 |
| 1:F:638:MET:H | 1:F:682:VAL:HG12 | 1.42 | 0.84 |
| 1:D:695:VAL:O | 1:D:699:MET:N | 2.10 | 0.84 |
| 1:D:834:ASN:OD1 | 1:D:835:GLU:N | 2.10 | 0.84 |
| 1:E:218:LYS:NZ | 1:E:387:ARG:HH12 | 1.75 | 0.84 |
| 1:F:839:LYS:HA | 1:F:842:LEU:HB3 | 1.57 | 0.84 |
| 1:B:298:ALA:HA | 1:B:301:LEU:HD11 | 1.60 | 0.84 |
| 1:C:718:CYS:SG | 1:C:720:ASN:ND2 | 2.50 | 0.84 |
| 1:E:747:LYS:H | 1:E:747:LYS:HZ3 | 1.25 | 0.84 |
| 1:F:832:ILE:HA | 1:F:835:GLU:OE2 | 1.78 | 0.84 |
| 1:B:176:GLU:OE2 | 1:B:180:GLN:N | 2.10 | 0.84 |
| 1:B:228:ARG:HD2 | 1:B:231:ASP:OD2 | 1.78 | 0.84 |
| 1:B:285:GLU:O | 1:B:289:LEU:N | 2.10 | 0.84 |
| 1:C:169:LYS:HD2 | 1:C:264:ARG:HH11 | 1.39 | 0.84 |
| 1:D:210:LEU:HG | 1:D:338:ILE:C | 2.03 | 0.84 |
| 1:F:176:GLU:O | 1:F:180:GLN:N | 2.11 | 0.84 |
| 1:B:646:LEU:HD11 | 1:B:690:LYS:NZ | 1.93 | 0.83 |
| 1:B:686:ASP:OD1 | 1:B:687:GLU:N | 2.10 | 0.83 |
| 1:C:842:LEU:O | 1:C:846:LYS:N | 2.09 | 0.83 |
| 1:D:218:LYS:O | 1:D:222:ILE:N | 2.11 | 0.83 |
| 1:E:349:VAL:HG11 | 1:E:373:VAL:HG22 | 1.60 | 0.83 |
| 1:F:205:LYS:NZ | 1:F:334:ARG:O | 2.10 | 0.83 |
| 1:A:777:ARG:NH2 | 1:A:812:ASP:OD1 | 2.11 | 0.83 |
| 1:B:191:GLU:HA | 1:B:194:ARG:HB2 | 1.60 | 0.83 |
| 1:C:191:GLU:O | 1:C:195:SER:N | 2.11 | 0.83 |
| 1:D:417:LYS:NZ | 1:D:420:GLN:OE1 | 2.10 | 0.83 |
| 1:D:543:SER:O | 1:D:547:SER:N | 2.10 | 0.83 |
| 1:E:270:LYS:HG3 | 1:E:274:GLU:HB3 | 1.60 | 0.83 |
| 1:F:285:GLU:HB2 | 1:F:288:MET:N | 1.94 | 0.83 |
| 1:C:476:LEU:HA | 1:C:520:LEU:HB3 | 1.58 | 0.83 |
| 1:D:684:LEU:HG | 1:D:725:MET:HA | 1.58 | 0.83 |
| 2:D:1001:AGS:O1B | 2:D:1001:AGS:O3G | 1.86 | 0.83 |
| 1:E:216:ILE:HG22 | 1:E:218:LYS:NZ | 1.92 | 0.83 |
| 1:E:319:ASN:HA | 1:E:322:ARG:HH12 | 1.41 | 0.83 |
| 1:F:216:ILE:HG12 | 1:F:218:LYS:HZ3 | 1.43 | 0.83 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:848:GLU:OE1 | 1:F:882:ASN:ND2 | 2.11 | 0.83 |
| 1:A:254:GLY:O | 1:A:264:ARG:NH1 | 2.11 | 0.83 |
| 1:A:777:ARG:CZ | 1:A:816:LYS:HG3 | 2.08 | 0.83 |
| 1:C:218:LYS:NZ | 2:C:1001:AGS:S1G | 2.50 | 0.83 |
| 1:C:548:GLU:N | 1:C:548:GLU:OE1 | 2.10 | 0.83 |
| 1:C:587:ILE:O | 1:C:591:SER:N | 2.11 | 0.83 |
| 1:D:196:THR:O | 1:D:200:LEU:N | 2.11 | 0.83 |
| 1:D:317:THR:N | 1:D:321:TYR:CG | 2.46 | 0.83 |
| 1:D:650:TYR:CD2 | 1:D:654:LYS:HB3 | 2.13 | 0.83 |
| 1:E:198:ARG:HD3 | 1:F:401:ALA:HB1 | 1.57 | 0.83 |
| 1:E:544:ASP:O | 1:E:548:GLU:N | 2.12 | 0.83 |
| 1:C:227:GLN:O | 1:C:231:ASP:N | 2.10 | 0.83 |
| 1:D:593:ALA:O | 1:D:597:SER:N | 2.10 | 0.83 |
| 1:E:746:THR:N | 1:E:747:LYS:HZ1 | 1.77 | 0.83 |
| 1:F:557:PRO:O | 1:F:561:LEU:N | 2.11 | 0.83 |
| 1:A:272:ILE:O | 1:A:276:LYS:NZ | 2.09 | 0.83 |
| 1:B:658:THR:HG21 | 1:B:711:GLY:HA3 | 1.59 | 0.83 |
| 1:B:751:MET:HB3 | 1:B:755:ARG:HH12 | 1.44 | 0.83 |
| 1:C:356:GLN:HG3 | 1:C:367:ILE:HD13 | 1.60 | 0.83 |
| 1:E:654:LYS:NZ | 1:E:694:ASP:OD2 | 2.10 | 0.83 |
| 1:F:347:GLN:NE2 | 1:F:348:THR:OG1 | 2.10 | 0.83 |
| 1:A:699:MET:O | 1:A:703:LEU:N | 2.12 | 0.83 |
| 1:C:203:ARG:HH12 | 1:D:359:TYR:CB | 1.92 | 0.83 |
| 1:E:640:ARG:HA | 1:E:684:LEU:HD13 | 1.61 | 0.83 |
| 1:A:169:LYS:HZ2 | 1:A:264:ARG:CZ | 1.91 | 0.83 |
| 1:A:826:ARG:NH2 | 1:F:304:ALA:O | 2.12 | 0.83 |
| 1:B:404:ALA:O | 1:B:408:ASP:N | 2.11 | 0.83 |
| 1:B:674:GLN:O | 1:B:678:LYS:N | 2.11 | 0.83 |
| 1:B:793:GLU:OE2 | 1:B:802:TYR:OH | 1.97 | 0.83 |
| 1:D:639:ILE:HG22 | 1:D:674:GLN:HE21 | 1.44 | 0.83 |
| 1:E:343:PRO:HG2 | 1:E:388:LEU:HD23 | 1.59 | 0.83 |
| 1:E:627:VAL:O | 1:E:631:LEU:HG | 1.78 | 0.83 |
| 1:E:687:GLU:O | 1:E:728:ALA:N | 2.12 | 0.83 |
| 1:E:701:GLN:HB3 | 1:E:702:MET:HE2 | 1.59 | 0.83 |
| 1:F:175:THR:O | 1:F:179:ARG:N | 2.12 | 0.83 |
| 1:F:656:LEU:CD1 | 1:F:711:GLY:HA3 | 2.09 | 0.83 |
| 1:A:777:ARG:O | 1:A:781:HIS:ND1 | 2.12 | 0.83 |
| 1:B:330:ALA:O | 1:B:333:ARG:NE | 2.12 | 0.83 |
| 1:C:621:THR:HB | 1:C:826:ARG:NH1 | 1.93 | 0.83 |
| 1:F:263:GLU:O | 1:F:267:GLY:N | 2.11 | 0.83 |
| 1:E:330:ALA:O | 1:E:334:ARG:N | 2.12 | 0.83 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:617:GLY:HA2 | 1:A:620:LYS:HD3 | 1.60 | 0.82 |
| 1:A:830:ARG:HH12 | 1:F:309:GLN:HG2 | 1.43 | 0.82 |
| 1:D:722:ILE:HG22 | 1:D:723:VAL:H | 1.41 | 0.82 |
| 1:E:215:GLY:C | 1:E:218:LYS:HZ3 | 1.86 | 0.82 |
| 1:F:651:ALA:H | 1:F:654:LYS:NZ | 1.76 | 0.82 |
| 1:A:685:PHE:HB2 | 1:A:725:MET:HG2 | 1.61 | 0.82 |
| 1:B:211:ILE:HD11 | 1:B:320:GLU:OE2 | 1.78 | 0.82 |
| 1:D:613:LEU:O | 1:D:772:PHE:N | 2.12 | 0.82 |
| 1:E:658:THR:N | 1:E:666:ASP:O | 2.10 | 0.82 |
| 1:C:218:LYS:HA | 1:C:221:ILE:HD12 | 1.60 | 0.82 |
| 1:C:317:THR:O | 1:C:321:TYR:N | 2.11 | 0.82 |
| 1:C:694:ASP:O | 1:C:697:THR:OG1 | 1.96 | 0.82 |
| 1:D:620:LYS:HG3 | 1:D:621:THR:H | 1.42 | 0.82 |
| 1:D:731:ALA:O | 1:D:735:ASN:N | 2.08 | 0.82 |
| 1:D:843:ARG:O | 1:D:847:ASN:N | 2.12 | 0.82 |
| 1:E:169:LYS:HZ1 | 1:E:267:GLY:HA3 | 1.44 | 0.82 |
| 1:C:245:SER:OG | 1:C:283:ILE:O | 1.96 | 0.82 |
| 1:C:577:SER:O | 1:C:580:VAL:N | 2.13 | 0.82 |
| 1:D:174:MET:O | 1:D:178:ALA:N | 2.11 | 0.82 |
| 1:D:369:ASP:HA | 1:D:372:LEU:HD13 | 1.60 | 0.82 |
| 1:E:594:VAL:O | 1:E:597:SER:OG | 1.97 | 0.82 |
| 1:E:625:LYS:HB3 | 1:E:635:GLU:OE1 | 1.77 | 0.82 |
| 1:F:858:VAL:HA | 1:F:878:GLU:HA | 1.59 | 0.82 |
| 1:B:834:ASN:O | 1:B:838:ASN:N | 2.12 | 0.82 |
| 1:C:473:HIS:NE2 | 1:C:538:GLN:O | 2.12 | 0.82 |
| 1:D:792:GLU:HA | 1:D:795:PHE:CE2 | 2.13 | 0.82 |
| 1:D:802:TYR:HE2 | 1:D:804:LEU:HB2 | 1.44 | 0.82 |
| 1:E:174:MET:O | 1:E:178:ALA:N | 2.11 | 0.82 |
| 1:C:210:LEU:HB3 | 1:C:338:ILE:O | 1.78 | 0.82 |
| 1:C:285:GLU:HA | 1:C:287:HIS:NE2 | 1.94 | 0.82 |
| 1:C:366:ARG:HH12 | 1:C:538:GLN:HB2 | 1.43 | 0.82 |
| 1:E:477:THR:HA | 1:E:480:LYS:HD2 | 1.59 | 0.82 |
| 1:A:283:ILE:H | 1:A:312:VAL:HG23 | 1.43 | 0.82 |
| 1:B:592:ASN:O | 1:B:596:LEU:N | 2.12 | 0.82 |
| 2:C:1001:AGS:O2A | 2:C:1001:AGS:O3G | 1.96 | 0.82 |
| 1:E:205:LYS:HZ2 | 1:E:334:ARG:C | 1.87 | 0.82 |
| 1:E:786:ILE:O | 1:E:790:GLU:N | 2.11 | 0.82 |
| 1:A:777:ARG:HH12 | 1:A:816:LYS:N | 1.78 | 0.82 |
| 1:A:858:VAL:H | 1:A:877:LEU:HB3 | 1.45 | 0.82 |
| 1:B:210:LEU:HG | 1:B:338:ILE:O | 1.79 | 0.82 |
| 1:C:407:ARG:NH1 | 1:C:539:ASN:O | 2.12 | 0.82 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:568:LYS:HZ1 | 1:C:630:PHE:C | 1.88 | 0.82 |
| 1:C:785:ASP:OD2 | 1:C:811:LYS:NZ | 2.12 | 0.82 |
| 1:D:585:ASP:CG | 1:D:588:LYS:HZ1 | 1.86 | 0.82 |
| 1:D:609:SER:H | 1:D:767:SER:HB3 | 1.45 | 0.82 |
| 1:E:194:ARG:HB3 | 1:E:198:ARG:HH12 | 1.42 | 0.82 |
| 1:E:787:ARG:NH1 | 1:E:829:ASN:HB3 | 1.95 | 0.82 |
| 1:B:878:GLU:CD | 1:B:879:VAL:H | 1.88 | 0.82 |
| 1:D:262:GLU:OE1 | 1:D:262:GLU:N | 2.12 | 0.82 |
| 1:D:344:SER:N | 1:D:347:GLN:OE1 | 2.13 | 0.82 |
| 1:E:190:GLU:O | 1:E:194:ARG:N | 2.09 | 0.82 |
| 1:E:366:ARG:HH11 | 1:E:539:ASN:CG | 1.87 | 0.82 |
| 1:A:267:GLY:O | 1:A:271:GLU:N | 2.13 | 0.82 |
| 1:C:545:THR:O | 1:C:549:THR:OG1 | 1.96 | 0.82 |
| 1:D:231:ASP:O | 1:D:495:ARG:NE | 2.12 | 0.82 |
| 1:D:299:ASN:O | 1:D:303:PRO:HD2 | 1.78 | 0.82 |
| 1:D:809:GLU:OE2 | 1:D:811:LYS:NZ | 2.13 | 0.82 |
| 1:E:858:VAL:H | 1:E:878:GLU:H | 1.28 | 0.82 |
| 1:F:331:PHE:CD1 | 1:F:334:ARG:HG3 | 2.14 | 0.82 |
| 1:A:179:ARG:HD2 | 1:A:242:LYS:HZ1 | 1.43 | 0.81 |
| 1:B:191:GLU:OE1 | 1:B:191:GLU:N | 2.12 | 0.81 |
| 1:C:777:ARG:O | 1:C:781:HIS:N | 2.10 | 0.81 |
| 1:D:470:LYS:HA | 1:D:473:HIS:HB3 | 1.61 | 0.81 |
| 1:D:556:ILE:HG22 | 1:D:559:LYS:NZ | 1.93 | 0.81 |
| 1:A:549:THR:HA | 1:A:552:ARG:NH1 | 1.95 | 0.81 |
| 1:B:859:LEU:HD12 | 1:B:875:GLU:HG2 | 1.61 | 0.81 |
| 1:D:671:LEU:O | 1:D:674:GLN:HB3 | 1.80 | 0.81 |
| 1:D:785:ASP:O | 1:D:789:LYS:N | 2.12 | 0.81 |
| 1:D:792:GLU:OE2 | 1:D:801:HIS:ND1 | 2.13 | 0.81 |
| 1:D:809:GLU:OE1 | 1:D:809:GLU:N | 2.12 | 0.81 |
| 1:E:227:GLN:HG3 | 1:E:231:ASP:OD2 | 1.80 | 0.81 |
| 1:E:228:ARG:NH2 | 1:E:233:ASP:O | 2.13 | 0.81 |
| 1:E:271:GLU:HA | 1:E:274:GLU:OE2 | 1.79 | 0.81 |
| 1:E:637:MET:HE3 | 1:E:682:VAL:HG12 | 1.62 | 0.81 |
| 1:A:378:LEU:O | 1:A:381:ARG:N | 2.12 | 0.81 |
| 1:C:174:MET:N | 1:C:242:LYS:HZ3 | 1.78 | 0.81 |
| 1:C:191:GLU:HA | 1:C:194:ARG:HB2 | 1.60 | 0.81 |
| 1:C:650:TYR:OH | 1:C:655:LEU:O | 1.96 | 0.81 |
| 1:C:672:THR:OG1 | 1:C:673:ASN:N | 2.11 | 0.81 |
| 1:C:699:MET:O | 1:C:703:LEU:N | 2.11 | 0.81 |
| 1:D:190:GLU:OE1 | 1:D:190:GLU:N | 2.12 | 0.81 |
| 1:D:240:GLY:O | 1:D:277:THR:OG1 | 1.97 | 0.81 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:461:PRO:O | 1:D:465:ARG:N | 2.13 | 0.81 |
| 1:D:545:THR:O | 1:D:549:THR:N | 2.13 | 0.81 |
| 1:D:590:VAL:HG12 | 1:D:594:VAL:HG23 | 1.61 | 0.81 |
| 1:D:618:SER:C | 1:D:826:ARG:HH11 | 1.87 | 0.81 |
| 1:D:839:LYS:HZ3 | 1:D:878:GLU:HB3 | 1.43 | 0.81 |
| 1:E:385:TYR:HD1 | 1:E:386:ARG:NH1 | 1.77 | 0.81 |
| 1:E:548:GLU:CB | 1:E:552:ARG:HH12 | 1.89 | 0.81 |
| 1:E:803:LYS:H | 1:E:852:LYS:HB3 | 1.45 | 0.81 |
| 1:F:751:MET:O | 1:F:755:ARG:N | 2.13 | 0.81 |
| 1:A:682:VAL:HG22 | 1:A:721:CYS:HA | 1.60 | 0.81 |
| 1:A:842:LEU:HB3 | 1:A:846:LYS:NZ | 1.95 | 0.81 |
| 1:B:700:LEU:HD12 | 1:B:703:LEU:HB2 | 1.61 | 0.81 |
| 1:C:168:SER:CA | 1:C:264:ARG:NH2 | 2.00 | 0.81 |
| 1:C:374:THR:O | 1:C:377:GLN:HG2 | 1.79 | 0.81 |
| 1:C:720:ASN:OD1 | 1:C:721:CYS:N | 2.13 | 0.81 |
| 1:A:348:THR:HG23 | 1:A:351:ILE:HD12 | 1.62 | 0.81 |
| 1:B:223:GLU:OE1 | 1:B:223:GLU:N | 2.12 | 0.81 |
| 1:B:744:GLU:HA | 1:B:747:LYS:HB2 | 1.61 | 0.81 |
| 1:D:486:LEU:O | 1:D:490:ALA:N | 2.13 | 0.81 |
| 1:D:605:ARG:NH1 | 1:D:707:ARG:HE | 1.79 | 0.81 |
| 1:E:534:ASN:HD21 | 1:E:538:GLN:H | 1.25 | 0.81 |
| 1:F:217:GLY:HA3 | 2:F:1001:AGS:H1' | 1.62 | 0.81 |
| 1:B:593:ALA:O | 1:B:597:SER:N | 2.11 | 0.81 |
| 1:C:641:VAL:HG23 | 1:C:683:LEU:HD11 | 1.63 | 0.81 |
| 1:D:807:THR:OG1 | 1:D:809:GLU:OE1 | 1.98 | 0.81 |
| 1:F:640:ARG:HD2 | 1:F:684:LEU:HB2 | 1.61 | 0.81 |
| 1:B:545:THR:O | 1:B:549:THR:N | 2.13 | 0.81 |
| 1:B:820:SER:H | 1:B:824:GLY:HA2 | 1.45 | 0.81 |
| 1:C:221:ILE:O | 1:C:225:VAL:N | 2.12 | 0.81 |
| 1:C:281:LEU:HD12 | 1:C:312:VAL:HB | 1.61 | 0.81 |
| 1:C:377:GLN:O | 1:C:380:LYS:HG2 | 1.80 | 0.81 |
| 1:C:612:PHE:HA | 1:C:726:THR:HA | 1.62 | 0.81 |
| 1:D:236:THR:O | 1:D:240:GLY:N | 2.14 | 0.81 |
| 1:D:316:THR:O | 1:D:321:TYR:CD2 | 2.33 | 0.81 |
| 1:D:329:GLY:O | 1:D:333:ARG:N | 2.14 | 0.81 |
| 1:D:530:ARG:HH22 | 1:D:538:GLN:H | 1.28 | 0.81 |
| 1:D:672:THR:O | 1:D:676:GLN:N | 2.14 | 0.81 |
| 1:E:699:MET:HA | 1:E:702:MET:HB2 | 1.63 | 0.81 |
| 1:C:349:VAL:HG22 | 1:C:373:VAL:HG11 | 1.63 | 0.81 |
| 1:C:597:SER:C | 1:C:598:ARG:HH11 | 1.87 | 0.81 |
| 1:C:695:VAL:O | 1:C:699:MET:N | 2.11 | 0.81 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:700:LEU:O | 1:C:704:ASP:N | 2.13 | 0.81 |
| 1:C:764:ASN:O | 1:D:830:ARG:NH2 | 2.14 | 0.81 |
| 1:C:786:ILE:HG13 | 1:C:789:LYS:HZ3 | 1.45 | 0.81 |
| 1:D:746:THR:O | 1:D:749:LEU:N | 2.13 | 0.81 |
| 1:E:671:LEU:HG | 1:E:675:LEU:HD13 | 1.63 | 0.81 |
| 1:F:211:ILE:HG23 | 1:F:317:THR:HA | 1.63 | 0.81 |
| 1:F:286:ILE:HD12 | 1:F:322:ARG:HE | 1.39 | 0.81 |
| 1:C:169:LYS:CD | 1:C:264:ARG:CD | 0.89 | 0.81 |
| 1:C:173:ASP:OD2 | 1:C:177:GLN:N | 2.14 | 0.81 |
| 1:D:643:CYS:HB3 | 1:D:646:LEU:HD23 | 1.63 | 0.81 |
| 1:E:302:LYS:HE3 | 1:E:331:PHE:HA | 1.63 | 0.81 |
| 1:E:545:THR:O | 1:E:549:THR:N | 2.14 | 0.81 |
| 1:B:639:ILE:N | 1:B:682:VAL:O | 2.14 | 0.81 |
| 1:C:175:THR:HG23 | 1:C:242:LYS:HD3 | 1.62 | 0.81 |
| 1:C:407:ARG:NH2 | 1:C:538:GLN:H | 1.78 | 0.81 |
| 1:C:566:ASN:O | 1:C:569:LEU:HB3 | 1.81 | 0.81 |
| 1:E:189:ARG:HH22 | 1:E:341:ALA:H | 1.25 | 0.81 |
| 1:F:556:ILE:HD12 | 1:F:558:VAL:HB | 1.63 | 0.81 |
| 1:A:226:ALA:O | 1:A:230:ILE:N | 2.14 | 0.80 |
| 1:C:576:LEU:O | 1:C:580:VAL:N | 2.14 | 0.80 |
| 1:C:731:ALA:O | 1:C:735:ASN:N | 2.13 | 0.80 |
| 1:D:202:ARG:HH12 | 1:D:205:LYS:CG | 1.94 | 0.80 |
| 1:E:791:ILE:O | 1:E:795:PHE:N | 2.14 | 0.80 |
| 1:F:211:ILE:H | 1:F:339:GLU:HG2 | 1.45 | 0.80 |
| 1:F:666:ASP:OD2 | 1:F:672:THR:OG1 | 1.99 | 0.80 |
| 1:C:565:GLU:HA | 1:C:568:LYS:HB3 | 1.63 | 0.80 |
| 1:D:175:THR:O | 1:D:179:ARG:N | 2.13 | 0.80 |
| 1:D:650:TYR:HA | 1:D:653:SER:OG | 1.81 | 0.80 |
| 1:E:607:PRO:HD3 | 1:E:707:ARG:HH12 | 1.43 | 0.80 |
| 1:E:747:LYS:NZ | 1:E:747:LYS:H | 1.79 | 0.80 |
| 1:F:563:GLU:HB3 | 1:F:568:LYS:HB3 | 1.64 | 0.80 |
| 1:F:581:VAL:HG12 | 1:F:582:GLY:H | 1.47 | 0.80 |
| 1:B:191:GLU:O | 1:B:195:SER:N | 2.12 | 0.80 |
| 1:B:202:ARG:HD3 | 1:B:206:SER:HA | 1.61 | 0.80 |
| 1:C:284:ASP:HB3 | 1:C:285:GLU:OE2 | 1.82 | 0.80 |
| 1:C:639:ILE:HG13 | 1:C:678:LYS:NZ | 1.95 | 0.80 |
| 1:D:839:LYS:NZ | 1:D:879:VAL:O | 2.10 | 0.80 |
| 1:E:351:ILE:O | 1:E:355:LEU:N | 2.13 | 0.80 |
| 1:F:287:HIS:NE2 | 1:F:322:ARG:CD | 2.44 | 0.80 |
| 1:F:714:LYS:C | 1:F:716:ILE:H | 1.89 | 0.80 |
| 1:F:802:TYR:O | 1:F:853:GLU:N | 2.14 | 0.80 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:285:GLU:OE1 | 1:B:288:MET:N | 2.14 | 0.80 |
| 1:B:761:GLU:OE1 | 1:B:761:GLU:N | 2.14 | 0.80 |
| 1:C:195:SER:HA | 1:C:198:ARG:NE | 1.94 | 0.80 |
| 1:C:710:SER:N | 1:C:714:LYS:O | 2.13 | 0.80 |
| 1:D:512:ASP:OD1 | 1:D:513:ILE:N | 2.14 | 0.80 |
| 1:D:839:LYS:HZ3 | 1:D:879:VAL:N | 1.78 | 0.80 |
| 1:F:283:ILE:HG12 | 1:F:312:VAL:HG21 | 1.62 | 0.80 |
| 1:F:749:LEU:O | 1:F:753:ALA:N | 2.13 | 0.80 |
| 1:A:625:LYS:HE3 | 1:A:635:GLU:HB3 | 1.63 | 0.80 |
| 1:E:543:SER:O | 1:E:546:ILE:N | 2.13 | 0.80 |
| 1:F:592:ASN:O | 1:F:595:ARG:NH1 | 2.15 | 0.80 |
| 1:B:677:TYR:HB2 | 1:B:678:LYS:NZ | 1.96 | 0.80 |
| 1:C:144:ALA:O | 1:C:148:ARG:N | 2.15 | 0.80 |
| 1:C:465:ARG:HH12 | 1:C:529:ARG:NH1 | 1.79 | 0.80 |
| 1:D:466:TYR:HE1 | 1:D:538:GLN:HE21 | 1.26 | 0.80 |
| 1:D:547:SER:O | 1:D:551:ALA:N | 2.14 | 0.80 |
| 1:D:790:GLU:HA | 1:D:793:GLU:CD | 2.06 | 0.80 |
| 1:E:319:ASN:CA | 1:E:322:ARG:HH12 | 1.93 | 0.80 |
| 1:F:199:VAL:O | 1:F:202:ARG:N | 2.14 | 0.80 |
| 1:F:285:GLU:HA | 1:F:315:ALA:O | 1.82 | 0.80 |
| 1:F:792:GLU:N | 1:F:792:GLU:OE1 | 2.14 | 0.80 |
| 1:C:349:VAL:HA | 1:C:352:LEU:HD12 | 1.64 | 0.80 |
| 1:C:843:ARG:NH2 | 1:C:882:ASN:OD1 | 2.15 | 0.80 |
| 1:D:229:ILE:HA | 1:D:233:ASP:H | 1.47 | 0.80 |
| 1:D:843:ARG:NH2 | 1:D:880:LEU:O | 2.14 | 0.80 |
| 1:E:695:VAL:O | 1:E:699:MET:N | 2.15 | 0.80 |
| 1:A:169:LYS:NZ | 1:A:264:ARG:CZ | 2.45 | 0.80 |
| 1:A:839:LYS:NZ | 1:A:879:VAL:HA | 1.96 | 0.80 |
| 1:B:812:ASP:O | 1:B:816:LYS:N | 2.13 | 0.80 |
| 1:C:191:GLU:OE1 | 1:C:194:ARG:NE | 2.13 | 0.80 |
| 1:D:284:ASP:OD1 | 1:D:285:GLU:HG2 | 1.82 | 0.80 |
| 1:D:358:LYS:HA | 1:D:361:ILE:HD12 | 1.64 | 0.80 |
| 1:D:485:GLU:O | 1:D:489:LYS:N | 2.13 | 0.80 |
| 1:D:644:SER:OG | 1:D:687:GLU:OE1 | 2.00 | 0.80 |
| 1:D:708:ILE:N | 1:D:716:ILE:H | 1.80 | 0.80 |
| 1:E:408:ASP:HB3 | 1:E:411:PRO:HG3 | 1.63 | 0.80 |
| 1:E:840:LEU:O | 1:E:844:ILE:N | 2.15 | 0.80 |
| 1:A:839:LYS:HZ3 | 1:A:879:VAL:HA | 1.46 | 0.80 |
| 1:B:620:LYS:HG3 | 1:B:621:THR:N | 1.94 | 0.80 |
| 1:C:613:LEU:H | 1:C:726:THR:HB | 1.46 | 0.80 |
| 1:D:486:LEU:HD23 | 1:D:489:LYS:HD2 | 1.64 | 0.80 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:668:GLY:O | 1:D:672:THR:N | 2.13 | 0.80 |
| 1:D:797:GLN:NE2 | 1:D:800:LYS:HZ1 | 1.78 | 0.80 |
| 1:E:168:SER:OG | 1:E:264:ARG:NH2 | 2.14 | 0.80 |
| 1:E:203:ARG:HB3 | 1:E:203:ARG:CZ | 2.11 | 0.80 |
| 1:A:595:ARG:HH11 | 1:B:841:ALA:HB3 | 1.47 | 0.80 |
| 1:A:739:GLY:HA3 | 1:A:742:ILE:HD13 | 1.63 | 0.80 |
| 1:C:617:GLY:N | 1:C:620:LYS:HE3 | 1.96 | 0.80 |
| 1:A:319:ASN:ND2 | 1:A:712:GLN:OE1 | 2.14 | 0.79 |
| 1:C:416:SER:O | 1:C:420:GLN:N | 2.11 | 0.79 |
| 1:C:557:PRO:HA | 1:C:560:LYS:NZ | 1.97 | 0.79 |
| 1:C:630:PHE:HB3 | 1:C:631:LEU:HD12 | 1.63 | 0.79 |
| 1:D:319:ASN:HB3 | 1:D:712:GLN:HG2 | 1.64 | 0.79 |
| 1:D:488:ASN:O | 1:D:492:ASP:N | 2.15 | 0.79 |
| 1:E:485:GLU:C | 1:E:489:LYS:HZ3 | 1.90 | 0.79 |
| 1:E:828:LEU:HA | 1:E:831:LEU:HB2 | 1.63 | 0.79 |
| 1:F:568:LYS:O | 1:F:572:MET:N | 2.11 | 0.79 |
| 1:F:702:MET:SD | 1:F:708:ILE:HG23 | 2.22 | 0.79 |
| 1:B:250:ALA:H | 1:B:264:ARG:HH12 | 1.26 | 0.79 |
| 1:B:812:ASP:HA | 1:B:815:ALA:HB3 | 1.64 | 0.79 |
| 1:C:465:ARG:HH12 | 1:C:529:ARG:HH11 | 1.30 | 0.79 |
| 1:C:549:THR:O | 1:C:553:LEU:N | 2.14 | 0.79 |
| 1:C:636:ASP:OD1 | 1:C:637:MET:N | 2.15 | 0.79 |
| 1:D:216:ILE:N | 2:D:1001:AGS:O3G | 2.11 | 0.79 |
| 1:D:452:GLU:O | 1:D:456:GLN:N | 2.13 | 0.79 |
| 1:D:686:ASP:HA | 1:D:688:VAL:HG12 | 1.64 | 0.79 |
| 1:A:272:ILE:C | 1:A:276:LYS:HZ3 | 1.89 | 0.79 |
| 1:A:569:LEU:O | 1:A:572:MET:N | 2.15 | 0.79 |
| 1:B:393:LEU:HA | 1:B:396:VAL:HB | 1.64 | 0.79 |
| 1:B:697:THR:O | 1:B:701:GLN:N | 2.12 | 0.79 |
| 1:C:571:HIS:HA | 1:C:574:ARG:HG2 | 1.64 | 0.79 |
| 1:C:850:LYS:NZ | 1:C:851:ASP:OD1 | 2.14 | 0.79 |
| 1:D:570:ILE:O | 1:D:595:ARG:NH2 | 2.13 | 0.79 |
| 1:D:696:LEU:HA | 1:D:699:MET:HB3 | 1.62 | 0.79 |
| 1:D:785:ASP:O | 1:D:788:LEU:N | 2.15 | 0.79 |
| 1:E:476:LEU:HD22 | 1:E:520:LEU:HB2 | 1.62 | 0.79 |
| 1:E:834:ASN:N | 1:E:834:ASN:OD1 | 2.12 | 0.79 |
| 1:F:216:ILE:HG12 | 1:F:218:LYS:NZ | 1.97 | 0.79 |
| 1:A:786:ILE:HA | 1:A:789:LYS:HZ3 | 1.46 | 0.79 |
| 1:B:214:PRO:HD2 | 1:B:387:ARG:NE | 1.97 | 0.79 |
| 1:B:242:LYS:N | 1:B:278:LEU:O | 2.11 | 0.79 |
| 1:C:203:ARG:HH12 | 1:D:359:TYR:HB3 | 1.47 | 0.79 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:262:GLU:HA | 1:C:265:PHE:HD2 | 1.48 | 0.79 |
| 1:F:307:ARG:NH1 | 1:F:333:ARG:NH1 | 2.30 | 0.79 |
| 1:F:678:LYS:HZ3 | 1:F:680:TYR:C | 1.89 | 0.79 |
| 1:C:286:ILE:HG12 | 1:C:290:MET:HG3 | 1.65 | 0.79 |
| 1:E:407:ARG:HH12 | 1:E:538:GLN:CD | 1.90 | 0.79 |
| 1:E:543:SER:OG | 1:E:544:ASP:N | 2.14 | 0.79 |
| 1:E:802:TYR:HA | 1:E:852:LYS:HG2 | 1.63 | 0.79 |
| 1:F:242:LYS:HZ3 | 1:F:277:THR:HG21 | 1.48 | 0.79 |
| 1:F:620:LYS:NZ | 2:F:1002:AGS:O3G | 2.15 | 0.79 |
| 1:B:170:TYR:HD1 | 1:B:250:ALA:HB1 | 1.48 | 0.79 |
| 1:B:351:ILE:O | 1:B:355:LEU:N | 2.15 | 0.79 |
| 1:D:265:PHE:CE2 | 1:D:298:ALA:HB1 | 2.18 | 0.79 |
| 1:D:754:VAL:O | 1:D:758:PHE:N | 2.13 | 0.79 |
| 1:E:825:ALA:HB1 | 1:E:828:LEU:HB3 | 1.63 | 0.79 |
| 1:F:683:LEU:HD23 | 1:F:684:LEU:H | 1.46 | 0.79 |
| 1:F:844:ILE:O | 1:F:847:ASN:ND2 | 2.14 | 0.79 |
| 1:A:206:SER:O | 1:A:207:ASN:ND2 | 2.16 | 0.79 |
| 1:A:223:GLU:O | 1:A:226:ALA:N | 2.15 | 0.79 |
| 1:B:353:ARG:NH1 | 1:B:372:LEU:HB2 | 1.97 | 0.79 |
| 1:B:646:LEU:HD12 | 1:B:690:LYS:H | 1.48 | 0.79 |
| 1:C:743:GLN:HB2 | 1:C:746:THR:H | 1.48 | 0.79 |
| 1:D:644:SER:HB2 | 1:D:691:ALA:HA | 1.63 | 0.79 |
| 1:E:365:VAL:HG12 | 1:E:407:ARG:HH11 | 1.47 | 0.79 |
| 1:F:731:ALA:HA | 1:F:734:ILE:HB | 1.65 | 0.79 |
| 1:A:322:ARG:HH22 | 1:A:337:LYS:HD3 | 1.47 | 0.79 |
| 1:B:625:LYS:O | 1:B:628:ALA:N | 2.11 | 0.79 |
| 1:D:387:ARG:O | 1:D:391:SER:N | 2.14 | 0.79 |
| 1:F:363:HIS:NE2 | 1:F:400:CYS:SG | 2.56 | 0.79 |
| 1:B:379:ALA:O | 1:B:383:LEU:N | 2.13 | 0.79 |
| 1:C:173:ASP:OD1 | 1:C:174:MET:N | 2.16 | 0.79 |
| 1:C:319:ASN:O | 1:C:323:SER:N | 2.16 | 0.79 |
| 1:D:216:ILE:HD13 | 1:D:390:ASP:OD2 | 1.82 | 0.79 |
| 1:D:820:SER:N | 1:D:823:MET:O | 2.16 | 0.79 |
| 1:E:593:ALA:O | 1:E:597:SER:N | 2.16 | 0.79 |
| 1:F:348:THR:HA | 1:F:351:ILE:HD12 | 1.65 | 0.79 |
| 1:A:167:LEU:O | 1:A:171:ALA:N | 2.15 | 0.79 |
| 1:A:213:GLU:HB2 | 1:A:218:LYS:NZ | 1.97 | 0.79 |
| 1:B:342:GLU:OE2 | 1:B:388:LEU:HB2 | 1.83 | 0.79 |
| 1:B:646:LEU:HB2 | 1:B:690:LYS:N | 1.97 | 0.79 |
| 1:B:699:MET:O | 1:B:703:LEU:N | 2.16 | 0.79 |
| 1:D:369:ASP:OD1 | 1:D:372:LEU:HD22 | 1.83 | 0.79 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:596:LEU:O | 1:D:599:SER:OG | 2.01 | 0.79 |
| 1:F:565:GLU:O | 1:F:569:LEU:N | 2.13 | 0.79 |
| 1:F:710:SER:OG | 1:F:713:GLY:HA2 | 1.83 | 0.79 |
| 1:C:189:ARG:HB3 | 1:C:192:GLU:HB2 | 1.63 | 0.78 |
| 1:C:686:ASP:CB | 1:C:690:LYS:HZ1 | 1.95 | 0.78 |
| 1:D:363:HIS:HB3 | 1:D:407:ARG:HH22 | 1.48 | 0.78 |
| 1:D:558:VAL:O | 1:D:562:SER:OG | 2.01 | 0.78 |
| 1:E:512:ASP:HA | 1:E:515:LYS:HB2 | 1.62 | 0.78 |
| 1:E:620:LYS:NZ | 2:E:1002:AGS:O2B | 2.15 | 0.78 |
| 1:E:839:LYS:HZ2 | 1:E:879:VAL:HA | 1.48 | 0.78 |
| 1:F:207:ASN:HD21 | 1:F:311:LYS:HE3 | 1.47 | 0.78 |
| 1:F:395:LEU:HD13 | 1:F:546:ILE:HG12 | 1.66 | 0.78 |
| 1:C:579:GLU:HB2 | 1:C:626:LYS:HZ3 | 1.46 | 0.78 |
| 1:C:843:ARG:HG2 | 1:C:846:LYS:HB2 | 1.64 | 0.78 |
| 1:C:843:ARG:HH11 | 1:C:848:GLU:HB2 | 1.47 | 0.78 |
| 1:D:258:LYS:HZ2 | 1:D:262:GLU:HB3 | 1.47 | 0.78 |
| 1:D:377:GLN:H | 1:D:377:GLN:CD | 1.85 | 0.78 |
| 1:D:579:GLU:C | 1:D:626:LYS:HZ3 | 1.92 | 0.78 |
| 1:E:221:ILE:O | 1:E:225:VAL:N | 2.15 | 0.78 |
| 1:E:762:PHE:HA | 1:E:765:ARG:HB3 | 1.63 | 0.78 |
| 1:F:552:ARG:HB2 | 1:F:552:ARG:NH1 | 1.98 | 0.78 |
| 1:D:191:GLU:O | 1:D:195:SER:N | 2.16 | 0.78 |
| 1:D:271:GLU:HG2 | 1:D:276:LYS:HZ2 | 1.45 | 0.78 |
| 1:D:548:GLU:O | 1:D:552:ARG:N | 2.16 | 0.78 |
| 1:D:585:ASP:O | 1:D:589:ALA:N | 2.12 | 0.78 |
| 1:D:637:MET:C | 1:D:678:LYS:HZ3 | 1.90 | 0.78 |
| 1:E:465:ARG:HA | 1:E:468:GLU:HB3 | 1.63 | 0.78 |
| 1:E:571:HIS:O | 1:E:574:ARG:HG2 | 1.84 | 0.78 |
| 1:B:234:VAL:HG22 | 1:B:236:THR:H | 1.48 | 0.78 |
| 1:B:344:SER:O | 1:B:348:THR:OG1 | 2.00 | 0.78 |
| 1:C:143:GLN:O | 1:C:147:LEU:N | 2.17 | 0.78 |
| 1:C:622:GLU:O | 1:C:626:LYS:N | 2.15 | 0.78 |
| 1:D:316:THR:C | 1:D:321:TYR:CD1 | 2.61 | 0.78 |
| 1:D:467:ASN:O | 1:D:471:HIS:N | 2.14 | 0.78 |
| 1:D:673:ASN:OD1 | 1:D:674:GLN:N | 2.15 | 0.78 |
| 1:D:791:ILE:HG22 | 1:D:795:PHE:HZ | 1.48 | 0.78 |
| 1:E:676:GLN:OE1 | 1:E:676:GLN:N | 2.16 | 0.78 |
| 1:F:680:TYR:HB3 | 1:F:720:ASN:HB2 | 1.64 | 0.78 |
| 1:F:806:LEU:HB2 | 1:F:811:LYS:HZ2 | 1.47 | 0.78 |
| 1:A:210:LEU:HD23 | 1:A:211:ILE:HB | 1.66 | 0.78 |
| 1:A:218:LYS:HZ1 | 1:A:387:ARG:HE | 1.31 | 0.78 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:610:PHE:N | 1:A:724:ILE:HG12 | 1.97 | 0.78 |
| 1:B:761:GLU:HA | 1:B:764:ASN:HB3 | 1.64 | 0.78 |
| 1:C:643:CYS:HA | 1:C:646:LEU:HD12 | 1.64 | 0.78 |
| 1:C:672:THR:O | 1:C:676:GLN:N | 2.12 | 0.78 |
| 1:D:537:ILE:O | 1:D:540:VAL:N | 2.15 | 0.78 |
| 1:D:755:ARG:O | 1:D:759:ARG:N | 2.15 | 0.78 |
| 1:E:218:LYS:NZ | 1:E:387:ARG:NH1 | 2.31 | 0.78 |
| 1:F:640:ARG:HA | 1:F:684:LEU:HB3 | 1.65 | 0.78 |
| 1:F:833:GLN:HE21 | 1:F:834:ASN:HD21 | 1.28 | 0.78 |
| 1:A:810:ALA:HA | 1:A:813:PHE:CD1 | 2.19 | 0.78 |
| 1:A:872:GLU:HB3 | 1:F:201:ALA:HB3 | 1.64 | 0.78 |
| 1:B:776:SER:OG | 1:B:777:ARG:N | 2.14 | 0.78 |
| 1:C:259:GLY:O | 1:C:262:GLU:N | 2.16 | 0.78 |
| 1:C:465:ARG:NH1 | 1:C:529:ARG:HH11 | 1.82 | 0.78 |
| 1:C:770:VAL:HG22 | 1:C:771:ILE:H | 1.48 | 0.78 |
| 1:F:609:SER:HB3 | 1:F:722:ILE:HG22 | 1.64 | 0.78 |
| 1:B:637:MET:HG2 | 1:B:680:TYR:O | 1.83 | 0.78 |
| 1:C:169:LYS:HD3 | 1:C:264:ARG:CD | 0.46 | 0.78 |
| 1:C:550:ALA:O | 1:C:554:THR:N | 2.16 | 0.78 |
| 1:D:362:HIS:HD2 | 1:D:363:HIS:CG | 2.02 | 0.78 |
| 1:D:556:ILE:HD13 | 1:D:633:ASN:HD21 | 1.47 | 0.78 |
| 1:D:794:ARG:HH11 | 1:D:795:PHE:HE1 | 1.32 | 0.78 |
| 1:E:766:ILE:O | 1:F:830:ARG:NH2 | 2.17 | 0.78 |
| 1:A:244:PHE:HB3 | 1:A:281:LEU:HD23 | 1.66 | 0.78 |
| 1:A:609:SER:HB3 | 1:A:724:ILE:HG13 | 1.64 | 0.78 |
| 1:C:302:LYS:HA | 1:C:305:LEU:HB2 | 1.64 | 0.78 |
| 1:C:575:ASP:O | 1:C:578:SER:N | 2.16 | 0.78 |
| 1:D:210:LEU:O | 1:D:316:THR:N | 2.14 | 0.78 |
| 1:D:274:GLU:O | 1:D:276:LYS:HG3 | 1.84 | 0.78 |
| 1:D:326:GLU:OE1 | 1:D:326:GLU:N | 2.15 | 0.78 |
| 1:D:357:PRO:CG | 1:D:358:LYS:HZ2 | 1.96 | 0.78 |
| 1:D:403:VAL:O | 1:D:407:ARG:N | 2.17 | 0.78 |
| 1:E:176:GLU:OE1 | 1:E:176:GLU:N | 2.16 | 0.78 |
| 1:E:187:ILE:HD12 | 2:E:1001:AGS:HN62 | 1.49 | 0.78 |
| 1:E:478:GLN:O | 1:E:482:LYS:N | 2.16 | 0.78 |
| 1:B:544:ASP:O | 1:B:560:LYS:NZ | 2.17 | 0.78 |
| 1:C:168:SER:CA | 1:C:264:ARG:HE | 1.97 | 0.78 |
| 1:D:357:PRO:HG2 | 1:D:358:LYS:HZ2 | 1.49 | 0.78 |
| 1:D:524:VAL:O | 1:D:534:ASN:ND2 | 2.17 | 0.78 |
| 1:D:626:LYS:O | 1:D:630:PHE:N | 2.16 | 0.78 |
| 1:E:689:GLU:OE2 | 1:E:757:HIS:CD2 | 2.36 | 0.78 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:701:GLN:HG2 | 1:E:707:ARG:HB2 | 1.65 | 0.78 |
| 1:F:699:MET:SD | 1:F:708:ILE:CG2 | 2.72 | 0.78 |
| 1:A:751:MET:SD | 1:A:755:ARG:NH2 | 2.55 | 0.78 |
| 1:B:190:GLU:O | 1:B:193:ILE:HG13 | 1.84 | 0.78 |
| 1:B:225:VAL:O | 1:B:229:ILE:N | 2.16 | 0.78 |
| 1:B:648:GLU:N | 1:B:693:PRO:HD3 | 1.99 | 0.78 |
| 1:C:543:SER:OG | 1:C:544:ASP:OD1 | 2.00 | 0.78 |
| 1:F:331:PHE:C | 1:F:334:ARG:HG2 | 2.09 | 0.78 |
| 1:F:755:ARG:NH1 | 1:F:763:LEU:HB3 | 1.99 | 0.78 |
| 1:A:251:LEU:O | 1:A:255:ALA:N | 2.17 | 0.77 |
| 1:A:786:ILE:HA | 1:A:789:LYS:NZ | 1.99 | 0.77 |
| 1:B:223:GLU:H | 1:B:223:GLU:CD | 1.90 | 0.77 |
| 1:B:654:LYS:HZ1 | 1:B:694:ASP:CG | 1.92 | 0.77 |
| 1:C:168:SER:CB | 1:C:271:GLU:CD | 2.54 | 0.77 |
| 1:C:245:SER:OG | 1:C:284:ASP:OD1 | 2.02 | 0.77 |
| 1:C:843:ARG:HH12 | 1:C:848:GLU:CD | 1.92 | 0.77 |
| 1:D:281:LEU:HD12 | 1:D:312:VAL:HG12 | 1.66 | 0.77 |
| 1:D:408:ASP:CG | 1:D:409:SER:H | 1.91 | 0.77 |
| 1:D:784:VAL:HG13 | 1:D:785:ASP:H | 1.49 | 0.77 |
| 1:E:358:LYS:NZ | 1:E:362:HIS:CE1 | 2.52 | 0.77 |
| 1:E:390:ASP:HA | 1:E:393:LEU:HD12 | 1.65 | 0.77 |
| 1:E:484:ASP:N | 1:E:484:ASP:OD1 | 2.15 | 0.77 |
| 1:F:612:PHE:HB2 | 1:F:724:ILE:HG13 | 1.66 | 0.77 |
| 1:F:623:LEU:HD12 | 1:F:626:LYS:HB2 | 1.66 | 0.77 |
| 1:A:708:ILE:O | 1:A:716:ILE:N | 2.17 | 0.77 |
| 1:B:545:THR:HA | 1:B:548:GLU:HB2 | 1.65 | 0.77 |
| 1:B:666:ASP:OD2 | 1:B:672:THR:OG1 | 2.01 | 0.77 |
| 1:B:857:VAL:HG12 | 1:B:878:GLU:H | 1.47 | 0.77 |
| 1:C:710:SER:OG | 1:C:714:LYS:N | 2.17 | 0.77 |
| 1:E:469:GLU:O | 1:E:473:HIS:ND1 | 2.17 | 0.77 |
| 1:E:703:LEU:HD13 | 1:E:765:ARG:HG3 | 1.66 | 0.77 |
| 1:F:174:MET:O | 1:F:177:GLN:N | 2.17 | 0.77 |
| 1:F:644:SER:HA | 1:F:690:LYS:HD2 | 1.66 | 0.77 |
| 1:B:166:TYR:HA | 1:B:169:LYS:HG2 | 1.65 | 0.77 |
| 1:B:238:LEU:HA | 1:B:241:ALA:HB3 | 1.65 | 0.77 |
| 1:B:540:VAL:HG12 | 1:B:542:ASP:H | 1.48 | 0.77 |
| 1:B:621:THR:H | 1:B:826:ARG:HH22 | 1.30 | 0.77 |
| 1:C:400:CYS:O | 1:C:404:ALA:N | 2.12 | 0.77 |
| 1:C:825:ALA:O | 1:C:829:ASN:N | 2.17 | 0.77 |
| 1:D:172:ILE:H | 1:D:245:SER:N | 1.82 | 0.77 |
| 1:D:177:GLN:O | 1:D:181:GLY:N | 2.17 | 0.77 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:219:THR:O | 1:D:223:GLU:N | 2.16 | 0.77 |
| 1:E:177:GLN:O | 1:E:181:GLY:N | 2.17 | 0.77 |
| 1:E:246:LEU:HB3 | 1:E:283:ILE:HD11 | 1.65 | 0.77 |
| 1:E:371:ALA:O | 1:E:375:ALA:N | 2.10 | 0.77 |
| 1:E:820:SER:HB3 | 1:E:824:GLY:N | 1.98 | 0.77 |
| 1:E:830:ARG:O | 1:E:833:GLN:NE2 | 2.17 | 0.77 |
| 1:F:785:ASP:HB3 | 1:F:789:LYS:NZ | 1.95 | 0.77 |
| 1:A:603:ASN:HB3 | 1:A:605:ARG:NE | 1.99 | 0.77 |
| 1:B:764:ASN:HB3 | 1:B:765:ARG:HH12 | 1.47 | 0.77 |
| 1:C:818:GLY:HA3 | 1:C:828:LEU:HD21 | 1.64 | 0.77 |
| 1:D:646:LEU:HD22 | 1:D:649:LYS:HB3 | 1.66 | 0.77 |
| 1:E:814:LEU:O | 1:E:818:GLY:N | 2.17 | 0.77 |
| 1:F:701:GLN:OE1 | 1:F:709:THR:CB | 2.31 | 0.77 |
| 1:A:396:VAL:HA | 1:A:399:SER:HB2 | 1.64 | 0.77 |
| 1:A:794:ARG:O | 1:A:797:GLN:NE2 | 2.17 | 0.77 |
| 1:D:362:HIS:HD2 | 1:D:363:HIS:CD2 | 2.02 | 0.77 |
| 1:D:391:SER:HA | 1:D:394:ASP:OD2 | 1.83 | 0.77 |
| 1:F:210:LEU:HD12 | 1:F:339:GLU:HA | 1.65 | 0.77 |
| 1:F:290:MET:HG2 | 1:F:293:GLY:HA2 | 1.66 | 0.77 |
| 1:F:666:ASP:OD2 | 1:F:669:GLY:HA2 | 1.83 | 0.77 |
| 1:F:699:MET:C | 1:F:703:LEU:CG | 2.40 | 0.77 |
| 1:A:179:ARG:HD2 | 1:A:242:LYS:NZ | 1.99 | 0.77 |
| 1:B:228:ARG:HH12 | 1:B:233:ASP:HB2 | 1.47 | 0.77 |
| 1:C:620:LYS:HG3 | 1:C:621:THR:N | 1.99 | 0.77 |
| 1:D:358:LYS:HD2 | 1:D:358:LYS:N | 1.99 | 0.77 |
| 1:D:560:LYS:HA | 1:D:563:GLU:OE2 | 1.85 | 0.77 |
| 1:E:654:LYS:HZ3 | 1:E:698:VAL:HG22 | 1.50 | 0.77 |
| 1:A:176:GLU:O | 1:A:180:GLN:N | 2.11 | 0.77 |
| 1:A:643:CYS:H | 1:A:686:ASP:H | 1.30 | 0.77 |
| 1:B:304:ALA:O | 1:B:308:GLY:N | 2.18 | 0.77 |
| 1:C:647:SER:OG | 1:C:649:LYS:O | 2.02 | 0.77 |
| 1:D:180:GLN:HB3 | 1:D:182:LYS:HG3 | 1.64 | 0.77 |
| 1:D:759:ARG:HB3 | 1:D:763:LEU:HD11 | 1.66 | 0.77 |
| 1:E:303:PRO:HB2 | 1:E:307:ARG:NH1 | 1.98 | 0.77 |
| 1:E:304:ALA:N | 1:E:307:ARG:NH1 | 2.33 | 0.77 |
| 1:E:654:LYS:HZ1 | 1:E:694:ASP:CG | 1.92 | 0.77 |
| 1:F:217:GLY:N | 2:F:1001:AGS:O2B | 2.18 | 0.77 |
| 1:F:302:LYS:HD2 | 1:F:305:LEU:HD11 | 1.67 | 0.77 |
| 1:C:197:ILE:HA | 1:C:200:LEU:HD12 | 1.67 | 0.77 |
| 1:C:215:GLY:N | 2:C:1001:AGS:S1G | 2.53 | 0.77 |
| 1:C:733:PHE:CZ | 1:C:749:LEU:HB2 | 2.18 | 0.77 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:798:ASN:OD1 | 1:C:799:ASP:N | 2.16 | 0.77 |
| 1:D:710:SER:OG | 1:D:714:LYS:N | 2.15 | 0.77 |
| 1:F:358:LYS:HG2 | 1:F:359:TYR:N | 1.98 | 0.77 |
| 1:A:236:THR:O | 1:A:239:GLN:N | 2.16 | 0.77 |
| 1:B:286:ILE:HD13 | 1:B:289:LEU:HD12 | 1.65 | 0.77 |
| 1:B:617:GLY:HA2 | 1:B:620:LYS:NZ | 2.00 | 0.77 |
| 1:B:787:ARG:HA | 1:B:790:GLU:HB3 | 1.64 | 0.77 |
| 1:C:15:LEU:N | 1:C:160:THR:H | 1.83 | 0.77 |
| 1:D:218:LYS:HZ2 | 2:D:1001:AGS:PB | 2.07 | 0.77 |
| 1:D:696:LEU:O | 1:D:700:LEU:N | 2.18 | 0.77 |
| 1:E:223:GLU:O | 1:E:227:GLN:N | 2.18 | 0.77 |
| 1:F:704:ASP:OD1 | 1:F:765:ARG:CD | 2.32 | 0.77 |
| 1:F:704:ASP:CA | 1:F:765:ARG:NE | 2.48 | 0.77 |
| 1:F:836:ILE:HA | 1:F:839:LYS:HZ3 | 1.49 | 0.77 |
| 1:A:843:ARG:HD3 | 1:A:846:LYS:HD2 | 1.66 | 0.77 |
| 1:B:643:CYS:C | 1:B:645:GLU:H | 1.93 | 0.77 |
| 1:D:344:SER:H | 1:D:347:GLN:HB2 | 1.50 | 0.77 |
| 1:D:408:ASP:OD1 | 1:D:409:SER:N | 2.18 | 0.77 |
| 1:D:839:LYS:NZ | 1:D:878:GLU:HB3 | 1.99 | 0.77 |
| 1:E:349:VAL:HG12 | 1:E:353:ARG:HG3 | 1.67 | 0.77 |
| 1:E:621:THR:O | 1:E:625:LYS:N | 2.16 | 0.77 |
| 1:E:646:LEU:N | 1:E:649:LYS:HD2 | 1.99 | 0.77 |
| 1:F:627:VAL:HA | 1:F:630:PHE:HB3 | 1.66 | 0.77 |
| 1:A:837:LEU:O | 1:A:841:ALA:N | 2.16 | 0.76 |
| 1:B:219:THR:O | 1:B:221:ILE:N | 2.18 | 0.76 |
| 1:B:682:VAL:HA | 1:B:723:VAL:HG21 | 1.67 | 0.76 |
| 1:D:345:VAL:O | 1:D:349:VAL:N | 2.16 | 0.76 |
| 1:D:701:GLN:OE1 | 1:D:701:GLN:N | 2.17 | 0.76 |
| 1:E:242:LYS:H | 1:E:279:ILE:HA | 1.49 | 0.76 |
| 1:E:789:LYS:O | 1:E:793:GLU:N | 2.12 | 0.76 |
| 1:A:205:LYS:N | 1:A:334:ARG:HD2 | 2.00 | 0.76 |
| 1:B:173:ASP:CG | 1:B:177:GLN:HG3 | 2.10 | 0.76 |
| 1:B:222:ILE:O | 1:B:226:ALA:N | 2.13 | 0.76 |
| 1:C:838:ASN:OD1 | 1:C:839:LYS:N | 2.18 | 0.76 |
| 1:D:372:LEU:HD12 | 1:D:542:ASP:HB3 | 1.65 | 0.76 |
| 1:D:566:ASN:O | 1:D:569:LEU:HG | 1.85 | 0.76 |
| 1:F:197:ILE:CG1 | 1:F:228:ARG:HH11 | 1.99 | 0.76 |
| 1:F:363:HIS:HE1 | 1:F:397:ASP:OD1 | 1.64 | 0.76 |
| 1:F:593:ALA:O | 1:F:597:SER:N | 2.17 | 0.76 |
| 1:B:646:LEU:H | 1:B:691:ALA:N | 1.83 | 0.76 |
| 1:B:693:PRO:HD2 | 1:B:694:ASP:H | 1.48 | 0.76 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:414:LEU:O | 1:C:418:GLU:N | 2.17 | 0.76 |
| 1:D:248:LEU:HA | 1:D:251:LEU:HG | 1.67 | 0.76 |
| 1:D:300:ILE:HA | 1:D:303:PRO:HG2 | 1.68 | 0.76 |
| 1:D:761:GLU:OE1 | 1:D:764:ASN:ND2 | 2.17 | 0.76 |
| 1:E:786:ILE:HG22 | 1:E:790:GLU:HB2 | 1.68 | 0.76 |
| 1:F:628:ALA:HB1 | 1:F:637:MET:HE2 | 1.67 | 0.76 |
| 1:F:804:LEU:HB3 | 1:F:855:VAL:HG23 | 1.66 | 0.76 |
| 1:F:818:GLY:HA3 | 1:F:828:LEU:HD21 | 1.68 | 0.76 |
| 1:A:191:GLU:O | 1:A:195:SER:N | 2.16 | 0.76 |
| 1:B:228:ARG:NH1 | 1:B:233:ASP:HB2 | 2.00 | 0.76 |
| 1:B:290:MET:O | 1:B:299:ASN:ND2 | 2.17 | 0.76 |
| 1:B:848:GLU:HB2 | 1:B:882:ASN:ND2 | 2.00 | 0.76 |
| 1:C:247:ASP:OD1 | 1:C:248:LEU:N | 2.18 | 0.76 |
| 1:C:519:LYS:O | 1:C:523:GLN:N | 2.18 | 0.76 |
| 1:C:763:LEU:HA | 1:C:766:ILE:HD12 | 1.66 | 0.76 |
| 1:D:576:LEU:HA | 1:D:579:GLU:HG2 | 1.68 | 0.76 |
| 1:E:302:LYS:NZ | 1:E:334:ARG:HB2 | 2.00 | 0.76 |
| 1:E:470:LYS:HG2 | 1:E:474:GLU:OE2 | 1.86 | 0.76 |
| 1:F:653:SER:HA | 1:F:667:GLU:HG2 | 1.68 | 0.76 |
| 1:F:755:ARG:HA | 1:F:763:LEU:HD13 | 1.68 | 0.76 |
| 1:F:812:ASP:C | 1:F:816:LYS:HZ3 | 1.93 | 0.76 |
| 1:B:620:LYS:HZ2 | 1:B:826:ARG:HH12 | 1.27 | 0.76 |
| 1:B:634:ASP:OD1 | 1:B:636:ASP:N | 2.15 | 0.76 |
| 1:B:801:HIS:ND1 | 1:B:851:ASP:OD1 | 2.18 | 0.76 |
| 1:C:169:LYS:CD | 1:C:264:ARG:NH1 | 2.42 | 0.76 |
| 1:C:356:GLN:O | 1:C:360:GLU:N | 2.19 | 0.76 |
| 1:D:617:GLY:N | 1:D:620:LYS:HE3 | 1.98 | 0.76 |
| 1:E:240:GLY:O | 1:E:277:THR:OG1 | 2.02 | 0.76 |
| 1:E:246:LEU:O | 1:E:283:ILE:HG12 | 1.86 | 0.76 |
| 1:E:703:LEU:C | 1:E:707:ARG:HH11 | 1.93 | 0.76 |
| 1:F:218:LYS:HA | 1:F:221:ILE:HD12 | 1.67 | 0.76 |
| 1:F:839:LYS:O | 1:F:843:ARG:N | 2.17 | 0.76 |
| 1:A:317:THR:OG1 | 1:A:322:ARG:N | 2.16 | 0.76 |
| 1:B:695:VAL:O | 1:B:699:MET:N | 2.15 | 0.76 |
| 1:C:702:MET:SD | 1:C:708:ILE:HG21 | 2.26 | 0.76 |
| 1:C:767:SER:HA | 1:D:830:ARG:NH1 | 2.00 | 0.76 |
| 1:D:799:ASP:H | 1:D:801:HIS:HD2 | 1.30 | 0.76 |
| 1:D:809:GLU:CD | 1:D:811:LYS:HZ2 | 1.94 | 0.76 |
| 1:F:548:GLU:OE1 | 1:F:552:ARG:NH1 | 2.14 | 0.76 |
| 1:A:700:LEU:HD12 | 1:A:703:LEU:HB3 | 1.67 | 0.76 |
| 1:B:207:ASN:HB2 | 1:B:335:PHE:CE1 | 2.20 | 0.76 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:622:GLU:H | 1:B:826:ARG:HH21 | 1.33 | 0.76 |
| 1:C:704:ASP:OD1 | 1:C:705:ASP:N | 2.18 | 0.76 |
| 1:D:303:PRO:O | 1:D:306:SER:OG | 2.04 | 0.76 |
| 1:D:785:ASP:OD1 | 1:D:788:LEU:HB2 | 1.86 | 0.76 |
| 1:E:248:LEU:HA | 1:E:251:LEU:HB2 | 1.65 | 0.76 |
| 1:E:256:LYS:HE2 | 1:E:260:ASP:OD2 | 1.85 | 0.76 |
| 1:E:642:ASP:C | 1:E:649:LYS:HZ3 | 1.93 | 0.76 |
| 1:E:833:GLN:O | 1:E:836:ILE:N | 2.18 | 0.76 |
| 1:F:176:GLU:OE2 | 1:F:177:GLN:HG3 | 1.84 | 0.76 |
| 1:F:655:LEU:HD21 | 1:F:671:LEU:HD12 | 1.67 | 0.76 |
| 1:F:708:ILE:HD12 | 1:F:708:ILE:N | 2.01 | 0.76 |
| 1:A:286:ILE:HG21 | 1:A:316:THR:HA | 1.67 | 0.76 |
| 1:B:348:THR:HG21 | 1:B:388:LEU:HG | 1.66 | 0.76 |
| 1:C:169:LYS:HD2 | 1:C:264:ARG:CD | 1.72 | 0.76 |
| 1:C:203:ARG:NH1 | 1:D:359:TYR:HB3 | 2.00 | 0.76 |
| 1:C:639:ILE:HG22 | 1:C:640:ARG:H | 1.51 | 0.76 |
| 1:C:681:SER:N | 1:C:721:CYS:SG | 2.59 | 0.76 |
| 1:C:828:LEU:O | 1:C:832:ILE:N | 2.19 | 0.76 |
| 1:D:563:GLU:HG3 | 1:D:568:LYS:NZ | 2.00 | 0.76 |
| 1:D:617:GLY:H | 1:D:620:LYS:CE | 1.96 | 0.76 |
| 1:E:203:ARG:HG3 | 1:F:363:HIS:ND1 | 2.00 | 0.76 |
| 1:E:285:GLU:HA | 1:E:287:HIS:CE1 | 2.20 | 0.76 |
| 1:E:534:ASN:HB2 | 1:E:536:MET:HB3 | 1.68 | 0.76 |
| 1:A:218:LYS:HZ1 | 1:A:387:ARG:NE | 1.84 | 0.76 |
| 1:B:215:GLY:O | 1:B:219:THR:N | 2.17 | 0.76 |
| 1:C:591:SER:HB2 | 1:C:595:ARG:HH12 | 1.51 | 0.76 |
| 1:D:390:ASP:HA | 1:D:393:LEU:HB2 | 1.68 | 0.76 |
| 1:D:636:ASP:C | 1:D:678:LYS:HZ1 | 1.93 | 0.76 |
| 1:E:323:SER:C | 1:E:327:LYS:HZ3 | 1.93 | 0.76 |
| 1:E:478:GLN:HA | 1:E:481:LYS:HB3 | 1.66 | 0.76 |
| 1:E:685:PHE:O | 1:E:726:THR:OG1 | 2.04 | 0.76 |
| 1:E:808:GLN:N | 1:E:811:LYS:NZ | 2.34 | 0.76 |
| 1:B:857:VAL:HB | 1:B:876:CYS:HB3 | 1.68 | 0.76 |
| 1:C:302:LYS:NZ | 1:C:306:SER:HA | 2.01 | 0.76 |
| 1:C:349:VAL:HB | 1:C:353:ARG:HH12 | 1.51 | 0.76 |
| 1:D:694:ASP:O | 1:D:698:VAL:N | 2.18 | 0.76 |
| 1:E:175:THR:HA | 1:E:178:ALA:HB3 | 1.67 | 0.76 |
| 1:E:747:LYS:O | 1:E:751:MET:N | 2.18 | 0.76 |
| 1:F:280:VAL:HG22 | 1:F:311:LYS:H | 1.51 | 0.76 |
| 1:A:718:CYS:SG | 1:A:720:ASN:ND2 | 2.59 | 0.75 |
| 1:A:820:SER:HB2 | 1:A:827:PRO:HG3 | 1.68 | 0.75 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:202:ARG:O | 1:B:206:SER:OG | 2.04 | 0.75 |
| 1:D:299:ASN:O | 1:D:302:LYS:N | 2.18 | 0.75 |
| 1:D:425:GLN:HB2 | 1:D:452:GLU:OE2 | 1.86 | 0.75 |
| 1:E:176:GLU:HG2 | 1:E:177:GLN:H | 1.51 | 0.75 |
| 1:E:565:GLU:O | 1:E:569:LEU:N | 2.19 | 0.75 |
| 1:F:273:GLU:HG3 | 1:F:274:GLU:H | 1.51 | 0.75 |
| 1:F:810:ALA:O | 1:F:814:LEU:N | 2.13 | 0.75 |
| 1:B:287:HIS:HA | 1:B:290:MET:HB3 | 1.68 | 0.75 |
| 1:B:646:LEU:HD21 | 1:B:686:ASP:CG | 2.11 | 0.75 |
| 1:C:180:GLN:HB2 | 1:C:182:LYS:HG3 | 1.67 | 0.75 |
| 1:C:420:GLN:HA | 1:C:423:LEU:HB2 | 1.68 | 0.75 |
| 1:C:465:ARG:NH1 | 1:C:529:ARG:HD2 | 2.02 | 0.75 |
| 1:D:186:VAL:HB | 2:D:1001:AGS:C4 | 2.16 | 0.75 |
| 1:D:530:ARG:NH1 | 1:D:537:ILE:HG23 | 2.01 | 0.75 |
| 1:D:530:ARG:NH1 | 1:D:539:ASN:N | 2.30 | 0.75 |
| 1:D:800:LYS:HZ3 | 1:D:801:HIS:CD2 | 2.04 | 0.75 |
| 1:E:704:ASP:C | 1:E:707:ARG:HH11 | 1.95 | 0.75 |
| 1:E:709:THR:O | 1:E:716:ILE:N | 2.20 | 0.75 |
| 1:A:298:ALA:O | 1:A:301:LEU:N | 2.20 | 0.75 |
| 1:A:346:ARG:O | 1:A:350:ALA:N | 2.19 | 0.75 |
| 1:B:209:CYS:HA | 1:B:314:GLY:HA2 | 1.67 | 0.75 |
| 1:C:217:GLY:H | 2:C:1001:AGS:PB | 2.10 | 0.75 |
| 1:C:376:ALA:O | 1:C:380:LYS:N | 2.19 | 0.75 |
| 1:C:621:THR:HB | 1:C:826:ARG:HH11 | 1.51 | 0.75 |
| 1:C:634:ASP:HB2 | 1:C:636:ASP:OD2 | 1.85 | 0.75 |
| 1:E:218:LYS:CE | 1:E:387:ARG:HH12 | 1.98 | 0.75 |
| 1:E:536:MET:HG3 | 1:E:538:GLN:HB3 | 1.68 | 0.75 |
| 1:E:572:MET:O | 1:E:576:LEU:HG | 1.87 | 0.75 |
| 1:F:166:TYR:N | 1:F:267:GLY:O | 2.20 | 0.75 |
| 1:A:708:ILE:HB | 1:A:716:ILE:HB | 1.66 | 0.75 |
| 1:B:195:SER:HB2 | 1:B:198:ARG:HH12 | 1.51 | 0.75 |
| 1:B:770:VAL:HG12 | 1:B:771:ILE:H | 1.51 | 0.75 |
| 1:C:565:GLU:O | 1:C:569:LEU:N | 2.19 | 0.75 |
| 1:D:688:VAL:HA | 1:D:691:ALA:HB2 | 1.69 | 0.75 |
| 1:F:784:VAL:O | 1:F:788:LEU:N | 2.16 | 0.75 |
| 1:A:403:VAL:HA | 1:A:406:ALA:HB3 | 1.68 | 0.75 |
| 1:C:189:ARG:HH22 | 1:C:342:GLU:CA | 2.00 | 0.75 |
| 1:C:712:GLN:C | 1:C:714:LYS:NZ | 2.45 | 0.75 |
| 1:D:282:PHE:HD1 | 1:D:313:ILE:HD11 | 1.49 | 0.75 |
| 1:D:733:PHE:CZ | 1:D:749:LEU:HB3 | 2.17 | 0.75 |
| 1:E:496:ARG:O | 1:E:499:THR:OG1 | 2.04 | 0.75 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:356:GLN:CB | 1:F:357:PRO:CD | 2.57 | 0.75 |
| 1:A:830:ARG:NH1 | 1:F:309:GLN:HA | 2.02 | 0.75 |
| 1:B:718:CYS:SG | 1:B:720:ASN:HB3 | 2.26 | 0.75 |
| 1:C:258:LYS:O | 1:C:263:GLU:OE2 | 2.05 | 0.75 |
| 1:D:195:SER:O | 1:D:199:VAL:N | 2.17 | 0.75 |
| 1:D:246:LEU:HD11 | 1:D:249:ALA:HB3 | 1.69 | 0.75 |
| 1:E:831:LEU:HA | 1:E:834:ASN:HD21 | 1.51 | 0.75 |
| 1:F:702:MET:HB3 | 1:F:708:ILE:HA | 1.68 | 0.75 |
| 1:C:168:SER:HA | 1:C:264:ARG:NE | 2.02 | 0.75 |
| 1:C:261:PHE:C | 1:C:265:PHE:HB3 | 2.11 | 0.75 |
| 1:D:198:ARG:NH1 | 1:E:401:ALA:O | 2.18 | 0.75 |
| 1:E:618:SER:H | 2:E:1002:AGS:PB | 2.10 | 0.75 |
| 1:F:344:SER:O | 1:F:348:THR:OG1 | 2.04 | 0.75 |
| 1:F:655:LEU:HA | 1:F:668:GLY:HA3 | 1.69 | 0.75 |
| 1:F:699:MET:HA | 1:F:702:MET:HG2 | 1.69 | 0.75 |
| 1:A:575:ASP:HA | 1:A:578:SER:HB3 | 1.68 | 0.75 |
| 1:B:407:ARG:NH2 | 1:B:538:GLN:O | 2.16 | 0.75 |
| 1:B:549:THR:C | 1:B:552:ARG:NH1 | 2.44 | 0.75 |
| 1:B:587:ILE:HA | 1:B:590:VAL:HB | 1.68 | 0.75 |
| 1:B:674:GLN:HA | 1:B:678:LYS:HE2 | 1.69 | 0.75 |
| 1:C:583:GLN:HG3 | 1:C:773:ASN:HD22 | 1.51 | 0.75 |
| 1:C:761:GLU:OE1 | 1:C:764:ASN:ND2 | 2.20 | 0.75 |
| 1:D:342:GLU:OE2 | 1:D:389:PRO:HD3 | 1.87 | 0.75 |
| 1:E:189:ARG:NH2 | 1:E:341:ALA:H | 1.85 | 0.75 |
| 1:A:265:PHE:O | 1:A:269:LEU:N | 2.18 | 0.75 |
| 1:B:305:LEU:O | 1:B:309:GLN:N | 2.20 | 0.75 |
| 1:B:322:ARG:HA | 1:B:325:VAL:HB | 1.69 | 0.75 |
| 1:B:615:LEU:O | 1:B:618:SER:OG | 2.05 | 0.75 |
| 1:D:248:LEU:O | 1:D:251:LEU:N | 2.19 | 0.75 |
| 1:E:394:ASP:O | 1:E:398:ILE:N | 2.13 | 0.75 |
| 1:E:802:TYR:CB | 1:E:852:LYS:HA | 2.17 | 0.75 |
| 1:E:839:LYS:HA | 1:E:842:LEU:HB3 | 1.67 | 0.75 |
| 1:A:641:VAL:HG23 | 1:A:683:LEU:HD11 | 1.68 | 0.74 |
| 1:A:830:ARG:CZ | 1:F:309:GLN:HA | 2.17 | 0.74 |
| 1:C:365:VAL:HG12 | 1:C:366:ARG:H | 1.52 | 0.74 |
| 1:D:849:ILE:HG22 | 1:D:851:ASP:H | 1.52 | 0.74 |
| 1:E:802:TYR:HB3 | 1:E:852:LYS:HA | 1.68 | 0.74 |
| 1:A:205:LYS:NZ | 1:B:397:ASP:HB3 | 2.01 | 0.74 |
| 1:A:287:HIS:CD2 | 1:A:290:MET:HB2 | 2.23 | 0.74 |
| 1:A:357:PRO:HA | 1:A:360:GLU:HB3 | 1.68 | 0.74 |
| 1:A:596:LEU:HA | 1:A:601:LEU:HD12 | 1.68 | 0.74 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:292:ASN:HB3 | 1:B:295:ASP:OD2 | 1.87 | 0.74 |
| 1:C:14:ILE:C | 1:C:160:THR:H | 1.95 | 0.74 |
| 1:C:333:ARG:NH1 | 1:C:334:ARG:CZ | 2.50 | 0.74 |
| 1:C:470:LYS:O | 1:C:474:GLU:N | 2.19 | 0.74 |
| 1:C:611:LEU:HD13 | 1:C:770:VAL:HG12 | 1.69 | 0.74 |
| 1:D:350:ALA:O | 1:D:354:GLY:N | 2.13 | 0.74 |
| 1:D:570:ILE:CA | 1:D:595:ARG:HH12 | 2.00 | 0.74 |
| 1:F:629:GLY:O | 1:F:633:ASN:N | 2.20 | 0.74 |
| 1:F:699:MET:O | 1:F:703:LEU:N | 2.18 | 0.74 |
| 1:A:857:VAL:HG22 | 1:A:878:GLU:HA | 1.69 | 0.74 |
| 1:B:804:LEU:HA | 1:B:855:VAL:HG23 | 1.67 | 0.74 |
| 1:C:203:ARG:HH11 | 1:D:363:HIS:CD2 | 2.05 | 0.74 |
| 1:C:542:ASP:OD1 | 1:C:543:SER:N | 2.20 | 0.74 |
| 1:D:172:ILE:O | 1:D:245:SER:N | 2.18 | 0.74 |
| 1:D:799:ASP:OD2 | 1:D:850:LYS:HB3 | 1.87 | 0.74 |
| 1:E:196:THR:O | 1:E:200:LEU:HG | 1.86 | 0.74 |
| 1:A:589:ALA:O | 1:A:593:ALA:N | 2.17 | 0.74 |
| 1:B:352:LEU:O | 1:B:356:GLN:N | 2.21 | 0.74 |
| 1:B:610:PHE:H | 1:B:724:ILE:HD12 | 1.52 | 0.74 |
| 1:B:736:SER:HB3 | 1:B:742:ILE:HG23 | 1.69 | 0.74 |
| 1:C:583:GLN:HE21 | 1:C:773:ASN:N | 1.86 | 0.74 |
| 1:D:400:CYS:O | 1:D:404:ALA:N | 2.18 | 0.74 |
| 1:D:466:TYR:O | 1:D:470:LYS:N | 2.13 | 0.74 |
| 1:E:191:GLU:OE1 | 1:E:191:GLU:N | 2.20 | 0.74 |
| 1:E:398:ILE:HG21 | 1:E:549:THR:HG23 | 1.70 | 0.74 |
| 1:E:569:LEU:O | 1:E:595:ARG:NH2 | 2.20 | 0.74 |
| 1:F:843:ARG:NH2 | 1:F:882:ASN:HA | 2.01 | 0.74 |
| 1:B:848:GLU:HG3 | 1:B:849:ILE:H | 1.52 | 0.74 |
| 1:D:216:ILE:N | 2:D:1001:AGS:O1B | 2.20 | 0.74 |
| 1:D:218:LYS:HZ2 | 2:D:1001:AGS:PA | 2.09 | 0.74 |
| 1:D:530:ARG:CZ | 1:D:539:ASN:H | 2.01 | 0.74 |
| 1:D:685:PHE:HB3 | 1:D:725:MET:HE3 | 1.69 | 0.74 |
| 1:D:843:ARG:HA | 1:D:846:LYS:HZ3 | 1.51 | 0.74 |
| 1:E:216:ILE:O | 2:E:1001:AGS:O1B | 2.05 | 0.74 |
| 1:E:802:TYR:OH | 1:E:850:LYS:O | 2.05 | 0.74 |
| 1:B:629:GLY:HA2 | 1:B:634:ASP:HA | 1.70 | 0.74 |
| 1:E:476:LEU:HG | 1:E:480:LYS:HE3 | 1.70 | 0.74 |
| 1:E:509:ALA:HB1 | 1:E:511:PRO:HD2 | 1.68 | 0.74 |
| 1:E:617:GLY:O | 1:E:826:ARG:NH2 | 2.20 | 0.74 |
| 1:E:802:TYR:CG | 1:E:852:LYS:HA | 2.23 | 0.74 |
| 1:F:805:ASN:N | 1:F:855:VAL:H | 1.86 | 0.74 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:377:GLN:OE1 | 1:A:377:GLN:N | 2.15 | 0.74 |
| 1:A:580:VAL:HG21 | 1:A:623:LEU:HD11 | 1.69 | 0.74 |
| 1:A:629:GLY:O | 1:A:633:ASN:N | 2.20 | 0.74 |
| 1:C:527:GLU:HG3 | 1:C:533:ALA:HA | 1.67 | 0.74 |
| 1:D:218:LYS:NZ | 2:D:1001:AGS:PB | 2.60 | 0.74 |
| 1:D:681:SER:O | 1:D:722:ILE:N | 2.20 | 0.74 |
| 1:D:805:ASN:OD1 | 1:D:856:ASN:HA | 1.87 | 0.74 |
| 1:E:583:GLN:HB3 | 1:E:586:ALA:HB3 | 1.68 | 0.74 |
| 1:E:637:MET:HA | 1:E:678:LYS:HZ1 | 1.48 | 0.74 |
| 1:F:239:GLN:H | 1:F:278:LEU:HD12 | 1.51 | 0.74 |
| 1:F:377:GLN:O | 1:F:381:ARG:N | 2.20 | 0.74 |
| 1:F:584:MET:HB3 | 1:F:588:LYS:HZ2 | 1.50 | 0.74 |
| 1:F:623:LEU:HG | 1:F:627:VAL:HG13 | 1.68 | 0.74 |
| 1:F:707:ARG:HG3 | 1:F:715:THR:CG2 | 2.15 | 0.74 |
| 1:F:843:ARG:NE | 1:F:882:ASN:OD1 | 2.21 | 0.74 |
| 1:A:319:ASN:O | 1:A:323:SER:N | 2.21 | 0.74 |
| 1:B:250:ALA:N | 1:B:264:ARG:HH12 | 1.83 | 0.74 |
| 1:C:262:GLU:HG3 | 1:C:266:LYS:HE2 | 1.70 | 0.74 |
| 1:C:469:GLU:O | 1:C:473:HIS:N | 2.21 | 0.74 |
| 1:C:583:GLN:HE22 | 1:C:775:LEU:HD11 | 1.52 | 0.74 |
| 1:D:194:ARG:HA | 1:D:197:ILE:HD12 | 1.68 | 0.74 |
| 1:D:879:VAL:HG12 | 1:D:880:LEU:H | 1.53 | 0.74 |
| 1:E:169:LYS:HE2 | 1:E:264:ARG:HB3 | 1.70 | 0.74 |
| 1:E:366:ARG:HG2 | 1:E:367:ILE:N | 2.01 | 0.74 |
| 1:E:543:SER:HG | 1:E:544:ASP:H | 1.33 | 0.74 |
| 1:F:656:LEU:CD1 | 1:F:711:GLY:CA | 2.66 | 0.74 |
| 1:A:228:ARG:NH1 | 1:A:233:ASP:OD1 | 2.20 | 0.74 |
| 1:B:272:ILE:O | 1:B:275:SER:N | 2.12 | 0.74 |
| 1:B:347:GLN:OE1 | 1:B:347:GLN:N | 2.21 | 0.74 |
| 1:B:371:ALA:O | 1:B:375:ALA:N | 2.16 | 0.74 |
| 1:B:594:VAL:O | 1:B:598:ARG:N | 2.15 | 0.74 |
| 1:B:607:PRO:HG2 | 1:B:703:LEU:HD23 | 1.70 | 0.74 |
| 1:B:765:ARG:HH11 | 1:B:765:ARG:N | 1.86 | 0.74 |
| 1:C:217:GLY:O | 1:C:221:ILE:N | 2.20 | 0.74 |
| 1:D:404:ALA:HA | 1:D:407:ARG:HB2 | 1.68 | 0.74 |
| 1:D:844:ILE:O | 1:D:847:ASN:ND2 | 2.21 | 0.74 |
| 1:E:205:LYS:HZ2 | 1:E:335:PHE:N | 1.86 | 0.74 |
| 1:E:534:ASN:ND2 | 1:E:538:GLN:H | 1.85 | 0.74 |
| 1:F:563:GLU:CB | 1:F:568:LYS:HB3 | 2.17 | 0.74 |
| 1:F:713:GLY:O | 1:F:714:LYS:HB3 | 1.86 | 0.74 |
| 1:A:213:GLU:HB2 | 1:A:218:LYS:HZ3 | 1.53 | 0.74 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:710:SER:OG | 1:A:714:LYS:N | 2.21 | 0.74 |
| 1:B:207:ASN:OD1 | 1:B:336:GLN:N | 2.17 | 0.74 |
| 1:B:246:LEU:N | 1:B:283:ILE:HB | 2.03 | 0.74 |
| 1:B:324:ILE:HA | 1:B:327:LYS:HB2 | 1.69 | 0.74 |
| 1:B:371:ALA:O | 1:B:374:THR:OG1 | 2.06 | 0.74 |
| 1:B:583:GLN:H | 1:B:773:ASN:ND2 | 1.86 | 0.74 |
| 1:B:619:GLY:HA2 | 1:B:622:GLU:HB3 | 1.69 | 0.74 |
| 1:B:646:LEU:HD11 | 1:B:690:LYS:HZ1 | 1.53 | 0.74 |
| 1:C:172:ILE:C | 1:C:244:PHE:HD1 | 1.96 | 0.74 |
| 1:C:318:ASN:O | 1:C:322:ARG:N | 2.19 | 0.74 |
| 1:C:371:ALA:O | 1:C:374:THR:OG1 | 2.05 | 0.74 |
| 1:D:174:MET:HE2 | 1:D:183:LEU:HD11 | 1.68 | 0.74 |
| 1:D:673:ASN:O | 1:D:677:TYR:N | 2.17 | 0.74 |
| 1:E:338:ILE:HG22 | 1:E:339:GLU:H | 1.53 | 0.74 |
| 1:A:595:ARG:NH2 | 1:B:838:ASN:O | 2.12 | 0.73 |
| 1:C:708:ILE:HG13 | 1:C:717:ASP:OD2 | 1.88 | 0.73 |
| 1:E:262:GLU:HB2 | 1:E:297:ALA:HB1 | 1.70 | 0.73 |
| 1:E:687:GLU:OE2 | 1:E:728:ALA:HB3 | 1.88 | 0.73 |
| 1:F:219:THR:O | 1:F:223:GLU:N | 2.17 | 0.73 |
| 1:F:828:LEU:O | 1:F:832:ILE:N | 2.21 | 0.73 |
| 1:A:393:LEU:HA | 1:A:396:VAL:HB | 1.70 | 0.73 |
| 1:B:605:ARG:HG3 | 1:B:606:GLN:N | 2.03 | 0.73 |
| 1:C:282:PHE:HB2 | 1:C:313:ILE:H | 1.54 | 0.73 |
| 1:C:374:THR:O | 1:C:378:LEU:N | 2.20 | 0.73 |
| 1:D:203:ARG:NH1 | 1:E:363:HIS:CE1 | 2.55 | 0.73 |
| 1:D:365:VAL:HG22 | 1:D:538:GLN:NE2 | 2.03 | 0.73 |
| 1:D:683:LEU:H | 1:D:723:VAL:HA | 1.53 | 0.73 |
| 1:D:804:LEU:HA | 1:D:854:THR:HA | 1.70 | 0.73 |
| 1:E:573:GLU:OE2 | 1:E:595:ARG:NE | 2.20 | 0.73 |
| 1:F:547:SER:O | 1:F:551:ALA:N | 2.19 | 0.73 |
| 1:F:702:MET:CG | 1:F:708:ILE:HG23 | 2.18 | 0.73 |
| 1:A:644:SER:N | 1:A:686:ASP:O | 2.21 | 0.73 |
| 1:C:783:ILE:O | 1:C:787:ARG:N | 2.18 | 0.73 |
| 1:D:272:ILE:HA | 1:D:276:LYS:NZ | 2.03 | 0.73 |
| 1:D:456:GLN:HA | 1:D:459:LEU:HG | 1.71 | 0.73 |
| 1:D:563:GLU:HA | 1:D:568:LYS:NZ | 2.03 | 0.73 |
| 1:E:385:TYR:O | 1:E:386:ARG:NH1 | 2.21 | 0.73 |
| 1:E:569:LEU:HD21 | 1:E:595:ARG:HG2 | 1.67 | 0.73 |
| 1:F:564:SER:H | 1:F:568:LYS:CD | 2.01 | 0.73 |
| 1:A:374:THR:O | 1:A:378:LEU:N | 2.18 | 0.73 |
| 1:B:398:ILE:O | 1:B:402:GLY:N | 2.15 | 0.73 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:785:ASP:O | 1:C:789:LYS:HG3 | 1.88 | 0.73 |
| 1:E:481:LYS:HG2 | 1:E:485:GLU:OE2 | 1.88 | 0.73 |
| 1:E:654:LYS:NZ | 1:E:694:ASP:O | 2.21 | 0.73 |
| 1:E:859:LEU:HA | 1:E:876:CYS:HA | 1.70 | 0.73 |
| 1:F:281:LEU:HD12 | 1:F:312:VAL:HG23 | 1.71 | 0.73 |
| 1:F:389:PRO:O | 1:F:393:LEU:N | 2.19 | 0.73 |
| 1:F:556:ILE:N | 1:F:559:LYS:HZ3 | 1.86 | 0.73 |
| 1:F:605:ARG:CG | 1:F:707:ARG:N | 2.50 | 0.73 |
| 1:F:707:ARG:CG | 1:F:715:THR:HG21 | 2.17 | 0.73 |
| 1:F:731:ALA:O | 1:F:735:ASN:N | 2.20 | 0.73 |
| 1:F:843:ARG:NH1 | 1:F:881:PRO:O | 2.21 | 0.73 |
| 1:B:244:PHE:N | 1:B:281:LEU:HB3 | 2.00 | 0.73 |
| 1:B:611:LEU:N | 1:B:768:SER:O | 2.21 | 0.73 |
| 1:B:621:THR:HA | 1:B:624:ALA:HB3 | 1.70 | 0.73 |
| 1:B:843:ARG:NH1 | 1:B:846:LYS:HB3 | 2.03 | 0.73 |
| 1:C:168:SER:C | 1:C:264:ARG:HE | 1.97 | 0.73 |
| 1:C:371:ALA:O | 1:C:375:ALA:N | 2.17 | 0.73 |
| 1:C:576:LEU:HD23 | 1:C:579:GLU:OE2 | 1.87 | 0.73 |
| 1:D:218:LYS:HG2 | 2:D:1001:AGS:O2B | 1.89 | 0.73 |
| 1:D:544:ASP:O | 1:D:548:GLU:N | 2.17 | 0.73 |
| 1:D:697:THR:O | 1:D:700:LEU:HB3 | 1.89 | 0.73 |
| 1:D:809:GLU:OE2 | 1:D:856:ASN:HB2 | 1.88 | 0.73 |
| 1:E:602:ALA:HB1 | 1:E:606:GLN:HB2 | 1.69 | 0.73 |
| 1:E:611:LEU:HG | 1:E:612:PHE:O | 1.88 | 0.73 |
| 1:E:641:VAL:H | 1:E:684:LEU:HD22 | 1.52 | 0.73 |
| 1:A:843:ARG:HG3 | 1:A:849:ILE:HD13 | 1.71 | 0.73 |
| 1:B:170:TYR:HB2 | 1:B:250:ALA:C | 2.14 | 0.73 |
| 1:B:282:PHE:HB3 | 1:B:313:ILE:N | 2.03 | 0.73 |
| 1:C:639:ILE:HG13 | 1:C:678:LYS:HZ2 | 1.53 | 0.73 |
| 1:E:311:LYS:HZ2 | 1:E:313:ILE:HD11 | 1.54 | 0.73 |
| 1:E:358:LYS:HZ2 | 1:E:359:TYR:HA | 1.53 | 0.73 |
| 1:E:591:SER:O | 1:E:595:ARG:N | 2.15 | 0.73 |
| 1:E:606:GLN:OE1 | 1:F:794:ARG:NH1 | 2.22 | 0.73 |
| 1:E:610:PHE:N | 1:E:724:ILE:HA | 2.04 | 0.73 |
| 1:F:710:SER:OG | 1:F:714:LYS:N | 2.21 | 0.73 |
| 1:B:650:TYR:H | 1:B:692:HIS:HE1 | 1.33 | 0.73 |
| 1:C:235:PRO:O | 1:C:239:GLN:N | 2.22 | 0.73 |
| 1:C:390:ASP:O | 1:C:393:LEU:N | 2.21 | 0.73 |
| 1:C:392:ALA:O | 1:C:395:LEU:HG | 1.89 | 0.73 |
| 1:C:697:THR:OG1 | 1:C:698:VAL:N | 2.13 | 0.73 |
| 1:C:833:GLN:HA | 1:C:836:ILE:HG12 | 1.69 | 0.73 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:811:LYS:HD2 | 1:D:811:LYS:N | 2.00 | 0.73 |
| 1:D:811:LYS:HA | 1:D:814:LEU:HD12 | 1.70 | 0.73 |
| 1:D:815:ALA:C | 1:D:818:GLY:H | 1.96 | 0.73 |
| 1:E:302:LYS:NZ | 1:E:334:ARG:HD3 | 2.02 | 0.73 |
| 1:E:319:ASN:HA | 1:E:322:ARG:NH1 | 2.04 | 0.73 |
| 1:F:209:CYS:N | 1:F:336:GLN:O | 2.21 | 0.73 |
| 1:F:356:GLN:HE21 | 1:F:367:ILE:HD13 | 1.48 | 0.73 |
| 1:F:742:ILE:HG22 | 1:F:747:LYS:NZ | 2.03 | 0.73 |
| 1:F:804:LEU:HD23 | 1:F:853:GLU:HB3 | 1.69 | 0.73 |
| 1:A:390:ASP:O | 1:A:394:ASP:N | 2.22 | 0.73 |
| 1:B:646:LEU:N | 1:B:691:ALA:H | 1.86 | 0.73 |
| 1:C:275:SER:N | 1:C:276:LYS:HZ3 | 1.87 | 0.73 |
| 1:C:737:GLN:HA | 1:C:774:LYS:HZ1 | 1.54 | 0.73 |
| 1:D:723:VAL:HG13 | 1:D:725:MET:HG3 | 1.68 | 0.73 |
| 1:E:839:LYS:NZ | 1:E:879:VAL:HA | 2.04 | 0.73 |
| 1:F:625:LYS:HE2 | 1:F:637:MET:HB2 | 1.71 | 0.73 |
| 1:F:640:ARG:HA | 1:F:684:LEU:CB | 2.19 | 0.73 |
| 1:A:287:HIS:NE2 | 1:A:291:GLY:O | 2.21 | 0.73 |
| 1:A:381:ARG:HG2 | 1:A:382:TYR:HD1 | 1.54 | 0.73 |
| 1:A:619:GLY:HA2 | 1:A:623:LEU:HD23 | 1.68 | 0.73 |
| 1:B:265:PHE:HA | 1:B:268:VAL:HB | 1.71 | 0.73 |
| 1:B:296:ASP:OD1 | 1:B:301:LEU:N | 2.21 | 0.73 |
| 1:B:572:MET:HE3 | 1:B:576:LEU:HB2 | 1.70 | 0.73 |
| 1:C:255:ALA:HB1 | 1:C:256:LYS:HZ3 | 1.53 | 0.73 |
| 1:C:564:SER:O | 1:C:565:GLU:HG2 | 1.89 | 0.73 |
| 1:C:605:ARG:HH12 | 1:C:765:ARG:CZ | 2.01 | 0.73 |
| 1:D:172:ILE:C | 1:D:245:SER:H | 1.97 | 0.73 |
| 1:D:572:MET:HA | 1:D:575:ASP:HB2 | 1.70 | 0.73 |
| 1:D:755:ARG:HG3 | 1:D:756:GLN:N | 2.01 | 0.73 |
| 1:F:189:ARG:NH2 | 1:F:342:GLU:O | 2.22 | 0.73 |
| 1:F:700:LEU:N | 1:F:703:LEU:HD21 | 1.94 | 0.73 |
| 1:F:777:ARG:HG3 | 1:F:778:LYS:H | 1.52 | 0.73 |
| 1:B:235:PRO:HD3 | 1:C:409:SER:HA | 1.69 | 0.73 |
| 1:B:285:GLU:O | 1:B:289:LEU:HG | 1.89 | 0.73 |
| 1:B:648:GLU:CA | 1:B:693:PRO:HD3 | 2.18 | 0.73 |
| 1:C:568:LYS:HG2 | 1:C:630:PHE:CE2 | 2.24 | 0.73 |
| 1:D:634:ASP:OD1 | 1:D:636:ASP:HB3 | 1.89 | 0.73 |
| 1:E:639:ILE:HB | 1:E:683:LEU:HA | 1.70 | 0.73 |
| 1:E:651:ALA:O | 1:E:657:GLY:N | 2.19 | 0.73 |
| 1:E:693:PRO:O | 1:E:696:LEU:N | 2.22 | 0.73 |
| 1:A:274:GLU:O | 1:A:276:LYS:NZ | 2.22 | 0.72 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:659:THR:HG22 | 1:A:660:ALA:H | 1.54 | 0.72 |
| 1:B:173:ASP:OD1 | 1:B:176:GLU:N | 2.21 | 0.72 |
| 1:B:215:GLY:O | 1:B:218:LYS:HG2 | 1.89 | 0.72 |
| 1:B:819:TYR:CE2 | 1:B:821:ASP:HA | 2.24 | 0.72 |
| 1:C:211:ILE:HG21 | 1:C:315:ALA:HA | 1.71 | 0.72 |
| 1:C:298:ALA:O | 1:C:301:LEU:N | 2.22 | 0.72 |
| 1:C:786:ILE:CG1 | 1:C:789:LYS:HZ3 | 2.02 | 0.72 |
| 1:C:839:LYS:HZ1 | 1:C:879:VAL:C | 1.97 | 0.72 |
| 1:D:302:LYS:HZ2 | 1:D:306:SER:HA | 1.50 | 0.72 |
| 1:D:524:VAL:HG12 | 1:D:526:GLU:H | 1.54 | 0.72 |
| 1:E:833:GLN:HG2 | 1:E:837:LEU:HD11 | 1.69 | 0.72 |
| 1:F:241:ALA:O | 1:F:242:LYS:NZ | 2.17 | 0.72 |
| 1:F:714:LYS:O | 1:F:716:ILE:N | 2.20 | 0.72 |
| 1:A:173:ASP:HA | 1:A:245:SER:N | 2.04 | 0.72 |
| 1:B:620:LYS:HZ3 | 1:B:826:ARG:NH1 | 1.86 | 0.72 |
| 1:C:592:ASN:N | 1:C:595:ARG:NH1 | 2.37 | 0.72 |
| 1:C:693:PRO:HA | 1:C:696:LEU:HD12 | 1.70 | 0.72 |
| 1:D:171:ALA:HA | 1:D:246:LEU:HB2 | 1.70 | 0.72 |
| 1:D:217:GLY:N | 2:D:1001:AGS:O1B | 2.21 | 0.72 |
| 1:D:789:LYS:HG2 | 1:D:793:GLU:OE2 | 1.89 | 0.72 |
| 1:E:785:ASP:C | 1:E:789:LYS:HZ2 | 1.96 | 0.72 |
| 1:F:280:VAL:HG13 | 1:F:311:LYS:C | 2.14 | 0.72 |
| 1:F:363:HIS:CE1 | 1:F:400:CYS:SG | 2.82 | 0.72 |
| 1:F:592:ASN:HD22 | 1:F:768:SER:HB2 | 1.54 | 0.72 |
| 1:A:193:ILE:O | 1:A:197:ILE:N | 2.17 | 0.72 |
| 1:B:250:ALA:H | 1:B:264:ARG:NH1 | 1.86 | 0.72 |
| 1:C:384:PRO:HG2 | 1:C:679:PRO:HG2 | 1.70 | 0.72 |
| 1:D:699:MET:HE1 | 1:D:759:ARG:HH22 | 1.54 | 0.72 |
| 1:D:763:LEU:O | 1:D:766:ILE:N | 2.22 | 0.72 |
| 1:E:588:LYS:O | 1:E:592:ASN:ND2 | 2.22 | 0.72 |
| 1:F:214:PRO:O | 2:F:1001:AGS:O2G | 2.07 | 0.72 |
| 1:A:248:LEU:HD11 | 1:A:253:ALA:HB3 | 1.71 | 0.72 |
| 1:A:542:ASP:HA | 1:A:546:ILE:HD12 | 1.71 | 0.72 |
| 1:B:216:ILE:HG13 | 1:B:220:ALA:HB2 | 1.69 | 0.72 |
| 1:B:359:TYR:OH | 1:B:397:ASP:OD1 | 2.07 | 0.72 |
| 1:C:303:PRO:O | 1:C:334:ARG:NH2 | 2.23 | 0.72 |
| 1:D:226:ALA:HA | 1:D:229:ILE:HD12 | 1.71 | 0.72 |
| 1:D:543:SER:OG | 1:D:544:ASP:OD1 | 2.07 | 0.72 |
| 1:D:681:SER:HG | 1:D:721:CYS:HG | 0.76 | 0.72 |
| 1:E:512:ASP:O | 1:E:516:GLN:N | 2.19 | 0.72 |
| 1:E:629:GLY:HA2 | 1:E:634:ASP:N | 2.04 | 0.72 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:642:ASP:HB3 | 1:E:649:LYS:NZ | 2.03 | 0.72 |
| 1:F:572:MET:HG3 | 1:F:630:PHE:CE2 | 2.24 | 0.72 |
| 1:B:203:ARG:HE | 1:C:359:TYR:HE1 | 1.36 | 0.72 |
| 1:B:252:THR:O | 1:B:264:ARG:NE | 2.21 | 0.72 |
| 1:C:113:GLN:O | 1:C:117:LEU:N | 2.22 | 0.72 |
| 1:C:459:LEU:O | 1:C:463:ARG:N | 2.16 | 0.72 |
| 1:C:820:SER:H | 1:C:824:GLY:HA3 | 1.55 | 0.72 |
| 1:C:820:SER:N | 1:C:824:GLY:HA3 | 2.05 | 0.72 |
| 1:C:843:ARG:HA | 1:C:846:LYS:HB2 | 1.71 | 0.72 |
| 1:D:165:GLU:OE1 | 1:D:170:TYR:OH | 2.07 | 0.72 |
| 1:D:231:ASP:HB3 | 1:D:495:ARG:HG3 | 1.70 | 0.72 |
| 1:D:240:GLY:O | 1:D:278:LEU:N | 2.17 | 0.72 |
| 1:D:791:ILE:HG22 | 1:D:795:PHE:CZ | 2.24 | 0.72 |
| 1:E:166:TYR:O | 1:E:170:TYR:N | 2.21 | 0.72 |
| 1:E:607:PRO:HG3 | 1:E:707:ARG:NH1 | 2.04 | 0.72 |
| 1:E:609:SER:OG | 1:E:724:ILE:O | 2.07 | 0.72 |
| 1:F:347:GLN:O | 1:F:351:ILE:N | 2.19 | 0.72 |
| 1:F:700:LEU:CB | 1:F:703:LEU:HD22 | 2.09 | 0.72 |
| 1:F:835:GLU:HA | 1:F:838:ASN:ND2 | 2.04 | 0.72 |
| 1:A:246:LEU:HB2 | 1:A:281:LEU:HB3 | 1.70 | 0.72 |
| 1:B:620:LYS:CG | 1:B:826:ARG:HH12 | 2.02 | 0.72 |
| 1:B:673:ASN:O | 1:B:677:TYR:N | 2.18 | 0.72 |
| 1:C:222:ILE:O | 1:C:225:VAL:HB | 1.89 | 0.72 |
| 1:C:789:LYS:O | 1:C:793:GLU:N | 2.19 | 0.72 |
| 1:D:332:GLU:HA | 1:D:335:PHE:CZ | 2.24 | 0.72 |
| 1:F:793:GLU:N | 1:F:793:GLU:OE1 | 2.22 | 0.72 |
| 1:F:803:LYS:NZ | 1:F:852:LYS:C | 2.48 | 0.72 |
| 1:C:390:ASP:OD1 | 1:C:390:ASP:N | 2.18 | 0.72 |
| 1:C:576:LEU:HA | 1:C:579:GLU:OE2 | 1.90 | 0.72 |
| 1:D:563:GLU:N | 1:D:563:GLU:OE1 | 2.22 | 0.72 |
| 1:D:737:GLN:H | 1:D:774:LYS:HE2 | 1.55 | 0.72 |
| 1:D:827:PRO:HB2 | 1:D:831:LEU:HD11 | 1.72 | 0.72 |
| 1:E:510:ILE:HD13 | 1:E:514:LYS:HZ1 | 1.54 | 0.72 |
| 1:E:704:ASP:O | 1:E:707:ARG:NH1 | 2.23 | 0.72 |
| 1:E:858:VAL:HB | 1:E:877:LEU:HB2 | 1.72 | 0.72 |
| 1:A:344:SER:H | 1:A:347:GLN:HB2 | 1.53 | 0.72 |
| 1:A:563:GLU:OE1 | 1:A:568:LYS:HB2 | 1.90 | 0.72 |
| 1:B:324:ILE:N | 1:B:327:LYS:HZ1 | 1.87 | 0.72 |
| 1:B:621:THR:N | 1:B:826:ARG:HH22 | 1.87 | 0.72 |
| 1:C:186:VAL:HG13 | 2:C:1001:AGS:C5 | 2.19 | 0.72 |
| 1:C:548:GLU:O | 1:C:552:ARG:N | 2.15 | 0.72 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:C:787:ARG:O | 1:C:791:ILE:HG12 | 1.90 | 0.72 |
| 1:E:833:GLN:C | 1:E:837:LEU:HG | 2.14 | 0.72 |
| 1:F:785:ASP:CB | 1:F:789:LYS:HZ1 | 1.96 | 0.72 |
| 1:F:859:LEU:HD12 | 1:F:876:CYS:HA | 1.72 | 0.72 |
| 1:A:316:THR:HG21 | 1:A:322:ARG:NH1 | 2.00 | 0.72 |
| 1:B:274:GLU:N | 1:B:274:GLU:OE1 | 2.19 | 0.72 |
| 1:B:282:PHE:HD1 | 1:B:313:ILE:HB | 1.53 | 0.72 |
| 1:C:567:GLU:H | 1:C:567:GLU:CD | 1.96 | 0.72 |
| 1:C:782:LYS:O | 1:C:784:VAL:N | 2.23 | 0.72 |
| 1:E:303:PRO:HA | 1:E:334:ARG:HH22 | 1.54 | 0.72 |
| 1:E:707:ARG:HG3 | 1:E:716:ILE:HG21 | 1.72 | 0.72 |
| 1:E:743:GLN:OE1 | 1:E:744:GLU:N | 2.23 | 0.72 |
| 1:E:842:LEU:O | 1:E:845:LEU:HG | 1.90 | 0.72 |
| 1:F:803:LYS:HZ2 | 1:F:852:LYS:C | 1.98 | 0.72 |
| 1:F:857:VAL:HG11 | 1:F:880:LEU:HA | 1.72 | 0.72 |
| 1:A:787:ARG:O | 1:A:790:GLU:HB3 | 1.90 | 0.72 |
| 1:B:543:SER:OG | 1:B:544:ASP:N | 2.22 | 0.72 |
| 1:C:205:LYS:HZ2 | 1:C:334:ARG:H | 0.74 | 0.72 |
| 1:C:452:GLU:HA | 1:C:455:LEU:HG | 1.72 | 0.72 |
| 1:C:749:LEU:O | 1:C:753:ALA:N | 2.18 | 0.72 |
| 1:D:777:ARG:HA | 1:D:780:ILE:HB | 1.70 | 0.72 |
| 1:E:651:ALA:C | 1:E:657:GLY:H | 1.98 | 0.72 |
| 1:F:345:VAL:HA | 1:F:380:LYS:HE3 | 1.72 | 0.72 |
| 1:F:363:HIS:NE2 | 1:F:396:VAL:C | 2.48 | 0.72 |
| 1:A:244:PHE:HD2 | 1:A:281:LEU:N | 1.88 | 0.71 |
| 1:A:802:TYR:CE2 | 1:A:804:LEU:HB2 | 2.24 | 0.71 |
| 1:C:365:VAL:HA | 1:C:473:HIS:HE1 | 1.53 | 0.71 |
| 1:D:203:ARG:NH1 | 1:E:363:HIS:CD2 | 2.58 | 0.71 |
| 1:D:286:ILE:HA | 1:D:289:LEU:HB2 | 1.70 | 0.71 |
| 1:D:530:ARG:HH22 | 1:D:536:MET:H | 1.35 | 0.71 |
| 1:E:228:ARG:HA | 1:E:231:ASP:OD2 | 1.89 | 0.71 |
| 1:E:347:GLN:H | 1:E:347:GLN:CD | 1.97 | 0.71 |
| 1:E:686:ASP:HA | 1:E:726:THR:OG1 | 1.90 | 0.71 |
| 1:E:732:GLU:N | 1:E:732:GLU:OE1 | 2.23 | 0.71 |
| 1:F:395:LEU:O | 1:F:399:SER:N | 2.22 | 0.71 |
| 1:F:627:VAL:O | 1:F:631:LEU:N | 2.22 | 0.71 |
| 1:B:282:PHE:CD1 | 1:B:313:ILE:HB | 2.25 | 0.71 |
| 1:E:671:LEU:O | 1:E:675:LEU:N | 2.23 | 0.71 |
| 1:E:825:ALA:O | 1:E:829:ASN:N | 2.23 | 0.71 |
| 1:F:187:ILE:C | 2:F:1001:AGS:HN62 | 1.98 | 0.71 |
| 1:F:287:HIS:NE2 | 1:F:322:ARG:HD2 | 2.04 | 0.71 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:307:ARG:H | 1:A:310:LEU:CD1 | 2.00 | 0.71 |
| 1:B:202:ARG:HG3 | 1:B:206:SER:OG | 1.91 | 0.71 |
| 1:B:352:LEU:HA | 1:B:355:LEU:HB2 | 1.71 | 0.71 |
| 1:C:168:SER:HB2 | 1:C:268:VAL:HG22 | 1.72 | 0.71 |
| 1:C:191:GLU:HB2 | 1:C:194:ARG:NH2 | 2.04 | 0.71 |
| 1:C:733:PHE:HB3 | 1:C:746:THR:HG23 | 1.72 | 0.71 |
| 1:D:459:LEU:HB3 | 1:D:463:ARG:HH22 | 1.54 | 0.71 |
| 1:D:777:ARG:O | 1:D:781:HIS:N | 2.23 | 0.71 |
| 1:D:845:LEU:O | 1:D:847:ASN:ND2 | 2.23 | 0.71 |
| 1:E:195:SER:HA | 1:E:198:ARG:HD2 | 1.73 | 0.71 |
| 1:E:642:ASP:HB3 | 1:E:649:LYS:HZ1 | 1.55 | 0.71 |
| 1:F:209:CYS:H | 1:F:337:LYS:HA | 1.54 | 0.71 |
| 1:F:574:ARG:O | 1:F:577:SER:OG | 2.08 | 0.71 |
| 1:F:654:LYS:HE2 | 1:F:694:ASP:OD2 | 1.90 | 0.71 |
| 1:A:647:SER:HA | 1:A:692:HIS:HB2 | 1.71 | 0.71 |
| 1:A:828:LEU:HD12 | 1:A:831:LEU:HB3 | 1.73 | 0.71 |
| 1:B:285:GLU:C | 1:B:289:LEU:HG | 2.15 | 0.71 |
| 1:B:650:TYR:N | 1:B:692:HIS:HE1 | 1.87 | 0.71 |
| 1:C:168:SER:CA | 1:C:264:ARG:NE | 2.53 | 0.71 |
| 1:C:464:GLN:O | 1:C:468:GLU:N | 2.15 | 0.71 |
| 1:E:356:GLN:O | 1:E:360:GLU:N | 2.17 | 0.71 |
| 1:E:689:GLU:OE2 | 1:E:754:VAL:HG22 | 1.90 | 0.71 |
| 1:E:710:SER:O | 1:E:714:LYS:HD3 | 1.91 | 0.71 |
| 1:E:831:LEU:HA | 1:E:834:ASN:ND2 | 2.04 | 0.71 |
| 1:F:704:ASP:CA | 1:F:765:ARG:CZ | 2.68 | 0.71 |
| 2:F:1001:AGS:O2A | 2:F:1001:AGS:O3B | 2.07 | 0.71 |
| 1:B:263:GLU:HA | 1:B:266:LYS:HZ2 | 1.53 | 0.71 |
| 1:C:373:VAL:O | 1:C:377:GLN:N | 2.22 | 0.71 |
| 1:C:543:SER:O | 1:C:547:SER:OG | 2.09 | 0.71 |
| 1:C:748:ASN:O | 1:C:751:MET:N | 2.24 | 0.71 |
| 1:C:751:MET:O | 1:C:755:ARG:N | 2.18 | 0.71 |
| 1:D:258:LYS:HD2 | 1:D:261:PHE:HB3 | 1.72 | 0.71 |
| 1:D:503:ALA:HA | 1:D:506:ARG:HB3 | 1.73 | 0.71 |
| 1:E:272:ILE:O | 1:E:276:LYS:HB3 | 1.91 | 0.71 |
| 1:E:302:LYS:HA | 1:E:305:LEU:HD12 | 1.72 | 0.71 |
| 1:E:794:ARG:NH1 | 1:E:796:GLU:C | 2.39 | 0.71 |
| 1:F:219:THR:HA | 1:F:222:ILE:HG12 | 1.71 | 0.71 |
| 1:B:803:LYS:N | 1:B:853:GLU:HG2 | 2.06 | 0.71 |
| 1:C:203:ARG:HE | 1:D:362:HIS:CD2 | 2.08 | 0.71 |
| 1:C:210:LEU:HD13 | 1:C:337:LYS:HA | 1.73 | 0.71 |
| 1:C:219:THR:N | 2:C:1001:AGS:O1B | 2.23 | 0.71 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:588:LYS:O | 1:C:591:SER:N | 2.23 | 0.71 |
| 1:D:302:LYS:HA | 1:D:305:LEU:HB2 | 1.72 | 0.71 |
| 1:D:456:GLN:HG3 | 1:D:459:LEU:HD12 | 1.73 | 0.71 |
| 1:D:482:LYS:O | 1:D:486:LEU:N | 2.17 | 0.71 |
| 1:D:565:GLU:HG2 | 1:D:566:ASN:H | 1.55 | 0.71 |
| 1:E:432:GLU:O | 1:E:442:LYS:NZ | 2.19 | 0.71 |
| 1:E:496:ARG:NH1 | 1:E:499:THR:OG1 | 2.23 | 0.71 |
| 1:F:390:ASP:O | 1:F:394:ASP:N | 2.23 | 0.71 |
| 1:B:296:ASP:HA | 1:B:300:ILE:H | 1.54 | 0.71 |
| 1:C:228:ARG:HH22 | 1:D:409:SER:HB2 | 1.56 | 0.71 |
| 1:C:301:LEU:HD12 | 1:C:302:LYS:N | 2.05 | 0.71 |
| 1:D:462:LEU:HD23 | 1:D:465:ARG:HD2 | 1.73 | 0.71 |
| 1:D:833:GLN:O | 1:D:837:LEU:HG | 1.89 | 0.71 |
| 1:E:547:SER:O | 1:E:551:ALA:N | 2.18 | 0.71 |
| 1:F:392:ALA:HA | 1:F:395:LEU:HB2 | 1.72 | 0.71 |
| 1:F:704:ASP:CB | 1:F:765:ARG:NH2 | 2.30 | 0.71 |
| 1:A:655:LEU:HA | 1:A:671:LEU:HD12 | 1.72 | 0.71 |
| 1:A:828:LEU:O | 1:A:832:ILE:N | 2.18 | 0.71 |
| 1:B:296:ASP:CG | 1:B:300:ILE:HB | 2.16 | 0.71 |
| 1:B:648:GLU:HA | 1:B:692:HIS:HA | 1.71 | 0.71 |
| 1:B:790:GLU:OE1 | 1:B:791:ILE:HG13 | 1.90 | 0.71 |
| 1:C:417:LYS:HG2 | 1:C:456:GLN:HE22 | 1.56 | 0.71 |
| 1:D:218:LYS:NZ | 2:D:1001:AGS:O1A | 2.23 | 0.71 |
| 1:D:417:LYS:HE3 | 1:D:421:LEU:HB2 | 1.72 | 0.71 |
| 1:D:823:MET:SD | 1:D:827:PRO:HD3 | 2.30 | 0.71 |
| 1:E:272:ILE:HA | 1:E:276:LYS:HD3 | 1.73 | 0.71 |
| 1:E:638:MET:SD | 1:E:640:ARG:NH2 | 2.64 | 0.71 |
| 1:E:686:ASP:OD1 | 1:E:690:LYS:HG3 | 1.90 | 0.71 |
| 1:E:698:VAL:C | 1:E:702:MET:HG2 | 2.16 | 0.71 |
| 1:F:241:ALA:N | 1:F:277:THR:HB | 2.05 | 0.71 |
| 1:F:548:GLU:O | 1:F:552:ARG:N | 2.24 | 0.71 |
| 1:F:683:LEU:CD2 | 1:F:684:LEU:H | 2.03 | 0.71 |
| 1:A:583:GLN:HB3 | 1:A:586:ALA:HB3 | 1.73 | 0.71 |
| 1:B:609:SER:OG | 1:B:767:SER:N | 2.23 | 0.71 |
| 1:B:848:GLU:HB2 | 1:B:882:ASN:HD22 | 1.56 | 0.71 |
| 1:C:285:GLU:HB3 | 1:C:288:MET:HE2 | 1.72 | 0.71 |
| 1:C:342:GLU:CD | 1:C:388:LEU:H | 1.98 | 0.71 |
| 1:C:809:GLU:OE1 | 1:C:809:GLU:N | 2.22 | 0.71 |
| 1:D:213:GLU:O | 2:D:1001:AGS:O2G | 2.08 | 0.71 |
| 1:D:351:ILE:HG22 | 1:D:355:LEU:HD23 | 1.72 | 0.71 |
| 1:D:526:GLU:CB | 1:D:529:ARG:H | 2.03 | 0.71 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:718:CYS:SG | 1:D:719:SER:N | 2.61 | 0.71 |
| 1:E:574:ARG:O | 1:E:577:SER:OG | 2.08 | 0.71 |
| 1:E:623:LEU:O | 1:E:627:VAL:N | 2.21 | 0.71 |
| 1:B:208:PRO:HG2 | 1:B:313:ILE:HG23 | 1.73 | 0.71 |
| 1:B:302:LYS:NZ | 1:B:306:SER:N | 2.39 | 0.71 |
| 1:C:168:SER:CB | 1:C:271:GLU:OE2 | 2.38 | 0.71 |
| 1:C:186:VAL:HA | 2:C:1001:AGS:C6 | 2.21 | 0.71 |
| 1:C:372:LEU:O | 1:C:376:ALA:N | 2.14 | 0.71 |
| 1:C:473:HIS:CG | 1:C:538:GLN:HB3 | 2.26 | 0.71 |
| 1:C:605:ARG:NH2 | 1:C:704:ASP:OD1 | 2.21 | 0.71 |
| 1:C:779:ALA:O | 1:C:783:ILE:N | 2.22 | 0.71 |
| 1:D:198:ARG:HG3 | 1:E:404:ALA:HB3 | 1.71 | 0.71 |
| 1:F:381:ARG:O | 1:F:383:LEU:N | 2.23 | 0.71 |
| 1:F:607:PRO:CG | 1:F:703:LEU:O | 2.38 | 0.71 |
| 1:F:612:PHE:HB3 | 1:F:726:THR:HA | 1.72 | 0.71 |
| 1:F:702:MET:HB2 | 1:F:708:ILE:CG1 | 2.12 | 0.71 |
| 1:B:195:SER:O | 1:B:198:ARG:HG2 | 1.91 | 0.70 |
| 1:B:766:ILE:O | 1:C:830:ARG:NH2 | 2.24 | 0.70 |
| 1:C:205:LYS:HG2 | 1:C:336:GLN:HE21 | 1.56 | 0.70 |
| 1:C:242:LYS:O | 1:C:280:VAL:N | 2.24 | 0.70 |
| 1:C:759:ARG:HD3 | 1:C:760:PRO:HD2 | 1.73 | 0.70 |
| 1:D:284:ASP:CG | 1:D:285:GLU:HG2 | 2.16 | 0.70 |
| 1:D:459:LEU:O | 1:D:463:ARG:N | 2.16 | 0.70 |
| 1:D:486:LEU:HA | 1:D:489:LYS:HB2 | 1.73 | 0.70 |
| 1:D:622:GLU:HG3 | 1:D:826:ARG:NH1 | 2.04 | 0.70 |
| 1:E:211:ILE:HG13 | 1:E:339:GLU:HG3 | 1.73 | 0.70 |
| 1:E:283:ILE:HB | 1:E:286:ILE:HG21 | 1.73 | 0.70 |
| 1:E:564:SER:O | 1:E:568:LYS:N | 2.22 | 0.70 |
| 1:E:694:ASP:O | 1:E:697:THR:HB | 1.91 | 0.70 |
| 1:A:575:ASP:O | 1:A:579:GLU:N | 2.20 | 0.70 |
| 1:B:191:GLU:HB3 | 1:B:194:ARG:NH2 | 2.06 | 0.70 |
| 1:B:348:THR:HG22 | 1:B:352:LEU:HD11 | 1.73 | 0.70 |
| 1:C:36:LEU:O | 1:C:40:ILE:N | 2.23 | 0.70 |
| 1:C:708:ILE:HG22 | 1:C:709:THR:N | 2.05 | 0.70 |
| 1:C:839:LYS:O | 1:C:842:LEU:HB3 | 1.91 | 0.70 |
| 1:D:179:ARG:HH22 | 1:D:230:ILE:HG21 | 1.57 | 0.70 |
| 1:E:176:GLU:CD | 1:E:176:GLU:H | 1.98 | 0.70 |
| 1:E:571:HIS:HD2 | 1:E:574:ARG:NH1 | 1.88 | 0.70 |
| 1:E:688:VAL:O | 1:E:690:LYS:HG2 | 1.91 | 0.70 |
| 1:F:742:ILE:HG22 | 1:F:747:LYS:HZ2 | 1.55 | 0.70 |
| 1:F:855:VAL:HG22 | 1:F:880:LEU:HD22 | 1.71 | 0.70 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:A:222:ILE:HG22 | 1:A:282:PHE:HE2 | 1.55 | 0.70 |
| 1:A:339:GLU:N | 1:A:339:GLU:OE1 | 2.24 | 0.70 |
| 1:B:259:GLY:O | 1:B:263:GLU:N | 2.19 | 0.70 |
| 1:C:744:GLU:O | 1:C:747:LYS:HG2 | 1.90 | 0.70 |
| 1:D:265:PHE:CE1 | 1:D:269:LEU:HD21 | 2.25 | 0.70 |
| 1:D:669:GLY:O | 1:D:673:ASN:N | 2.24 | 0.70 |
| 1:D:721:CYS:SG | 1:D:722:ILE:N | 2.64 | 0.70 |
| 2:D:1001:AGS:H5'2 | 2:D:1001:AGS:C8 | 2.21 | 0.70 |
| 1:F:643:CYS:HA | 1:F:646:LEU:HD12 | 1.73 | 0.70 |
| 1:A:551:ALA:O | 1:A:555:GLY:N | 2.20 | 0.70 |
| 1:A:822:ASP:HB2 | 1:F:333:ARG:NH1 | 2.05 | 0.70 |
| 1:B:296:ASP:C | 1:B:299:ASN:HB3 | 2.15 | 0.70 |
| 1:B:555:GLY:O | 1:B:556:ILE:HG12 | 1.92 | 0.70 |
| 1:B:641:VAL:H | 1:B:684:LEU:HB3 | 1.57 | 0.70 |
| 1:C:568:LYS:NZ | 1:C:630:PHE:CG | 2.59 | 0.70 |
| 1:C:827:PRO:HA | 1:C:830:ARG:HB3 | 1.73 | 0.70 |
| 1:D:282:PHE:HA | 1:D:313:ILE:HG13 | 1.73 | 0.70 |
| 1:D:366:ARG:H | 1:D:536:MET:HG3 | 1.56 | 0.70 |
| 1:D:624:ALA:O | 1:D:628:ALA:N | 2.14 | 0.70 |
| 1:D:718:CYS:O | 1:D:719:SER:OG | 2.08 | 0.70 |
| 1:E:304:ALA:N | 1:E:307:ARG:HH11 | 1.88 | 0.70 |
| 1:E:368:LEU:H | 1:E:540:VAL:HB | 1.55 | 0.70 |
| 1:E:445:LEU:O | 1:E:449:ARG:NE | 2.24 | 0.70 |
| 1:E:613:LEU:HB3 | 1:E:771:ILE:HG12 | 1.73 | 0.70 |
| 1:E:832:ILE:O | 1:E:835:GLU:HB3 | 1.92 | 0.70 |
| 1:E:833:GLN:O | 1:E:837:LEU:N | 2.24 | 0.70 |
| 1:F:704:ASP:HA | 1:F:765:ARG:NE | 2.06 | 0.70 |
| 1:F:794:ARG:NH1 | 1:F:795:PHE:CE1 | 2.51 | 0.70 |
| 1:F:811:LYS:HA | 1:F:814:LEU:HD12 | 1.74 | 0.70 |
| 1:F:835:GLU:HG3 | 1:F:878:GLU:OE2 | 1.91 | 0.70 |
| 1:A:573:GLU:HG3 | 1:A:574:ARG:H | 1.56 | 0.70 |
| 1:A:817:TYR:OH | 1:A:875:GLU:O | 2.09 | 0.70 |
| 1:B:704:ASP:HB2 | 1:B:707:ARG:NH1 | 2.05 | 0.70 |
| 1:B:761:GLU:O | 1:B:765:ARG:N | 2.24 | 0.70 |
| 1:D:302:LYS:HZ3 | 1:D:306:SER:HA | 1.55 | 0.70 |
| 1:D:655:LEU:HD22 | 1:D:710:SER:HA | 1.73 | 0.70 |
| 1:E:358:LYS:HZ3 | 1:E:362:HIS:CE1 | 2.09 | 0.70 |
| 1:E:462:LEU:HD12 | 1:E:465:ARG:HH11 | 1.56 | 0.70 |
| 1:E:645:GLU:OE1 | 1:E:645:GLU:N | 2.23 | 0.70 |
| 1:E:645:GLU:H | 1:E:649:LYS:HZ2 | 1.38 | 0.70 |
| 1:E:705:ASP:OD2 | 1:F:794:ARG:NH2 | 2.24 | 0.70 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:198:ARG:HB2 | 1:F:202:ARG:HH21 | 1.55 | 0.70 |
| 1:A:172:ILE:C | 1:A:245:SER:HB3 | 2.17 | 0.70 |
| 1:B:12:LEU:O | 1:B:17:LEU:N | 2.19 | 0.70 |
| 1:B:266:LYS:HA | 1:B:269:LEU:HD22 | 1.72 | 0.70 |
| 1:B:547:SER:HB3 | 1:B:560:LYS:NZ | 2.07 | 0.70 |
| 1:B:740:SER:OG | 1:B:774:LYS:O | 2.09 | 0.70 |
| 1:B:856:ASN:H | 1:B:880:LEU:HD11 | 1.56 | 0.70 |
| 1:D:620:LYS:HG3 | 1:D:621:THR:N | 2.05 | 0.70 |
| 1:D:835:GLU:OE2 | 1:D:878:GLU:HB3 | 1.92 | 0.70 |
| 1:E:497:TYR:O | 1:E:501:THR:HG23 | 1.91 | 0.70 |
| 1:E:602:ALA:HB1 | 1:E:606:GLN:CB | 2.20 | 0.70 |
| 1:E:710:SER:OG | 1:E:714:LYS:N | 2.25 | 0.70 |
| 1:E:808:GLN:N | 1:E:808:GLN:OE1 | 2.25 | 0.70 |
| 1:F:302:LYS:O | 1:F:306:SER:OG | 2.05 | 0.70 |
| 1:F:363:HIS:HE1 | 1:F:397:ASP:CA | 1.87 | 0.70 |
| 1:F:715:THR:C | 1:F:717:ASP:N | 2.49 | 0.70 |
| 1:F:813:PHE:N | 1:F:816:LYS:HZ3 | 1.88 | 0.70 |
| 1:A:620:LYS:O | 1:A:624:ALA:N | 2.21 | 0.70 |
| 1:A:800:LYS:HE3 | 1:A:851:ASP:HB2 | 1.73 | 0.70 |
| 1:B:348:THR:O | 1:B:352:LEU:HG | 1.91 | 0.70 |
| 1:B:359:TYR:HA | 1:B:362:HIS:HB3 | 1.74 | 0.70 |
| 1:B:743:GLN:NE2 | 1:B:744:GLU:H | 1.90 | 0.70 |
| 1:C:613:LEU:HG | 1:C:772:PHE:H | 1.55 | 0.70 |
| 1:C:815:ALA:O | 1:C:819:TYR:N | 2.24 | 0.70 |
| 1:C:850:LYS:NZ | 1:C:851:ASP:CG | 2.50 | 0.70 |
| 1:D:175:THR:HA | 1:D:178:ALA:HB3 | 1.74 | 0.70 |
| 1:D:572:MET:HG2 | 1:D:576:LEU:HG | 1.74 | 0.70 |
| 1:D:765:ARG:HH21 | 1:E:640:ARG:NH1 | 1.90 | 0.70 |
| 1:E:328:ASP:OD2 | 1:E:331:PHE:HB2 | 1.91 | 0.70 |
| 1:E:382:TYR:OH | 1:E:560:LYS:O | 2.06 | 0.70 |
| 1:E:786:ILE:N | 1:E:789:LYS:HZ3 | 1.90 | 0.70 |
| 1:F:654:LYS:HB2 | 1:F:657:GLY:H | 1.55 | 0.70 |
| 1:F:781:HIS:CE1 | 1:F:782:LYS:HG3 | 2.26 | 0.70 |
| 1:C:169:LYS:CD | 1:C:264:ARG:HD2 | 0.29 | 0.70 |
| 1:C:210:LEU:HB2 | 1:C:338:ILE:N | 2.03 | 0.70 |
| 1:C:262:GLU:HA | 1:C:265:PHE:CD2 | 2.27 | 0.70 |
| 1:C:417:LYS:HZ3 | 1:C:463:ARG:CG | 2.05 | 0.70 |
| 1:C:489:LYS:O | 1:C:493:ALA:N | 2.25 | 0.70 |
| 1:C:583:GLN:HG2 | 1:C:772:PHE:O | 1.91 | 0.70 |
| 1:D:281:LEU:O | 1:D:313:ILE:N | 2.25 | 0.70 |
| 1:D:348:THR:O | 1:D:352:LEU:HG | 1.91 | 0.70 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:809:GLU:CD | 1:D:811:LYS:NZ | 2.50 | 0.70 |
| 1:E:242:LYS:CB | 1:E:279:ILE:HG12 | 2.22 | 0.70 |
| 1:E:762:PHE:O | 1:E:766:ILE:N | 2.24 | 0.70 |
| 1:F:189:ARG:HD2 | 1:F:340:VAL:HB | 1.73 | 0.70 |
| 1:F:209:CYS:O | 1:F:338:ILE:N | 2.17 | 0.70 |
| 1:A:178:ALA:HA | 1:A:182:LYS:HB2 | 1.74 | 0.70 |
| 1:A:747:LYS:O | 1:A:751:MET:N | 2.21 | 0.70 |
| 1:B:270:LYS:O | 1:B:273:GLU:N | 2.25 | 0.70 |
| 1:C:366:ARG:CZ | 1:C:539:ASN:HB3 | 2.22 | 0.70 |
| 1:C:428:ILE:O | 1:C:449:ARG:NH2 | 2.25 | 0.70 |
| 1:C:625:LYS:O | 1:C:627:VAL:N | 2.24 | 0.70 |
| 1:D:218:LYS:O | 1:D:222:ILE:HG12 | 1.91 | 0.70 |
| 1:D:437:ALA:HB2 | 1:D:443:ASP:OD2 | 1.92 | 0.70 |
| 1:D:781:HIS:NE2 | 1:D:808:GLN:OE1 | 2.25 | 0.70 |
| 1:E:202:ARG:NH1 | 1:E:205:LYS:H | 1.90 | 0.70 |
| 1:F:696:LEU:O | 1:F:700:LEU:N | 2.24 | 0.70 |
| 1:A:274:GLU:C | 1:A:276:LYS:HZ2 | 1.99 | 0.70 |
| 1:A:569:LEU:HD12 | 1:A:572:MET:HG2 | 1.73 | 0.70 |
| 1:A:781:HIS:CE1 | 1:A:782:LYS:NZ | 2.59 | 0.70 |
| 1:B:391:SER:O | 1:B:395:LEU:N | 2.22 | 0.70 |
| 1:C:175:THR:H | 1:C:242:LYS:HE2 | 1.55 | 0.70 |
| 1:C:228:ARG:NH1 | 1:D:408:ASP:OD1 | 2.24 | 0.70 |
| 1:C:251:LEU:HD12 | 1:C:252:THR:H | 1.56 | 0.70 |
| 1:C:834:ASN:HD22 | 1:C:837:LEU:HD21 | 1.57 | 0.70 |
| 1:C:875:GLU:O | 1:C:877:LEU:HG | 1.91 | 0.70 |
| 1:D:672:THR:HA | 1:D:675:LEU:CG | 2.20 | 0.70 |
| 1:E:645:GLU:HB2 | 1:E:649:LYS:NZ | 2.07 | 0.70 |
| 1:F:638:MET:SD | 1:F:683:LEU:HA | 2.32 | 0.70 |
| 1:F:838:ASN:O | 1:F:842:LEU:N | 2.19 | 0.70 |
| 1:C:625:LYS:HG2 | 1:C:635:GLU:OE1 | 1.92 | 0.69 |
| 1:C:743:GLN:CB | 1:C:746:THR:H | 2.05 | 0.69 |
| 1:D:537:ILE:O | 1:D:540:VAL:HG12 | 1.92 | 0.69 |
| 1:D:612:PHE:H | 1:D:770:VAL:HB | 1.56 | 0.69 |
| 1:D:642:ASP:O | 1:D:644:SER:N | 2.25 | 0.69 |
| 1:E:173:ASP:HA | 1:E:244:PHE:HA | 1.72 | 0.69 |
| 1:E:305:LEU:O | 1:E:309:GLN:N | 2.23 | 0.69 |
| 1:E:576:LEU:CA | 1:E:579:GLU:HG2 | 2.22 | 0.69 |
| 1:E:632:PHE:CE1 | 1:E:680:TYR:HB3 | 2.27 | 0.69 |
| 1:E:645:GLU:HB2 | 1:E:649:LYS:HZ1 | 1.55 | 0.69 |
| 1:E:698:VAL:HB | 1:E:702:MET:HE3 | 1.74 | 0.69 |
| 1:E:746:THR:O | 1:E:750:VAL:N | 2.23 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:E:785:ASP:OD1 | 1:E:786:ILE:HD12 | 1.92 | 0.69 |
| 1:E:805:ASN:OD1 | 1:E:805:ASN:N | 2.23 | 0.69 |
| 1:F:827:PRO:O | 1:F:830:ARG:N | 2.24 | 0.69 |
| 1:B:190:GLU:O | 1:B:194:ARG:N | 2.16 | 0.69 |
| 1:C:170:TYR:OH | 1:C:250:ALA:H | 1.07 | 0.69 |
| 1:C:351:ILE:HG12 | 2:C:1001:AGS:HN61 | 1.57 | 0.69 |
| 1:D:475:GLU:O | 1:D:479:ALA:N | 2.26 | 0.69 |
| 1:E:395:LEU:O | 1:E:399:SER:N | 2.17 | 0.69 |
| 1:E:523:GLN:NE2 | 1:E:527:GLU:OE2 | 2.14 | 0.69 |
| 1:E:618:SER:OG | 2:E:1002:AGS:O3A | 2.06 | 0.69 |
| 1:E:619:GLY:N | 2:E:1002:AGS:O4' | 2.25 | 0.69 |
| 1:E:622:GLU:O | 1:E:626:LYS:HG2 | 1.92 | 0.69 |
| 1:E:626:LYS:HD3 | 1:E:635:GLU:OE2 | 1.93 | 0.69 |
| 1:F:814:LEU:O | 1:F:818:GLY:N | 2.23 | 0.69 |
| 1:A:191:GLU:N | 1:A:191:GLU:OE1 | 2.24 | 0.69 |
| 1:A:802:TYR:HB2 | 1:A:853:GLU:HB3 | 1.73 | 0.69 |
| 1:A:843:ARG:HA | 1:A:846:LYS:HB2 | 1.73 | 0.69 |
| 1:B:172:ILE:HD12 | 1:B:174:MET:H | 1.57 | 0.69 |
| 1:B:280:VAL:HG12 | 1:B:310:LEU:HA | 1.72 | 0.69 |
| 1:C:262:GLU:OE2 | 1:C:263:GLU:OE2 | 2.10 | 0.69 |
| 1:C:379:ALA:O | 1:C:382:TYR:N | 2.22 | 0.69 |
| 1:C:784:VAL:HG22 | 1:C:811:LYS:NZ | 2.08 | 0.69 |
| 1:D:228:ARG:HD3 | 1:D:231:ASP:OD2 | 1.91 | 0.69 |
| 1:D:787:ARG:O | 1:D:790:GLU:HB3 | 1.93 | 0.69 |
| 1:E:303:PRO:HB2 | 1:E:307:ARG:CZ | 2.22 | 0.69 |
| 1:E:698:VAL:O | 1:E:702:MET:N | 2.19 | 0.69 |
| 1:F:392:ALA:O | 1:F:396:VAL:N | 2.17 | 0.69 |
| 1:F:801:HIS:HB2 | 1:F:852:LYS:HG2 | 1.72 | 0.69 |
| 1:A:168:SER:O | 1:A:171:ALA:N | 2.26 | 0.69 |
| 1:A:541:VAL:HG12 | 1:A:543:SER:H | 1.57 | 0.69 |
| 1:A:543:SER:O | 1:A:548:GLU:N | 2.25 | 0.69 |
| 1:A:563:GLU:OE1 | 1:A:568:LYS:HE3 | 1.92 | 0.69 |
| 1:B:344:SER:C | 1:B:347:GLN:HE22 | 2.01 | 0.69 |
| 1:B:559:LYS:NZ | 1:B:630:PHE:C | 2.50 | 0.69 |
| 1:C:190:GLU:HG2 | 1:C:191:GLU:N | 2.03 | 0.69 |
| 1:C:628:ALA:N | 1:C:635:GLU:OE2 | 2.26 | 0.69 |
| 1:C:754:VAL:HB | 1:C:755:ARG:NH1 | 2.07 | 0.69 |
| 1:D:573:GLU:CD | 1:D:573:GLU:H | 2.00 | 0.69 |
| 1:D:609:SER:O | 1:D:768:SER:N | 2.25 | 0.69 |
| 1:E:262:GLU:OE2 | 1:E:300:ILE:HB | 1.91 | 0.69 |
| 1:E:359:TYR:HA | 1:E:362:HIS:CE1 | 2.27 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:232:ASP:HA | 1:B:238:LEU:HD11 | 1.74 | 0.69 |
| 1:C:323:SER:HA | 1:C:326:GLU:OE2 | 1.92 | 0.69 |
| 1:C:428:ILE:HG23 | 1:C:449:ARG:NH1 | 2.06 | 0.69 |
| 1:C:454:SER:HA | 1:C:457:GLU:HB3 | 1.74 | 0.69 |
| 1:D:173:ASP:HB2 | 1:D:244:PHE:CD1 | 2.28 | 0.69 |
| 1:D:765:ARG:HH21 | 1:E:640:ARG:HH12 | 1.40 | 0.69 |
| 1:E:166:TYR:N | 1:E:169:LYS:HB2 | 2.07 | 0.69 |
| 1:E:442:LYS:HA | 1:E:445:LEU:HB3 | 1.72 | 0.69 |
| 1:E:584:MET:O | 1:E:588:LYS:N | 2.19 | 0.69 |
| 1:E:826:ARG:HA | 1:E:829:ASN:ND2 | 2.08 | 0.69 |
| 1:F:217:GLY:N | 2:F:1001:AGS:O3G | 2.25 | 0.69 |
| 1:F:363:HIS:HE2 | 1:F:400:CYS:HG | 1.38 | 0.69 |
| 1:F:572:MET:HG3 | 1:F:630:PHE:CD2 | 2.27 | 0.69 |
| 1:A:199:VAL:HG11 | 1:A:208:PRO:HD3 | 1.74 | 0.69 |
| 1:B:202:ARG:HH12 | 1:B:205:LYS:HB2 | 1.55 | 0.69 |
| 1:B:758:PHE:HB2 | 1:B:763:LEU:HD11 | 1.74 | 0.69 |
| 1:B:839:LYS:NZ | 1:B:877:LEU:HA | 2.07 | 0.69 |
| 1:C:169:LYS:H | 1:C:264:ARG:NH2 | 1.89 | 0.69 |
| 1:C:169:LYS:CD | 1:C:264:ARG:HH11 | 1.98 | 0.69 |
| 1:C:185:PRO:HG2 | 1:C:355:LEU:HD11 | 1.75 | 0.69 |
| 1:C:534:ASN:HB3 | 1:C:537:ILE:HA | 1.75 | 0.69 |
| 1:C:800:LYS:HE2 | 1:C:850:LYS:HA | 1.73 | 0.69 |
| 1:D:18:ALA:O | 1:D:37:ALA:N | 2.14 | 0.69 |
| 1:D:203:ARG:NH1 | 1:E:362:HIS:C | 2.51 | 0.69 |
| 1:E:332:GLU:OE2 | 1:E:337:LYS:HG3 | 1.93 | 0.69 |
| 1:E:610:PHE:HA | 1:E:768:SER:O | 1.92 | 0.69 |
| 1:E:795:PHE:CG | 1:E:796:GLU:N | 2.61 | 0.69 |
| 1:F:363:HIS:NE2 | 1:F:397:ASP:CA | 2.50 | 0.69 |
| 1:F:805:ASN:OD1 | 1:F:806:LEU:N | 2.26 | 0.69 |
| 1:A:572:MET:HB2 | 1:A:630:PHE:CE1 | 2.27 | 0.69 |
| 1:B:226:ALA:HA | 1:B:229:ILE:HB | 1.75 | 0.69 |
| 1:B:324:ILE:O | 1:B:328:ASP:N | 2.25 | 0.69 |
| 1:B:397:ASP:O | 1:B:401:ALA:N | 2.21 | 0.69 |
| 1:B:634:ASP:OD1 | 1:B:635:GLU:N | 2.25 | 0.69 |
| 1:B:831:LEU:O | 1:B:835:GLU:N | 2.24 | 0.69 |
| 1:C:228:ARG:NH1 | 1:C:233:ASP:O | 2.26 | 0.69 |
| 1:C:368:LEU:HB2 | 1:C:540:VAL:O | 1.92 | 0.69 |
| 1:C:626:LYS:C | 1:C:635:GLU:OE2 | 2.35 | 0.69 |
| 1:D:686:ASP:C | 1:D:688:VAL:H | 2.01 | 0.69 |
| 1:D:806:LEU:C | 1:D:811:LYS:HZ3 | 1.98 | 0.69 |
| 1:E:646:LEU:HB2 | 1:E:649:LYS:HB2 | 1.74 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:200:LEU:HD13 | 1:A:238:LEU:HD21 | 1.73 | 0.69 |
| 1:A:649:LYS:O | 1:A:653:SER:OG | 2.06 | 0.69 |
| 1:C:302:LYS:HZ2 | 1:C:306:SER:HA | 1.56 | 0.69 |
| 1:C:374:THR:OG1 | 1:C:375:ALA:N | 2.24 | 0.69 |
| 1:C:483:LEU:HD11 | 1:C:513:ILE:HA | 1.75 | 0.69 |
| 1:C:746:THR:O | 1:C:748:ASN:N | 2.26 | 0.69 |
| 1:C:787:ARG:CZ | 1:C:826:ARG:HH21 | 2.06 | 0.69 |
| 1:D:214:PRO:HD2 | 1:D:387:ARG:NH2 | 2.08 | 0.69 |
| 1:D:220:ALA:O | 1:D:224:GLY:N | 2.24 | 0.69 |
| 1:D:260:ASP:HA | 1:D:263:GLU:HB2 | 1.75 | 0.69 |
| 1:D:460:GLU:HA | 1:D:463:ARG:HH11 | 1.57 | 0.69 |
| 1:D:610:PHE:H | 1:D:724:ILE:HG23 | 1.58 | 0.69 |
| 1:D:703:LEU:HG | 1:D:704:ASP:OD1 | 1.92 | 0.69 |
| 1:D:755:ARG:HH12 | 1:D:756:GLN:HB3 | 1.56 | 0.69 |
| 1:E:344:SER:OG | 1:E:347:GLN:HB2 | 1.92 | 0.69 |
| 1:E:585:ASP:N | 1:E:585:ASP:OD1 | 2.23 | 0.69 |
| 1:E:611:LEU:O | 1:E:769:ILE:HG23 | 1.92 | 0.69 |
| 1:E:807:THR:OG1 | 1:E:808:GLN:OE1 | 2.06 | 0.69 |
| 1:E:833:GLN:H | 1:E:833:GLN:CD | 1.98 | 0.69 |
| 1:F:284:ASP:O | 1:F:315:ALA:N | 2.25 | 0.69 |
| 1:F:708:ILE:HD11 | 1:F:718:CYS:HB2 | 1.74 | 0.69 |
| 1:A:658:THR:HG22 | 1:A:659:THR:H | 1.57 | 0.69 |
| 1:D:763:LEU:O | 1:D:766:ILE:HG12 | 1.92 | 0.69 |
| 1:D:802:TYR:CZ | 1:D:853:GLU:HG3 | 2.28 | 0.69 |
| 1:E:202:ARG:HG3 | 1:F:397:ASP:OD2 | 1.93 | 0.69 |
| 1:E:215:GLY:C | 1:E:218:LYS:NZ | 2.46 | 0.69 |
| 1:E:366:ARG:HH12 | 1:E:368:LEU:N | 1.91 | 0.69 |
| 1:A:280:VAL:HG13 | 1:A:311:LYS:O | 1.93 | 0.69 |
| 1:A:326:GLU:H | 1:A:326:GLU:CD | 1.99 | 0.69 |
| 1:A:674:GLN:HA | 1:A:677:TYR:CD2 | 2.28 | 0.69 |
| 1:A:742:ILE:HG23 | 1:A:746:THR:HB | 1.75 | 0.69 |
| 1:B:198:ARG:HB2 | 1:C:401:ALA:HB1 | 1.72 | 0.69 |
| 1:B:351:ILE:HG13 | 1:B:355:LEU:HD13 | 1.74 | 0.69 |
| 1:B:647:SER:H | 1:B:691:ALA:N | 1.91 | 0.69 |
| 1:C:203:ARG:HG2 | 1:C:204:ILE:H | 1.58 | 0.69 |
| 1:C:687:GLU:O | 1:C:688:VAL:HG12 | 1.93 | 0.69 |
| 1:C:750:VAL:O | 1:C:754:VAL:N | 2.20 | 0.69 |
| 1:D:823:MET:SD | 1:D:826:ARG:HB2 | 2.33 | 0.69 |
| 1:E:205:LYS:O | 1:E:336:GLN:NE2 | 2.26 | 0.69 |
| 1:E:216:ILE:O | 2:E:1001:AGS:O1A | 2.10 | 0.69 |
| 1:E:285:GLU:O | 1:E:288:MET:N | 2.26 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:365:VAL:HG23 | 1:E:366:ARG:O | 1.92 | 0.69 |
| 1:E:615:LEU:O | 2:E:1002:AGS:O2B | 2.11 | 0.69 |
| 2:E:1002:AGS:O1B | 2:E:1002:AGS:H4' | 1.92 | 0.69 |
| 1:A:689:GLU:HA | 1:A:757:HIS:CE1 | 2.28 | 0.68 |
| 1:B:242:LYS:NZ | 1:B:277:THR:HG21 | 2.08 | 0.68 |
| 1:B:391:SER:HA | 1:B:394:ASP:HB2 | 1.75 | 0.68 |
| 1:B:743:GLN:HG3 | 1:B:745:SER:H | 1.58 | 0.68 |
| 1:B:841:ALA:HA | 1:B:844:ILE:HD12 | 1.76 | 0.68 |
| 1:C:785:ASP:CG | 1:C:789:LYS:NZ | 2.51 | 0.68 |
| 1:D:218:LYS:HA | 1:D:221:ILE:HB | 1.75 | 0.68 |
| 1:D:776:SER:O | 1:D:780:ILE:N | 2.24 | 0.68 |
| 1:E:205:LYS:HB2 | 1:E:336:GLN:NE2 | 2.07 | 0.68 |
| 1:E:647:SER:HB2 | 1:E:692:HIS:HD2 | 1.57 | 0.68 |
| 1:E:823:MET:HG2 | 1:E:826:ARG:HB2 | 1.74 | 0.68 |
| 1:F:167:LEU:N | 1:F:169:LYS:HZ3 | 1.82 | 0.68 |
| 1:F:262:GLU:O | 1:F:266:LYS:N | 2.26 | 0.68 |
| 1:A:250:ALA:HA | 1:A:264:ARG:CZ | 2.24 | 0.68 |
| 1:A:345:VAL:O | 1:A:349:VAL:N | 2.23 | 0.68 |
| 1:A:376:ALA:O | 1:A:380:LYS:N | 2.20 | 0.68 |
| 1:A:611:LEU:HD21 | 1:A:726:THR:HG22 | 1.74 | 0.68 |
| 1:A:834:ASN:OD1 | 1:A:838:ASN:ND2 | 2.25 | 0.68 |
| 1:B:401:ALA:O | 1:B:405:VAL:N | 2.21 | 0.68 |
| 1:B:582:GLY:HA2 | 1:B:773:ASN:HD21 | 1.58 | 0.68 |
| 1:C:413:GLU:O | 1:C:417:LYS:N | 2.21 | 0.68 |
| 1:C:568:LYS:NZ | 1:C:630:PHE:O | 2.25 | 0.68 |
| 1:D:203:ARG:NH1 | 1:E:363:HIS:CG | 2.58 | 0.68 |
| 1:D:281:LEU:HD11 | 1:D:310:LEU:HB3 | 1.75 | 0.68 |
| 1:D:641:VAL:HB | 1:D:685:PHE:CD2 | 2.29 | 0.68 |
| 1:E:284:ASP:C | 1:E:315:ALA:H | 2.01 | 0.68 |
| 1:F:363:HIS:HE1 | 1:F:397:ASP:CG | 2.01 | 0.68 |
| 1:F:379:ALA:HA | 1:F:383:LEU:HD12 | 1.74 | 0.68 |
| 1:B:332:GLU:HA | 1:B:335:PHE:HB2 | 1.75 | 0.68 |
| 1:C:167:LEU:C | 1:C:167:LEU:HD12 | 2.17 | 0.68 |
| 1:C:370:SER:O | 1:C:373:VAL:N | 2.26 | 0.68 |
| 1:C:819:TYR:HA | 1:C:824:GLY:O | 1.92 | 0.68 |
| 1:D:124:SER:C | 1:D:126:ILE:H | 2.01 | 0.68 |
| 1:D:503:ALA:O | 1:D:507:TYR:N | 2.24 | 0.68 |
| 1:D:767:SER:HA | 1:E:830:ARG:HH12 | 1.57 | 0.68 |
| 1:E:228:ARG:HD2 | 1:E:231:ASP:HB2 | 1.75 | 0.68 |
| 1:E:242:LYS:O | 1:E:279:ILE:HA | 1.93 | 0.68 |
| 1:E:265:PHE:HA | 1:E:268:VAL:HB | 1.74 | 0.68 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:571:HIS:HD2 | 1:E:574:ARG:HH11 | 1.41 | 0.68 |
| 1:E:652:VAL:O | 1:E:669:GLY:N | 2.26 | 0.68 |
| 1:E:787:ARG:NH2 | 1:E:829:ASN:O | 2.26 | 0.68 |
| 1:F:360:GLU:OE1 | 1:F:367:ILE:HB | 1.93 | 0.68 |
| 1:F:605:ARG:NH1 | 1:F:706:GLY:N | 2.41 | 0.68 |
| 1:A:251:LEU:O | 1:A:254:GLY:N | 2.26 | 0.68 |
| 1:B:248:LEU:HB3 | 1:B:253:ALA:HB2 | 1.74 | 0.68 |
| 1:B:353:ARG:NH1 | 1:B:373:VAL:H | 1.91 | 0.68 |
| 1:B:353:ARG:CZ | 1:B:369:ASP:HB2 | 2.23 | 0.68 |
| 1:B:544:ASP:OD1 | 1:B:545:THR:N | 2.27 | 0.68 |
| 1:C:14:ILE:N | 1:C:160:THR:H | 1.91 | 0.68 |
| 1:C:222:ILE:C | 1:C:225:VAL:HB | 2.18 | 0.68 |
| 1:C:564:SER:C | 1:C:566:ASN:H | 2.01 | 0.68 |
| 1:C:754:VAL:HB | 1:C:755:ARG:HH11 | 1.58 | 0.68 |
| 1:C:846:LYS:NZ | 1:C:882:ASN:HD21 | 1.91 | 0.68 |
| 1:D:198:ARG:HH22 | 1:E:406:ALA:N | 1.92 | 0.68 |
| 1:D:226:ALA:O | 1:D:230:ILE:N | 2.26 | 0.68 |
| 1:D:520:LEU:HA | 1:D:523:GLN:CD | 2.18 | 0.68 |
| 1:D:691:ALA:HB3 | 1:D:696:LEU:HD11 | 1.75 | 0.68 |
| 1:E:411:PRO:HA | 1:E:414:LEU:HD12 | 1.74 | 0.68 |
| 1:E:833:GLN:O | 1:E:837:LEU:HG | 1.94 | 0.68 |
| 1:F:207:ASN:HB2 | 1:F:335:PHE:CG | 2.28 | 0.68 |
| 1:F:568:LYS:HG2 | 1:F:571:HIS:HD2 | 1.58 | 0.68 |
| 1:F:744:GLU:CA | 1:F:747:LYS:HZ3 | 2.04 | 0.68 |
| 1:A:378:LEU:O | 1:A:381:ARG:HG2 | 1.92 | 0.68 |
| 1:B:302:LYS:HD2 | 1:B:305:LEU:HD12 | 1.75 | 0.68 |
| 1:B:385:TYR:CZ | 1:B:386:ARG:NH1 | 2.61 | 0.68 |
| 1:C:401:ALA:O | 1:C:405:VAL:N | 2.25 | 0.68 |
| 1:C:605:ARG:HG3 | 1:C:606:GLN:N | 2.08 | 0.68 |
| 1:D:597:SER:O | 1:D:600:GLY:N | 2.26 | 0.68 |
| 1:D:837:LEU:HA | 1:D:840:LEU:HD11 | 1.76 | 0.68 |
| 1:E:196:THR:O | 1:E:200:LEU:N | 2.24 | 0.68 |
| 1:E:218:LYS:HD3 | 1:E:387:ARG:HH22 | 1.58 | 0.68 |
| 1:E:296:ASP:O | 1:E:300:ILE:N | 2.23 | 0.68 |
| 1:F:378:LEU:HA | 1:F:381:ARG:HB3 | 1.74 | 0.68 |
| 1:F:878:GLU:HG2 | 1:F:879:VAL:H | 1.57 | 0.68 |
| 1:A:192:GLU:N | 1:A:192:GLU:OE1 | 2.27 | 0.68 |
| 1:A:325:VAL:O | 1:A:329:GLY:N | 2.27 | 0.68 |
| 1:C:416:SER:OG | 1:C:420:GLN:OE1 | 2.12 | 0.68 |
| 1:D:262:GLU:OE2 | 1:D:263:GLU:HG2 | 1.94 | 0.68 |
| 1:D:576:LEU:O | 1:D:580:VAL:N | 2.27 | 0.68 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:611:LEU:H | 1:D:769:ILE:HA | 1.58 | 0.68 |
| 1:D:775:LEU:O | 1:D:780:ILE:HG13 | 1.92 | 0.68 |
| 1:E:597:SER:O | 1:E:601:LEU:HA | 1.93 | 0.68 |
| 1:E:712:GLN:N | 1:E:714:LYS:NZ | 2.36 | 0.68 |
| 1:F:552:ARG:HB2 | 1:F:552:ARG:CZ | 2.24 | 0.68 |
| 1:A:777:ARG:HA | 1:A:780:ILE:CG1 | 2.23 | 0.68 |
| 1:C:198:ARG:O | 1:C:201:ALA:N | 2.22 | 0.68 |
| 1:C:275:SER:N | 1:C:276:LYS:NZ | 2.42 | 0.68 |
| 1:C:613:LEU:N | 1:C:726:THR:HB | 2.09 | 0.68 |
| 1:C:751:MET:O | 1:C:755:ARG:HG2 | 1.94 | 0.68 |
| 1:D:216:ILE:HB | 2:D:1001:AGS:O2A | 1.94 | 0.68 |
| 1:D:317:THR:C | 1:D:321:TYR:CG | 2.67 | 0.68 |
| 1:E:476:LEU:HD12 | 1:E:479:ALA:HB3 | 1.76 | 0.68 |
| 1:E:522:ASP:O | 1:E:526:GLU:N | 2.24 | 0.68 |
| 1:E:571:HIS:CD2 | 1:E:574:ARG:NH1 | 2.62 | 0.68 |
| 1:B:613:LEU:HG | 1:B:771:ILE:HA | 1.75 | 0.68 |
| 1:C:260:ASP:CA | 1:C:263:GLU:HG2 | 2.18 | 0.68 |
| 1:C:287:HIS:NE2 | 1:C:315:ALA:O | 2.27 | 0.68 |
| 1:C:496:ARG:HB2 | 1:C:498:ASP:OD1 | 1.93 | 0.68 |
| 1:C:789:LYS:HB3 | 1:C:793:GLU:OE2 | 1.93 | 0.68 |
| 1:C:835:GLU:HA | 1:C:838:ASN:ND2 | 2.06 | 0.68 |
| 1:D:403:VAL:HG22 | 1:D:540:VAL:HG21 | 1.74 | 0.68 |
| 1:E:212:GLY:H | 1:E:317:THR:HA | 1.59 | 0.68 |
| 1:E:558:VAL:HA | 1:E:561:LEU:HB2 | 1.76 | 0.68 |
| 1:E:843:ARG:NE | 1:E:881:PRO:O | 2.26 | 0.68 |
| 1:F:263:GLU:HA | 1:F:266:LYS:HB3 | 1.74 | 0.68 |
| 1:A:222:ILE:HG22 | 1:A:282:PHE:CE2 | 2.27 | 0.68 |
| 1:A:346:ARG:HD2 | 1:A:349:VAL:HB | 1.75 | 0.68 |
| 1:B:673:ASN:OD1 | 1:B:674:GLN:N | 2.27 | 0.68 |
| 1:C:386:ARG:HG3 | 1:C:390:ASP:OD2 | 1.94 | 0.68 |
| 1:D:202:ARG:HH12 | 1:D:205:LYS:CB | 2.07 | 0.68 |
| 1:D:229:ILE:HG12 | 1:D:233:ASP:HB2 | 1.76 | 0.68 |
| 1:D:251:LEU:HA | 1:D:261:PHE:CZ | 2.29 | 0.68 |
| 1:D:262:GLU:O | 1:D:265:PHE:HD2 | 1.76 | 0.68 |
| 1:D:799:ASP:N | 1:D:801:HIS:CD2 | 2.60 | 0.68 |
| 1:D:800:LYS:NZ | 1:D:801:HIS:NE2 | 2.42 | 0.68 |
| 1:E:270:LYS:O | 1:E:273:GLU:N | 2.27 | 0.68 |
| 1:E:270:LYS:O | 1:E:274:GLU:N | 2.27 | 0.68 |
| 1:E:281:LEU:HD23 | 1:E:282:PHE:N | 2.09 | 0.68 |
| 1:A:617:GLY:O | 1:A:620:LYS:NZ | 2.27 | 0.68 |
| 1:A:758:PHE:HZ | 1:A:763:LEU:HB2 | 1.59 | 0.68 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:777:ARG:O | 1:A:781:HIS:N | 2.26 | 0.68 |
| 1:A:842:LEU:HB3 | 1:A:846:LYS:HZ2 | 1.56 | 0.68 |
| 1:B:645:GLU:HA | 1:B:691:ALA:CB | 2.15 | 0.68 |
| 1:C:222:ILE:O | 1:C:226:ALA:N | 2.25 | 0.68 |
| 1:D:235:PRO:HD3 | 1:E:408:ASP:HB2 | 1.76 | 0.68 |
| 1:D:269:LEU:HA | 1:D:272:ILE:HD11 | 1.75 | 0.68 |
| 1:D:566:ASN:OD1 | 1:D:566:ASN:N | 2.27 | 0.68 |
| 1:E:556:ILE:HB | 1:E:560:LYS:HD3 | 1.75 | 0.68 |
| 1:E:620:LYS:HA | 1:E:623:LEU:HB3 | 1.76 | 0.68 |
| 1:E:737:GLN:OE1 | 1:E:743:GLN:N | 2.20 | 0.68 |
| 1:F:542:ASP:OD2 | 1:F:544:ASP:OD2 | 2.12 | 0.68 |
| 1:F:544:ASP:O | 1:F:547:SER:OG | 2.11 | 0.68 |
| 1:F:622:GLU:HB2 | 2:F:1002:AGS:H5'2 | 1.76 | 0.68 |
| 1:F:683:LEU:HD23 | 1:F:684:LEU:HG | 1.76 | 0.68 |
| 1:F:880:LEU:HD12 | 1:F:881:PRO:HD2 | 1.76 | 0.68 |
| 1:B:785:ASP:C | 1:B:789:LYS:HZ1 | 1.99 | 0.67 |
| 1:C:226:ALA:HA | 1:C:229:ILE:HD12 | 1.76 | 0.67 |
| 1:C:402:GLY:O | 1:C:406:ALA:N | 2.18 | 0.67 |
| 1:D:328:ASP:HB3 | 1:D:331:PHE:HB3 | 1.74 | 0.67 |
| 1:D:743:GLN:C | 1:D:747:LYS:HZ1 | 2.03 | 0.67 |
| 1:E:237:ILE:HG22 | 1:E:278:LEU:HD22 | 1.75 | 0.67 |
| 1:E:302:LYS:HG2 | 1:E:334:ARG:NH1 | 2.09 | 0.67 |
| 1:E:348:THR:HG22 | 1:E:352:LEU:HD11 | 1.76 | 0.67 |
| 1:E:358:LYS:NZ | 1:E:359:TYR:HA | 2.09 | 0.67 |
| 1:E:442:LYS:O | 1:E:446:LYS:N | 2.26 | 0.67 |
| 1:F:286:ILE:HG13 | 1:F:322:ARG:HD3 | 1.74 | 0.67 |
| 1:F:611:LEU:HD11 | 1:F:725:MET:HB3 | 1.77 | 0.67 |
| 1:F:695:VAL:HA | 1:F:698:VAL:HB | 1.76 | 0.67 |
| 1:F:715:THR:O | 1:F:716:ILE:C | 2.37 | 0.67 |
| 1:B:18:ALA:O | 1:B:22:ALA:N | 2.27 | 0.67 |
| 1:B:645:GLU:HB3 | 1:B:692:HIS:CD2 | 2.30 | 0.67 |
| 1:B:671:LEU:O | 1:B:675:LEU:HG | 1.94 | 0.67 |
| 1:C:333:ARG:NH1 | 1:C:334:ARG:NE | 2.41 | 0.67 |
| 1:C:333:ARG:HH11 | 1:C:334:ARG:CG | 2.06 | 0.67 |
| 1:C:754:VAL:O | 1:C:756:GLN:N | 2.27 | 0.67 |
| 1:D:202:ARG:NH1 | 1:D:205:LYS:C | 2.52 | 0.67 |
| 1:D:619:GLY:HA2 | 1:D:622:GLU:HB2 | 1.76 | 0.67 |
| 1:D:790:GLU:C | 1:D:794:ARG:HH22 | 2.01 | 0.67 |
| 1:E:202:ARG:HG2 | 1:E:204:ILE:H | 1.60 | 0.67 |
| 1:E:207:ASN:HA | 1:E:313:ILE:HD11 | 1.74 | 0.67 |
| 1:E:365:VAL:HG12 | 1:E:538:GLN:HB2 | 1.75 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:654:LYS:HZ3 | 1:E:698:VAL:CG2 | 2.07 | 0.67 |
| 1:E:817:TYR:OH | 1:E:874:GLU:HB3 | 1.94 | 0.67 |
| 1:F:174:MET:SD | 1:F:177:GLN:HB2 | 2.34 | 0.67 |
| 1:F:584:MET:HB3 | 1:F:588:LYS:HZ3 | 1.56 | 0.67 |
| 1:F:743:GLN:O | 1:F:747:LYS:NZ | 2.27 | 0.67 |
| 1:A:169:LYS:HG2 | 1:A:264:ARG:NH2 | 2.08 | 0.67 |
| 1:A:622:GLU:O | 1:A:626:LYS:N | 2.20 | 0.67 |
| 1:B:202:ARG:NE | 1:B:204:ILE:O | 2.26 | 0.67 |
| 1:B:222:ILE:N | 1:B:223:GLU:OE1 | 2.26 | 0.67 |
| 1:C:212:GLY:O | 1:C:318:ASN:N | 2.23 | 0.67 |
| 1:C:217:GLY:N | 2:C:1001:AGS:O1A | 2.27 | 0.67 |
| 1:E:203:ARG:N | 1:F:397:ASP:OD2 | 2.26 | 0.67 |
| 1:F:192:GLU:O | 1:F:196:THR:N | 2.23 | 0.67 |
| 1:F:613:LEU:H | 1:F:770:VAL:HB | 1.58 | 0.67 |
| 1:A:197:ILE:HG23 | 1:A:235:PRO:HG3 | 1.76 | 0.67 |
| 1:B:392:ALA:O | 1:B:395:LEU:HB2 | 1.95 | 0.67 |
| 1:B:691:ALA:O | 1:B:692:HIS:ND1 | 2.26 | 0.67 |
| 1:B:743:GLN:HE21 | 1:B:744:GLU:H | 1.39 | 0.67 |
| 1:C:168:SER:C | 1:C:264:ARG:NE | 2.53 | 0.67 |
| 1:C:286:ILE:HA | 1:C:289:LEU:HB2 | 1.77 | 0.67 |
| 1:C:387:ARG:HB2 | 1:C:390:ASP:OD2 | 1.94 | 0.67 |
| 1:C:607:PRO:HB2 | 1:C:722:ILE:HD12 | 1.74 | 0.67 |
| 1:D:262:GLU:HG2 | 1:D:263:GLU:OE2 | 1.93 | 0.67 |
| 1:D:612:PHE:CB | 1:D:726:THR:HG21 | 2.24 | 0.67 |
| 1:E:265:PHE:O | 1:E:269:LEU:N | 2.27 | 0.67 |
| 1:E:358:LYS:HZ3 | 1:E:362:HIS:HE1 | 1.41 | 0.67 |
| 1:E:429:LYS:O | 1:E:432:GLU:N | 2.27 | 0.67 |
| 1:E:625:LYS:C | 1:E:635:GLU:OE2 | 2.38 | 0.67 |
| 1:F:199:VAL:HG22 | 1:F:207:ASN:HA | 1.75 | 0.67 |
| 1:A:822:ASP:CG | 1:F:307:ARG:HH12 | 2.03 | 0.67 |
| 1:B:214:PRO:HD2 | 1:B:387:ARG:HE | 1.56 | 0.67 |
| 1:B:620:LYS:HG2 | 1:B:826:ARG:NH1 | 2.10 | 0.67 |
| 1:B:637:MET:HE3 | 1:B:639:ILE:HD11 | 1.76 | 0.67 |
| 1:B:777:ARG:O | 1:B:781:HIS:N | 2.21 | 0.67 |
| 1:C:172:ILE:HD11 | 1:C:245:SER:H | 1.57 | 0.67 |
| 1:C:191:GLU:N | 1:C:192:GLU:OE1 | 2.27 | 0.67 |
| 1:C:328:ASP:HA | 1:C:331:PHE:HD2 | 1.59 | 0.67 |
| 1:C:606:GLN:HG3 | 1:C:607:PRO:HD2 | 1.77 | 0.67 |
| 1:C:759:ARG:O | 1:C:762:PHE:HB3 | 1.94 | 0.67 |
| 1:D:167:LEU:O | 1:D:170:TYR:HB2 | 1.94 | 0.67 |
| 1:D:177:GLN:HA | 1:D:180:GLN:HB2 | 1.76 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:388:LEU:O | 1:D:392:ALA:N | 2.19 | 0.67 |
| 1:D:718:CYS:C | 1:D:720:ASN:H | 2.00 | 0.67 |
| 1:E:194:ARG:HB3 | 1:E:198:ARG:NH1 | 2.09 | 0.67 |
| 1:A:174:MET:HA | 1:A:177:GLN:NE2 | 2.10 | 0.67 |
| 1:A:611:LEU:O | 1:A:769:ILE:HG23 | 1.94 | 0.67 |
| 1:A:669:GLY:O | 1:A:672:THR:N | 2.28 | 0.67 |
| 1:A:788:LEU:O | 1:A:792:GLU:N | 2.27 | 0.67 |
| 1:B:274:GLU:CD | 1:B:274:GLU:H | 2.01 | 0.67 |
| 1:B:402:GLY:O | 1:B:406:ALA:N | 2.16 | 0.67 |
| 1:B:764:ASN:CB | 1:B:765:ARG:HH12 | 2.06 | 0.67 |
| 1:D:260:ASP:O | 1:D:263:GLU:N | 2.28 | 0.67 |
| 1:D:579:GLU:C | 1:D:626:LYS:NZ | 2.52 | 0.67 |
| 1:E:349:VAL:HA | 1:E:352:LEU:HD12 | 1.77 | 0.67 |
| 1:E:822:ASP:OD1 | 1:E:823:MET:N | 2.28 | 0.67 |
| 1:F:331:PHE:HD1 | 1:F:334:ARG:HG3 | 1.60 | 0.67 |
| 1:A:625:LYS:HA | 1:A:628:ALA:HB3 | 1.77 | 0.67 |
| 1:A:634:ASP:CG | 1:A:637:MET:HB2 | 2.20 | 0.67 |
| 1:B:195:SER:HB2 | 1:B:198:ARG:NH1 | 2.09 | 0.67 |
| 1:B:350:ALA:O | 1:B:354:GLY:N | 2.25 | 0.67 |
| 1:B:615:LEU:H | 1:B:772:PHE:HD2 | 1.41 | 0.67 |
| 1:C:272:ILE:HA | 1:C:276:LYS:HE3 | 1.75 | 0.67 |
| 1:C:410:LYS:HD3 | 1:C:470:LYS:NZ | 2.09 | 0.67 |
| 1:D:510:ILE:HB | 1:D:511:PRO:HD3 | 1.77 | 0.67 |
| 1:D:530:ARG:CZ | 1:D:537:ILE:HG23 | 2.24 | 0.67 |
| 1:D:570:ILE:HG12 | 1:D:595:ARG:NH1 | 2.10 | 0.67 |
| 1:D:617:GLY:O | 1:D:621:THR:OG1 | 2.12 | 0.67 |
| 1:D:705:ASP:OD1 | 1:D:707:ARG:NH1 | 2.28 | 0.67 |
| 1:E:286:ILE:O | 1:E:289:LEU:N | 2.27 | 0.67 |
| 1:E:302:LYS:HZ1 | 1:E:334:ARG:HB2 | 1.59 | 0.67 |
| 1:E:448:ALA:HA | 1:E:451:LYS:HG2 | 1.77 | 0.67 |
| 1:E:476:LEU:HB3 | 1:E:521:GLU:OE2 | 1.94 | 0.67 |
| 1:E:777:ARG:HA | 1:E:780:ILE:HG22 | 1.75 | 0.67 |
| 1:E:819:TYR:CE2 | 1:E:821:ASP:HA | 2.30 | 0.67 |
| 1:F:605:ARG:CD | 1:F:707:ARG:H | 2.07 | 0.67 |
| 1:B:198:ARG:HG3 | 1:B:199:VAL:N | 2.10 | 0.67 |
| 1:B:808:GLN:NE2 | 1:B:811:LYS:HB3 | 2.09 | 0.67 |
| 1:C:217:GLY:HA3 | 2:C:1001:AGS:H1' | 1.76 | 0.67 |
| 1:D:380:LYS:HZ2 | 1:D:381:ARG:N | 1.92 | 0.67 |
| 1:D:550:ALA:O | 1:D:553:LEU:N | 2.28 | 0.67 |
| 1:D:794:ARG:NH1 | 1:D:795:PHE:CE1 | 2.62 | 0.67 |
| 1:E:311:LYS:HZ2 | 1:E:313:ILE:CD1 | 2.08 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:431:LEU:HD13 | 1:E:444:ARG:HG3 | 1.76 | 0.67 |
| 1:E:777:ARG:HG3 | 1:E:778:LYS:H | 1.58 | 0.67 |
| 1:F:176:GLU:HA | 1:F:179:ARG:HB3 | 1.77 | 0.67 |
| 1:F:623:LEU:HA | 1:F:626:LYS:HB2 | 1.76 | 0.67 |
| 1:C:215:GLY:C | 2:C:1001:AGS:O2B | 2.38 | 0.67 |
| 1:C:456:GLN:HA | 1:C:459:LEU:HD12 | 1.77 | 0.67 |
| 1:C:579:GLU:OE1 | 1:C:579:GLU:N | 2.28 | 0.67 |
| 1:C:591:SER:C | 1:C:595:ARG:NH1 | 2.52 | 0.67 |
| 1:C:808:GLN:HG3 | 1:C:812:ASP:OD2 | 1.95 | 0.67 |
| 1:D:202:ARG:NH1 | 1:D:205:LYS:HG2 | 2.09 | 0.67 |
| 1:D:229:ILE:C | 1:D:232:ASP:H | 2.02 | 0.67 |
| 1:D:514:LYS:HA | 1:D:517:ILE:HD12 | 1.77 | 0.67 |
| 1:D:743:GLN:C | 1:D:747:LYS:NZ | 2.52 | 0.67 |
| 1:D:744:GLU:O | 1:D:746:THR:OG1 | 2.13 | 0.67 |
| 1:D:812:ASP:HA | 1:D:815:ALA:HB3 | 1.77 | 0.67 |
| 1:E:215:GLY:N | 1:E:218:LYS:HZ1 | 1.92 | 0.67 |
| 1:F:172:ILE:CG1 | 1:F:245:SER:H | 2.06 | 0.67 |
| 1:F:213:GLU:O | 1:F:218:LYS:NZ | 2.27 | 0.67 |
| 1:F:625:LYS:HZ1 | 1:F:636:ASP:C | 2.03 | 0.67 |
| 1:F:714:LYS:C | 1:F:716:ILE:N | 2.51 | 0.67 |
| 1:B:611:LEU:HG | 1:B:769:ILE:HA | 1.76 | 0.67 |
| 1:B:631:LEU:HD12 | 1:B:632:PHE:HB2 | 1.75 | 0.67 |
| 1:C:546:ILE:O | 1:C:550:ALA:N | 2.28 | 0.67 |
| 1:C:576:LEU:HD12 | 1:C:587:ILE:HG23 | 1.76 | 0.67 |
| 1:C:594:VAL:O | 1:C:598:ARG:N | 2.21 | 0.67 |
| 1:C:658:THR:O | 1:C:712:GLN:NE2 | 2.27 | 0.67 |
| 1:C:815:ALA:HA | 1:C:828:LEU:HD11 | 1.77 | 0.67 |
| 1:D:210:LEU:C | 1:D:316:THR:HG22 | 2.20 | 0.67 |
| 1:D:338:ILE:HG22 | 1:D:339:GLU:H | 1.60 | 0.67 |
| 1:D:362:HIS:CD2 | 1:D:363:HIS:CG | 2.83 | 0.67 |
| 1:D:585:ASP:OD1 | 1:D:585:ASP:N | 2.23 | 0.67 |
| 1:D:859:LEU:HB3 | 1:D:876:CYS:C | 2.20 | 0.67 |
| 1:E:175:THR:O | 1:E:179:ARG:HB2 | 1.95 | 0.67 |
| 1:E:219:THR:OG1 | 2:E:1001:AGS:O2G | 2.12 | 0.67 |
| 1:E:431:LEU:HB2 | 1:E:445:LEU:HD12 | 1.77 | 0.67 |
| 1:E:496:ARG:HH12 | 1:E:499:THR:HG21 | 1.60 | 0.67 |
| 1:E:629:GLY:HA2 | 1:E:633:ASN:C | 2.20 | 0.67 |
| 1:A:285:GLU:O | 1:A:288:MET:N | 2.27 | 0.66 |
| 1:A:558:VAL:O | 1:A:561:LEU:HB3 | 1.95 | 0.66 |
| 1:A:595:ARG:NH1 | 1:B:841:ALA:HB3 | 2.10 | 0.66 |
| 1:A:873:ALA:H | 1:F:201:ALA:HB3 | 1.58 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:837:LEU:HA | 1:B:840:LEU:HD12 | 1.75 | 0.66 |
| 1:C:168:SER:CB | 1:C:268:VAL:HG22 | 2.24 | 0.66 |
| 1:C:279:ILE:O | 1:C:311:LYS:HD2 | 1.95 | 0.66 |
| 1:C:629:GLY:H | 1:C:635:GLU:CD | 2.02 | 0.66 |
| 1:D:198:ARG:NH1 | 1:E:404:ALA:N | 2.42 | 0.66 |
| 1:D:322:ARG:O | 1:D:325:VAL:N | 2.28 | 0.66 |
| 1:D:329:GLY:HA2 | 1:D:332:GLU:HB3 | 1.76 | 0.66 |
| 1:D:708:ILE:HB | 1:D:716:ILE:N | 2.09 | 0.66 |
| 1:D:761:GLU:CD | 1:D:764:ASN:HD22 | 2.03 | 0.66 |
| 1:E:193:ILE:HG23 | 1:E:225:VAL:HG22 | 1.76 | 0.66 |
| 1:E:407:ARG:NH1 | 1:E:538:GLN:CD | 2.52 | 0.66 |
| 1:F:554:THR:HG22 | 1:F:559:LYS:HE2 | 1.75 | 0.66 |
| 1:A:207:ASN:O | 1:A:336:GLN:N | 2.27 | 0.66 |
| 1:B:277:THR:HG22 | 1:B:278:LEU:H | 1.60 | 0.66 |
| 1:B:548:GLU:N | 1:B:560:LYS:NZ | 2.42 | 0.66 |
| 1:B:640:ARG:HG3 | 1:B:684:LEU:HD13 | 1.76 | 0.66 |
| 1:B:744:GLU:OE2 | 1:B:751:MET:HE1 | 1.95 | 0.66 |
| 1:C:192:GLU:H | 1:C:192:GLU:CD | 1.99 | 0.66 |
| 1:C:614:GLY:N | 1:C:727:SER:O | 2.27 | 0.66 |
| 1:C:803:LYS:HA | 1:C:853:GLU:O | 1.96 | 0.66 |
| 1:D:206:SER:O | 1:D:336:GLN:N | 2.26 | 0.66 |
| 1:D:221:ILE:HG22 | 1:D:222:ILE:HD13 | 1.75 | 0.66 |
| 1:D:255:ALA:HB3 | 1:D:261:PHE:HD1 | 1.60 | 0.66 |
| 1:D:613:LEU:N | 1:D:770:VAL:O | 2.27 | 0.66 |
| 1:D:673:ASN:O | 1:D:676:GLN:HB2 | 1.94 | 0.66 |
| 1:D:841:ALA:O | 1:D:845:LEU:N | 2.15 | 0.66 |
| 1:E:858:VAL:HB | 1:E:877:LEU:HD12 | 1.77 | 0.66 |
| 1:F:215:GLY:HA2 | 2:F:1001:AGS:O1B | 1.94 | 0.66 |
| 1:C:14:ILE:H | 1:C:159:ASP:CA | 2.08 | 0.66 |
| 1:C:351:ILE:HG12 | 2:C:1001:AGS:N6 | 2.09 | 0.66 |
| 1:C:671:LEU:O | 1:C:674:GLN:HB3 | 1.94 | 0.66 |
| 1:D:203:ARG:HH12 | 1:E:363:HIS:CD2 | 2.12 | 0.66 |
| 1:D:242:LYS:HG2 | 1:D:278:LEU:O | 1.96 | 0.66 |
| 1:D:378:LEU:O | 1:D:381:ARG:HG2 | 1.95 | 0.66 |
| 1:D:786:ILE:O | 1:D:789:LYS:HE3 | 1.96 | 0.66 |
| 1:D:815:ALA:O | 1:D:818:GLY:N | 2.29 | 0.66 |
| 1:E:247:ASP:O | 1:E:250:ALA:HB3 | 1.94 | 0.66 |
| 1:E:301:LEU:HG | 1:E:305:LEU:HG | 1.76 | 0.66 |
| 1:E:504:ASP:OD1 | 1:E:505:LEU:N | 2.27 | 0.66 |
| 1:E:829:ASN:HA | 1:E:832:ILE:HD12 | 1.75 | 0.66 |
| 1:E:833:GLN:O | 1:E:836:ILE:HG12 | 1.94 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:214:PRO:C | 1:F:218:LYS:HZ1 | 2.03 | 0.66 |
| 1:A:324:ILE:O | 1:A:328:ASP:N | 2.24 | 0.66 |
| 1:B:195:SER:HB2 | 1:B:198:ARG:HH22 | 1.61 | 0.66 |
| 1:B:203:ARG:HB2 | 1:C:359:TYR:OH | 1.95 | 0.66 |
| 1:B:353:ARG:HH22 | 1:B:372:LEU:HD12 | 1.60 | 0.66 |
| 1:B:700:LEU:O | 1:B:703:LEU:N | 2.28 | 0.66 |
| 1:B:783:ILE:O | 1:B:787:ARG:HG2 | 1.95 | 0.66 |
| 1:C:203:ARG:HH11 | 1:D:363:HIS:HD2 | 1.43 | 0.66 |
| 1:C:551:ALA:O | 1:C:554:THR:N | 2.28 | 0.66 |
| 1:C:571:HIS:O | 1:C:574:ARG:HG2 | 1.95 | 0.66 |
| 1:D:363:HIS:HB3 | 1:D:407:ARG:NH2 | 2.10 | 0.66 |
| 1:D:563:GLU:HG3 | 1:D:568:LYS:HZ1 | 1.59 | 0.66 |
| 1:D:623:LEU:O | 1:D:627:VAL:N | 2.24 | 0.66 |
| 1:E:332:GLU:OE1 | 1:E:337:LYS:NZ | 2.28 | 0.66 |
| 1:E:638:MET:C | 1:E:682:VAL:HG11 | 2.21 | 0.66 |
| 1:F:571:HIS:HA | 1:F:574:ARG:HG2 | 1.76 | 0.66 |
| 1:F:609:SER:HB2 | 1:F:724:ILE:HG22 | 1.75 | 0.66 |
| 1:A:268:VAL:HA | 1:A:271:GLU:HB3 | 1.78 | 0.66 |
| 1:A:654:LYS:HG2 | 1:A:656:LEU:H | 1.60 | 0.66 |
| 1:A:876:CYS:SG | 1:A:877:LEU:N | 2.68 | 0.66 |
| 1:B:208:PRO:HD3 | 1:B:311:LYS:HE3 | 1.77 | 0.66 |
| 1:B:576:LEU:O | 1:B:579:GLU:N | 2.29 | 0.66 |
| 1:C:274:GLU:N | 1:C:276:LYS:HZ1 | 1.92 | 0.66 |
| 1:C:276:LYS:HB3 | 1:C:279:ILE:HD12 | 1.78 | 0.66 |
| 1:C:567:GLU:OE1 | 1:C:567:GLU:N | 2.16 | 0.66 |
| 1:C:648:GLU:N | 1:C:648:GLU:OE1 | 2.28 | 0.66 |
| 1:C:857:VAL:HG13 | 1:C:879:VAL:N | 2.11 | 0.66 |
| 1:D:429:LYS:HD3 | 1:D:445:LEU:HD21 | 1.78 | 0.66 |
| 1:E:460:GLU:HA | 1:E:463:ARG:CZ | 2.24 | 0.66 |
| 1:E:543:SER:HG | 1:E:547:SER:HG | 1.43 | 0.66 |
| 1:E:617:GLY:HA2 | 1:E:826:ARG:HE | 1.61 | 0.66 |
| 1:E:710:SER:OG | 1:E:715:THR:N | 2.28 | 0.66 |
| 1:F:242:LYS:NZ | 1:F:277:THR:HG21 | 2.11 | 0.66 |
| 1:F:299:ASN:HB3 | 1:F:302:LYS:CE | 2.23 | 0.66 |
| 1:F:685:PHE:HB2 | 1:F:726:THR:OG1 | 1.96 | 0.66 |
| 1:F:687:GLU:O | 1:F:727:SER:OG | 2.12 | 0.66 |
| 1:B:167:LEU:HD13 | 1:B:271:GLU:HG2 | 1.78 | 0.66 |
| 1:B:172:ILE:HG23 | 1:B:246:LEU:HG | 1.76 | 0.66 |
| 1:B:216:ILE:HA | 1:B:219:THR:OG1 | 1.95 | 0.66 |
| 1:B:731:ALA:O | 1:B:735:ASN:N | 2.28 | 0.66 |
| 1:B:843:ARG:HD3 | 1:B:846:LYS:HB2 | 1.76 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:299:ASN:OD1 | 1:C:300:ILE:N | 2.29 | 0.66 |
| 1:D:273:GLU:CG | 1:D:274:GLU:HG3 | 2.21 | 0.66 |
| 1:D:542:ASP:O | 1:D:545:THR:OG1 | 2.12 | 0.66 |
| 1:E:189:ARG:HH22 | 1:E:341:ALA:N | 1.94 | 0.66 |
| 1:E:571:HIS:CD2 | 1:E:574:ARG:HD3 | 2.31 | 0.66 |
| 1:E:671:LEU:C | 1:E:675:LEU:HB2 | 2.21 | 0.66 |
| 1:F:363:HIS:HE2 | 1:F:397:ASP:HA | 1.60 | 0.66 |
| 1:F:819:TYR:OH | 1:F:826:ARG:O | 2.06 | 0.66 |
| 1:A:255:ALA:HA | 1:A:260:ASP:OD2 | 1.95 | 0.66 |
| 1:B:207:ASN:ND2 | 1:B:331:PHE:HZ | 1.94 | 0.66 |
| 1:B:244:PHE:HD1 | 1:B:279:ILE:HG22 | 1.61 | 0.66 |
| 1:B:296:ASP:O | 1:B:299:ASN:N | 2.27 | 0.66 |
| 1:B:674:GLN:HG3 | 1:B:678:LYS:HE2 | 1.77 | 0.66 |
| 1:B:843:ARG:HH11 | 1:B:848:GLU:HG2 | 1.61 | 0.66 |
| 1:C:733:PHE:O | 1:C:736:SER:OG | 2.09 | 0.66 |
| 1:C:782:LYS:O | 1:C:785:ASP:OD1 | 2.14 | 0.66 |
| 1:D:599:SER:HG | 1:D:600:GLY:N | 1.93 | 0.66 |
| 1:E:268:VAL:HA | 1:E:271:GLU:HB2 | 1.77 | 0.66 |
| 1:E:748:ASN:CA | 1:E:751:MET:HG2 | 2.21 | 0.66 |
| 1:F:704:ASP:HA | 1:F:765:ARG:HD3 | 1.67 | 0.66 |
| 1:A:708:ILE:H | 1:A:717:ASP:H | 1.41 | 0.66 |
| 1:B:315:ALA:O | 1:B:316:THR:OG1 | 2.14 | 0.66 |
| 1:C:47:SER:O | 1:C:52:GLN:N | 2.27 | 0.66 |
| 1:C:170:TYR:CE1 | 1:C:249:ALA:HB1 | 2.29 | 0.66 |
| 1:C:261:PHE:O | 1:C:265:PHE:N | 2.23 | 0.66 |
| 1:C:390:ASP:OD1 | 1:C:391:SER:N | 2.29 | 0.66 |
| 1:C:786:ILE:N | 1:C:789:LYS:NZ | 2.43 | 0.66 |
| 1:D:201:ALA:HA | 1:D:238:LEU:HD21 | 1.78 | 0.66 |
| 1:D:855:VAL:HG23 | 1:D:880:LEU:HD22 | 1.78 | 0.66 |
| 1:E:746:THR:HA | 1:E:749:LEU:HD12 | 1.78 | 0.66 |
| 1:F:610:PHE:HB2 | 1:F:724:ILE:HG21 | 1.77 | 0.66 |
| 1:F:614:GLY:O | 1:F:728:ALA:HB3 | 1.95 | 0.66 |
| 1:A:565:GLU:H | 1:A:568:LYS:HD2 | 1.60 | 0.66 |
| 1:B:654:LYS:HD3 | 1:B:692:HIS:CB | 2.24 | 0.66 |
| 1:B:782:LYS:HD2 | 1:B:785:ASP:OD2 | 1.96 | 0.66 |
| 1:B:793:GLU:O | 1:B:798:ASN:ND2 | 2.29 | 0.66 |
| 1:C:205:LYS:HG2 | 1:C:336:GLN:NE2 | 2.10 | 0.66 |
| 1:C:366:ARG:NH1 | 1:C:538:GLN:O | 2.29 | 0.66 |
| 1:C:371:ALA:C | 1:C:374:THR:HG1 | 2.02 | 0.66 |
| 1:C:841:ALA:O | 1:C:845:LEU:N | 2.20 | 0.66 |
| 1:D:285:GLU:O | 1:D:289:LEU:HG | 1.95 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:355:LEU:O | 1:D:358:LYS:N | 2.22 | 0.66 |
| 1:D:358:LYS:O | 1:D:361:ILE:HB | 1.96 | 0.66 |
| 1:D:366:ARG:O | 1:D:537:ILE:HB | 1.96 | 0.66 |
| 1:D:510:ILE:HG23 | 1:D:514:LYS:HD2 | 1.77 | 0.66 |
| 2:D:1001:AGS:O3G | 2:D:1001:AGS:O2A | 2.14 | 0.66 |
| 1:E:202:ARG:NH1 | 1:E:205:LYS:HB2 | 2.10 | 0.66 |
| 1:E:569:LEU:HA | 1:E:630:PHE:CZ | 2.23 | 0.66 |
| 1:E:704:ASP:C | 1:E:707:ARG:NH1 | 2.54 | 0.66 |
| 1:E:830:ARG:C | 1:E:833:GLN:HE22 | 2.04 | 0.66 |
| 1:F:214:PRO:O | 1:F:218:LYS:NZ | 2.24 | 0.66 |
| 1:F:301:LEU:HG | 1:F:303:PRO:HD2 | 1.77 | 0.66 |
| 1:F:564:SER:N | 1:F:568:LYS:HD2 | 2.06 | 0.66 |
| 1:F:632:PHE:HZ | 1:F:720:ASN:HB3 | 1.61 | 0.66 |
| 1:F:783:ILE:O | 1:F:787:ARG:HG2 | 1.95 | 0.66 |
| 1:A:208:PRO:O | 1:A:338:ILE:N | 2.29 | 0.66 |
| 1:A:287:HIS:ND1 | 1:A:287:HIS:O | 2.29 | 0.66 |
| 1:A:732:GLU:HA | 1:A:735:ASN:HB2 | 1.78 | 0.66 |
| 1:B:685:PHE:CE2 | 1:B:687:GLU:HA | 2.31 | 0.66 |
| 1:C:173:ASP:OD2 | 1:C:176:GLU:C | 2.39 | 0.66 |
| 1:C:243:LEU:HD23 | 1:C:245:SER:HB2 | 1.78 | 0.66 |
| 1:C:360:GLU:O | 1:C:363:HIS:N | 2.29 | 0.66 |
| 1:C:768:SER:OG | 1:C:769:ILE:N | 2.28 | 0.66 |
| 1:D:369:ASP:O | 1:D:372:LEU:HB3 | 1.96 | 0.66 |
| 1:D:799:ASP:OD1 | 1:D:800:LYS:HG2 | 1.96 | 0.66 |
| 1:E:387:ARG:O | 1:E:390:ASP:N | 2.29 | 0.66 |
| 1:F:320:GLU:OE1 | 1:F:320:GLU:HA | 1.95 | 0.66 |
| 1:F:609:SER:OG | 1:F:723:VAL:O | 2.13 | 0.66 |
| 1:F:639:ILE:HG22 | 1:F:640:ARG:H | 1.61 | 0.66 |
| 1:F:699:MET:SD | 1:F:708:ILE:HG21 | 2.35 | 0.66 |
| 1:A:612:PHE:CG | 1:A:769:ILE:HG22 | 2.30 | 0.65 |
| 1:A:843:ARG:O | 1:A:847:ASN:N | 2.27 | 0.65 |
| 1:B:803:LYS:H | 1:B:853:GLU:HG2 | 1.60 | 0.65 |
| 1:C:208:PRO:HD3 | 1:C:313:ILE:HG23 | 1.78 | 0.65 |
| 1:C:583:GLN:HG3 | 1:C:773:ASN:ND2 | 2.11 | 0.65 |
| 1:C:650:TYR:OH | 1:C:656:LEU:HB3 | 1.95 | 0.65 |
| 1:C:778:LYS:O | 1:C:782:LYS:HG2 | 1.96 | 0.65 |
| 1:D:187:ILE:O | 2:D:1001:AGS:N6 | 2.19 | 0.65 |
| 1:D:210:LEU:HA | 1:D:338:ILE:O | 1.97 | 0.65 |
| 1:D:565:GLU:H | 1:D:565:GLU:CD | 2.03 | 0.65 |
| 1:D:605:ARG:NE | 1:D:707:ARG:HH21 | 1.94 | 0.65 |
| 1:D:702:MET:HA | 1:D:706:GLY:HA2 | 1.78 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:805:ASN:HA | 1:D:855:VAL:O | 1.95 | 0.65 |
| 1:E:803:LYS:HG3 | 1:E:804:LEU:N | 2.10 | 0.65 |
| 1:E:820:SER:H | 1:E:824:GLY:HA2 | 1.60 | 0.65 |
| 1:F:282:PHE:HD1 | 1:F:313:ILE:HB | 1.62 | 0.65 |
| 1:F:640:ARG:NH1 | 1:F:686:ASP:CG | 2.54 | 0.65 |
| 1:A:605:ARG:O | 1:A:706:GLY:N | 2.28 | 0.65 |
| 1:C:173:ASP:CG | 1:C:176:GLU:HG3 | 2.21 | 0.65 |
| 1:C:465:ARG:HH12 | 1:C:529:ARG:CD | 2.07 | 0.65 |
| 1:D:146:GLU:O | 1:D:164:LEU:N | 2.29 | 0.65 |
| 1:D:175:THR:O | 1:D:179:ARG:HG2 | 1.97 | 0.65 |
| 1:D:810:ALA:O | 1:D:814:LEU:HG | 1.96 | 0.65 |
| 1:E:374:THR:HA | 1:E:377:GLN:CD | 2.21 | 0.65 |
| 1:E:707:ARG:HG2 | 1:E:718:CYS:SG | 2.36 | 0.65 |
| 1:E:745:SER:O | 1:E:749:LEU:HG | 1.95 | 0.65 |
| 1:A:218:LYS:HG3 | 1:A:219:THR:N | 2.10 | 0.65 |
| 1:A:227:GLN:HG3 | 1:A:228:ARG:H | 1.60 | 0.65 |
| 1:A:259:GLY:H | 1:A:261:PHE:HB2 | 1.59 | 0.65 |
| 1:A:700:LEU:O | 1:A:704:ASP:N | 2.29 | 0.65 |
| 1:B:231:ASP:OD1 | 1:B:232:ASP:N | 2.29 | 0.65 |
| 1:C:298:ALA:HB1 | 1:C:302:LYS:HB2 | 1.79 | 0.65 |
| 1:C:434:ASP:OD2 | 1:C:445:LEU:HD11 | 1.97 | 0.65 |
| 1:C:672:THR:HG1 | 1:C:673:ASN:H | 1.42 | 0.65 |
| 1:C:826:ARG:O | 1:C:830:ARG:N | 2.21 | 0.65 |
| 1:D:566:ASN:O | 1:D:570:ILE:N | 2.27 | 0.65 |
| 1:D:842:LEU:O | 1:D:845:LEU:HB3 | 1.96 | 0.65 |
| 1:F:283:ILE:N | 1:F:313:ILE:O | 2.28 | 0.65 |
| 1:F:603:ASN:HB3 | 1:F:605:ARG:N | 2.12 | 0.65 |
| 1:A:247:ASP:OD1 | 1:A:284:ASP:N | 2.20 | 0.65 |
| 1:A:380:LYS:HZ2 | 1:A:381:ARG:HA | 1.61 | 0.65 |
| 1:A:569:LEU:HA | 1:A:572:MET:HG2 | 1.77 | 0.65 |
| 1:B:210:LEU:HD11 | 1:B:337:LYS:NZ | 2.12 | 0.65 |
| 1:B:220:ALA:O | 1:B:223:GLU:HB2 | 1.97 | 0.65 |
| 1:B:619:GLY:O | 1:B:623:LEU:N | 2.26 | 0.65 |
| 1:B:684:LEU:HD23 | 1:B:685:PHE:H | 1.62 | 0.65 |
| 1:B:751:MET:CB | 1:B:755:ARG:HH12 | 2.08 | 0.65 |
| 1:B:784:VAL:O | 1:B:787:ARG:N | 2.29 | 0.65 |
| 1:C:95:VAL:O | 1:C:99:ALA:N | 2.30 | 0.65 |
| 1:C:167:LEU:C | 1:C:264:ARG:NH2 | 2.54 | 0.65 |
| 1:C:802:TYR:N | 1:C:853:GLU:OE2 | 2.29 | 0.65 |
| 1:D:397:ASP:O | 1:D:400:CYS:N | 2.29 | 0.65 |
| 1:E:786:ILE:N | 1:E:789:LYS:NZ | 2.45 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:810:ALA:HA | 1:E:857:VAL:HG21 | 1.78 | 0.65 |
| 1:E:828:LEU:O | 1:E:832:ILE:N | 2.27 | 0.65 |
| 1:F:708:ILE:CD1 | 1:F:718:CYS:HB2 | 2.27 | 0.65 |
| 1:F:855:VAL:HA | 1:F:880:LEU:HD13 | 1.76 | 0.65 |
| 1:A:202:ARG:O | 1:B:397:ASP:OD2 | 2.13 | 0.65 |
| 1:B:859:LEU:HB2 | 1:B:876:CYS:SG | 2.36 | 0.65 |
| 1:C:180:GLN:OE1 | 1:C:180:GLN:N | 2.23 | 0.65 |
| 1:C:348:THR:HG22 | 1:C:352:LEU:HD21 | 1.79 | 0.65 |
| 1:C:417:LYS:HE2 | 1:C:459:LEU:HB3 | 1.79 | 0.65 |
| 1:C:686:ASP:C | 1:C:688:VAL:N | 2.53 | 0.65 |
| 1:D:207:ASN:OD1 | 1:D:311:LYS:HB3 | 1.97 | 0.65 |
| 1:D:295:ASP:C | 1:D:297:ALA:H | 2.02 | 0.65 |
| 1:F:605:ARG:CG | 1:F:706:GLY:HA3 | 2.24 | 0.65 |
| 1:A:402:GLY:O | 1:A:406:ALA:N | 2.30 | 0.65 |
| 1:B:251:LEU:H | 1:B:264:ARG:HH12 | 1.42 | 0.65 |
| 1:C:165:GLU:OE1 | 1:C:165:GLU:N | 2.20 | 0.65 |
| 1:C:170:TYR:CE2 | 1:C:249:ALA:C | 2.70 | 0.65 |
| 1:C:219:THR:O | 1:C:222:ILE:N | 2.29 | 0.65 |
| 1:C:628:ALA:O | 1:C:631:LEU:N | 2.30 | 0.65 |
| 1:C:723:VAL:O | 1:C:724:ILE:HG13 | 1.97 | 0.65 |
| 1:D:248:LEU:HD12 | 1:D:251:LEU:HD12 | 1.78 | 0.65 |
| 1:E:710:SER:O | 1:E:714:LYS:HA | 1.96 | 0.65 |
| 1:F:209:CYS:SG | 1:F:210:LEU:N | 2.67 | 0.65 |
| 1:F:557:PRO:O | 1:F:560:LYS:N | 2.29 | 0.65 |
| 1:A:373:VAL:HG12 | 1:A:377:GLN:HE22 | 1.62 | 0.65 |
| 1:A:596:LEU:O | 1:A:601:LEU:HB2 | 1.97 | 0.65 |
| 1:A:635:GLU:O | 1:A:638:MET:N | 2.28 | 0.65 |
| 1:A:642:ASP:OD1 | 1:A:644:SER:N | 2.27 | 0.65 |
| 1:A:734:ILE:HG13 | 1:A:738:GLN:H | 1.62 | 0.65 |
| 1:C:583:GLN:CD | 1:C:583:GLN:H | 2.05 | 0.65 |
| 1:C:785:ASP:C | 1:C:789:LYS:HZ2 | 2.04 | 0.65 |
| 1:C:850:LYS:NZ | 1:C:851:ASP:OD2 | 2.29 | 0.65 |
| 1:D:203:ARG:HH11 | 1:E:362:HIS:HB3 | 1.62 | 0.65 |
| 1:D:205:LYS:HE3 | 1:D:335:PHE:N | 2.11 | 0.65 |
| 1:D:579:GLU:HB2 | 1:D:626:LYS:NZ | 2.12 | 0.65 |
| 1:D:605:ARG:CZ | 1:D:707:ARG:HE | 2.09 | 0.65 |
| 1:D:687:GLU:O | 1:D:691:ALA:N | 2.30 | 0.65 |
| 1:D:759:ARG:HB3 | 1:D:763:LEU:CD1 | 2.26 | 0.65 |
| 1:D:811:LYS:O | 1:D:815:ALA:N | 2.29 | 0.65 |
| 1:E:191:GLU:HA | 1:E:194:ARG:HD3 | 1.78 | 0.65 |
| 1:E:647:SER:HA | 1:E:692:HIS:HB2 | 1.78 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:787:ARG:HA | 1:F:790:GLU:CD | 2.22 | 0.65 |
| 1:B:842:LEU:CB | 1:B:846:LYS:HZ3 | 2.10 | 0.65 |
| 1:C:177:GLN:O | 1:C:182:LYS:HB2 | 1.96 | 0.65 |
| 1:C:224:GLY:O | 1:C:227:GLN:HB3 | 1.95 | 0.65 |
| 1:C:671:LEU:O | 1:C:675:LEU:HG | 1.97 | 0.65 |
| 1:C:751:MET:SD | 1:C:755:ARG:NH2 | 2.69 | 0.65 |
| 1:C:839:LYS:HE3 | 1:C:857:VAL:HG22 | 1.79 | 0.65 |
| 1:D:687:GLU:O | 1:D:690:LYS:N | 2.30 | 0.65 |
| 1:D:710:SER:OG | 1:D:713:GLY:N | 2.29 | 0.65 |
| 1:D:859:LEU:O | 1:D:878:GLU:N | 2.27 | 0.65 |
| 1:E:202:ARG:HH12 | 1:E:205:LYS:HB2 | 1.62 | 0.65 |
| 1:E:213:GLU:O | 1:E:387:ARG:NH1 | 2.30 | 0.65 |
| 1:E:385:TYR:CD1 | 1:E:386:ARG:NH1 | 2.64 | 0.65 |
| 1:E:799:ASP:OD1 | 1:E:800:LYS:N | 2.26 | 0.65 |
| 1:E:820:SER:H | 1:E:824:GLY:CA | 2.09 | 0.65 |
| 1:E:833:GLN:HA | 1:E:836:ILE:HG23 | 1.77 | 0.65 |
| 1:F:294:LYS:HE2 | 1:F:325:VAL:CG1 | 2.25 | 0.65 |
| 1:F:331:PHE:CA | 1:F:334:ARG:HG3 | 2.08 | 0.65 |
| 1:F:651:ALA:H | 1:F:654:LYS:HZ2 | 1.43 | 0.65 |
| 1:A:326:GLU:OE1 | 1:A:326:GLU:N | 2.16 | 0.65 |
| 1:A:785:ASP:O | 1:A:788:LEU:HG | 1.97 | 0.65 |
| 1:B:376:ALA:O | 1:B:380:LYS:N | 2.15 | 0.65 |
| 1:B:587:ILE:O | 1:B:591:SER:N | 2.17 | 0.65 |
| 1:B:757:HIS:HB3 | 1:B:758:PHE:CE1 | 2.32 | 0.65 |
| 1:C:825:ALA:H | 1:C:827:PRO:HG2 | 1.61 | 0.65 |
| 1:C:857:VAL:HG13 | 1:C:879:VAL:H | 1.61 | 0.65 |
| 1:D:167:LEU:HA | 1:D:170:TYR:CD2 | 2.31 | 0.65 |
| 1:D:485:GLU:HB3 | 1:D:489:LYS:HE3 | 1.79 | 0.65 |
| 1:D:556:ILE:HD13 | 1:D:633:ASN:ND2 | 2.12 | 0.65 |
| 1:E:214:PRO:C | 1:E:387:ARG:HH11 | 2.00 | 0.65 |
| 1:E:575:ASP:OD1 | 1:E:575:ASP:N | 2.28 | 0.65 |
| 1:E:668:GLY:O | 1:E:672:THR:N | 2.29 | 0.65 |
| 1:E:826:ARG:HE | 2:E:1002:AGS:H1' | 1.61 | 0.65 |
| 1:F:778:LYS:O | 1:F:781:HIS:N | 2.24 | 0.65 |
| 1:A:216:ILE:O | 1:A:220:ALA:N | 2.24 | 0.65 |
| 1:A:248:LEU:HD13 | 1:A:251:LEU:H | 1.59 | 0.65 |
| 1:A:262:GLU:OE2 | 1:A:297:ALA:N | 2.29 | 0.65 |
| 1:A:813:PHE:CD2 | 1:A:857:VAL:HG11 | 2.32 | 0.65 |
| 1:B:189:ARG:NH1 | 1:B:341:ALA:C | 2.47 | 0.65 |
| 1:B:226:ALA:O | 1:B:230:ILE:N | 2.21 | 0.65 |
| 1:B:637:MET:HE1 | 1:B:678:LYS:O | 1.96 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:298:ALA:HA | 1:C:301:LEU:HG | 1.79 | 0.65 |
| 1:C:356:GLN:HG2 | 1:C:357:PRO:HD3 | 1.78 | 0.65 |
| 1:C:368:LEU:HD13 | 1:C:540:VAL:H | 1.61 | 0.65 |
| 1:C:713:GLY:C | 1:C:714:LYS:HZ3 | 2.05 | 0.65 |
| 1:D:369:ASP:HA | 1:D:372:LEU:HB3 | 1.79 | 0.65 |
| 1:D:381:ARG:NH1 | 1:D:382:TYR:HE1 | 1.94 | 0.65 |
| 1:E:410:LYS:HB3 | 1:E:413:GLU:HB2 | 1.78 | 0.65 |
| 1:E:581:VAL:HG11 | 1:E:772:PHE:CE1 | 2.32 | 0.65 |
| 1:E:711:GLY:O | 1:E:713:GLY:N | 2.28 | 0.65 |
| 1:F:218:LYS:O | 1:F:221:ILE:HB | 1.97 | 0.65 |
| 1:F:742:ILE:CG2 | 1:F:747:LYS:HZ2 | 2.09 | 0.65 |
| 1:A:192:GLU:O | 1:A:196:THR:N | 2.28 | 0.64 |
| 1:A:596:LEU:HD21 | 1:B:838:ASN:HA | 1.78 | 0.64 |
| 1:B:770:VAL:C | 1:B:771:ILE:HG13 | 2.21 | 0.64 |
| 1:C:242:LYS:H | 1:C:279:ILE:HA | 1.62 | 0.64 |
| 1:C:275:SER:OG | 1:C:276:LYS:N | 2.26 | 0.64 |
| 1:D:420:GLN:O | 1:D:424:ILE:N | 2.27 | 0.64 |
| 1:E:512:ASP:OD1 | 1:E:516:GLN:N | 2.30 | 0.64 |
| 1:E:618:SER:N | 2:E:1002:AGS:O1B | 2.27 | 0.64 |
| 1:E:858:VAL:O | 1:E:877:LEU:N | 2.30 | 0.64 |
| 1:F:176:GLU:OE1 | 1:F:176:GLU:N | 2.28 | 0.64 |
| 1:F:250:ALA:HB1 | 1:F:264:ARG:HG2 | 1.78 | 0.64 |
| 1:A:229:ILE:CA | 1:A:233:ASP:HB2 | 2.20 | 0.64 |
| 1:B:648:GLU:HB3 | 1:B:693:PRO:HD3 | 1.79 | 0.64 |
| 1:C:214:PRO:HA | 1:C:218:LYS:HE3 | 1.80 | 0.64 |
| 1:C:228:ARG:HA | 1:C:231:ASP:OD2 | 1.97 | 0.64 |
| 1:C:630:PHE:C | 1:C:633:ASN:HD21 | 2.05 | 0.64 |
| 1:C:681:SER:OG | 1:C:682:VAL:N | 2.31 | 0.64 |
| 1:C:731:ALA:O | 1:C:734:ILE:N | 2.30 | 0.64 |
| 1:C:752:GLY:O | 1:C:756:GLN:HG3 | 1.98 | 0.64 |
| 1:C:807:THR:HG23 | 1:C:856:ASN:HD21 | 1.63 | 0.64 |
| 1:D:372:LEU:HA | 1:D:546:ILE:HD11 | 1.79 | 0.64 |
| 1:D:375:ALA:HB2 | 1:D:546:ILE:HD13 | 1.79 | 0.64 |
| 1:D:843:ARG:HA | 1:D:846:LYS:NZ | 2.11 | 0.64 |
| 1:E:321:TYR:O | 1:E:325:VAL:N | 2.20 | 0.64 |
| 1:E:812:ASP:HA | 1:E:815:ALA:HB3 | 1.80 | 0.64 |
| 1:F:369:ASP:O | 1:F:372:LEU:N | 2.29 | 0.64 |
| 1:F:699:MET:CA | 1:F:702:MET:HG2 | 2.27 | 0.64 |
| 1:F:708:ILE:H | 1:F:715:THR:HG23 | 1.62 | 0.64 |
| 1:F:778:LYS:C | 1:F:781:HIS:HD2 | 2.05 | 0.64 |
| 1:A:196:THR:HA | 1:A:199:VAL:HB | 1.79 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:377:GLN:O | 1:A:380:LYS:HB3 | 1.96 | 0.64 |
| 1:B:170:TYR:CD1 | 1:B:250:ALA:HB1 | 2.30 | 0.64 |
| 1:B:744:GLU:HA | 1:B:747:LYS:HE3 | 1.77 | 0.64 |
| 1:C:213:GLU:OE2 | 1:C:387:ARG:CZ | 2.45 | 0.64 |
| 1:C:353:ARG:O | 1:C:356:GLN:HG2 | 1.97 | 0.64 |
| 1:C:572:MET:O | 1:C:576:LEU:HG | 1.97 | 0.64 |
| 1:C:671:LEU:HD12 | 1:C:672:THR:N | 2.13 | 0.64 |
| 1:D:218:LYS:NZ | 2:D:1001:AGS:PA | 2.71 | 0.64 |
| 1:D:363:HIS:CG | 1:D:407:ARG:HH12 | 2.14 | 0.64 |
| 1:F:193:ILE:HG23 | 1:F:225:VAL:HG22 | 1.79 | 0.64 |
| 1:A:208:PRO:HD2 | 1:A:313:ILE:HG12 | 1.79 | 0.64 |
| 1:B:369:ASP:OD1 | 1:B:370:SER:N | 2.29 | 0.64 |
| 1:C:173:ASP:HA | 1:C:244:PHE:CE1 | 2.33 | 0.64 |
| 1:C:606:GLN:OE1 | 1:C:706:GLY:N | 2.30 | 0.64 |
| 1:C:686:ASP:HB3 | 1:C:690:LYS:NZ | 2.07 | 0.64 |
| 1:D:332:GLU:HA | 1:D:335:PHE:CE2 | 2.32 | 0.64 |
| 1:D:785:ASP:HA | 1:D:788:LEU:HD12 | 1.80 | 0.64 |
| 1:E:228:ARG:HH22 | 1:E:233:ASP:N | 1.95 | 0.64 |
| 1:E:298:ALA:O | 1:E:302:LYS:N | 2.31 | 0.64 |
| 1:E:571:HIS:CD2 | 1:E:574:ARG:HH11 | 2.15 | 0.64 |
| 1:E:623:LEU:HG | 1:E:624:ALA:N | 2.11 | 0.64 |
| 1:F:639:ILE:H | 1:F:674:GLN:HE22 | 1.43 | 0.64 |
| 1:F:710:SER:OG | 1:F:713:GLY:CA | 2.46 | 0.64 |
| 1:F:802:TYR:O | 1:F:804:LEU:N | 2.24 | 0.64 |
| 1:A:259:GLY:H | 1:A:261:PHE:CB | 2.09 | 0.64 |
| 1:A:803:LYS:HB2 | 1:A:852:LYS:HE3 | 1.80 | 0.64 |
| 1:B:590:VAL:HG13 | 1:B:610:PHE:CD2 | 2.33 | 0.64 |
| 1:B:742:ILE:HG22 | 1:B:743:GLN:H | 1.61 | 0.64 |
| 1:B:808:GLN:HE22 | 1:B:811:LYS:HB3 | 1.62 | 0.64 |
| 1:C:459:LEU:HD23 | 1:C:462:LEU:HD12 | 1.78 | 0.64 |
| 1:C:563:GLU:OE2 | 1:C:565:GLU:OE2 | 2.16 | 0.64 |
| 1:C:688:VAL:HB | 1:C:725:MET:HB3 | 1.79 | 0.64 |
| 1:C:785:ASP:CG | 1:C:789:LYS:HZ1 | 2.06 | 0.64 |
| 1:D:654:LYS:HE2 | 1:D:656:LEU:HB2 | 1.80 | 0.64 |
| 1:D:673:ASN:HB2 | 1:D:677:TYR:CE2 | 2.32 | 0.64 |
| 1:D:685:PHE:H | 1:D:725:MET:HG2 | 1.63 | 0.64 |
| 1:E:172:ILE:O | 1:E:245:SER:N | 2.30 | 0.64 |
| 1:E:607:PRO:CD | 1:E:707:ARG:HH12 | 2.08 | 0.64 |
| 1:E:609:SER:O | 1:E:767:SER:HB2 | 1.97 | 0.64 |
| 1:F:283:ILE:HB | 1:F:289:LEU:HD23 | 1.79 | 0.64 |
| 1:F:576:LEU:HD21 | 1:F:630:PHE:CD2 | 2.32 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:807:THR:O | 1:A:811:LYS:N | 2.28 | 0.64 |
| 1:B:142:GLN:O | 1:B:146:GLU:N | 2.30 | 0.64 |
| 1:C:167:LEU:C | 1:C:264:ARG:HH21 | 2.04 | 0.64 |
| 1:C:262:GLU:HG2 | 1:C:263:GLU:N | 2.13 | 0.64 |
| 1:C:366:ARG:HH11 | 1:C:473:HIS:CD2 | 2.16 | 0.64 |
| 1:C:788:LEU:O | 1:C:791:ILE:N | 2.31 | 0.64 |
| 1:C:829:ASN:HA | 1:C:832:ILE:HB | 1.79 | 0.64 |
| 1:D:258:LYS:HZ2 | 1:D:262:GLU:H | 1.45 | 0.64 |
| 1:E:210:LEU:HD11 | 1:E:338:ILE:HB | 1.79 | 0.64 |
| 1:E:803:LYS:HG3 | 1:E:804:LEU:H | 1.61 | 0.64 |
| 1:E:879:VAL:HG12 | 1:E:880:LEU:N | 2.13 | 0.64 |
| 1:F:819:TYR:OH | 1:F:828:LEU:N | 2.31 | 0.64 |
| 1:A:543:SER:O | 1:A:547:SER:N | 2.30 | 0.64 |
| 1:A:641:VAL:O | 1:A:685:PHE:HA | 1.98 | 0.64 |
| 1:B:251:LEU:HD12 | 1:B:252:THR:N | 2.11 | 0.64 |
| 1:B:358:LYS:HG3 | 1:B:359:TYR:H | 1.62 | 0.64 |
| 1:B:549:THR:HG22 | 1:B:552:ARG:HH11 | 1.63 | 0.64 |
| 1:B:617:GLY:C | 1:B:826:ARG:HD2 | 2.23 | 0.64 |
| 1:B:621:THR:HG22 | 1:B:625:LYS:HG3 | 1.80 | 0.64 |
| 1:C:572:MET:O | 1:C:576:LEU:N | 2.30 | 0.64 |
| 1:C:605:ARG:NH2 | 1:C:705:ASP:H | 1.95 | 0.64 |
| 1:C:619:GLY:HA2 | 1:C:826:ARG:NH2 | 2.13 | 0.64 |
| 1:D:190:GLU:CD | 1:D:191:GLU:H | 2.05 | 0.64 |
| 1:D:349:VAL:HA | 1:D:352:LEU:HD12 | 1.79 | 0.64 |
| 1:D:590:VAL:HG12 | 1:D:594:VAL:CG2 | 2.27 | 0.64 |
| 1:D:668:GLY:O | 1:D:671:LEU:N | 2.31 | 0.64 |
| 1:D:833:GLN:C | 1:D:837:LEU:HG | 2.23 | 0.64 |
| 1:E:493:ALA:O | 1:E:496:ARG:HB3 | 1.97 | 0.64 |
| 1:E:730:GLY:O | 1:E:734:ILE:N | 2.26 | 0.64 |
| 1:F:565:GLU:HG2 | 1:F:598:ARG:NH1 | 2.11 | 0.64 |
| 1:A:224:GLY:O | 1:A:227:GLN:HG2 | 1.98 | 0.64 |
| 1:A:395:LEU:O | 1:A:399:SER:N | 2.30 | 0.64 |
| 1:B:202:ARG:CD | 1:B:206:SER:HA | 2.27 | 0.64 |
| 1:B:803:LYS:H | 1:B:853:GLU:CG | 2.10 | 0.64 |
| 1:C:609:SER:O | 1:C:767:SER:OG | 2.12 | 0.64 |
| 1:C:742:ILE:HG22 | 1:C:743:GLN:H | 1.62 | 0.64 |
| 1:D:214:PRO:HD2 | 1:D:387:ARG:HH21 | 1.62 | 0.64 |
| 1:D:259:GLY:HA2 | 1:D:262:GLU:OE2 | 1.96 | 0.64 |
| 1:D:267:GLY:O | 1:D:270:LYS:N | 2.27 | 0.64 |
| 1:D:370:SER:O | 1:D:373:VAL:HB | 1.98 | 0.64 |
| 1:E:256:LYS:HB2 | 1:E:260:ASP:OD2 | 1.97 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:699:MET:HE2 | 1:E:762:PHE:CZ | 2.33 | 0.64 |
| 1:E:777:ARG:O | 1:E:780:ILE:N | 2.31 | 0.64 |
| 1:E:785:ASP:O | 1:E:789:LYS:HG2 | 1.97 | 0.64 |
| 1:E:855:VAL:HA | 1:E:880:LEU:HD23 | 1.80 | 0.64 |
| 1:F:286:ILE:HA | 1:F:289:LEU:HD12 | 1.79 | 0.64 |
| 1:A:830:ARG:NH1 | 1:F:309:GLN:HG2 | 2.12 | 0.64 |
| 1:B:286:ILE:HG12 | 1:B:316:THR:OG1 | 1.98 | 0.64 |
| 1:C:196:THR:O | 1:C:200:LEU:N | 2.29 | 0.64 |
| 1:C:591:SER:O | 1:C:595:ARG:HG3 | 1.98 | 0.64 |
| 1:C:792:GLU:OE2 | 1:C:802:TYR:HB3 | 1.98 | 0.64 |
| 1:D:203:ARG:NH2 | 1:E:362:HIS:O | 2.31 | 0.64 |
| 1:D:639:ILE:HG22 | 1:D:674:GLN:NE2 | 2.12 | 0.64 |
| 1:E:285:GLU:OE2 | 1:E:320:GLU:OE2 | 2.15 | 0.64 |
| 1:E:344:SER:O | 1:E:348:THR:OG1 | 2.10 | 0.64 |
| 1:E:476:LEU:HD13 | 1:E:520:LEU:HD12 | 1.78 | 0.64 |
| 1:E:623:LEU:O | 1:E:627:VAL:HG23 | 1.98 | 0.64 |
| 1:E:696:LEU:HA | 1:E:699:MET:HG2 | 1.78 | 0.64 |
| 1:E:760:PRO:O | 1:E:764:ASN:N | 2.23 | 0.64 |
| 1:F:312:VAL:HG22 | 1:F:313:ILE:H | 1.63 | 0.64 |
| 1:F:626:LYS:O | 1:F:630:PHE:N | 2.21 | 0.64 |
| 1:F:837:LEU:HA | 1:F:840:LEU:HB2 | 1.78 | 0.64 |
| 1:A:205:LYS:HE2 | 1:B:398:ILE:HG13 | 1.79 | 0.64 |
| 1:A:258:LYS:HZ2 | 1:A:295:ASP:HB3 | 1.62 | 0.64 |
| 1:A:573:GLU:HG3 | 1:A:574:ARG:N | 2.13 | 0.64 |
| 1:A:655:LEU:O | 1:A:669:GLY:HA2 | 1.98 | 0.64 |
| 1:A:685:PHE:HE2 | 1:A:723:VAL:HG11 | 1.62 | 0.64 |
| 1:B:178:ALA:HB3 | 1:B:230:ILE:HG21 | 1.80 | 0.64 |
| 1:B:244:PHE:HE1 | 1:B:280:VAL:HA | 1.61 | 0.64 |
| 1:B:798:ASN:O | 1:B:801:HIS:N | 2.19 | 0.64 |
| 1:C:174:MET:H | 1:C:242:LYS:NZ | 1.96 | 0.64 |
| 1:C:189:ARG:NH1 | 1:C:341:ALA:O | 2.25 | 0.64 |
| 1:C:597:SER:C | 1:C:598:ARG:NH1 | 2.51 | 0.64 |
| 1:C:650:TYR:HH | 1:C:654:LYS:NZ | 1.92 | 0.64 |
| 1:C:708:ILE:CG2 | 1:C:709:THR:H | 2.07 | 0.64 |
| 1:C:786:ILE:N | 1:C:789:LYS:HZ2 | 1.96 | 0.64 |
| 1:D:248:LEU:HD12 | 1:D:251:LEU:HB2 | 1.78 | 0.64 |
| 1:D:417:LYS:HD2 | 1:D:420:GLN:HB2 | 1.79 | 0.64 |
| 1:D:622:GLU:HG3 | 1:D:826:ARG:HH12 | 1.63 | 0.64 |
| 1:D:743:GLN:O | 1:D:747:LYS:NZ | 2.28 | 0.64 |
| 1:D:779:ALA:C | 1:D:782:LYS:NZ | 2.56 | 0.64 |
| 1:E:244:PHE:O | 1:E:281:LEU:HA | 1.98 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:332:GLU:OE2 | 1:E:337:LYS:NZ | 2.31 | 0.64 |
| 1:E:542:ASP:N | 1:E:544:ASP:OD2 | 2.31 | 0.64 |
| 1:E:813:PHE:HA | 1:E:816:LYS:HD2 | 1.80 | 0.64 |
| 1:F:287:HIS:NE2 | 1:F:322:ARG:HA | 2.13 | 0.64 |
| 1:F:363:HIS:HE1 | 1:F:397:ASP:CB | 2.11 | 0.64 |
| 1:F:651:ALA:O | 1:F:654:LYS:NZ | 2.28 | 0.64 |
| 1:F:752:GLY:HA2 | 1:F:755:ARG:HB2 | 1.80 | 0.64 |
| 1:A:796:GLU:OE2 | 1:A:799:ASP:N | 2.31 | 0.63 |
| 1:B:572:MET:HE2 | 1:B:630:PHE:CD1 | 2.32 | 0.63 |
| 1:B:654:LYS:HZ1 | 1:B:694:ASP:CB | 2.09 | 0.63 |
| 1:B:751:MET:O | 1:B:754:VAL:HB | 1.98 | 0.63 |
| 1:B:758:PHE:HB3 | 1:B:763:LEU:HD21 | 1.80 | 0.63 |
| 1:B:787:ARG:HH11 | 1:B:790:GLU:CD | 2.06 | 0.63 |
| 1:B:835:GLU:O | 1:B:839:LYS:HG3 | 1.98 | 0.63 |
| 1:C:209:CYS:HB2 | 1:C:336:GLN:H | 1.62 | 0.63 |
| 1:C:215:GLY:O | 2:C:1001:AGS:O1A | 2.15 | 0.63 |
| 1:C:458:GLU:HA | 1:C:461:PRO:HD2 | 1.78 | 0.63 |
| 1:C:571:HIS:O | 1:C:575:ASP:N | 2.31 | 0.63 |
| 1:D:203:ARG:NH1 | 1:E:362:HIS:HB3 | 2.13 | 0.63 |
| 1:D:839:LYS:HG2 | 1:D:879:VAL:HA | 1.80 | 0.63 |
| 1:E:242:LYS:C | 1:E:279:ILE:HA | 2.23 | 0.63 |
| 1:E:296:ASP:CA | 1:E:299:ASN:HB3 | 2.27 | 0.63 |
| 1:E:462:LEU:CD1 | 1:E:465:ARG:HH11 | 2.11 | 0.63 |
| 1:F:395:LEU:O | 1:F:399:SER:OG | 2.16 | 0.63 |
| 1:F:569:LEU:HA | 1:F:572:MET:HE2 | 1.79 | 0.63 |
| 1:F:792:GLU:HG2 | 1:F:797:GLN:HG2 | 1.80 | 0.63 |
| 1:A:777:ARG:HH12 | 1:A:815:ALA:C | 2.05 | 0.63 |
| 1:B:371:ALA:HB2 | 1:B:542:ASP:HA | 1.80 | 0.63 |
| 1:C:216:ILE:HG23 | 1:C:387:ARG:HD2 | 1.79 | 0.63 |
| 1:C:700:LEU:CA | 1:C:703:LEU:HB2 | 2.20 | 0.63 |
| 1:D:258:LYS:HZ1 | 1:D:262:GLU:HB3 | 1.61 | 0.63 |
| 1:D:299:ASN:OD1 | 1:D:300:ILE:HG13 | 1.97 | 0.63 |
| 1:D:305:LEU:HA | 1:D:307:ARG:HG2 | 1.80 | 0.63 |
| 1:D:732:GLU:HG3 | 1:D:733:PHE:CD1 | 2.34 | 0.63 |
| 1:D:804:LEU:HD12 | 1:D:855:VAL:N | 2.09 | 0.63 |
| 1:D:819:TYR:HA | 1:D:825:ALA:HB2 | 1.81 | 0.63 |
| 1:E:256:LYS:NZ | 1:E:264:ARG:HD3 | 2.14 | 0.63 |
| 1:E:605:ARG:HB3 | 1:E:705:ASP:OD1 | 1.98 | 0.63 |
| 1:E:674:GLN:OE1 | 1:E:678:LYS:HG3 | 1.99 | 0.63 |
| 1:E:683:LEU:HD23 | 1:E:723:VAL:HB | 1.79 | 0.63 |
| 1:F:197:ILE:HG12 | 1:F:228:ARG:HH11 | 1.62 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:198:ARG:O | 1:F:202:ARG:HB2 | 1.97 | 0.63 |
| 1:F:356:GLN:NE2 | 1:F:367:ILE:HG21 | 2.03 | 0.63 |
| 1:A:572:MET:O | 1:A:576:LEU:N | 2.22 | 0.63 |
| 1:A:843:ARG:HD2 | 1:A:849:ILE:HG21 | 1.80 | 0.63 |
| 1:B:173:ASP:OD1 | 1:B:173:ASP:C | 2.40 | 0.63 |
| 1:B:375:ALA:O | 1:B:379:ALA:N | 2.27 | 0.63 |
| 1:B:610:PHE:O | 1:B:724:ILE:HG21 | 1.98 | 0.63 |
| 1:B:637:MET:O | 1:B:674:GLN:NE2 | 2.32 | 0.63 |
| 1:C:296:ASP:OD2 | 1:C:300:ILE:HD12 | 1.99 | 0.63 |
| 1:C:365:VAL:HA | 1:C:473:HIS:CE1 | 2.33 | 0.63 |
| 1:C:542:ASP:HA | 1:C:545:THR:HB | 1.80 | 0.63 |
| 1:D:258:LYS:HZ2 | 1:D:262:GLU:CB | 2.11 | 0.63 |
| 1:D:320:GLU:O | 1:D:324:ILE:HD12 | 1.99 | 0.63 |
| 1:D:564:SER:OG | 1:D:566:ASN:OD1 | 2.11 | 0.63 |
| 1:D:565:GLU:OE1 | 1:D:565:GLU:N | 2.20 | 0.63 |
| 1:D:733:PHE:HA | 1:D:736:SER:HB3 | 1.80 | 0.63 |
| 1:D:839:LYS:NZ | 1:D:879:VAL:N | 2.45 | 0.63 |
| 1:E:476:LEU:HD11 | 1:E:517:ILE:HG12 | 1.81 | 0.63 |
| 1:E:606:GLN:N | 1:E:705:ASP:OD2 | 2.31 | 0.63 |
| 2:E:1002:AGS:PB | 2:E:1002:AGS:H4' | 2.38 | 0.63 |
| 1:F:279:ILE:O | 1:F:310:LEU:HD21 | 1.98 | 0.63 |
| 1:B:797:GLN:HB3 | 1:B:799:ASP:CG | 2.23 | 0.63 |
| 1:B:800:LYS:N | 1:B:800:LYS:HD2 | 2.12 | 0.63 |
| 1:C:286:ILE:HG13 | 1:C:289:LEU:HB2 | 1.81 | 0.63 |
| 1:C:392:ALA:C | 1:C:396:VAL:HG23 | 2.24 | 0.63 |
| 1:C:691:ALA:HB3 | 1:C:696:LEU:HD21 | 1.81 | 0.63 |
| 1:D:271:GLU:HG2 | 1:D:276:LYS:HZ1 | 1.63 | 0.63 |
| 1:D:363:HIS:CB | 1:D:407:ARG:HH22 | 2.09 | 0.63 |
| 1:D:614:GLY:HA2 | 1:D:772:PHE:CG | 2.33 | 0.63 |
| 1:D:671:LEU:O | 1:D:675:LEU:HG | 1.97 | 0.63 |
| 1:D:728:ALA:C | 1:D:730:GLY:H | 2.07 | 0.63 |
| 1:D:744:GLU:C | 1:D:747:LYS:NZ | 2.55 | 0.63 |
| 1:E:273:GLU:OE2 | 1:E:308:GLY:HA2 | 1.99 | 0.63 |
| 1:E:324:ILE:O | 1:E:328:ASP:N | 2.25 | 0.63 |
| 1:E:351:ILE:HD13 | 2:E:1001:AGS:H2 | 1.79 | 0.63 |
| 1:E:365:VAL:HG12 | 1:E:407:ARG:NH1 | 2.11 | 0.63 |
| 1:E:828:LEU:O | 1:E:832:ILE:HG13 | 1.98 | 0.63 |
| 1:F:170:TYR:HD2 | 1:F:248:LEU:HB2 | 1.63 | 0.63 |
| 1:F:207:ASN:HB2 | 1:F:335:PHE:CD1 | 2.33 | 0.63 |
| 1:A:740:SER:HB3 | 1:A:774:LYS:NZ | 2.13 | 0.63 |
| 1:B:226:ALA:HA | 1:B:229:ILE:HD12 | 1.80 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:236:THR:OG1 | 1:B:237:ILE:N | 2.30 | 0.63 |
| 1:B:649:LYS:HB3 | 1:B:692:HIS:CE1 | 2.34 | 0.63 |
| 1:C:345:VAL:HG11 | 1:C:377:GLN:HB3 | 1.79 | 0.63 |
| 1:C:427:GLU:HB3 | 1:C:452:GLU:OE2 | 1.99 | 0.63 |
| 1:C:544:ASP:OD1 | 1:C:544:ASP:N | 2.24 | 0.63 |
| 1:C:683:LEU:H | 1:C:723:VAL:HG22 | 1.63 | 0.63 |
| 1:D:365:VAL:HG22 | 1:D:538:GLN:HE22 | 1.62 | 0.63 |
| 1:D:558:VAL:HG22 | 1:D:561:LEU:HD22 | 1.79 | 0.63 |
| 1:F:273:GLU:CD | 1:F:309:GLN:HE22 | 2.05 | 0.63 |
| 1:F:605:ARG:HD2 | 1:F:707:ARG:H | 1.63 | 0.63 |
| 1:F:842:LEU:O | 1:F:845:LEU:N | 2.22 | 0.63 |
| 1:A:211:ILE:HG12 | 1:A:317:THR:O | 1.99 | 0.63 |
| 1:A:566:ASN:OD1 | 1:A:566:ASN:N | 2.31 | 0.63 |
| 1:A:802:TYR:HE2 | 1:A:804:LEU:HB2 | 1.63 | 0.63 |
| 1:A:831:LEU:O | 1:A:834:ASN:N | 2.29 | 0.63 |
| 1:B:10:ARG:O | 1:B:14:ILE:N | 2.30 | 0.63 |
| 1:B:176:GLU:CD | 1:B:179:ARG:HB3 | 2.24 | 0.63 |
| 1:B:176:GLU:OE1 | 1:B:179:ARG:HB3 | 1.99 | 0.63 |
| 1:B:196:THR:O | 1:B:199:VAL:N | 2.31 | 0.63 |
| 1:B:549:THR:C | 1:B:552:ARG:HH11 | 2.06 | 0.63 |
| 1:B:613:LEU:HB2 | 1:B:732:GLU:OE2 | 1.97 | 0.63 |
| 1:B:646:LEU:HB2 | 1:B:690:LYS:H | 1.63 | 0.63 |
| 1:B:829:ASN:CA | 1:B:832:ILE:HB | 2.17 | 0.63 |
| 1:C:203:ARG:NE | 1:D:362:HIS:CD2 | 2.67 | 0.63 |
| 1:C:404:ALA:HA | 1:C:408:ASP:H | 1.63 | 0.63 |
| 1:C:599:SER:OG | 1:C:602:ALA:N | 2.31 | 0.63 |
| 1:C:613:LEU:HD21 | 1:C:772:PHE:CG | 2.34 | 0.63 |
| 1:C:777:ARG:HB3 | 1:C:781:HIS:CE1 | 2.33 | 0.63 |
| 1:C:827:PRO:O | 1:C:831:LEU:N | 2.30 | 0.63 |
| 1:D:462:LEU:HA | 1:D:465:ARG:HD2 | 1.81 | 0.63 |
| 1:D:546:ILE:O | 1:D:549:THR:HB | 1.98 | 0.63 |
| 1:D:611:LEU:CB | 1:D:770:VAL:H | 2.12 | 0.63 |
| 1:D:759:ARG:HE | 1:D:763:LEU:HD21 | 1.63 | 0.63 |
| 1:E:274:GLU:O | 1:E:276:LYS:N | 2.32 | 0.63 |
| 1:E:483:LEU:HG | 1:E:508:PHE:CZ | 2.34 | 0.63 |
| 1:E:667:GLU:CD | 1:E:711:GLY:HA3 | 2.24 | 0.63 |
| 1:E:695:VAL:HG12 | 1:E:699:MET:SD | 2.38 | 0.63 |
| 1:E:737:GLN:HB3 | 1:E:774:LYS:HD3 | 1.81 | 0.63 |
| 1:E:785:ASP:OD1 | 1:E:786:ILE:N | 2.32 | 0.63 |
| 1:F:211:ILE:HB | 1:F:339:GLU:CD | 2.24 | 0.63 |
| 1:A:346:ARG:HA | 1:A:349:VAL:HB | 1.80 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:592:ASN:HA | 1:A:595:ARG:HB3 | 1.79 | 0.63 |
| 1:B:378:LEU:HA | 1:B:381:ARG:HG2 | 1.79 | 0.63 |
| 1:B:819:TYR:CZ | 1:B:821:ASP:HA | 2.33 | 0.63 |
| 1:B:830:ARG:NH1 | 1:B:834:ASN:OD1 | 2.31 | 0.63 |
| 1:C:428:ILE:HG23 | 1:C:449:ARG:HH12 | 1.62 | 0.63 |
| 1:D:190:GLU:OE2 | 1:D:191:GLU:HG2 | 1.99 | 0.63 |
| 1:D:227:GLN:HE21 | 1:D:231:ASP:CG | 2.05 | 0.63 |
| 1:D:352:LEU:HD13 | 1:D:373:VAL:HG13 | 1.81 | 0.63 |
| 1:D:714:LYS:HD2 | 1:D:715:THR:H | 1.63 | 0.63 |
| 1:E:216:ILE:CG2 | 1:E:218:LYS:HZ2 | 2.09 | 0.63 |
| 1:E:528:GLU:OE1 | 1:E:528:GLU:N | 2.31 | 0.63 |
| 1:E:572:MET:O | 1:E:576:LEU:N | 2.25 | 0.63 |
| 1:E:613:LEU:HG | 1:E:728:ALA:HA | 1.81 | 0.63 |
| 1:E:724:ILE:O | 1:E:725:MET:HB3 | 1.99 | 0.63 |
| 1:F:743:GLN:C | 1:F:747:LYS:NZ | 2.57 | 0.63 |
| 1:A:817:TYR:HD1 | 1:A:874:GLU:HB3 | 1.63 | 0.63 |
| 1:B:855:VAL:O | 1:B:856:ASN:ND2 | 2.31 | 0.63 |
| 1:C:349:VAL:HB | 1:C:353:ARG:NH1 | 2.13 | 0.63 |
| 1:C:837:LEU:HD12 | 1:C:838:ASN:N | 2.14 | 0.63 |
| 1:D:321:TYR:O | 1:D:325:VAL:HG23 | 1.98 | 0.63 |
| 1:D:751:MET:O | 1:D:755:ARG:HG2 | 1.98 | 0.63 |
| 1:D:843:ARG:O | 1:D:846:LYS:N | 2.32 | 0.63 |
| 1:E:784:VAL:HG11 | 1:E:815:ALA:HB2 | 1.80 | 0.63 |
| 1:E:845:LEU:HD12 | 1:E:846:LYS:N | 2.13 | 0.63 |
| 1:F:584:MET:HE3 | 1:F:588:LYS:NZ | 2.14 | 0.63 |
| 1:A:217:GLY:HA2 | 1:A:220:ALA:HB3 | 1.81 | 0.63 |
| 1:A:736:SER:O | 1:A:738:GLN:HG2 | 1.99 | 0.63 |
| 1:B:251:LEU:HG | 1:B:264:ARG:HG2 | 1.81 | 0.63 |
| 1:B:319:ASN:OD1 | 1:B:320:GLU:N | 2.32 | 0.63 |
| 1:B:557:PRO:HB2 | 1:B:561:LEU:HD11 | 1.80 | 0.63 |
| 1:C:168:SER:N | 1:C:271:GLU:OE2 | 2.31 | 0.63 |
| 1:C:290:MET:C | 1:C:294:LYS:HG2 | 2.24 | 0.63 |
| 1:C:585:ASP:HA | 1:C:588:LYS:HG3 | 1.81 | 0.63 |
| 1:D:170:TYR:OH | 1:D:271:GLU:OE1 | 2.11 | 0.63 |
| 1:D:198:ARG:HH12 | 1:E:403:VAL:C | 2.07 | 0.63 |
| 1:D:530:ARG:NH2 | 1:D:536:MET:H | 1.97 | 0.63 |
| 1:D:798:ASN:HA | 1:D:801:HIS:CD2 | 2.34 | 0.63 |
| 1:D:803:LYS:HB3 | 1:D:806:LEU:HD11 | 1.81 | 0.63 |
| 1:E:643:CYS:N | 1:E:649:LYS:HZ3 | 1.96 | 0.63 |
| 1:F:360:GLU:OE1 | 1:F:367:ILE:CD1 | 2.47 | 0.63 |
| 1:F:607:PRO:HD3 | 1:F:705:ASP:C | 2.24 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:549:THR:HA | 1:A:552:ARG:HH11 | 1.63 | 0.62 |
| 1:A:612:PHE:CD2 | 1:A:769:ILE:HG22 | 2.34 | 0.62 |
| 1:B:191:GLU:H | 1:B:191:GLU:CD | 2.06 | 0.62 |
| 1:B:228:ARG:HA | 1:B:231:ASP:OD2 | 1.99 | 0.62 |
| 1:B:329:GLY:HA2 | 1:B:332:GLU:HB2 | 1.81 | 0.62 |
| 1:B:708:ILE:HG22 | 1:B:709:THR:H | 1.61 | 0.62 |
| 1:B:710:SER:HB3 | 1:B:714:LYS:N | 2.14 | 0.62 |
| 1:C:323:SER:HA | 1:C:326:GLU:CD | 2.24 | 0.62 |
| 1:C:324:ILE:HG23 | 1:C:327:LYS:HB2 | 1.81 | 0.62 |
| 1:C:712:GLN:C | 1:C:714:LYS:HZ3 | 2.05 | 0.62 |
| 1:D:176:GLU:O | 1:D:180:GLN:N | 2.23 | 0.62 |
| 1:D:639:ILE:HD11 | 1:D:682:VAL:C | 2.23 | 0.62 |
| 1:D:708:ILE:O | 1:D:715:THR:HA | 1.99 | 0.62 |
| 1:D:842:LEU:HG | 1:D:846:LYS:HZ1 | 1.64 | 0.62 |
| 1:E:464:GLN:O | 1:E:467:ASN:N | 2.31 | 0.62 |
| 1:E:508:PHE:CE2 | 1:E:510:ILE:HD11 | 2.34 | 0.62 |
| 1:E:694:ASP:O | 1:E:698:VAL:HG22 | 1.99 | 0.62 |
| 1:E:794:ARG:NH1 | 1:E:794:ARG:O | 2.32 | 0.62 |
| 1:F:344:SER:O | 1:F:347:GLN:NE2 | 2.27 | 0.62 |
| 1:F:646:LEU:HB3 | 1:F:691:ALA:HA | 1.81 | 0.62 |
| 1:F:781:HIS:NE2 | 1:F:782:LYS:NZ | 2.46 | 0.62 |
| 1:A:766:ILE:O | 1:B:830:ARG:NH2 | 2.32 | 0.62 |
| 1:A:830:ARG:NH2 | 1:F:275:SER:H | 1.91 | 0.62 |
| 1:B:203:ARG:HH11 | 1:C:362:HIS:HB2 | 1.61 | 0.62 |
| 1:B:346:ARG:HG3 | 1:B:347:GLN:H | 1.64 | 0.62 |
| 1:B:669:GLY:O | 1:B:672:THR:N | 2.32 | 0.62 |
| 1:B:689:GLU:OE1 | 1:B:689:GLU:N | 2.31 | 0.62 |
| 1:B:784:VAL:HG21 | 1:B:811:LYS:HG3 | 1.80 | 0.62 |
| 1:C:265:PHE:O | 1:C:269:LEU:HG | 1.98 | 0.62 |
| 1:C:318:ASN:HA | 1:C:321:TYR:HB3 | 1.81 | 0.62 |
| 1:D:316:THR:HA | 1:D:321:TYR:CD1 | 2.34 | 0.62 |
| 1:D:746:THR:O | 1:D:747:LYS:C | 2.42 | 0.62 |
| 1:D:762:PHE:CE1 | 1:D:766:ILE:HG21 | 2.33 | 0.62 |
| 1:E:302:LYS:HZ3 | 1:E:334:ARG:CD | 2.07 | 0.62 |
| 1:E:302:LYS:CE | 1:E:331:PHE:HA | 2.29 | 0.62 |
| 1:E:318:ASN:HA | 1:E:321:TYR:HE2 | 1.64 | 0.62 |
| 1:E:523:GLN:O | 1:E:527:GLU:N | 2.21 | 0.62 |
| 1:E:618:SER:HG | 1:E:620:LYS:NZ | 1.95 | 0.62 |
| 1:E:745:SER:HA | 1:E:748:ASN:OD1 | 1.99 | 0.62 |
| 1:F:702:MET:HB3 | 1:F:708:ILE:CB | 2.28 | 0.62 |
| 1:A:228:ARG:HG2 | 1:A:233:ASP:OD2 | 2.00 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:290:MET:O | 1:A:294:LYS:N | 2.24 | 0.62 |
| 1:A:693:PRO:HA | 1:A:696:LEU:HD21 | 1.81 | 0.62 |
| 1:A:696:LEU:CA | 1:A:699:MET:HB3 | 2.27 | 0.62 |
| 1:B:211:ILE:HG12 | 1:B:317:THR:C | 2.24 | 0.62 |
| 1:B:320:GLU:N | 1:B:320:GLU:OE1 | 2.32 | 0.62 |
| 1:C:199:VAL:O | 1:C:202:ARG:N | 2.30 | 0.62 |
| 1:C:216:ILE:N | 1:C:218:LYS:NZ | 2.43 | 0.62 |
| 1:C:554:THR:OG1 | 1:C:555:GLY:N | 2.32 | 0.62 |
| 1:C:577:SER:OG | 1:C:578:SER:N | 2.29 | 0.62 |
| 1:C:671:LEU:C | 1:C:675:LEU:HG | 2.24 | 0.62 |
| 1:C:696:LEU:HA | 1:C:699:MET:HG2 | 1.82 | 0.62 |
| 1:D:202:ARG:NH2 | 1:D:205:LYS:HB3 | 2.12 | 0.62 |
| 1:D:441:THR:HG22 | 1:D:442:LYS:H | 1.64 | 0.62 |
| 1:D:813:PHE:CE2 | 1:D:817:TYR:HE2 | 2.17 | 0.62 |
| 1:E:209:CYS:SG | 1:E:315:ALA:HA | 2.39 | 0.62 |
| 1:E:256:LYS:HZ1 | 1:E:264:ARG:HD3 | 1.64 | 0.62 |
| 1:E:597:SER:O | 1:E:599:SER:N | 2.32 | 0.62 |
| 1:E:645:GLU:H | 1:E:649:LYS:NZ | 1.97 | 0.62 |
| 1:E:686:ASP:CG | 1:E:690:LYS:HE2 | 2.25 | 0.62 |
| 1:E:800:LYS:HB3 | 1:E:802:TYR:CE1 | 2.33 | 0.62 |
| 1:E:807:THR:C | 1:E:811:LYS:NZ | 2.55 | 0.62 |
| 1:F:242:LYS:HG2 | 1:F:277:THR:OG1 | 1.99 | 0.62 |
| 1:F:350:ALA:HA | 1:F:353:ARG:HG2 | 1.80 | 0.62 |
| 1:F:583:GLN:O | 1:F:587:ILE:HD12 | 1.99 | 0.62 |
| 1:F:615:LEU:HD21 | 1:F:734:ILE:HD13 | 1.81 | 0.62 |
| 1:F:828:LEU:HA | 1:F:831:LEU:HB2 | 1.81 | 0.62 |
| 1:A:204:ILE:HB | 1:A:334:ARG:HE | 1.63 | 0.62 |
| 1:A:218:LYS:NZ | 1:A:387:ARG:HE | 1.97 | 0.62 |
| 1:B:171:ALA:CA | 1:B:246:LEU:HD21 | 2.28 | 0.62 |
| 1:B:176:GLU:O | 1:B:178:ALA:N | 2.32 | 0.62 |
| 1:B:348:THR:OG1 | 1:B:388:LEU:HD21 | 2.00 | 0.62 |
| 1:B:825:ALA:HA | 1:B:828:LEU:HB2 | 1.82 | 0.62 |
| 1:B:839:LYS:NZ | 1:B:877:LEU:HD23 | 2.14 | 0.62 |
| 1:C:169:LYS:N | 1:C:264:ARG:NH2 | 2.45 | 0.62 |
| 1:C:208:PRO:HG3 | 1:C:313:ILE:HG23 | 1.81 | 0.62 |
| 1:C:241:ALA:HB1 | 1:C:280:VAL:HG23 | 1.81 | 0.62 |
| 1:C:291:GLY:H | 1:C:294:LYS:HZ2 | 1.48 | 0.62 |
| 1:C:390:ASP:HA | 1:C:393:LEU:HD12 | 1.80 | 0.62 |
| 1:D:192:GLU:OE2 | 1:D:193:ILE:HG13 | 1.98 | 0.62 |
| 1:D:530:ARG:NH1 | 1:D:537:ILE:C | 2.51 | 0.62 |
| 1:D:583:GLN:OE1 | 1:D:773:ASN:N | 2.31 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:840:LEU:HD13 | 1:D:844:ILE:HD12 | 1.81 | 0.62 |
| 1:E:243:LEU:HA | 1:E:280:VAL:H | 1.64 | 0.62 |
| 1:E:298:ALA:HA | 1:E:301:LEU:HB3 | 1.82 | 0.62 |
| 1:E:637:MET:SD | 1:E:678:LYS:HE2 | 2.39 | 0.62 |
| 1:F:367:ILE:HD11 | 1:F:372:LEU:HD11 | 1.81 | 0.62 |
| 1:F:651:ALA:N | 1:F:654:LYS:NZ | 2.47 | 0.62 |
| 1:A:347:GLN:OE1 | 1:A:347:GLN:N | 2.30 | 0.62 |
| 1:B:196:THR:HA | 1:B:199:VAL:HG23 | 1.80 | 0.62 |
| 1:B:638:MET:SD | 1:B:640:ARG:NH2 | 2.72 | 0.62 |
| 1:B:683:LEU:HB3 | 1:B:723:VAL:HB | 1.82 | 0.62 |
| 1:C:190:GLU:O | 1:C:193:ILE:HB | 1.99 | 0.62 |
| 1:C:219:THR:OG1 | 2:C:1001:AGS:O3B | 2.14 | 0.62 |
| 1:C:407:ARG:NH2 | 1:C:538:GLN:N | 2.48 | 0.62 |
| 1:C:599:SER:C | 1:C:601:LEU:H | 2.07 | 0.62 |
| 1:C:839:LYS:HA | 1:C:842:LEU:HD13 | 1.81 | 0.62 |
| 1:D:48:VAL:O | 1:D:50:TYR:N | 2.33 | 0.62 |
| 1:D:265:PHE:CZ | 1:D:269:LEU:HD11 | 2.34 | 0.62 |
| 1:D:282:PHE:HA | 1:D:313:ILE:CG1 | 2.28 | 0.62 |
| 1:D:294:LYS:HZ1 | 1:D:327:LYS:HD2 | 1.65 | 0.62 |
| 1:D:461:PRO:O | 1:D:465:ARG:HG3 | 1.99 | 0.62 |
| 1:D:656:LEU:HD11 | 1:D:709:THR:HB | 1.81 | 0.62 |
| 1:D:819:TYR:CE2 | 1:D:821:ASP:HA | 2.35 | 0.62 |
| 1:E:209:CYS:H | 1:E:337:LYS:HA | 1.63 | 0.62 |
| 1:E:241:ALA:HB2 | 1:E:278:LEU:HB3 | 1.81 | 0.62 |
| 1:E:400:CYS:O | 1:E:404:ALA:N | 2.32 | 0.62 |
| 1:E:655:LEU:O | 1:E:659:THR:OG1 | 2.17 | 0.62 |
| 1:E:841:ALA:HA | 1:E:844:ILE:HD12 | 1.81 | 0.62 |
| 1:F:647:SER:HA | 1:F:690:LYS:HG2 | 1.82 | 0.62 |
| 1:A:266:LYS:O | 1:A:270:LYS:N | 2.28 | 0.62 |
| 1:A:388:LEU:HB2 | 1:A:389:PRO:HD3 | 1.82 | 0.62 |
| 1:A:777:ARG:HH22 | 1:A:815:ALA:HB3 | 1.64 | 0.62 |
| 1:A:822:ASP:OD1 | 1:A:822:ASP:N | 2.31 | 0.62 |
| 1:C:344:SER:OG | 1:C:346:ARG:HB3 | 1.99 | 0.62 |
| 1:D:177:GLN:HG3 | 1:D:182:LYS:HB2 | 1.82 | 0.62 |
| 1:D:246:LEU:CD1 | 1:D:249:ALA:HB3 | 2.30 | 0.62 |
| 1:D:272:ILE:HB | 1:D:279:ILE:HG21 | 1.81 | 0.62 |
| 1:D:316:THR:CA | 1:D:321:TYR:CD1 | 2.83 | 0.62 |
| 1:D:637:MET:HG3 | 1:D:681:SER:HB2 | 1.82 | 0.62 |
| 1:D:797:GLN:HG3 | 1:D:801:HIS:CE1 | 2.34 | 0.62 |
| 1:E:189:ARG:HE | 1:E:192:GLU:CD | 2.04 | 0.62 |
| 1:E:669:GLY:O | 1:E:673:ASN:ND2 | 2.32 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:803:LYS:HG2 | 1:E:852:LYS:HB3 | 1.80 | 0.62 |
| 1:F:190:GLU:HB3 | 1:F:228:ARG:HH21 | 1.64 | 0.62 |
| 1:F:205:LYS:HD2 | 1:F:336:GLN:HG2 | 1.80 | 0.62 |
| 1:F:812:ASP:O | 1:F:816:LYS:N | 2.28 | 0.62 |
| 1:A:175:THR:OG1 | 1:A:243:LEU:O | 2.18 | 0.62 |
| 1:A:317:THR:HG23 | 1:A:321:TYR:HB2 | 1.82 | 0.62 |
| 1:A:548:GLU:O | 1:A:552:ARG:N | 2.31 | 0.62 |
| 1:A:813:PHE:HB2 | 1:A:817:TYR:HE2 | 1.63 | 0.62 |
| 1:B:650:TYR:HD1 | 1:B:652:VAL:H | 1.48 | 0.62 |
| 1:C:367:ILE:HG22 | 1:C:368:LEU:O | 2.00 | 0.62 |
| 1:C:673:ASN:O | 1:C:676:GLN:HB3 | 2.00 | 0.62 |
| 1:D:94:LYS:O | 1:D:97:GLN:N | 2.33 | 0.62 |
| 1:D:301:LEU:HD12 | 1:D:302:LYS:N | 2.14 | 0.62 |
| 1:D:408:ASP:CG | 1:D:409:SER:N | 2.56 | 0.62 |
| 1:D:722:ILE:HG22 | 1:D:723:VAL:N | 2.14 | 0.62 |
| 1:E:428:ILE:HA | 1:E:449:ARG:HD3 | 1.82 | 0.62 |
| 1:E:827:PRO:O | 1:E:831:LEU:HG | 1.99 | 0.62 |
| 1:E:828:LEU:HG | 1:E:832:ILE:HG13 | 1.80 | 0.62 |
| 1:F:703:LEU:HD12 | 1:F:703:LEU:N | 2.12 | 0.62 |
| 1:F:732:GLU:O | 1:F:735:ASN:HB3 | 1.99 | 0.62 |
| 1:F:805:ASN:HB2 | 1:F:854:THR:HB | 1.80 | 0.62 |
| 1:A:177:GLN:CB | 1:A:182:LYS:HZ1 | 2.10 | 0.62 |
| 1:A:274:GLU:OE2 | 1:A:275:SER:OG | 2.16 | 0.62 |
| 1:A:599:SER:HB2 | 1:A:601:LEU:HG | 1.82 | 0.62 |
| 1:A:812:ASP:OD2 | 1:A:816:LYS:HD3 | 2.00 | 0.62 |
| 1:B:113:GLN:N | 1:B:159:ASP:O | 2.17 | 0.62 |
| 1:B:268:VAL:HA | 1:B:271:GLU:HB2 | 1.82 | 0.62 |
| 1:B:378:LEU:O | 1:B:382:TYR:N | 2.29 | 0.62 |
| 1:C:374:THR:O | 1:C:377:GLN:N | 2.33 | 0.62 |
| 1:C:609:SER:OG | 1:C:767:SER:N | 2.31 | 0.62 |
| 1:D:507:TYR:CG | 1:E:429:LYS:HB2 | 2.35 | 0.62 |
| 1:E:270:LYS:HD2 | 1:E:273:GLU:HB2 | 1.82 | 0.62 |
| 1:E:276:LYS:HZ1 | 1:E:279:ILE:C | 2.07 | 0.62 |
| 1:E:573:GLU:OE2 | 1:E:595:ARG:CZ | 2.48 | 0.62 |
| 1:E:681:SER:O | 1:E:722:ILE:HB | 1.99 | 0.62 |
| 1:F:551:ALA:HB2 | 1:F:557:PRO:HD3 | 1.81 | 0.62 |
| 1:B:229:ILE:O | 1:B:232:ASP:N | 2.30 | 0.62 |
| 1:B:671:LEU:HD12 | 1:B:672:THR:HG23 | 1.80 | 0.62 |
| 1:C:216:ILE:N | 1:C:218:LYS:HZ2 | 1.85 | 0.62 |
| 1:C:242:LYS:NZ | 1:C:244:PHE:CE1 | 2.57 | 0.62 |
| 1:C:306:SER:OG | 1:C:334:ARG:NH2 | 2.32 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:C:372:LEU:N | 1:C:542:ASP:OD2 | 2.32 | 0.62 |
| 1:C:744:GLU:O | 1:C:748:ASN:ND2 | 2.33 | 0.62 |
| 1:D:345:VAL:HG12 | 1:D:346:ARG:HG3 | 1.82 | 0.62 |
| 1:E:483:LEU:HD12 | 1:E:513:ILE:HG22 | 1.82 | 0.62 |
| 1:E:564:SER:O | 1:E:567:GLU:N | 2.32 | 0.62 |
| 1:E:574:ARG:C | 1:E:577:SER:HG | 2.07 | 0.62 |
| 1:E:650:TYR:HB2 | 1:E:654:LYS:CG | 2.23 | 0.62 |
| 1:F:174:MET:HE1 | 1:F:183:LEU:HB2 | 1.81 | 0.62 |
| 1:F:331:PHE:HA | 1:F:334:ARG:HD2 | 1.79 | 0.62 |
| 1:F:765:ARG:HG3 | 1:F:766:ILE:HG13 | 1.82 | 0.62 |
| 1:A:169:LYS:HZ2 | 1:A:264:ARG:NH1 | 1.97 | 0.62 |
| 1:A:211:ILE:HA | 1:A:316:THR:O | 2.00 | 0.62 |
| 1:B:265:PHE:HE2 | 1:B:297:ALA:HA | 1.64 | 0.62 |
| 1:B:646:LEU:HD22 | 1:B:687:GLU:O | 2.00 | 0.62 |
| 1:B:675:LEU:HB3 | 1:B:717:ASP:OD2 | 2.00 | 0.62 |
| 1:C:333:ARG:HG3 | 1:C:334:ARG:HG2 | 1.82 | 0.62 |
| 1:C:417:LYS:HZ3 | 1:C:463:ARG:HG3 | 1.65 | 0.62 |
| 1:C:549:THR:O | 1:C:553:LEU:HG | 1.99 | 0.62 |
| 1:C:712:GLN:HG3 | 1:C:714:LYS:HZ1 | 1.65 | 0.62 |
| 1:C:833:GLN:HG3 | 1:C:834:ASN:N | 2.15 | 0.62 |
| 1:D:187:ILE:C | 2:D:1001:AGS:HN62 | 2.06 | 0.62 |
| 1:D:235:PRO:HG3 | 1:E:408:ASP:HA | 1.82 | 0.62 |
| 1:D:508:PHE:HA | 1:D:511:PRO:HD2 | 1.82 | 0.62 |
| 1:D:530:ARG:HH22 | 1:D:538:GLN:N | 1.96 | 0.62 |
| 1:F:175:THR:HG23 | 1:F:244:PHE:HE1 | 1.65 | 0.62 |
| 1:F:290:MET:HE1 | 1:F:325:VAL:HG21 | 1.81 | 0.62 |
| 1:F:316:THR:CG2 | 1:F:322:ARG:HG2 | 2.27 | 0.62 |
| 1:F:786:ILE:O | 1:F:790:GLU:HG3 | 1.99 | 0.62 |
| 1:F:814:LEU:HD13 | 1:F:832:ILE:HD13 | 1.81 | 0.62 |
| 1:A:218:LYS:O | 1:A:222:ILE:HG12 | 1.98 | 0.61 |
| 1:A:380:LYS:NZ | 1:A:680:TYR:OH | 2.33 | 0.61 |
| 1:A:382:TYR:CD2 | 1:A:383:LEU:HB2 | 2.36 | 0.61 |
| 1:A:582:GLY:O | 1:A:587:ILE:HD12 | 2.01 | 0.61 |
| 1:B:567:GLU:HA | 1:B:570:ILE:HD12 | 1.82 | 0.61 |
| 1:B:617:GLY:H | 1:B:620:LYS:HD3 | 1.65 | 0.61 |
| 1:C:172:ILE:HG13 | 1:C:244:PHE:HB3 | 1.82 | 0.61 |
| 1:D:753:ALA:O | 1:D:756:GLN:HG2 | 2.00 | 0.61 |
| 1:D:828:LEU:HA | 1:D:831:LEU:HD12 | 1.82 | 0.61 |
| 1:E:169:LYS:NZ | 1:E:268:VAL:N | 2.48 | 0.61 |
| 1:E:322:ARG:HA | 1:E:325:VAL:HG22 | 1.82 | 0.61 |
| 1:E:547:SER:HB3 | 1:E:561:LEU:HD13 | 1.81 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:E:647:SER:HB2 | 1:E:692:HIS:CD2 | 2.35 | 0.61 |
| 1:E:815:ALA:C | 1:E:818:GLY:H | 2.08 | 0.61 |
| 1:F:221:ILE:O | 1:F:225:VAL:N | 2.26 | 0.61 |
| 1:F:264:ARG:O | 1:F:268:VAL:HG23 | 2.00 | 0.61 |
| 1:F:556:ILE:CG1 | 1:F:559:LYS:HZ3 | 2.10 | 0.61 |
| 1:F:616:SER:CB | 1:F:620:LYS:HD3 | 2.20 | 0.61 |
| 1:F:683:LEU:HD22 | 1:F:685:PHE:CZ | 2.35 | 0.61 |
| 1:F:704:ASP:CG | 1:F:765:ARG:NH2 | 2.56 | 0.61 |
| 1:B:175:THR:HG22 | 1:B:243:LEU:HG | 1.81 | 0.61 |
| 1:C:210:LEU:HB2 | 1:C:337:LYS:HA | 1.82 | 0.61 |
| 1:C:841:ALA:O | 1:C:845:LEU:HG | 2.01 | 0.61 |
| 1:D:263:GLU:O | 1:D:266:LYS:N | 2.33 | 0.61 |
| 1:D:320:GLU:O | 1:D:324:ILE:N | 2.31 | 0.61 |
| 1:E:457:GLU:HA | 1:E:460:GLU:HB3 | 1.82 | 0.61 |
| 1:E:619:GLY:HA2 | 2:E:1002:AGS:H5'2 | 1.81 | 0.61 |
| 1:E:655:LEU:O | 1:E:667:GLU:HB2 | 2.00 | 0.61 |
| 1:E:702:MET:HA | 1:E:707:ARG:HD3 | 1.82 | 0.61 |
| 1:E:812:ASP:OD2 | 1:E:816:LYS:HE3 | 2.00 | 0.61 |
| 1:E:859:LEU:O | 1:E:877:LEU:N | 2.32 | 0.61 |
| 1:E:879:VAL:HG12 | 1:E:880:LEU:H | 1.64 | 0.61 |
| 1:F:393:LEU:O | 1:F:396:VAL:HB | 2.00 | 0.61 |
| 1:F:707:ARG:CA | 1:F:715:THR:HG21 | 2.30 | 0.61 |
| 1:F:710:SER:HG | 1:F:713:GLY:HA2 | 1.63 | 0.61 |
| 1:A:332:GLU:OE2 | 1:A:334:ARG:HG2 | 2.00 | 0.61 |
| 1:B:210:LEU:HD21 | 1:B:337:LYS:NZ | 2.12 | 0.61 |
| 1:B:759:ARG:O | 1:B:763:LEU:HG | 2.00 | 0.61 |
| 1:B:804:LEU:H | 1:B:853:GLU:CG | 2.13 | 0.61 |
| 1:C:333:ARG:C | 1:C:335:PHE:H | 2.06 | 0.61 |
| 1:C:789:LYS:O | 1:C:792:GLU:HB3 | 2.00 | 0.61 |
| 1:D:186:VAL:HB | 2:D:1001:AGS:C2 | 2.29 | 0.61 |
| 1:D:752:GLY:HA2 | 1:D:755:ARG:HH21 | 1.64 | 0.61 |
| 1:E:685:PHE:CB | 1:E:725:MET:HB2 | 2.30 | 0.61 |
| 1:F:705:ASP:OD1 | 1:F:705:ASP:N | 2.32 | 0.61 |
| 1:A:211:ILE:H | 1:A:316:THR:N | 1.97 | 0.61 |
| 1:A:244:PHE:HB3 | 1:A:281:LEU:CD2 | 2.29 | 0.61 |
| 1:A:777:ARG:NH2 | 1:A:815:ALA:HB3 | 2.16 | 0.61 |
| 1:B:370:SER:O | 1:B:373:VAL:HB | 2.01 | 0.61 |
| 1:B:547:SER:HB3 | 1:B:560:LYS:HZ1 | 1.63 | 0.61 |
| 1:C:473:HIS:CD2 | 1:C:538:GLN:HB3 | 2.35 | 0.61 |
| 1:C:708:ILE:O | 1:C:716:ILE:N | 2.30 | 0.61 |
| 1:D:198:ARG:HD3 | 1:E:401:ALA:C | 2.25 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:262:GLU:CD | 1:D:263:GLU:HG2 | 2.25 | 0.61 |
| 1:D:352:LEU:HD23 | 1:D:355:LEU:HD21 | 1.81 | 0.61 |
| 1:D:402:GLY:O | 1:D:405:VAL:HB | 2.01 | 0.61 |
| 1:D:630:PHE:O | 1:D:631:LEU:C | 2.43 | 0.61 |
| 1:D:799:ASP:N | 1:D:801:HIS:HD2 | 1.96 | 0.61 |
| 1:E:797:GLN:OE1 | 1:E:797:GLN:N | 2.33 | 0.61 |
| 1:F:166:TYR:HE2 | 1:F:264:ARG:HA | 1.65 | 0.61 |
| 1:F:331:PHE:CA | 1:F:334:ARG:CD | 2.70 | 0.61 |
| 1:F:828:LEU:HD22 | 1:F:832:ILE:HD11 | 1.82 | 0.61 |
| 1:A:758:PHE:CZ | 1:A:763:LEU:HB2 | 2.34 | 0.61 |
| 1:B:175:THR:OG1 | 1:B:176:GLU:N | 2.33 | 0.61 |
| 1:B:318:ASN:N | 1:B:318:ASN:OD1 | 2.32 | 0.61 |
| 1:B:396:VAL:O | 1:B:400:CYS:N | 2.26 | 0.61 |
| 1:C:169:LYS:H | 1:C:264:ARG:NE | 1.86 | 0.61 |
| 1:C:641:VAL:N | 1:C:684:LEU:O | 2.33 | 0.61 |
| 1:C:689:GLU:OE1 | 1:C:727:SER:OG | 2.17 | 0.61 |
| 1:C:706:GLY:O | 1:C:717:ASP:HB3 | 2.01 | 0.61 |
| 1:D:366:ARG:N | 1:D:536:MET:HE3 | 2.16 | 0.61 |
| 1:D:778:LYS:O | 1:D:782:LYS:NZ | 2.34 | 0.61 |
| 1:D:844:ILE:HA | 1:D:847:ASN:OD1 | 2.01 | 0.61 |
| 1:E:673:ASN:N | 1:E:673:ASN:OD1 | 2.33 | 0.61 |
| 1:E:859:LEU:HD23 | 1:E:876:CYS:HB3 | 1.82 | 0.61 |
| 1:F:640:ARG:HH21 | 1:F:641:VAL:H | 1.48 | 0.61 |
| 1:F:702:MET:CB | 1:F:708:ILE:CG1 | 2.76 | 0.61 |
| 1:A:872:GLU:OE2 | 1:F:200:LEU:HD12 | 2.01 | 0.61 |
| 1:B:180:GLN:HG3 | 1:B:182:LYS:NZ | 2.15 | 0.61 |
| 1:B:203:ARG:HB2 | 1:C:359:TYR:HH | 1.63 | 0.61 |
| 1:B:342:GLU:OE2 | 1:B:388:LEU:N | 2.33 | 0.61 |
| 1:B:551:ALA:HA | 1:B:554:THR:HG23 | 1.82 | 0.61 |
| 1:B:617:GLY:N | 1:B:620:LYS:HZ2 | 1.98 | 0.61 |
| 1:B:656:LEU:HD13 | 1:B:658:THR:HG23 | 1.82 | 0.61 |
| 1:C:483:LEU:HG | 1:C:486:LEU:HD12 | 1.83 | 0.61 |
| 1:C:764:ASN:OD1 | 1:C:764:ASN:N | 2.29 | 0.61 |
| 1:D:164:LEU:O | 1:D:165:GLU:HG2 | 2.00 | 0.61 |
| 1:D:198:ARG:NH1 | 1:E:402:GLY:O | 2.33 | 0.61 |
| 1:D:400:CYS:HA | 1:D:403:VAL:HB | 1.83 | 0.61 |
| 1:D:503:ALA:HB1 | 1:D:507:TYR:CE1 | 2.35 | 0.61 |
| 1:D:684:LEU:HA | 1:D:725:MET:HG2 | 1.81 | 0.61 |
| 1:F:171:ALA:HA | 1:F:246:LEU:HA | 1.80 | 0.61 |
| 1:F:640:ARG:HD2 | 1:F:684:LEU:CB | 2.30 | 0.61 |
| 1:A:583:GLN:HE22 | 1:A:773:ASN:H | 1.47 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:840:LEU:O | 1:A:844:ILE:N | 2.27 | 0.61 |
| 1:B:191:GLU:HG2 | 1:B:192:GLU:OE1 | 1.99 | 0.61 |
| 1:B:359:TYR:O | 1:B:362:HIS:HB3 | 1.99 | 0.61 |
| 1:B:648:GLU:CB | 1:B:693:PRO:HD3 | 2.30 | 0.61 |
| 1:B:783:ILE:O | 1:B:786:ILE:HB | 2.00 | 0.61 |
| 1:C:374:THR:HG1 | 1:C:375:ALA:H | 1.48 | 0.61 |
| 1:C:648:GLU:HA | 1:C:692:HIS:NE2 | 2.16 | 0.61 |
| 1:D:391:SER:HA | 1:D:394:ASP:CG | 2.26 | 0.61 |
| 1:D:429:LYS:HA | 1:D:445:LEU:HD11 | 1.82 | 0.61 |
| 1:E:323:SER:C | 1:E:327:LYS:NZ | 2.59 | 0.61 |
| 1:E:609:SER:HG | 1:E:723:VAL:HG13 | 1.64 | 0.61 |
| 1:E:645:GLU:HB2 | 1:E:649:LYS:HE3 | 1.81 | 0.61 |
| 1:E:828:LEU:O | 1:E:831:LEU:N | 2.33 | 0.61 |
| 1:F:584:MET:O | 1:F:588:LYS:N | 2.21 | 0.61 |
| 1:A:213:GLU:CB | 1:A:218:LYS:HZ3 | 2.14 | 0.61 |
| 1:A:379:ALA:HA | 1:A:382:TYR:CZ | 2.36 | 0.61 |
| 1:C:285:GLU:HA | 1:C:287:HIS:CD2 | 2.36 | 0.61 |
| 1:C:320:GLU:O | 1:C:323:SER:HB2 | 2.01 | 0.61 |
| 1:C:659:THR:HA | 1:C:712:GLN:NE2 | 2.16 | 0.61 |
| 1:C:785:ASP:OD1 | 1:C:785:ASP:N | 2.30 | 0.61 |
| 1:D:270:LYS:HA | 1:D:273:GLU:CD | 2.26 | 0.61 |
| 1:D:613:LEU:HB3 | 1:D:771:ILE:HG23 | 1.83 | 0.61 |
| 1:D:705:ASP:CG | 1:D:707:ARG:NH1 | 2.59 | 0.61 |
| 1:D:708:ILE:H | 1:D:716:ILE:N | 1.85 | 0.61 |
| 1:E:626:LYS:NZ | 1:E:635:GLU:OE2 | 2.34 | 0.61 |
| 1:F:351:ILE:O | 1:F:355:LEU:N | 2.25 | 0.61 |
| 1:F:613:LEU:HD13 | 1:F:770:VAL:N | 2.12 | 0.61 |
| 1:F:810:ALA:HB2 | 1:F:858:VAL:HG21 | 1.81 | 0.61 |
| 1:A:262:GLU:O | 1:A:266:LYS:N | 2.34 | 0.61 |
| 1:A:813:PHE:CE2 | 1:A:814:LEU:HB2 | 2.35 | 0.61 |
| 1:B:346:ARG:O | 1:B:350:ALA:N | 2.25 | 0.61 |
| 1:B:405:VAL:HA | 1:B:408:ASP:OD2 | 2.00 | 0.61 |
| 1:B:610:PHE:HA | 1:B:768:SER:HB3 | 1.81 | 0.61 |
| 1:B:786:ILE:C | 1:B:789:LYS:HZ3 | 2.06 | 0.61 |
| 1:C:301:LEU:HD12 | 1:C:302:LYS:H | 1.65 | 0.61 |
| 1:C:328:ASP:HA | 1:C:331:PHE:CD2 | 2.36 | 0.61 |
| 1:C:391:SER:HA | 1:C:394:ASP:OD2 | 2.00 | 0.61 |
| 1:C:639:ILE:O | 1:C:684:LEU:N | 2.33 | 0.61 |
| 1:C:686:ASP:C | 1:C:688:VAL:H | 2.09 | 0.61 |
| 1:D:210:LEU:O | 1:D:211:ILE:HG12 | 2.01 | 0.61 |
| 1:D:219:THR:O | 1:D:222:ILE:N | 2.34 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:557:PRO:HB2 | 1:D:558:VAL:HG23 | 1.81 | 0.61 |
| 1:D:686:ASP:CG | 1:D:727:SER:HA | 2.26 | 0.61 |
| 1:E:611:LEU:H | 1:E:769:ILE:HA | 1.66 | 0.61 |
| 1:E:744:GLU:HA | 1:E:747:LYS:HE3 | 1.82 | 0.61 |
| 1:F:170:TYR:CD2 | 1:F:248:LEU:HB2 | 2.36 | 0.61 |
| 1:F:175:THR:HG23 | 1:F:244:PHE:CE1 | 2.35 | 0.61 |
| 1:F:360:GLU:OE1 | 1:F:367:ILE:CB | 2.48 | 0.61 |
| 1:F:687:GLU:HA | 1:F:727:SER:CA | 2.28 | 0.61 |
| 1:F:774:LYS:HG2 | 1:F:775:LEU:H | 1.66 | 0.61 |
| 2:F:1002:AGS:O3A | 2:F:1002:AGS:H4' | 1.99 | 0.61 |
| 1:A:212:GLY:H | 1:A:315:ALA:C | 2.09 | 0.61 |
| 1:A:272:ILE:C | 1:A:276:LYS:NZ | 2.55 | 0.61 |
| 1:A:347:GLN:H | 1:A:347:GLN:CD | 2.09 | 0.61 |
| 1:A:571:HIS:HD2 | 1:A:574:ARG:HD2 | 1.65 | 0.61 |
| 1:B:170:TYR:CD1 | 1:B:251:LEU:HD23 | 2.36 | 0.61 |
| 1:B:198:ARG:O | 1:B:200:LEU:N | 2.34 | 0.61 |
| 1:B:745:SER:OG | 1:B:746:THR:N | 2.33 | 0.61 |
| 1:C:784:VAL:CG2 | 1:C:811:LYS:HZ2 | 2.14 | 0.61 |
| 1:C:839:LYS:HZ3 | 1:C:879:VAL:HG12 | 1.65 | 0.61 |
| 1:C:858:VAL:C | 1:C:878:GLU:HA | 2.25 | 0.61 |
| 1:D:198:ARG:NH1 | 1:E:405:VAL:N | 2.48 | 0.61 |
| 1:D:686:ASP:OD1 | 1:D:687:GLU:N | 2.33 | 0.61 |
| 1:E:174:MET:HE1 | 1:E:183:LEU:HB2 | 1.81 | 0.61 |
| 1:E:270:LYS:HZ3 | 1:E:274:GLU:CA | 2.05 | 0.61 |
| 1:E:378:LEU:HG | 1:E:381:ARG:HD2 | 1.81 | 0.61 |
| 1:E:445:LEU:HD23 | 1:E:449:ARG:HH21 | 1.64 | 0.61 |
| 1:E:643:CYS:N | 1:E:686:ASP:OD2 | 2.34 | 0.61 |
| 1:F:270:LYS:HA | 1:F:273:GLU:HB2 | 1.82 | 0.61 |
| 1:F:715:THR:O | 1:F:717:ASP:CA | 2.48 | 0.61 |
| 1:F:798:ASN:HA | 1:F:801:HIS:NE2 | 2.15 | 0.61 |
| 1:F:829:ASN:CG | 1:F:830:ARG:H | 2.07 | 0.61 |
| 1:B:294:LYS:O | 1:B:299:ASN:ND2 | 2.34 | 0.60 |
| 1:B:587:ILE:H | 1:B:587:ILE:HD12 | 1.64 | 0.60 |
| 1:C:12:LEU:O | 1:C:16:THR:N | 2.33 | 0.60 |
| 1:C:608:ALA:O | 1:C:722:ILE:HD11 | 2.01 | 0.60 |
| 1:D:469:GLU:OE2 | 1:D:533:ALA:HB1 | 2.00 | 0.60 |
| 1:D:524:VAL:HG13 | 1:D:533:ALA:N | 2.16 | 0.60 |
| 1:D:685:PHE:N | 1:D:725:MET:HG2 | 2.15 | 0.60 |
| 1:D:744:GLU:HB2 | 1:D:746:THR:CG2 | 2.28 | 0.60 |
| 1:D:763:LEU:HA | 1:D:766:ILE:HG12 | 1.83 | 0.60 |
| 1:E:302:LYS:O | 1:E:305:LEU:HB2 | 2.01 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:759:ARG:C | 1:E:763:LEU:HG | 2.26 | 0.60 |
| 1:F:714:LYS:O | 1:F:714:LYS:HG3 | 2.02 | 0.60 |
| 1:F:760:PRO:O | 1:F:764:ASN:N | 2.34 | 0.60 |
| 1:F:788:LEU:HD12 | 1:F:791:ILE:HD12 | 1.83 | 0.60 |
| 1:A:382:TYR:CD2 | 1:A:383:LEU:N | 2.69 | 0.60 |
| 1:A:612:PHE:HB2 | 1:A:771:ILE:HA | 1.84 | 0.60 |
| 1:A:673:ASN:ND2 | 1:A:676:GLN:OE1 | 2.33 | 0.60 |
| 1:A:760:PRO:O | 1:A:763:LEU:HB3 | 2.00 | 0.60 |
| 1:A:791:ILE:HA | 1:A:794:ARG:NH1 | 2.16 | 0.60 |
| 1:B:367:ILE:O | 1:B:368:LEU:HD12 | 2.01 | 0.60 |
| 1:B:565:GLU:N | 1:B:568:LYS:NZ | 2.47 | 0.60 |
| 1:B:617:GLY:CA | 1:B:620:LYS:HZ2 | 2.13 | 0.60 |
| 1:C:375:ALA:HA | 1:C:378:LEU:HD12 | 1.82 | 0.60 |
| 1:C:686:ASP:O | 1:C:689:GLU:N | 2.34 | 0.60 |
| 1:C:829:ASN:O | 1:C:832:ILE:N | 2.33 | 0.60 |
| 1:D:227:GLN:O | 1:D:231:ASP:N | 2.30 | 0.60 |
| 1:D:355:LEU:HD12 | 1:D:356:GLN:N | 2.16 | 0.60 |
| 1:D:453:ALA:O | 1:D:457:GLU:HG2 | 2.01 | 0.60 |
| 1:D:564:SER:C | 1:D:568:LYS:HE2 | 2.25 | 0.60 |
| 1:D:637:MET:O | 1:D:639:ILE:HG23 | 2.01 | 0.60 |
| 1:E:197:ILE:HA | 1:E:200:LEU:HD12 | 1.83 | 0.60 |
| 1:E:202:ARG:NH1 | 1:E:205:LYS:N | 2.49 | 0.60 |
| 1:E:366:ARG:NH1 | 1:E:367:ILE:C | 2.59 | 0.60 |
| 1:E:510:ILE:HD13 | 1:E:514:LYS:NZ | 2.15 | 0.60 |
| 1:E:581:VAL:HG11 | 1:E:772:PHE:HE1 | 1.65 | 0.60 |
| 1:E:620:LYS:HG2 | 2:E:1002:AGS:O1A | 2.01 | 0.60 |
| 1:E:689:GLU:HG3 | 1:E:758:PHE:CZ | 2.35 | 0.60 |
| 1:F:807:THR:HG23 | 1:F:810:ALA:HB3 | 1.83 | 0.60 |
| 1:F:813:PHE:N | 1:F:816:LYS:NZ | 2.49 | 0.60 |
| 1:A:274:GLU:N | 1:A:276:LYS:NZ | 2.50 | 0.60 |
| 1:B:362:HIS:HD2 | 1:B:363:HIS:CD2 | 2.19 | 0.60 |
| 1:C:570:ILE:HD11 | 1:D:845:LEU:HD13 | 1.82 | 0.60 |
| 1:C:634:ASP:HB2 | 1:C:636:ASP:CG | 2.26 | 0.60 |
| 1:C:683:LEU:N | 1:C:723:VAL:HG22 | 2.16 | 0.60 |
| 1:C:712:GLN:C | 1:C:714:LYS:HZ1 | 2.08 | 0.60 |
| 1:D:168:SER:OG | 1:D:169:LYS:N | 2.31 | 0.60 |
| 1:D:175:THR:OG1 | 1:D:223:GLU:OE2 | 2.14 | 0.60 |
| 1:D:205:LYS:HD2 | 1:D:333:ARG:O | 2.00 | 0.60 |
| 1:D:613:LEU:HD21 | 1:D:734:ILE:HD11 | 1.82 | 0.60 |
| 1:E:345:VAL:HA | 1:E:388:LEU:HD21 | 1.83 | 0.60 |
| 1:E:483:LEU:HG | 1:E:508:PHE:HZ | 1.66 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:606:GLN:HG3 | 1:F:794:ARG:NH2 | 2.17 | 0.60 |
| 1:E:611:LEU:HB2 | 1:E:725:MET:HG2 | 1.83 | 0.60 |
| 1:E:683:LEU:HB3 | 1:E:723:VAL:HB | 1.82 | 0.60 |
| 1:E:785:ASP:C | 1:E:789:LYS:NZ | 2.58 | 0.60 |
| 1:F:605:ARG:HG2 | 1:F:707:ARG:H | 1.65 | 0.60 |
| 1:F:730:GLY:O | 1:F:734:ILE:N | 2.27 | 0.60 |
| 1:F:802:TYR:O | 1:F:803:LYS:HG2 | 2.01 | 0.60 |
| 1:B:210:LEU:HD11 | 1:B:337:LYS:HZ3 | 1.66 | 0.60 |
| 1:B:263:GLU:HA | 1:B:266:LYS:HZ1 | 1.66 | 0.60 |
| 1:B:366:ARG:HE | 1:B:538:GLN:N | 1.98 | 0.60 |
| 1:B:366:ARG:C | 1:B:539:ASN:HB2 | 2.26 | 0.60 |
| 1:C:362:HIS:HD2 | 1:C:363:HIS:CE1 | 2.19 | 0.60 |
| 1:C:407:ARG:CZ | 1:C:539:ASN:H | 2.15 | 0.60 |
| 1:C:787:ARG:NH1 | 1:C:826:ARG:NH2 | 2.44 | 0.60 |
| 1:C:837:LEU:HD12 | 1:C:838:ASN:H | 1.66 | 0.60 |
| 1:C:841:ALA:HA | 1:C:844:ILE:HD13 | 1.83 | 0.60 |
| 1:D:468:GLU:O | 1:D:471:HIS:HB3 | 2.02 | 0.60 |
| 1:D:542:ASP:OD1 | 1:D:543:SER:N | 2.29 | 0.60 |
| 1:D:549:THR:O | 1:D:553:LEU:N | 2.34 | 0.60 |
| 1:D:642:ASP:HA | 1:D:685:PHE:CZ | 2.36 | 0.60 |
| 1:E:228:ARG:HH11 | 1:E:231:ASP:HB2 | 1.67 | 0.60 |
| 1:E:230:ILE:HG22 | 1:E:495:ARG:NH2 | 2.13 | 0.60 |
| 1:E:304:ALA:CA | 1:E:307:ARG:HH11 | 2.14 | 0.60 |
| 1:E:367:ILE:HA | 1:E:540:VAL:HG23 | 1.84 | 0.60 |
| 1:E:737:GLN:C | 1:E:774:LYS:HZ3 | 2.05 | 0.60 |
| 1:E:763:LEU:O | 1:E:766:ILE:HB | 2.00 | 0.60 |
| 1:F:190:GLU:HA | 1:F:193:ILE:HD12 | 1.83 | 0.60 |
| 1:F:646:LEU:CB | 1:F:691:ALA:HA | 2.32 | 0.60 |
| 1:F:819:TYR:HE1 | 1:F:828:LEU:H | 1.49 | 0.60 |
| 1:A:287:HIS:HB2 | 1:A:321:TYR:CE2 | 2.35 | 0.60 |
| 1:A:374:THR:O | 1:A:378:LEU:HG | 2.01 | 0.60 |
| 1:A:696:LEU:HD12 | 1:A:697:THR:N | 2.16 | 0.60 |
| 1:A:800:LYS:HE2 | 1:A:850:LYS:HB3 | 1.82 | 0.60 |
| 1:B:195:SER:HB2 | 1:B:198:ARG:NH2 | 2.16 | 0.60 |
| 1:B:541:VAL:H | 1:B:546:ILE:HD11 | 1.67 | 0.60 |
| 1:B:782:LYS:O | 1:B:785:ASP:N | 2.35 | 0.60 |
| 1:C:348:THR:O | 1:C:352:LEU:HG | 2.01 | 0.60 |
| 1:C:465:ARG:NH2 | 1:C:466:TYR:OH | 2.34 | 0.60 |
| 1:C:606:GLN:HE22 | 1:C:704:ASP:HA | 1.66 | 0.60 |
| 1:C:622:GLU:CG | 1:C:826:ARG:HH22 | 2.15 | 0.60 |
| 1:D:209:CYS:C | 1:D:210:LEU:HD12 | 2.27 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:D:461:PRO:C | 1:D:465:ARG:HG3 | 2.27 | 0.60 |
| 1:D:735:ASN:O | 1:D:737:GLN:N | 2.35 | 0.60 |
| 1:D:745:SER:HB2 | 1:D:748:ASN:OD1 | 2.01 | 0.60 |
| 1:D:748:ASN:HA | 1:D:751:MET:HE2 | 1.83 | 0.60 |
| 1:D:776:SER:HB3 | 1:D:779:ALA:HB3 | 1.83 | 0.60 |
| 1:E:366:ARG:HG2 | 1:E:367:ILE:H | 1.63 | 0.60 |
| 1:F:194:ARG:CA | 1:F:228:ARG:HH12 | 2.14 | 0.60 |
| 1:F:216:ILE:CG1 | 1:F:218:LYS:HG3 | 2.31 | 0.60 |
| 1:F:240:GLY:O | 1:F:279:ILE:N | 2.35 | 0.60 |
| 1:F:556:ILE:N | 1:F:559:LYS:NZ | 2.48 | 0.60 |
| 1:F:610:PHE:HA | 1:F:768:SER:CB | 2.28 | 0.60 |
| 1:A:207:ASN:HB2 | 1:A:335:PHE:CD1 | 2.37 | 0.60 |
| 1:A:268:VAL:O | 1:A:272:ILE:HG13 | 2.01 | 0.60 |
| 1:A:858:VAL:N | 1:A:877:LEU:HB3 | 2.14 | 0.60 |
| 1:B:244:PHE:CE1 | 1:B:280:VAL:HA | 2.36 | 0.60 |
| 1:B:366:ARG:O | 1:B:367:ILE:HG13 | 2.02 | 0.60 |
| 1:B:377:GLN:HA | 1:B:380:LYS:HB3 | 1.84 | 0.60 |
| 1:B:606:GLN:HB2 | 1:B:607:PRO:HD2 | 1.84 | 0.60 |
| 1:B:607:PRO:CB | 1:B:722:ILE:HG12 | 2.31 | 0.60 |
| 1:C:650:TYR:CZ | 1:C:656:LEU:HB3 | 2.37 | 0.60 |
| 1:D:199:VAL:O | 1:D:202:ARG:HG2 | 2.02 | 0.60 |
| 1:D:630:PHE:CE2 | 1:D:631:LEU:HD23 | 2.36 | 0.60 |
| 1:D:708:ILE:HD12 | 1:D:716:ILE:HB | 1.83 | 0.60 |
| 1:E:217:GLY:HA2 | 2:E:1001:AGS:C4' | 2.31 | 0.60 |
| 1:E:302:LYS:HG2 | 1:E:334:ARG:HH11 | 1.66 | 0.60 |
| 1:E:588:LYS:HG3 | 1:E:592:ASN:HD21 | 1.67 | 0.60 |
| 1:E:590:VAL:O | 1:E:594:VAL:N | 2.23 | 0.60 |
| 1:E:638:MET:CA | 1:E:682:VAL:HG11 | 2.31 | 0.60 |
| 1:E:845:LEU:HD12 | 1:E:846:LYS:H | 1.67 | 0.60 |
| 1:F:618:SER:HA | 2:F:1002:AGS:C2 | 2.31 | 0.60 |
| 1:F:855:VAL:HG13 | 1:F:880:LEU:HB2 | 1.84 | 0.60 |
| 2:F:1001:AGS:HO3' | 2:F:1001:AGS:PB | 2.25 | 0.60 |
| 1:A:620:LYS:HA | 1:A:772:PHE:CE2 | 2.37 | 0.60 |
| 1:A:820:SER:OG | 1:F:307:ARG:NH2 | 2.34 | 0.60 |
| 1:B:195:SER:CB | 1:B:198:ARG:HH12 | 2.15 | 0.60 |
| 1:B:739:GLY:O | 1:B:742:ILE:N | 2.29 | 0.60 |
| 1:B:744:GLU:CA | 1:B:747:LYS:HE3 | 2.32 | 0.60 |
| 1:C:208:PRO:HB2 | 1:C:338:ILE:HG12 | 1.84 | 0.60 |
| 1:C:285:GLU:O | 1:C:288:MET:N | 2.34 | 0.60 |
| 1:C:296:ASP:OD2 | 1:C:300:ILE:HB | 2.01 | 0.60 |
| 1:C:761:GLU:HA | 1:C:764:ASN:ND2 | 2.17 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:783:ILE:HA | 1:C:786:ILE:HB | 1.84 | 0.60 |
| 1:C:857:VAL:HG13 | 1:C:879:VAL:CA | 2.31 | 0.60 |
| 1:D:344:SER:O | 1:D:347:GLN:HB2 | 2.02 | 0.60 |
| 1:E:216:ILE:HD11 | 1:E:390:ASP:H | 1.65 | 0.60 |
| 1:E:282:PHE:O | 1:E:283:ILE:HG13 | 2.01 | 0.60 |
| 1:E:342:GLU:OE2 | 1:E:388:LEU:HB2 | 2.00 | 0.60 |
| 1:E:705:ASP:H | 1:E:765:ARG:NH1 | 1.98 | 0.60 |
| 1:E:800:LYS:HB3 | 1:E:802:TYR:CZ | 2.36 | 0.60 |
| 1:F:261:PHE:CE2 | 1:F:262:GLU:HB2 | 2.37 | 0.60 |
| 1:A:746:THR:O | 1:A:750:VAL:N | 2.17 | 0.60 |
| 1:B:548:GLU:HG2 | 1:B:560:LYS:NZ | 2.07 | 0.60 |
| 1:B:748:ASN:HA | 1:B:751:MET:SD | 2.42 | 0.60 |
| 1:B:759:ARG:O | 1:B:762:PHE:HB3 | 2.02 | 0.60 |
| 1:B:806:LEU:HD22 | 1:B:811:LYS:N | 2.16 | 0.60 |
| 1:C:264:ARG:HG2 | 1:C:268:VAL:HG23 | 1.82 | 0.60 |
| 1:C:350:ALA:N | 1:C:353:ARG:HH11 | 2.00 | 0.60 |
| 1:C:619:GLY:HA2 | 1:C:622:GLU:HG2 | 1.84 | 0.60 |
| 1:C:805:ASN:HB2 | 1:C:854:THR:HG22 | 1.83 | 0.60 |
| 1:D:229:ILE:HG13 | 1:D:233:ASP:OD2 | 2.01 | 0.60 |
| 1:D:367:ILE:HG22 | 1:D:369:ASP:H | 1.67 | 0.60 |
| 1:E:193:ILE:HA | 1:E:196:THR:HB | 1.84 | 0.60 |
| 1:E:434:ASP:OD1 | 1:E:435:GLU:N | 2.34 | 0.60 |
| 1:E:584:MET:O | 1:E:587:ILE:HB | 2.00 | 0.60 |
| 1:E:803:LYS:HZ1 | 1:E:854:THR:HG23 | 1.67 | 0.60 |
| 1:B:333:ARG:NH2 | 1:B:334:ARG:HE | 2.00 | 0.60 |
| 1:B:385:TYR:OH | 1:B:386:ARG:NH1 | 2.34 | 0.60 |
| 1:B:848:GLU:OE2 | 1:B:881:PRO:HA | 2.00 | 0.60 |
| 1:C:168:SER:OG | 1:C:268:VAL:CG2 | 2.50 | 0.60 |
| 1:C:375:ALA:O | 1:C:379:ALA:N | 2.23 | 0.60 |
| 1:C:592:ASN:O | 1:C:596:LEU:N | 2.24 | 0.60 |
| 1:C:751:MET:O | 1:C:754:VAL:HB | 2.01 | 0.60 |
| 1:C:784:VAL:HG23 | 1:C:785:ASP:N | 2.14 | 0.60 |
| 1:D:213:GLU:OE2 | 1:D:388:LEU:HG | 2.02 | 0.60 |
| 1:D:242:LYS:HG2 | 1:D:278:LEU:HB3 | 1.84 | 0.60 |
| 1:D:298:ALA:C | 1:D:301:LEU:HD11 | 2.26 | 0.60 |
| 1:D:848:GLU:OE1 | 1:D:882:ASN:ND2 | 2.31 | 0.60 |
| 1:E:207:ASN:OD1 | 1:E:311:LYS:HG3 | 2.00 | 0.60 |
| 1:E:583:GLN:O | 1:E:587:ILE:N | 2.30 | 0.60 |
| 1:E:804:LEU:HA | 1:E:854:THR:HA | 1.84 | 0.60 |
| 1:F:683:LEU:N | 1:F:723:VAL:HG11 | 2.16 | 0.60 |
| 1:A:205:LYS:NZ | 1:B:394:ASP:HA | 2.17 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:404:ALA:HA | 1:A:408:ASP:OD2 | 2.01 | 0.60 |
| 1:A:692:HIS:O | 1:A:694:ASP:N | 2.35 | 0.60 |
| 1:B:211:ILE:HG12 | 1:B:318:ASN:HA | 1.84 | 0.60 |
| 1:B:541:VAL:HG11 | 1:B:545:THR:OG1 | 2.01 | 0.60 |
| 1:B:605:ARG:HG3 | 1:B:606:GLN:H | 1.65 | 0.60 |
| 1:C:302:LYS:HD2 | 1:C:306:SER:N | 2.16 | 0.60 |
| 1:C:596:LEU:O | 1:C:599:SER:N | 2.35 | 0.60 |
| 1:C:677:TYR:C | 1:C:679:PRO:HD3 | 2.27 | 0.60 |
| 1:C:788:LEU:HG | 1:C:789:LYS:N | 2.16 | 0.60 |
| 1:D:570:ILE:HG12 | 1:D:595:ARG:HH12 | 1.65 | 0.60 |
| 1:E:202:ARG:N | 1:E:206:SER:OG | 2.35 | 0.60 |
| 1:E:378:LEU:HA | 1:E:381:ARG:CB | 2.27 | 0.60 |
| 1:E:459:LEU:HG | 1:E:463:ARG:HB3 | 1.84 | 0.60 |
| 1:E:646:LEU:HB2 | 1:E:649:LYS:CB | 2.32 | 0.60 |
| 1:E:708:ILE:HA | 1:E:716:ILE:O | 2.02 | 0.60 |
| 1:E:839:LYS:HE3 | 1:E:880:LEU:HD12 | 1.84 | 0.60 |
| 1:F:240:GLY:O | 1:F:279:ILE:HG12 | 2.02 | 0.60 |
| 1:B:189:ARG:O | 1:B:192:GLU:HB2 | 2.02 | 0.59 |
| 1:B:596:LEU:O | 1:B:602:ALA:HB2 | 2.02 | 0.59 |
| 1:B:752:GLY:O | 1:B:756:GLN:N | 2.33 | 0.59 |
| 1:C:362:HIS:CD2 | 1:C:363:HIS:CE1 | 2.90 | 0.59 |
| 1:C:397:ASP:HA | 1:C:400:CYS:HB2 | 1.84 | 0.59 |
| 1:D:281:LEU:HG | 1:D:311:LYS:O | 2.02 | 0.59 |
| 1:D:282:PHE:CD1 | 1:D:313:ILE:HD11 | 2.35 | 0.59 |
| 1:D:563:GLU:HA | 1:D:568:LYS:HZ3 | 1.65 | 0.59 |
| 1:D:752:GLY:HA2 | 1:D:755:ARG:NH2 | 2.17 | 0.59 |
| 1:D:825:ALA:H | 1:D:827:PRO:HD2 | 1.67 | 0.59 |
| 1:E:174:MET:O | 1:E:177:GLN:N | 2.35 | 0.59 |
| 1:E:582:GLY:O | 1:E:584:MET:N | 2.35 | 0.59 |
| 1:E:585:ASP:O | 1:E:589:ALA:N | 2.27 | 0.59 |
| 1:E:645:GLU:HB2 | 1:E:649:LYS:CE | 2.31 | 0.59 |
| 1:F:603:ASN:HB3 | 1:F:605:ARG:H | 1.65 | 0.59 |
| 1:A:316:THR:CG2 | 1:A:322:ARG:HH11 | 2.06 | 0.59 |
| 1:A:583:GLN:NE2 | 1:A:771:ILE:O | 2.35 | 0.59 |
| 1:B:38:ALA:O | 1:B:71:ARG:N | 2.35 | 0.59 |
| 1:B:208:PRO:HD2 | 1:B:313:ILE:CA | 2.26 | 0.59 |
| 1:B:644:SER:O | 1:B:690:LYS:HE2 | 2.02 | 0.59 |
| 1:B:696:LEU:HA | 1:B:699:MET:SD | 2.42 | 0.59 |
| 1:C:199:VAL:C | 1:C:202:ARG:H | 2.09 | 0.59 |
| 1:C:211:ILE:HG21 | 1:C:316:THR:N | 2.17 | 0.59 |
| 1:C:365:VAL:HG12 | 1:C:366:ARG:N | 2.16 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:526:GLU:HA | 1:C:532:GLY:HA2 | 1.84 | 0.59 |
| 1:C:557:PRO:HA | 1:C:560:LYS:HZ3 | 1.63 | 0.59 |
| 1:C:616:SER:HA | 1:C:620:LYS:CD | 2.30 | 0.59 |
| 1:C:650:TYR:HE2 | 1:C:657:GLY:H | 1.49 | 0.59 |
| 1:C:767:SER:HA | 1:D:830:ARG:HH11 | 1.66 | 0.59 |
| 1:C:842:LEU:O | 1:C:845:LEU:HB2 | 2.01 | 0.59 |
| 1:D:684:LEU:HA | 1:D:725:MET:HA | 1.84 | 0.59 |
| 1:E:217:GLY:HA2 | 2:E:1001:AGS:H4' | 1.83 | 0.59 |
| 1:F:287:HIS:NE2 | 1:F:322:ARG:CG | 2.65 | 0.59 |
| 2:F:1001:AGS:O2B | 2:F:1001:AGS:O3' | 2.14 | 0.59 |
| 1:A:170:TYR:HD1 | 1:A:264:ARG:HE | 1.50 | 0.59 |
| 1:A:173:ASP:OD2 | 1:A:175:THR:OG1 | 2.19 | 0.59 |
| 1:A:613:LEU:HD22 | 1:A:727:SER:C | 2.27 | 0.59 |
| 1:A:643:CYS:SG | 1:A:685:PHE:HB3 | 2.43 | 0.59 |
| 1:A:780:ILE:O | 1:A:784:VAL:HG12 | 2.02 | 0.59 |
| 1:B:258:LYS:HZ1 | 1:C:255:ALA:CB | 2.15 | 0.59 |
| 1:B:303:PRO:O | 1:B:307:ARG:HG2 | 2.01 | 0.59 |
| 1:B:792:GLU:HB3 | 1:B:802:TYR:CZ | 2.37 | 0.59 |
| 1:C:625:LYS:NZ | 1:C:635:GLU:HB2 | 2.17 | 0.59 |
| 1:C:708:ILE:C | 1:C:716:ILE:HB | 2.26 | 0.59 |
| 1:D:265:PHE:HA | 1:D:268:VAL:HB | 1.84 | 0.59 |
| 1:D:317:THR:HG23 | 1:D:321:TYR:CD1 | 2.38 | 0.59 |
| 1:D:317:THR:HG22 | 1:D:321:TYR:CE1 | 2.30 | 0.59 |
| 1:D:394:ASP:O | 1:D:397:ASP:HB3 | 2.02 | 0.59 |
| 1:D:453:ALA:O | 1:D:457:GLU:N | 2.27 | 0.59 |
| 1:D:460:GLU:CD | 1:D:463:ARG:NH1 | 2.61 | 0.59 |
| 1:D:682:VAL:HA | 1:D:722:ILE:O | 2.02 | 0.59 |
| 1:E:170:TYR:CE2 | 1:E:251:LEU:HD21 | 2.38 | 0.59 |
| 1:E:247:ASP:CG | 1:E:249:ALA:HB3 | 2.27 | 0.59 |
| 1:E:247:ASP:CB | 1:E:250:ALA:H | 2.09 | 0.59 |
| 1:E:358:LYS:HZ1 | 1:E:359:TYR:HB2 | 1.66 | 0.59 |
| 1:E:372:LEU:HD11 | 1:E:540:VAL:HG21 | 1.84 | 0.59 |
| 1:E:805:ASN:N | 1:E:854:THR:HA | 2.17 | 0.59 |
| 1:F:317:THR:HG22 | 1:F:318:ASN:H | 1.67 | 0.59 |
| 1:A:213:GLU:H | 1:A:218:LYS:HD3 | 1.68 | 0.59 |
| 1:A:354:GLY:HA2 | 1:A:361:ILE:HD11 | 1.84 | 0.59 |
| 1:B:208:PRO:HA | 1:B:337:LYS:HB2 | 1.83 | 0.59 |
| 1:B:302:LYS:HZ3 | 1:B:305:LEU:HB2 | 1.67 | 0.59 |
| 1:B:566:ASN:O | 1:B:569:LEU:N | 2.36 | 0.59 |
| 1:B:752:GLY:O | 1:B:756:GLN:HG3 | 2.02 | 0.59 |
| 1:C:577:SER:C | 1:C:580:VAL:H | 2.10 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:658:THR:HG23 | 1:C:662:TYR:HB2 | 1.83 | 0.59 |
| 1:D:338:ILE:HG22 | 1:D:339:GLU:N | 2.18 | 0.59 |
| 1:D:587:ILE:HD12 | 1:D:587:ILE:H | 1.68 | 0.59 |
| 1:D:705:ASP:HA | 1:D:707:ARG:CZ | 2.33 | 0.59 |
| 1:E:265:PHE:O | 1:E:269:LEU:HG | 2.02 | 0.59 |
| 1:E:332:GLU:C | 1:E:335:PHE:H | 2.10 | 0.59 |
| 1:E:573:GLU:O | 1:E:576:LEU:N | 2.35 | 0.59 |
| 1:F:261:PHE:CG | 1:F:262:GLU:N | 2.70 | 0.59 |
| 1:F:612:PHE:CE2 | 1:F:614:GLY:HA2 | 2.37 | 0.59 |
| 1:F:658:THR:N | 1:F:667:GLU:OE1 | 2.25 | 0.59 |
| 1:F:775:LEU:HD22 | 1:F:780:ILE:HG21 | 1.84 | 0.59 |
| 1:F:809:GLU:H | 1:F:809:GLU:CD | 2.08 | 0.59 |
| 1:F:813:PHE:HZ | 1:F:875:GLU:HA | 1.67 | 0.59 |
| 1:A:248:LEU:HD12 | 1:A:250:ALA:N | 2.18 | 0.59 |
| 1:A:393:LEU:O | 1:A:397:ASP:N | 2.30 | 0.59 |
| 1:A:771:ILE:HG22 | 1:A:772:PHE:C | 2.27 | 0.59 |
| 1:A:842:LEU:O | 1:A:846:LYS:HG3 | 2.01 | 0.59 |
| 1:C:170:TYR:CD1 | 1:C:249:ALA:HA | 2.34 | 0.59 |
| 1:C:334:ARG:C | 1:C:335:PHE:HD1 | 2.10 | 0.59 |
| 1:C:627:VAL:N | 1:C:635:GLU:OE2 | 2.35 | 0.59 |
| 1:D:265:PHE:O | 1:D:269:LEU:HG | 2.02 | 0.59 |
| 1:D:475:GLU:HA | 1:D:478:GLN:HB2 | 1.84 | 0.59 |
| 1:D:584:MET:C | 1:D:588:LYS:HZ3 | 2.09 | 0.59 |
| 1:E:172:ILE:N | 1:E:245:SER:O | 2.32 | 0.59 |
| 1:E:247:ASP:HB3 | 1:E:250:ALA:N | 2.09 | 0.59 |
| 1:E:410:LYS:C | 1:E:414:LEU:HG | 2.28 | 0.59 |
| 1:E:583:GLN:C | 1:E:585:ASP:OD1 | 2.46 | 0.59 |
| 1:E:611:LEU:HD11 | 1:E:727:SER:H | 1.67 | 0.59 |
| 1:F:172:ILE:O | 1:F:172:ILE:HG13 | 2.01 | 0.59 |
| 1:F:189:ARG:HH22 | 1:F:342:GLU:C | 2.10 | 0.59 |
| 1:F:379:ALA:O | 1:F:383:LEU:HB2 | 2.02 | 0.59 |
| 1:F:693:PRO:HA | 1:F:696:LEU:HB2 | 1.83 | 0.59 |
| 1:A:190:GLU:N | 1:A:191:GLU:OE1 | 2.35 | 0.59 |
| 1:A:279:ILE:O | 1:A:309:GLN:HB3 | 2.02 | 0.59 |
| 1:A:617:GLY:C | 1:A:620:LYS:HZ2 | 2.11 | 0.59 |
| 1:A:791:ILE:HA | 1:A:794:ARG:CZ | 2.33 | 0.59 |
| 1:B:222:ILE:O | 1:B:225:VAL:HB | 2.02 | 0.59 |
| 1:B:543:SER:HB2 | 1:B:547:SER:HB2 | 1.84 | 0.59 |
| 1:B:842:LEU:CB | 1:B:846:LYS:NZ | 2.65 | 0.59 |
| 1:C:333:ARG:C | 1:C:335:PHE:N | 2.61 | 0.59 |
| 1:C:387:ARG:O | 1:C:391:SER:OG | 2.21 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:636:ASP:O | 1:D:638:MET:N | 2.35 | 0.59 |
| 1:D:692:HIS:O | 1:D:695:VAL:HB | 2.02 | 0.59 |
| 1:D:744:GLU:O | 1:D:747:LYS:NZ | 2.22 | 0.59 |
| 1:E:214:PRO:C | 1:E:387:ARG:NH1 | 2.60 | 0.59 |
| 1:E:751:MET:O | 1:E:755:ARG:HG2 | 2.03 | 0.59 |
| 1:F:307:ARG:HH11 | 1:F:333:ARG:HH12 | 1.49 | 0.59 |
| 1:F:398:ILE:HG22 | 1:F:545:THR:HG23 | 1.83 | 0.59 |
| 1:F:640:ARG:HH21 | 1:F:684:LEU:HB2 | 1.67 | 0.59 |
| 1:A:210:LEU:HB3 | 1:A:338:ILE:C | 2.27 | 0.59 |
| 1:A:242:LYS:HG3 | 1:A:243:LEU:H | 1.67 | 0.59 |
| 1:A:298:ALA:H | 1:A:301:LEU:HD23 | 1.68 | 0.59 |
| 1:A:574:ARG:O | 1:A:577:SER:OG | 2.21 | 0.59 |
| 1:A:625:LYS:HZ3 | 1:A:638:MET:HG3 | 1.67 | 0.59 |
| 1:A:787:ARG:NE | 1:A:790:GLU:OE1 | 2.24 | 0.59 |
| 1:B:640:ARG:HA | 1:B:684:LEU:HB3 | 1.84 | 0.59 |
| 1:C:242:LYS:N | 1:C:279:ILE:HA | 2.17 | 0.59 |
| 1:C:568:LYS:HZ1 | 1:C:630:PHE:CA | 2.15 | 0.59 |
| 1:C:683:LEU:HG | 1:C:684:LEU:N | 2.18 | 0.59 |
| 1:D:369:ASP:OD1 | 1:D:373:VAL:HG23 | 2.02 | 0.59 |
| 1:D:397:ASP:O | 1:D:401:ALA:N | 2.29 | 0.59 |
| 1:D:413:GLU:O | 1:D:416:SER:HB2 | 2.02 | 0.59 |
| 1:D:464:GLN:O | 1:D:468:GLU:N | 2.34 | 0.59 |
| 1:D:679:PRO:HB2 | 1:D:680:TYR:CE2 | 2.38 | 0.59 |
| 1:D:855:VAL:HG11 | 1:D:881:PRO:HG2 | 1.83 | 0.59 |
| 1:E:206:SER:C | 1:E:311:LYS:HZ1 | 2.03 | 0.59 |
| 1:E:284:ASP:HB3 | 1:E:315:ALA:HB3 | 1.85 | 0.59 |
| 1:E:551:ALA:HA | 1:E:555:GLY:H | 1.68 | 0.59 |
| 1:E:789:LYS:HD2 | 1:E:793:GLU:OE2 | 2.03 | 0.59 |
| 1:E:841:ALA:HA | 1:E:844:ILE:HB | 1.85 | 0.59 |
| 1:F:312:VAL:HG22 | 1:F:313:ILE:N | 2.18 | 0.59 |
| 1:B:228:ARG:NH2 | 1:B:233:ASP:HB2 | 2.18 | 0.59 |
| 1:B:262:GLU:HA | 1:B:265:PHE:CD2 | 2.37 | 0.59 |
| 1:B:353:ARG:NH2 | 1:B:372:LEU:HB2 | 2.18 | 0.59 |
| 1:B:612:PHE:HA | 1:B:770:VAL:O | 2.02 | 0.59 |
| 1:B:764:ASN:HA | 1:C:830:ARG:CZ | 2.32 | 0.59 |
| 1:C:158:ALA:N | 1:C:165:GLU:OE2 | 2.31 | 0.59 |
| 1:C:191:GLU:CD | 1:C:194:ARG:HB2 | 2.27 | 0.59 |
| 1:C:287:HIS:ND1 | 1:C:288:MET:N | 2.50 | 0.59 |
| 1:C:713:GLY:O | 1:C:714:LYS:HG3 | 2.02 | 0.59 |
| 1:C:830:ARG:O | 1:C:833:GLN:NE2 | 2.36 | 0.59 |
| 1:C:859:LEU:N | 1:C:878:GLU:HA | 2.17 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:166:TYR:CE1 | 1:D:169:LYS:HB3 | 2.38 | 0.59 |
| 1:D:216:ILE:HD12 | 2:D:1001:AGS:O3G | 2.03 | 0.59 |
| 1:D:607:PRO:HB2 | 1:D:722:ILE:HG23 | 1.85 | 0.59 |
| 1:D:617:GLY:C | 1:D:826:ARG:NH1 | 2.60 | 0.59 |
| 1:D:812:ASP:N | 1:D:812:ASP:OD1 | 2.32 | 0.59 |
| 1:E:228:ARG:HH12 | 1:E:232:ASP:C | 2.11 | 0.59 |
| 1:E:448:ALA:HA | 1:E:451:LYS:HE3 | 1.85 | 0.59 |
| 1:E:704:ASP:HA | 1:E:765:ARG:CZ | 2.31 | 0.59 |
| 1:F:172:ILE:HG12 | 1:F:245:SER:N | 2.13 | 0.59 |
| 1:F:190:GLU:HB3 | 1:F:228:ARG:NH2 | 2.17 | 0.59 |
| 1:F:226:ALA:O | 1:F:230:ILE:N | 2.35 | 0.59 |
| 1:A:211:ILE:H | 1:A:316:THR:HG22 | 1.67 | 0.59 |
| 1:A:217:GLY:O | 1:A:221:ILE:HD12 | 2.03 | 0.59 |
| 1:A:244:PHE:CZ | 1:A:279:ILE:HB | 2.37 | 0.59 |
| 1:A:381:ARG:HG2 | 1:A:382:TYR:CD1 | 2.38 | 0.59 |
| 1:B:92:LEU:O | 1:B:96:LEU:N | 2.35 | 0.59 |
| 1:B:166:TYR:HA | 1:B:169:LYS:NZ | 2.18 | 0.59 |
| 1:B:205:LYS:HB3 | 1:B:336:GLN:HB3 | 1.85 | 0.59 |
| 1:B:353:ARG:HH22 | 1:B:372:LEU:HB2 | 1.66 | 0.59 |
| 1:B:764:ASN:ND2 | 1:B:765:ARG:HH12 | 1.99 | 0.59 |
| 1:C:482:LYS:O | 1:C:485:GLU:N | 2.35 | 0.59 |
| 1:C:583:GLN:HG2 | 1:C:772:PHE:C | 2.28 | 0.59 |
| 1:C:785:ASP:HA | 1:C:788:LEU:HB3 | 1.85 | 0.59 |
| 1:D:302:LYS:HZ3 | 1:D:306:SER:CA | 2.15 | 0.59 |
| 1:E:573:GLU:CD | 1:E:573:GLU:H | 2.11 | 0.59 |
| 1:E:660:ALA:HB3 | 1:E:662:TYR:HB2 | 1.85 | 0.59 |
| 1:E:795:PHE:HZ | 1:E:799:ASP:OD2 | 1.86 | 0.59 |
| 1:F:193:ILE:O | 1:F:197:ILE:HG12 | 2.03 | 0.59 |
| 1:F:280:VAL:HA | 1:F:310:LEU:HG | 1.85 | 0.59 |
| 1:F:356:GLN:NE2 | 1:F:367:ILE:CD1 | 2.60 | 0.59 |
| 1:F:587:ILE:O | 1:F:591:SER:N | 2.36 | 0.59 |
| 1:F:678:LYS:NZ | 1:F:680:TYR:C | 2.59 | 0.59 |
| 1:F:687:GLU:HG2 | 1:F:728:ALA:H | 1.68 | 0.59 |
| 1:F:783:ILE:O | 1:F:786:ILE:HB | 2.02 | 0.59 |
| 1:F:789:LYS:HA | 1:F:792:GLU:OE2 | 2.03 | 0.59 |
| 1:A:270:LYS:HG2 | 1:A:273:GLU:OE1 | 2.03 | 0.59 |
| 1:A:380:LYS:HG2 | 1:A:680:TYR:OH | 2.03 | 0.59 |
| 1:B:180:GLN:CG | 1:B:182:LYS:NZ | 2.66 | 0.59 |
| 1:B:235:PRO:HB3 | 1:C:408:ASP:O | 2.02 | 0.59 |
| 1:B:363:HIS:HB3 | 1:B:365:VAL:HG23 | 1.84 | 0.59 |
| 1:B:657:GLY:O | 1:B:667:GLU:HB3 | 2.03 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:778:LYS:O | 1:B:782:LYS:HG2 | 2.03 | 0.59 |
| 1:B:843:ARG:NH1 | 1:B:848:GLU:CD | 2.60 | 0.59 |
| 1:C:179:ARG:HD2 | 1:C:495:ARG:HD2 | 1.85 | 0.59 |
| 1:C:592:ASN:CA | 1:C:595:ARG:HH11 | 2.16 | 0.59 |
| 1:D:291:GLY:H | 1:D:294:LYS:HG2 | 1.66 | 0.59 |
| 1:D:390:ASP:O | 1:D:393:LEU:HB2 | 2.03 | 0.59 |
| 1:D:599:SER:OG | 1:D:600:GLY:N | 2.32 | 0.59 |
| 1:D:762:PHE:O | 1:D:766:ILE:HG23 | 2.02 | 0.59 |
| 1:D:801:HIS:N | 1:D:802:TYR:HD1 | 2.00 | 0.59 |
| 1:E:332:GLU:CD | 1:E:337:LYS:NZ | 2.60 | 0.59 |
| 1:E:606:GLN:HG3 | 1:E:705:ASP:OD2 | 2.03 | 0.59 |
| 1:E:629:GLY:N | 1:E:634:ASP:O | 2.36 | 0.59 |
| 1:F:211:ILE:HG13 | 1:F:318:ASN:OD1 | 2.03 | 0.59 |
| 1:F:744:GLU:CG | 1:F:747:LYS:HB2 | 2.31 | 0.59 |
| 1:A:198:ARG:HG2 | 1:B:401:ALA:HB1 | 1.85 | 0.58 |
| 1:B:625:LYS:C | 1:B:635:GLU:OE2 | 2.46 | 0.58 |
| 1:B:646:LEU:HD11 | 1:B:690:LYS:HZ3 | 1.68 | 0.58 |
| 1:C:214:PRO:HG2 | 1:C:387:ARG:NH2 | 2.18 | 0.58 |
| 1:C:737:GLN:HA | 1:C:774:LYS:NZ | 2.17 | 0.58 |
| 1:C:857:VAL:HG12 | 1:C:878:GLU:HB3 | 1.86 | 0.58 |
| 1:D:197:ILE:HA | 1:D:200:LEU:HD12 | 1.85 | 0.58 |
| 1:D:763:LEU:H | 1:D:763:LEU:HD12 | 1.66 | 0.58 |
| 1:D:810:ALA:C | 1:D:814:LEU:HG | 2.28 | 0.58 |
| 1:D:840:LEU:HD12 | 1:D:841:ALA:N | 2.18 | 0.58 |
| 1:D:842:LEU:C | 1:D:846:LYS:NZ | 2.61 | 0.58 |
| 1:E:211:ILE:HA | 1:E:316:THR:O | 2.03 | 0.58 |
| 1:F:743:GLN:C | 1:F:747:LYS:HZ1 | 2.11 | 0.58 |
| 1:A:651:ALA:HB1 | 1:A:658:THR:HG23 | 1.85 | 0.58 |
| 1:B:282:PHE:HA | 1:B:312:VAL:HB | 1.85 | 0.58 |
| 1:B:544:ASP:CG | 1:B:545:THR:H | 2.11 | 0.58 |
| 1:B:825:ALA:O | 1:B:828:LEU:N | 2.36 | 0.58 |
| 1:C:391:SER:O | 1:C:394:ASP:HB2 | 2.03 | 0.58 |
| 1:C:513:ILE:HD12 | 1:C:514:LYS:HG3 | 1.84 | 0.58 |
| 1:C:567:GLU:O | 1:C:571:HIS:N | 2.29 | 0.58 |
| 1:D:172:ILE:H | 1:D:245:SER:H | 1.51 | 0.58 |
| 1:D:266:LYS:HG2 | 1:D:270:LYS:NZ | 2.18 | 0.58 |
| 1:D:377:GLN:HA | 1:D:380:LYS:HE3 | 1.84 | 0.58 |
| 1:D:731:ALA:O | 1:D:734:ILE:N | 2.37 | 0.58 |
| 1:E:226:ALA:O | 1:E:229:ILE:HB | 2.02 | 0.58 |
| 1:E:228:ARG:NH1 | 1:E:231:ASP:HB2 | 2.18 | 0.58 |
| 1:E:367:ILE:HG12 | 1:E:540:VAL:HG23 | 1.85 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:405:VAL:O | 1:E:408:ASP:N | 2.35 | 0.58 |
| 1:E:504:ASP:HA | 1:E:507:TYR:CD2 | 2.38 | 0.58 |
| 1:E:616:SER:HA | 2:E:1002:AGS:PB | 2.43 | 0.58 |
| 1:E:813:PHE:O | 1:E:816:LYS:HB2 | 2.03 | 0.58 |
| 1:F:205:LYS:HZ3 | 1:F:334:ARG:N | 2.01 | 0.58 |
| 1:F:348:THR:O | 1:F:351:ILE:HB | 2.03 | 0.58 |
| 1:F:623:LEU:O | 1:F:627:VAL:N | 2.31 | 0.58 |
| 1:F:702:MET:O | 1:F:705:ASP:O | 2.21 | 0.58 |
| 1:F:758:PHE:O | 1:F:759:ARG:HG2 | 2.04 | 0.58 |
| 1:A:357:PRO:HA | 1:A:361:ILE:H | 1.67 | 0.58 |
| 1:A:684:LEU:HA | 1:A:723:VAL:HG21 | 1.86 | 0.58 |
| 1:B:612:PHE:H | 1:B:726:THR:HB | 1.67 | 0.58 |
| 1:B:683:LEU:CB | 1:B:723:VAL:HB | 2.33 | 0.58 |
| 1:C:325:VAL:HA | 1:C:331:PHE:CE2 | 2.37 | 0.58 |
| 1:C:490:ALA:HA | 1:C:493:ALA:HB3 | 1.84 | 0.58 |
| 1:C:680:TYR:HA | 1:C:721:CYS:HB2 | 1.84 | 0.58 |
| 2:C:1001:AGS:O1A | 2:C:1001:AGS:O3' | 2.19 | 0.58 |
| 1:D:165:GLU:O | 1:D:264:ARG:NH2 | 2.36 | 0.58 |
| 1:D:251:LEU:HA | 1:D:261:PHE:HZ | 1.67 | 0.58 |
| 1:D:371:ALA:O | 1:D:375:ALA:N | 2.36 | 0.58 |
| 1:D:377:GLN:O | 1:D:380:LYS:HB3 | 2.02 | 0.58 |
| 1:D:593:ALA:O | 1:D:597:SER:OG | 2.22 | 0.58 |
| 1:D:813:PHE:O | 1:D:817:TYR:N | 2.36 | 0.58 |
| 1:E:189:ARG:HA | 1:E:191:GLU:OE2 | 2.02 | 0.58 |
| 1:E:612:PHE:C | 1:E:771:ILE:HG13 | 2.28 | 0.58 |
| 1:E:643:CYS:N | 1:E:645:GLU:OE1 | 2.36 | 0.58 |
| 1:E:655:LEU:HG | 1:E:710:SER:HA | 1.85 | 0.58 |
| 1:F:283:ILE:O | 1:F:314:GLY:HA2 | 2.02 | 0.58 |
| 1:F:833:GLN:O | 1:F:837:LEU:N | 2.21 | 0.58 |
| 1:A:169:LYS:NZ | 1:A:170:TYR:CE1 | 2.70 | 0.58 |
| 1:A:200:LEU:HD21 | 1:A:235:PRO:HG2 | 1.86 | 0.58 |
| 1:A:624:ALA:O | 1:A:627:VAL:HB | 2.03 | 0.58 |
| 1:B:316:THR:HG22 | 1:B:317:THR:N | 2.18 | 0.58 |
| 1:B:759:ARG:HB3 | 1:B:762:PHE:HB3 | 1.85 | 0.58 |
| 1:C:286:ILE:HA | 1:C:289:LEU:HD12 | 1.85 | 0.58 |
| 1:D:202:ARG:O | 1:D:206:SER:HB2 | 2.02 | 0.58 |
| 1:D:425:GLN:HG3 | 1:D:428:ILE:HD12 | 1.84 | 0.58 |
| 1:D:645:GLU:H | 1:D:645:GLU:CD | 2.11 | 0.58 |
| 1:E:597:SER:O | 1:E:601:LEU:HG | 2.03 | 0.58 |
| 1:E:742:ILE:HG12 | 1:E:773:ASN:OD1 | 2.02 | 0.58 |
| 1:F:211:ILE:HG21 | 1:F:318:ASN:CG | 2.28 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:683:LEU:HB3 | 1:F:685:PHE:CE2 | 2.38 | 0.58 |
| 1:F:700:LEU:HD22 | 1:F:761:GLU:HG2 | 1.84 | 0.58 |
| 1:A:194:ARG:O | 1:A:198:ARG:HG3 | 2.02 | 0.58 |
| 1:A:217:GLY:C | 1:A:221:ILE:HD12 | 2.27 | 0.58 |
| 1:A:646:LEU:HD12 | 1:A:647:SER:H | 1.67 | 0.58 |
| 1:A:817:TYR:CD1 | 1:A:874:GLU:HB3 | 2.38 | 0.58 |
| 1:B:172:ILE:HG12 | 1:B:245:SER:O | 2.03 | 0.58 |
| 1:B:656:LEU:HD21 | 1:B:710:SER:HA | 1.85 | 0.58 |
| 1:B:806:LEU:O | 1:B:807:THR:OG1 | 2.20 | 0.58 |
| 1:B:846:LYS:HE3 | 1:B:879:VAL:HG13 | 1.86 | 0.58 |
| 1:C:255:ALA:HB1 | 1:C:256:LYS:NZ | 2.18 | 0.58 |
| 1:C:564:SER:O | 1:C:566:ASN:N | 2.29 | 0.58 |
| 1:D:283:ILE:O | 1:D:314:GLY:HA2 | 2.04 | 0.58 |
| 1:D:452:GLU:HG2 | 1:D:456:GLN:HB2 | 1.85 | 0.58 |
| 1:D:459:LEU:C | 1:D:463:ARG:NH1 | 2.62 | 0.58 |
| 1:E:270:LYS:NZ | 1:E:274:GLU:CA | 2.66 | 0.58 |
| 1:E:369:ASP:HA | 1:E:372:LEU:HD12 | 1.84 | 0.58 |
| 1:E:651:ALA:CA | 1:E:656:LEU:HB2 | 2.25 | 0.58 |
| 1:E:658:THR:HB | 1:E:665:TYR:HA | 1.85 | 0.58 |
| 1:E:767:SER:O | 1:F:830:ARG:NH2 | 2.31 | 0.58 |
| 1:F:548:GLU:HA | 1:F:551:ALA:HB3 | 1.85 | 0.58 |
| 1:F:605:ARG:HG3 | 1:F:707:ARG:N | 2.18 | 0.58 |
| 1:F:613:LEU:HB2 | 1:F:770:VAL:O | 2.03 | 0.58 |
| 1:F:704:ASP:OD1 | 1:F:765:ARG:HD3 | 2.01 | 0.58 |
| 1:F:833:GLN:HE21 | 1:F:834:ASN:ND2 | 2.01 | 0.58 |
| 1:A:213:GLU:CA | 1:A:218:LYS:HZ3 | 2.16 | 0.58 |
| 1:B:195:SER:OG | 1:B:196:THR:N | 2.35 | 0.58 |
| 1:B:649:LYS:N | 1:B:691:ALA:O | 2.36 | 0.58 |
| 1:C:172:ILE:HD11 | 1:C:245:SER:N | 2.18 | 0.58 |
| 1:C:197:ILE:HA | 1:C:200:LEU:CD1 | 2.34 | 0.58 |
| 1:C:350:ALA:HA | 1:C:353:ARG:HD2 | 1.84 | 0.58 |
| 1:C:587:ILE:O | 1:C:590:VAL:HB | 2.04 | 0.58 |
| 1:D:463:ARG:NH1 | 1:D:463:ARG:HB2 | 2.19 | 0.58 |
| 1:D:673:ASN:HA | 1:D:676:GLN:OE1 | 2.03 | 0.58 |
| 1:D:802:TYR:CE1 | 1:D:853:GLU:HG3 | 2.39 | 0.58 |
| 1:E:448:ALA:O | 1:E:452:GLU:N | 2.31 | 0.58 |
| 1:E:597:SER:OG | 1:E:598:ARG:N | 2.33 | 0.58 |
| 1:F:197:ILE:HG13 | 1:F:228:ARG:HH11 | 1.68 | 0.58 |
| 1:F:356:GLN:OE1 | 1:F:372:LEU:HD23 | 2.03 | 0.58 |
| 1:F:620:LYS:HD2 | 2:F:1002:AGS:C4' | 2.32 | 0.58 |
| 1:F:638:MET:HE2 | 1:F:671:LEU:HD21 | 1.86 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:549:THR:O | 1:A:552:ARG:NH1 | 2.36 | 0.58 |
| 1:A:801:HIS:N | 1:A:851:ASP:OD1 | 2.37 | 0.58 |
| 1:B:302:LYS:NZ | 1:B:305:LEU:HB2 | 2.18 | 0.58 |
| 1:B:669:GLY:C | 1:B:671:LEU:HG | 2.28 | 0.58 |
| 1:C:190:GLU:OE2 | 1:C:192:GLU:OE2 | 2.22 | 0.58 |
| 1:C:548:GLU:HG2 | 1:C:549:THR:N | 2.17 | 0.58 |
| 1:C:692:HIS:HE1 | 1:C:694:ASP:CG | 2.12 | 0.58 |
| 1:C:852:LYS:N | 1:C:853:GLU:OE1 | 2.36 | 0.58 |
| 1:D:89:SER:O | 1:D:93:GLY:N | 2.30 | 0.58 |
| 1:D:264:ARG:O | 1:D:268:VAL:N | 2.29 | 0.58 |
| 1:D:357:PRO:CD | 1:D:358:LYS:HZ2 | 2.17 | 0.58 |
| 1:D:733:PHE:CE2 | 1:D:750:VAL:HB | 2.39 | 0.58 |
| 1:D:778:LYS:O | 1:D:781:HIS:N | 2.36 | 0.58 |
| 1:E:216:ILE:HG23 | 1:E:217:GLY:H | 1.69 | 0.58 |
| 1:E:222:ILE:O | 1:E:225:VAL:HB | 2.03 | 0.58 |
| 1:E:300:ILE:O | 1:E:303:PRO:HD2 | 2.03 | 0.58 |
| 1:E:319:ASN:O | 1:E:322:ARG:NH1 | 2.36 | 0.58 |
| 1:E:416:SER:O | 1:E:419:ARG:NE | 2.37 | 0.58 |
| 1:F:331:PHE:CA | 1:F:334:ARG:HD2 | 2.33 | 0.58 |
| 1:A:606:GLN:HG3 | 1:A:703:LEU:HD21 | 1.85 | 0.58 |
| 1:A:790:GLU:HG2 | 1:A:794:ARG:NH2 | 2.18 | 0.58 |
| 1:A:839:LYS:HA | 1:A:842:LEU:HD12 | 1.85 | 0.58 |
| 1:A:843:ARG:NH1 | 1:A:846:LYS:HD2 | 2.18 | 0.58 |
| 1:B:353:ARG:HH22 | 1:B:372:LEU:CD1 | 2.17 | 0.58 |
| 1:B:643:CYS:O | 1:B:686:ASP:OD2 | 2.21 | 0.58 |
| 1:B:650:TYR:HD1 | 1:B:652:VAL:HG22 | 1.69 | 0.58 |
| 1:B:754:VAL:O | 1:B:756:GLN:N | 2.36 | 0.58 |
| 1:C:298:ALA:HB1 | 1:C:302:LYS:CB | 2.33 | 0.58 |
| 1:C:392:ALA:O | 1:C:393:LEU:C | 2.46 | 0.58 |
| 1:D:431:LEU:HB3 | 1:D:443:ASP:OD1 | 2.03 | 0.58 |
| 1:D:576:LEU:O | 1:D:580:VAL:HG23 | 2.04 | 0.58 |
| 1:E:170:TYR:HB2 | 1:E:246:LEU:HD13 | 1.86 | 0.58 |
| 1:E:189:ARG:HB3 | 1:E:192:GLU:OE1 | 2.03 | 0.58 |
| 1:E:389:PRO:O | 1:E:393:LEU:HG | 2.03 | 0.58 |
| 1:F:176:GLU:O | 1:F:179:ARG:N | 2.36 | 0.58 |
| 1:F:225:VAL:O | 1:F:229:ILE:HG12 | 2.04 | 0.58 |
| 1:F:245:SER:HA | 1:F:283:ILE:HD13 | 1.85 | 0.58 |
| 1:F:790:GLU:HA | 1:F:793:GLU:OE2 | 2.04 | 0.58 |
| 1:A:200:LEU:HD11 | 1:A:235:PRO:HG2 | 1.86 | 0.58 |
| 1:A:274:GLU:N | 1:A:276:LYS:HZ1 | 2.02 | 0.58 |
| 1:A:351:ILE:HG22 | 1:A:355:LEU:HD11 | 1.86 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:353:ARG:C | 1:A:360:GLU:OE2 | 2.46 | 0.58 |
| 1:A:583:GLN:HE21 | 1:A:771:ILE:C | 2.11 | 0.58 |
| 1:A:602:ALA:O | 1:A:605:ARG:NE | 2.18 | 0.58 |
| 1:A:634:ASP:OD2 | 1:A:637:MET:HE2 | 2.03 | 0.58 |
| 1:A:814:LEU:HA | 1:A:817:TYR:HB2 | 1.86 | 0.58 |
| 1:B:210:LEU:CD2 | 1:B:337:LYS:HZ3 | 2.13 | 0.58 |
| 1:B:215:GLY:HA2 | 1:B:218:LYS:HE3 | 1.85 | 0.58 |
| 1:B:228:ARG:NH1 | 1:B:231:ASP:OD2 | 2.36 | 0.58 |
| 1:B:348:THR:O | 1:B:351:ILE:N | 2.37 | 0.58 |
| 1:B:656:LEU:HA | 1:B:668:GLY:CA | 2.34 | 0.58 |
| 1:C:485:GLU:HG2 | 1:C:488:ASN:HD22 | 1.68 | 0.58 |
| 1:C:708:ILE:HB | 1:C:716:ILE:HB | 1.85 | 0.58 |
| 1:D:716:ILE:HG13 | 1:D:717:ASP:O | 2.04 | 0.58 |
| 1:D:784:VAL:HG13 | 1:D:785:ASP:N | 2.17 | 0.58 |
| 1:E:330:ALA:CA | 1:E:333:ARG:HB2 | 2.28 | 0.58 |
| 1:E:516:GLN:O | 1:E:520:LEU:HG | 2.04 | 0.58 |
| 1:A:177:GLN:HB2 | 1:A:182:LYS:NZ | 2.12 | 0.58 |
| 1:A:608:ALA:O | 1:A:722:ILE:HG23 | 2.04 | 0.58 |
| 1:B:215:GLY:O | 1:B:218:LYS:N | 2.37 | 0.58 |
| 1:B:700:LEU:HA | 1:B:703:LEU:CB | 2.27 | 0.58 |
| 1:D:459:LEU:C | 1:D:463:ARG:HH12 | 2.11 | 0.58 |
| 1:D:650:TYR:HB2 | 1:D:654:LYS:N | 2.19 | 0.58 |
| 1:D:857:VAL:CG1 | 1:D:878:GLU:HA | 2.29 | 0.58 |
| 1:E:274:GLU:C | 1:E:276:LYS:H | 2.12 | 0.58 |
| 1:E:323:SER:HA | 1:E:326:GLU:OE1 | 2.04 | 0.58 |
| 1:E:418:GLU:OE2 | 1:E:421:LEU:HD12 | 2.04 | 0.58 |
| 1:E:779:ALA:O | 1:E:782:LYS:N | 2.37 | 0.58 |
| 1:F:622:GLU:CD | 2:F:1002:AGS:H8 | 2.29 | 0.58 |
| 1:A:234:VAL:HB | 1:A:238:LEU:HB2 | 1.86 | 0.57 |
| 1:A:368:LEU:HD21 | 1:A:540:VAL:H | 1.69 | 0.57 |
| 1:B:175:THR:N | 1:B:243:LEU:HD11 | 2.19 | 0.57 |
| 1:B:374:THR:C | 1:B:378:LEU:HG | 2.29 | 0.57 |
| 1:B:399:SER:O | 1:B:403:VAL:N | 2.23 | 0.57 |
| 1:C:296:ASP:HA | 1:C:299:ASN:CG | 2.29 | 0.57 |
| 1:C:622:GLU:H | 1:C:826:ARG:NH1 | 1.99 | 0.57 |
| 1:C:788:LEU:O | 1:C:789:LYS:C | 2.46 | 0.57 |
| 1:D:192:GLU:N | 1:D:192:GLU:OE1 | 2.35 | 0.57 |
| 1:D:328:ASP:CG | 1:D:331:PHE:H | 2.12 | 0.57 |
| 1:D:369:ASP:OD1 | 1:D:369:ASP:O | 2.21 | 0.57 |
| 1:D:395:LEU:HD23 | 1:D:398:ILE:HD12 | 1.86 | 0.57 |
| 1:D:565:GLU:HG2 | 1:D:566:ASN:N | 2.18 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:377:GLN:O | 1:E:381:ARG:N | 2.32 | 0.57 |
| 1:E:383:LEU:HD21 | 1:E:385:TYR:CE1 | 2.39 | 0.57 |
| 1:E:622:GLU:HA | 1:E:625:LYS:HB2 | 1.86 | 0.57 |
| 1:E:629:GLY:O | 1:E:633:ASN:N | 2.33 | 0.57 |
| 1:E:681:SER:OG | 1:E:722:ILE:N | 2.37 | 0.57 |
| 1:E:683:LEU:C | 1:E:723:VAL:HG23 | 2.28 | 0.57 |
| 1:F:356:GLN:CB | 1:F:357:PRO:HD2 | 2.25 | 0.57 |
| 1:A:246:LEU:HG | 1:A:283:ILE:HD13 | 1.85 | 0.57 |
| 1:A:361:ILE:HA | 1:A:364:GLY:HA2 | 1.86 | 0.57 |
| 1:A:569:LEU:HA | 1:A:572:MET:CG | 2.33 | 0.57 |
| 1:A:833:GLN:HA | 1:A:836:ILE:HD12 | 1.85 | 0.57 |
| 1:B:320:GLU:HA | 1:B:323:SER:CB | 2.34 | 0.57 |
| 1:B:611:LEU:CG | 1:B:769:ILE:HA | 2.33 | 0.57 |
| 1:C:328:ASP:O | 1:C:331:PHE:HB3 | 2.04 | 0.57 |
| 1:C:350:ALA:N | 1:C:353:ARG:NH1 | 2.52 | 0.57 |
| 1:C:366:ARG:HG2 | 1:C:538:GLN:O | 2.03 | 0.57 |
| 1:C:611:LEU:O | 1:C:726:THR:HG22 | 2.05 | 0.57 |
| 1:D:378:LEU:HA | 1:D:381:ARG:HG2 | 1.86 | 0.57 |
| 1:D:537:ILE:HG13 | 1:D:540:VAL:CG1 | 2.34 | 0.57 |
| 1:D:606:GLN:C | 1:D:719:SER:HB3 | 2.28 | 0.57 |
| 1:D:803:LYS:HB3 | 1:D:806:LEU:CD1 | 2.33 | 0.57 |
| 1:E:304:ALA:HA | 1:E:307:ARG:HD2 | 1.86 | 0.57 |
| 1:F:240:GLY:O | 1:F:278:LEU:N | 2.37 | 0.57 |
| 1:F:648:GLU:O | 1:F:692:HIS:HA | 2.04 | 0.57 |
| 1:F:708:ILE:HD12 | 1:F:708:ILE:H | 1.69 | 0.57 |
| 1:B:166:TYR:O | 1:B:169:LYS:HG2 | 2.03 | 0.57 |
| 1:B:219:THR:O | 1:B:222:ILE:HD12 | 2.04 | 0.57 |
| 1:B:751:MET:HB3 | 1:B:755:ARG:NH1 | 2.16 | 0.57 |
| 1:C:48:VAL:O | 1:C:55:ILE:N | 2.37 | 0.57 |
| 1:C:317:THR:HB | 1:C:320:GLU:HB3 | 1.87 | 0.57 |
| 1:C:322:ARG:HG3 | 1:C:325:VAL:HB | 1.86 | 0.57 |
| 1:C:390:ASP:O | 1:C:394:ASP:N | 2.27 | 0.57 |
| 1:D:6:GLN:N | 1:D:153:ILE:O | 2.37 | 0.57 |
| 1:D:544:ASP:OD1 | 1:D:544:ASP:N | 2.35 | 0.57 |
| 1:D:791:ILE:CA | 1:D:794:ARG:HH12 | 2.16 | 0.57 |
| 1:D:832:ILE:O | 1:D:836:ILE:HG12 | 2.04 | 0.57 |
| 1:E:218:LYS:HZ2 | 1:E:387:ARG:NH1 | 2.00 | 0.57 |
| 1:E:221:ILE:O | 1:E:225:VAL:HG23 | 2.04 | 0.57 |
| 1:E:654:LYS:HZ2 | 1:E:698:VAL:HG13 | 1.70 | 0.57 |
| 1:E:668:GLY:HA3 | 1:E:672:THR:H | 1.68 | 0.57 |
| 1:E:856:ASN:N | 1:E:879:VAL:O | 2.30 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:305:LEU:HD12 | 1:F:306:SER:N | 2.20 | 0.57 |
| 1:F:803:LYS:HD3 | 1:F:852:LYS:HB3 | 1.85 | 0.57 |
| 1:A:320:GLU:HA | 1:A:323:SER:HB2 | 1.84 | 0.57 |
| 1:B:12:LEU:O | 1:B:16:THR:N | 2.37 | 0.57 |
| 1:B:345:VAL:O | 1:B:348:THR:HB | 2.05 | 0.57 |
| 1:B:777:ARG:HG3 | 1:B:778:LYS:N | 2.18 | 0.57 |
| 1:C:174:MET:CG | 1:C:242:LYS:HZ3 | 2.14 | 0.57 |
| 1:C:290:MET:HA | 1:C:294:LYS:HA | 1.84 | 0.57 |
| 1:C:610:PHE:CB | 1:C:724:ILE:HD13 | 2.34 | 0.57 |
| 1:C:655:LEU:HG | 1:C:656:LEU:N | 2.18 | 0.57 |
| 1:D:207:ASN:HD21 | 1:D:311:LYS:HA | 1.69 | 0.57 |
| 1:D:218:LYS:O | 1:D:221:ILE:HB | 2.05 | 0.57 |
| 1:D:225:VAL:HA | 1:D:228:ARG:HB2 | 1.85 | 0.57 |
| 1:D:321:TYR:HD1 | 1:D:324:ILE:HD13 | 1.69 | 0.57 |
| 1:D:707:ARG:HB2 | 1:D:716:ILE:O | 2.05 | 0.57 |
| 1:E:217:GLY:O | 1:E:220:ALA:HB3 | 2.05 | 0.57 |
| 1:E:348:THR:O | 1:E:352:LEU:HG | 2.03 | 0.57 |
| 1:E:409:SER:OG | 1:E:414:LEU:HD21 | 2.03 | 0.57 |
| 1:E:592:ASN:O | 1:E:593:ALA:C | 2.47 | 0.57 |
| 1:E:795:PHE:CD2 | 1:E:796:GLU:N | 2.72 | 0.57 |
| 1:F:265:PHE:O | 1:F:268:VAL:HB | 2.04 | 0.57 |
| 1:F:820:SER:HB3 | 1:F:823:MET:C | 2.29 | 0.57 |
| 1:A:210:LEU:HB2 | 1:A:337:LYS:C | 2.29 | 0.57 |
| 1:A:262:GLU:OE1 | 1:A:262:GLU:N | 2.37 | 0.57 |
| 1:A:331:PHE:CD2 | 1:A:332:GLU:HB3 | 2.40 | 0.57 |
| 1:A:584:MET:O | 1:A:588:LYS:N | 2.26 | 0.57 |
| 1:A:611:LEU:HB2 | 1:A:724:ILE:HG21 | 1.87 | 0.57 |
| 1:B:617:GLY:O | 1:B:826:ARG:HD2 | 2.03 | 0.57 |
| 1:B:683:LEU:H | 1:B:723:VAL:HG11 | 1.69 | 0.57 |
| 1:B:696:LEU:O | 1:B:699:MET:HB2 | 2.04 | 0.57 |
| 1:B:745:SER:O | 1:B:749:LEU:N | 2.30 | 0.57 |
| 1:C:557:PRO:HA | 1:C:560:LYS:CE | 2.34 | 0.57 |
| 1:D:213:GLU:CD | 1:D:387:ARG:HD2 | 2.28 | 0.57 |
| 1:D:225:VAL:HG13 | 1:D:233:ASP:OD2 | 2.04 | 0.57 |
| 1:D:613:LEU:H | 1:D:771:ILE:HA | 1.68 | 0.57 |
| 1:D:794:ARG:O | 1:D:796:GLU:OE2 | 2.23 | 0.57 |
| 1:D:842:LEU:HD12 | 1:D:846:LYS:HZ2 | 1.68 | 0.57 |
| 1:E:237:ILE:H | 1:E:237:ILE:HD12 | 1.68 | 0.57 |
| 1:E:383:LEU:HD11 | 1:E:385:TYR:CZ | 2.39 | 0.57 |
| 1:E:407:ARG:HA | 1:E:536:MET:SD | 2.44 | 0.57 |
| 1:E:513:ILE:HA | 1:E:516:GLN:CD | 2.29 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:549:THR:O | 1:E:553:LEU:HG | 2.04 | 0.57 |
| 1:E:657:GLY:HA3 | 1:E:667:GLU:HA | 1.86 | 0.57 |
| 1:E:667:GLU:OE1 | 1:E:711:GLY:HA3 | 2.05 | 0.57 |
| 1:E:786:ILE:CA | 1:E:789:LYS:HZ3 | 2.17 | 0.57 |
| 1:F:173:ASP:C | 1:F:176:GLU:OE2 | 2.48 | 0.57 |
| 1:F:257:TYR:CZ | 1:F:260:ASP:OD2 | 2.57 | 0.57 |
| 1:F:640:ARG:NE | 1:F:685:PHE:O | 2.38 | 0.57 |
| 1:A:344:SER:O | 1:A:348:THR:N | 2.34 | 0.57 |
| 1:A:617:GLY:C | 1:A:620:LYS:NZ | 2.62 | 0.57 |
| 1:A:700:LEU:HD21 | 1:A:765:ARG:HB2 | 1.86 | 0.57 |
| 1:B:550:ALA:HA | 1:B:552:ARG:NH1 | 2.20 | 0.57 |
| 1:B:659:THR:OG1 | 1:B:661:GLY:O | 2.14 | 0.57 |
| 1:B:830:ARG:O | 1:B:833:GLN:HB3 | 2.03 | 0.57 |
| 1:C:460:GLU:OE1 | 1:C:463:ARG:HD2 | 2.05 | 0.57 |
| 1:C:506:ARG:NH2 | 1:D:430:ALA:HB1 | 2.20 | 0.57 |
| 1:C:654:LYS:O | 1:C:671:LEU:HG | 2.04 | 0.57 |
| 1:C:857:VAL:HA | 1:C:880:LEU:H | 1.70 | 0.57 |
| 1:D:248:LEU:O | 1:D:251:LEU:HG | 2.05 | 0.57 |
| 1:D:493:ALA:HB3 | 1:D:498:ASP:OD2 | 2.04 | 0.57 |
| 1:D:559:LYS:HZ3 | 1:D:560:LYS:NZ | 2.02 | 0.57 |
| 1:D:650:TYR:HB2 | 1:D:654:LYS:HB3 | 1.87 | 0.57 |
| 1:D:777:ARG:CA | 1:D:780:ILE:HB | 2.34 | 0.57 |
| 1:D:879:VAL:HG12 | 1:D:880:LEU:N | 2.18 | 0.57 |
| 1:E:169:LYS:NZ | 1:E:268:VAL:H | 2.03 | 0.57 |
| 1:E:570:ILE:C | 1:E:595:ARG:HH22 | 2.13 | 0.57 |
| 1:E:762:PHE:O | 1:E:766:ILE:HG13 | 2.04 | 0.57 |
| 1:F:193:ILE:HG22 | 1:F:228:ARG:NH1 | 2.20 | 0.57 |
| 1:F:206:SER:OG | 1:F:207:ASN:ND2 | 2.37 | 0.57 |
| 1:F:707:ARG:HA | 1:F:715:THR:HG21 | 1.86 | 0.57 |
| 1:A:270:LYS:HA | 1:A:273:GLU:HB2 | 1.85 | 0.57 |
| 1:A:828:LEU:O | 1:A:832:ILE:HG13 | 2.04 | 0.57 |
| 1:B:563:GLU:O | 1:B:568:LYS:NZ | 2.36 | 0.57 |
| 1:B:673:ASN:HA | 1:B:676:GLN:HB3 | 1.86 | 0.57 |
| 1:C:170:TYR:OH | 1:C:249:ALA:C | 2.42 | 0.57 |
| 1:C:234:VAL:HB | 1:C:239:GLN:HA | 1.85 | 0.57 |
| 1:C:784:VAL:CG2 | 1:C:785:ASP:H | 2.13 | 0.57 |
| 1:D:297:ALA:HB3 | 1:D:299:ASN:ND2 | 2.20 | 0.57 |
| 1:D:650:TYR:HD2 | 1:D:654:LYS:CB | 2.14 | 0.57 |
| 1:D:723:VAL:CG1 | 1:D:725:MET:HG3 | 2.35 | 0.57 |
| 1:D:834:ASN:CG | 1:D:835:GLU:H | 2.07 | 0.57 |
| 1:E:179:ARG:HG2 | 1:E:492:ASP:OD2 | 2.04 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:209:CYS:SG | 1:E:210:LEU:N | 2.76 | 0.57 |
| 1:E:621:THR:HG22 | 1:E:625:LYS:CD | 2.35 | 0.57 |
| 1:E:659:THR:O | 1:E:714:LYS:NZ | 2.36 | 0.57 |
| 1:A:246:LEU:HB3 | 1:A:282:PHE:N | 2.20 | 0.57 |
| 1:A:283:ILE:H | 1:A:312:VAL:CG2 | 2.17 | 0.57 |
| 1:A:612:PHE:H | 1:A:770:VAL:C | 2.13 | 0.57 |
| 1:A:808:GLN:O | 1:A:811:LYS:HB2 | 2.05 | 0.57 |
| 1:A:818:GLY:O | 1:A:828:LEU:HB2 | 2.05 | 0.57 |
| 1:A:822:ASP:OD1 | 1:F:307:ARG:NH2 | 2.34 | 0.57 |
| 1:A:842:LEU:O | 1:A:845:LEU:HB3 | 2.05 | 0.57 |
| 1:B:320:GLU:HA | 1:B:323:SER:OG | 2.05 | 0.57 |
| 1:B:778:LYS:HA | 1:B:781:HIS:HB3 | 1.85 | 0.57 |
| 1:B:787:ARG:O | 1:B:790:GLU:N | 2.38 | 0.57 |
| 1:B:848:GLU:HG3 | 1:B:849:ILE:N | 2.18 | 0.57 |
| 1:C:568:LYS:NZ | 1:C:630:PHE:CD2 | 2.73 | 0.57 |
| 1:C:620:LYS:O | 1:C:623:LEU:HB3 | 2.04 | 0.57 |
| 1:C:718:CYS:O | 1:C:720:ASN:N | 2.32 | 0.57 |
| 1:C:813:PHE:CZ | 1:C:877:LEU:HA | 2.40 | 0.57 |
| 1:C:828:LEU:HD22 | 1:C:832:ILE:HD11 | 1.86 | 0.57 |
| 1:D:225:VAL:O | 1:D:229:ILE:HG13 | 2.05 | 0.57 |
| 1:D:234:VAL:HG12 | 1:D:235:PRO:O | 2.04 | 0.57 |
| 1:D:251:LEU:O | 1:D:253:ALA:N | 2.37 | 0.57 |
| 1:D:381:ARG:HH11 | 1:D:382:TYR:HE1 | 1.50 | 0.57 |
| 1:D:668:GLY:O | 1:D:671:LEU:HG | 2.05 | 0.57 |
| 1:D:682:VAL:HA | 1:D:722:ILE:C | 2.30 | 0.57 |
| 1:E:356:GLN:O | 1:E:359:TYR:N | 2.38 | 0.57 |
| 1:E:470:LYS:HA | 1:E:473:HIS:ND1 | 2.20 | 0.57 |
| 1:E:696:LEU:HD23 | 1:E:699:MET:SD | 2.45 | 0.57 |
| 1:F:783:ILE:HD12 | 1:F:786:ILE:HD12 | 1.86 | 0.57 |
| 1:F:807:THR:HB | 1:F:856:ASN:HA | 1.87 | 0.57 |
| 1:B:251:LEU:N | 1:B:264:ARG:HH12 | 2.00 | 0.57 |
| 1:B:646:LEU:N | 1:B:692:HIS:N | 2.47 | 0.57 |
| 1:B:839:LYS:HZ3 | 1:B:877:LEU:HD23 | 1.69 | 0.57 |
| 1:C:214:PRO:HG2 | 1:C:387:ARG:HH21 | 1.69 | 0.57 |
| 1:C:242:LYS:H | 1:C:280:VAL:H | 1.52 | 0.57 |
| 1:C:395:LEU:O | 1:C:399:SER:OG | 2.22 | 0.57 |
| 1:C:612:PHE:HA | 1:C:726:THR:CA | 2.32 | 0.57 |
| 1:C:648:GLU:HG3 | 1:C:692:HIS:CD2 | 2.40 | 0.57 |
| 1:C:733:PHE:HZ | 1:C:749:LEU:CB | 2.12 | 0.57 |
| 1:C:803:LYS:NZ | 1:C:854:THR:N | 2.53 | 0.57 |
| 1:C:857:VAL:CA | 1:C:880:LEU:HB3 | 2.31 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:200:LEU:HD23 | 1:D:208:PRO:HD2 | 1.86 | 0.57 |
| 1:D:260:ASP:OD2 | 1:D:264:ARG:HB2 | 2.04 | 0.57 |
| 1:D:460:GLU:OE2 | 1:D:463:ARG:NH1 | 2.38 | 0.57 |
| 1:D:461:PRO:HB2 | 1:D:465:ARG:HE | 1.69 | 0.57 |
| 1:D:609:SER:C | 1:D:768:SER:HG | 2.13 | 0.57 |
| 1:E:169:LYS:HZ2 | 1:E:268:VAL:N | 2.02 | 0.57 |
| 1:E:200:LEU:HB3 | 1:E:311:LYS:HE3 | 1.87 | 0.57 |
| 1:E:210:LEU:HG | 1:E:338:ILE:C | 2.30 | 0.57 |
| 1:E:268:VAL:O | 1:E:272:ILE:N | 2.24 | 0.57 |
| 1:E:611:LEU:N | 1:E:769:ILE:HG12 | 2.19 | 0.57 |
| 1:E:617:GLY:N | 2:E:1002:AGS:O2G | 2.21 | 0.57 |
| 1:E:626:LYS:NZ | 1:E:635:GLU:CD | 2.62 | 0.57 |
| 1:E:798:ASN:HA | 1:E:801:HIS:CB | 2.33 | 0.57 |
| 1:E:828:LEU:C | 1:E:831:LEU:H | 2.12 | 0.57 |
| 1:F:286:ILE:HA | 1:F:289:LEU:HB2 | 1.87 | 0.57 |
| 1:F:605:ARG:HD2 | 1:F:707:ARG:HB3 | 1.86 | 0.57 |
| 1:F:649:LYS:O | 1:F:694:ASP:HB2 | 2.05 | 0.57 |
| 1:F:748:ASN:C | 1:F:751:MET:HB3 | 2.30 | 0.57 |
| 1:A:583:GLN:O | 1:A:587:ILE:N | 2.20 | 0.57 |
| 1:B:176:GLU:OE2 | 1:B:179:ARG:HB3 | 2.05 | 0.57 |
| 1:B:617:GLY:CA | 1:B:620:LYS:NZ | 2.67 | 0.57 |
| 1:B:803:LYS:H | 1:B:853:GLU:HB3 | 1.70 | 0.57 |
| 1:B:804:LEU:H | 1:B:853:GLU:HG2 | 1.69 | 0.57 |
| 1:C:176:GLU:O | 1:C:180:GLN:NE2 | 2.35 | 0.57 |
| 1:C:212:GLY:HA3 | 1:C:340:VAL:HG22 | 1.87 | 0.57 |
| 1:C:678:LYS:HE2 | 1:C:681:SER:CB | 2.32 | 0.57 |
| 1:C:842:LEU:CD1 | 1:C:881:PRO:HB3 | 2.33 | 0.57 |
| 1:C:853:GLU:O | 1:C:853:GLU:HG2 | 2.04 | 0.57 |
| 1:D:124:SER:N | 1:D:126:ILE:O | 2.38 | 0.57 |
| 1:D:659:THR:HG22 | 1:D:660:ALA:H | 1.69 | 0.57 |
| 1:D:707:ARG:HA | 1:D:716:ILE:HG22 | 1.86 | 0.57 |
| 1:E:186:VAL:HG13 | 2:E:1001:AGS:C2 | 2.35 | 0.57 |
| 1:E:228:ARG:NH1 | 1:E:231:ASP:C | 2.63 | 0.57 |
| 1:E:596:LEU:O | 1:E:599:SER:OG | 2.16 | 0.57 |
| 1:E:611:LEU:O | 1:E:770:VAL:N | 2.38 | 0.57 |
| 1:E:637:MET:HG2 | 1:E:680:TYR:O | 2.04 | 0.57 |
| 1:E:747:LYS:HA | 1:E:750:VAL:HB | 1.86 | 0.57 |
| 1:F:245:SER:HB3 | 1:F:282:PHE:O | 2.05 | 0.57 |
| 1:F:363:HIS:ND1 | 1:F:397:ASP:OD1 | 2.37 | 0.57 |
| 1:F:363:HIS:HE2 | 1:F:396:VAL:C | 2.10 | 0.57 |
| 1:F:612:PHE:HA | 1:F:770:VAL:HG21 | 1.87 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:268:VAL:HA | 1:A:271:GLU:CB | 2.34 | 0.56 |
| 1:A:582:GLY:H | 1:A:584:MET:HE2 | 1.69 | 0.56 |
| 1:A:813:PHE:C | 1:A:817:TYR:HD2 | 2.12 | 0.56 |
| 1:B:246:LEU:H | 1:B:283:ILE:HB | 1.68 | 0.56 |
| 1:B:323:SER:C | 1:B:327:LYS:NZ | 2.63 | 0.56 |
| 1:B:385:TYR:CZ | 1:B:386:ARG:CZ | 2.87 | 0.56 |
| 1:B:751:MET:CA | 1:B:755:ARG:HH12 | 2.17 | 0.56 |
| 1:C:261:PHE:O | 1:C:263:GLU:N | 2.38 | 0.56 |
| 1:C:471:HIS:ND1 | 1:C:474:GLU:OE1 | 2.33 | 0.56 |
| 1:C:591:SER:HB2 | 1:C:595:ARG:NH1 | 2.19 | 0.56 |
| 1:C:593:ALA:HA | 1:C:596:LEU:HD12 | 1.87 | 0.56 |
| 1:D:342:GLU:HG3 | 1:D:343:PRO:O | 2.05 | 0.56 |
| 1:D:378:LEU:O | 1:D:382:TYR:N | 2.38 | 0.56 |
| 1:D:425:GLN:OE1 | 1:D:456:GLN:NE2 | 2.37 | 0.56 |
| 1:D:482:LYS:HA | 1:D:485:GLU:CD | 2.30 | 0.56 |
| 1:D:565:GLU:CD | 1:D:565:GLU:N | 2.63 | 0.56 |
| 1:D:755:ARG:NH2 | 1:D:756:GLN:OE1 | 2.38 | 0.56 |
| 1:D:853:GLU:HG2 | 1:D:854:THR:N | 2.20 | 0.56 |
| 1:E:325:VAL:O | 1:E:329:GLY:N | 2.29 | 0.56 |
| 1:E:541:VAL:C | 1:E:544:ASP:OD2 | 2.48 | 0.56 |
| 1:E:802:TYR:HB3 | 1:E:852:LYS:CA | 2.35 | 0.56 |
| 1:F:556:ILE:HG13 | 1:F:559:LYS:N | 2.17 | 0.56 |
| 1:F:569:LEU:HD22 | 1:F:598:ARG:HH21 | 1.70 | 0.56 |
| 1:F:572:MET:O | 1:F:576:LEU:HG | 2.04 | 0.56 |
| 1:F:708:ILE:H | 1:F:715:THR:CG2 | 2.18 | 0.56 |
| 1:F:806:LEU:HB3 | 1:F:811:LYS:HD3 | 1.87 | 0.56 |
| 1:F:834:ASN:O | 1:F:838:ASN:N | 2.35 | 0.56 |
| 1:A:210:LEU:HB3 | 1:A:338:ILE:O | 2.04 | 0.56 |
| 1:A:213:GLU:HG3 | 1:A:387:ARG:HH21 | 1.70 | 0.56 |
| 1:A:256:LYS:HE3 | 1:A:257:TYR:CZ | 2.40 | 0.56 |
| 1:A:387:ARG:O | 1:A:391:SER:N | 2.31 | 0.56 |
| 1:A:700:LEU:HD11 | 1:A:765:ARG:HB3 | 1.86 | 0.56 |
| 1:B:197:ILE:HA | 1:B:200:LEU:CD1 | 2.34 | 0.56 |
| 1:B:359:TYR:CZ | 1:B:363:HIS:NE2 | 2.73 | 0.56 |
| 1:B:559:LYS:NZ | 1:B:631:LEU:O | 2.38 | 0.56 |
| 1:B:650:TYR:N | 1:B:692:HIS:CE1 | 2.73 | 0.56 |
| 1:B:750:VAL:HA | 1:B:753:ALA:HB3 | 1.87 | 0.56 |
| 1:C:288:MET:HE3 | 1:C:289:LEU:HD21 | 1.86 | 0.56 |
| 1:C:403:VAL:O | 1:C:406:ALA:N | 2.38 | 0.56 |
| 1:D:380:LYS:HZ2 | 1:D:381:ARG:CA | 2.17 | 0.56 |
| 1:D:480:LYS:O | 1:D:484:ASP:N | 2.23 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:188:GLY:N | 1:E:190:GLU:OE2 | 2.38 | 0.56 |
| 1:E:211:ILE:HD13 | 1:E:337:LYS:HD2 | 1.85 | 0.56 |
| 1:E:474:GLU:HA | 1:E:477:THR:HB | 1.85 | 0.56 |
| 1:E:610:PHE:HD2 | 1:E:724:ILE:HD12 | 1.70 | 0.56 |
| 1:F:170:TYR:HB2 | 1:F:246:LEU:O | 2.05 | 0.56 |
| 1:F:294:LYS:CE | 1:F:325:VAL:HG12 | 2.27 | 0.56 |
| 1:F:353:ARG:HA | 1:F:356:GLN:HB2 | 1.87 | 0.56 |
| 1:F:356:GLN:HE22 | 1:F:372:LEU:CD2 | 2.11 | 0.56 |
| 1:F:394:ASP:O | 1:F:398:ILE:N | 2.24 | 0.56 |
| 1:A:290:MET:HB3 | 1:A:293:GLY:H | 1.68 | 0.56 |
| 1:A:332:GLU:OE2 | 1:A:333:ARG:C | 2.48 | 0.56 |
| 1:A:366:ARG:O | 1:A:367:ILE:HG22 | 2.05 | 0.56 |
| 1:A:583:GLN:HE22 | 1:A:773:ASN:N | 2.04 | 0.56 |
| 1:A:680:TYR:O | 1:A:720:ASN:HB3 | 2.06 | 0.56 |
| 1:A:813:PHE:CG | 1:A:814:LEU:N | 2.74 | 0.56 |
| 1:B:11:ALA:O | 1:B:15:LEU:N | 2.38 | 0.56 |
| 1:B:173:ASP:O | 1:B:175:THR:N | 2.37 | 0.56 |
| 1:B:610:PHE:N | 1:B:724:ILE:HD12 | 2.20 | 0.56 |
| 1:B:722:ILE:O | 1:B:723:VAL:HG23 | 2.05 | 0.56 |
| 1:B:820:SER:N | 1:B:824:GLY:HA2 | 2.19 | 0.56 |
| 1:C:218:LYS:O | 1:C:221:ILE:HB | 2.06 | 0.56 |
| 1:C:228:ARG:HA | 1:C:231:ASP:HB2 | 1.87 | 0.56 |
| 1:C:355:LEU:HD22 | 1:C:358:LYS:HD3 | 1.85 | 0.56 |
| 1:C:421:LEU:O | 1:C:424:ILE:HG22 | 2.05 | 0.56 |
| 1:C:541:VAL:HB | 1:C:544:ASP:OD2 | 2.04 | 0.56 |
| 1:C:646:LEU:HB3 | 1:C:695:VAL:HG21 | 1.86 | 0.56 |
| 1:C:753:ALA:HA | 1:C:756:GLN:CD | 2.30 | 0.56 |
| 1:C:788:LEU:HD11 | 1:C:792:GLU:HB2 | 1.87 | 0.56 |
| 1:C:825:ALA:HA | 1:C:828:LEU:HB2 | 1.86 | 0.56 |
| 1:C:839:LYS:HZ2 | 1:C:881:PRO:N | 2.03 | 0.56 |
| 1:D:165:GLU:OE2 | 1:D:167:LEU:HD12 | 2.05 | 0.56 |
| 1:D:178:ALA:C | 1:D:181:GLY:H | 2.12 | 0.56 |
| 1:D:243:LEU:HD21 | 1:D:282:PHE:CB | 2.32 | 0.56 |
| 1:D:266:LYS:HG2 | 1:D:270:LYS:HZ1 | 1.69 | 0.56 |
| 1:D:617:GLY:N | 1:D:620:LYS:HG2 | 2.20 | 0.56 |
| 1:D:620:LYS:CG | 1:D:621:THR:H | 2.15 | 0.56 |
| 1:D:779:ALA:CA | 1:D:782:LYS:HZ2 | 2.18 | 0.56 |
| 1:D:794:ARG:NH1 | 1:D:795:PHE:HE1 | 2.00 | 0.56 |
| 1:D:805:ASN:HA | 1:D:856:ASN:HB3 | 1.88 | 0.56 |
| 1:E:189:ARG:NH2 | 1:E:192:GLU:OE2 | 2.39 | 0.56 |
| 1:E:205:LYS:CB | 1:E:336:GLN:HE22 | 2.13 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:388:LEU:HB3 | 1:E:389:PRO:HD3 | 1.87 | 0.56 |
| 1:E:421:LEU:O | 1:E:425:GLN:N | 2.37 | 0.56 |
| 1:E:620:LYS:NZ | 2:E:1002:AGS:PB | 2.79 | 0.56 |
| 1:E:622:GLU:HA | 1:E:625:LYS:HD3 | 1.87 | 0.56 |
| 1:E:802:TYR:CD1 | 1:E:852:LYS:HA | 2.41 | 0.56 |
| 1:F:215:GLY:O | 2:F:1001:AGS:O2B | 2.22 | 0.56 |
| 1:F:219:THR:O | 1:F:222:ILE:N | 2.39 | 0.56 |
| 1:F:287:HIS:NE2 | 1:F:322:ARG:CA | 2.68 | 0.56 |
| 1:F:287:HIS:CE1 | 1:F:322:ARG:HA | 2.40 | 0.56 |
| 1:F:366:ARG:O | 1:F:367:ILE:HB | 2.03 | 0.56 |
| 1:F:609:SER:HG | 1:F:723:VAL:C | 2.13 | 0.56 |
| 1:F:674:GLN:O | 1:F:678:LYS:N | 2.33 | 0.56 |
| 1:F:685:PHE:CG | 1:F:725:MET:HA | 2.41 | 0.56 |
| 1:F:700:LEU:HG | 1:F:703:LEU:CD2 | 2.05 | 0.56 |
| 1:F:750:VAL:HA | 1:F:753:ALA:HB3 | 1.88 | 0.56 |
| 1:F:807:THR:O | 1:F:810:ALA:N | 2.38 | 0.56 |
| 1:A:213:GLU:OE2 | 1:A:318:ASN:N | 2.38 | 0.56 |
| 1:A:237:ILE:HA | 1:A:239:GLN:HE22 | 1.70 | 0.56 |
| 1:A:265:PHE:HA | 1:A:268:VAL:HG22 | 1.87 | 0.56 |
| 1:A:386:ARG:HB3 | 1:A:390:ASP:OD2 | 2.05 | 0.56 |
| 1:A:820:SER:OG | 1:A:823:MET:N | 2.37 | 0.56 |
| 1:A:829:ASN:HA | 1:A:832:ILE:HD12 | 1.87 | 0.56 |
| 1:B:211:ILE:O | 1:B:318:ASN:N | 2.39 | 0.56 |
| 1:B:228:ARG:CZ | 1:B:233:ASP:HB2 | 2.34 | 0.56 |
| 1:B:252:THR:HG21 | 1:B:256:LYS:NZ | 2.20 | 0.56 |
| 1:C:169:LYS:CG | 1:C:264:ARG:NE | 2.46 | 0.56 |
| 1:C:223:GLU:N | 1:C:223:GLU:CD | 2.58 | 0.56 |
| 1:C:265:PHE:CE1 | 1:C:269:LEU:HD21 | 2.39 | 0.56 |
| 1:C:280:VAL:HA | 1:C:311:LYS:HG3 | 1.87 | 0.56 |
| 1:C:785:ASP:C | 1:C:789:LYS:HG3 | 2.30 | 0.56 |
| 1:D:656:LEU:HD21 | 1:D:709:THR:HG22 | 1.88 | 0.56 |
| 1:D:701:GLN:O | 1:D:703:LEU:HB3 | 2.05 | 0.56 |
| 1:D:758:PHE:CD2 | 1:D:759:ARG:HG3 | 2.40 | 0.56 |
| 1:D:761:GLU:HA | 1:D:764:ASN:ND2 | 2.19 | 0.56 |
| 1:D:762:PHE:HD1 | 1:D:763:LEU:HD12 | 1.70 | 0.56 |
| 1:E:366:ARG:C | 1:E:539:ASN:HA | 2.31 | 0.56 |
| 1:E:535:SER:O | 1:E:537:ILE:HG12 | 2.05 | 0.56 |
| 1:E:541:VAL:HG12 | 1:E:544:ASP:OD2 | 2.05 | 0.56 |
| 1:E:653:SER:O | 1:E:668:GLY:HA2 | 2.05 | 0.56 |
| 1:F:268:VAL:HG12 | 1:F:272:ILE:HD13 | 1.87 | 0.56 |
| 1:F:629:GLY:O | 1:F:632:PHE:N | 2.38 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:698:VAL:O | 1:F:701:GLN:HB2 | 2.05 | 0.56 |
| 1:A:205:LYS:NZ | 1:B:393:LEU:O | 2.39 | 0.56 |
| 1:A:560:LYS:HZ1 | 1:A:633:ASN:HB2 | 1.71 | 0.56 |
| 1:A:643:CYS:SG | 1:A:688:VAL:N | 2.78 | 0.56 |
| 1:A:658:THR:HB | 1:A:667:GLU:HA | 1.87 | 0.56 |
| 1:A:786:ILE:CA | 1:A:789:LYS:HZ3 | 2.17 | 0.56 |
| 1:B:228:ARG:HH11 | 1:B:231:ASP:CG | 2.12 | 0.56 |
| 1:B:280:VAL:HG12 | 1:B:310:LEU:C | 2.30 | 0.56 |
| 1:B:331:PHE:HD1 | 1:B:334:ARG:CZ | 2.19 | 0.56 |
| 1:B:731:ALA:HB3 | 1:B:746:THR:HG23 | 1.87 | 0.56 |
| 1:B:755:ARG:HH11 | 1:B:755:ARG:HG3 | 1.71 | 0.56 |
| 1:B:799:ASP:O | 1:B:801:HIS:ND1 | 2.39 | 0.56 |
| 1:B:849:ILE:HG23 | 1:B:852:LYS:HB2 | 1.87 | 0.56 |
| 1:C:211:ILE:HG21 | 1:C:316:THR:H | 1.71 | 0.56 |
| 1:C:216:ILE:HG13 | 1:C:218:LYS:HG3 | 1.88 | 0.56 |
| 1:C:247:ASP:CG | 1:C:248:LEU:N | 2.63 | 0.56 |
| 1:C:302:LYS:HE2 | 1:C:310:LEU:HB3 | 1.88 | 0.56 |
| 1:C:366:ARG:NH1 | 1:C:538:GLN:C | 2.63 | 0.56 |
| 1:C:784:VAL:HG22 | 1:C:811:LYS:HZ1 | 1.70 | 0.56 |
| 1:C:831:LEU:HD12 | 1:C:834:ASN:OD1 | 2.05 | 0.56 |
| 1:D:173:ASP:CG | 1:D:175:THR:HB | 2.30 | 0.56 |
| 1:D:398:ILE:HA | 1:D:401:ALA:HB3 | 1.87 | 0.56 |
| 1:D:710:SER:CB | 1:D:714:LYS:H | 2.18 | 0.56 |
| 1:E:367:ILE:HG23 | 1:E:372:LEU:HD11 | 1.88 | 0.56 |
| 1:E:383:LEU:HD22 | 1:E:386:ARG:HG2 | 1.88 | 0.56 |
| 1:E:397:ASP:O | 1:E:400:CYS:N | 2.39 | 0.56 |
| 1:E:421:LEU:HA | 1:E:452:GLU:OE2 | 2.04 | 0.56 |
| 1:E:571:HIS:HD2 | 1:E:574:ARG:HD3 | 1.68 | 0.56 |
| 1:E:619:GLY:C | 2:E:1002:AGS:O1A | 2.48 | 0.56 |
| 1:F:337:LYS:HD2 | 1:F:339:GLU:OE2 | 2.06 | 0.56 |
| 1:F:632:PHE:CZ | 1:F:720:ASN:HB3 | 2.40 | 0.56 |
| 1:F:837:LEU:O | 1:F:840:LEU:HB2 | 2.05 | 0.56 |
| 1:A:269:LEU:HD23 | 1:A:270:LYS:HG3 | 1.87 | 0.56 |
| 1:A:274:GLU:O | 1:A:276:LYS:HG3 | 2.06 | 0.56 |
| 1:A:543:SER:HA | 1:A:547:SER:CB | 2.32 | 0.56 |
| 1:A:612:PHE:N | 1:A:770:VAL:O | 2.35 | 0.56 |
| 1:B:180:GLN:CG | 1:B:182:LYS:HZ3 | 2.18 | 0.56 |
| 1:B:194:ARG:HA | 1:B:197:ILE:CD1 | 2.33 | 0.56 |
| 1:B:302:LYS:HA | 1:B:305:LEU:HD12 | 1.88 | 0.56 |
| 1:B:343:PRO:HG2 | 1:B:388:LEU:HD23 | 1.87 | 0.56 |
| 1:B:609:SER:O | 1:B:767:SER:N | 2.39 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:291:GLY:H | 1:C:294:LYS:NZ | 2.03 | 0.56 |
| 1:C:308:GLY:O | 1:C:310:LEU:HG | 2.05 | 0.56 |
| 1:C:366:ARG:NH1 | 1:C:534:ASN:OD1 | 2.39 | 0.56 |
| 1:C:481:LYS:O | 1:C:484:ASP:HB3 | 2.06 | 0.56 |
| 1:C:576:LEU:HA | 1:C:579:GLU:CD | 2.31 | 0.56 |
| 1:C:686:ASP:CB | 1:C:690:LYS:NZ | 2.68 | 0.56 |
| 1:C:796:GLU:HG2 | 1:C:797:GLN:OE1 | 2.05 | 0.56 |
| 1:D:167:LEU:HA | 1:D:170:TYR:CG | 2.40 | 0.56 |
| 1:D:395:LEU:O | 1:D:399:SER:OG | 2.18 | 0.56 |
| 1:D:659:THR:HG22 | 1:D:660:ALA:N | 2.21 | 0.56 |
| 1:E:407:ARG:HH12 | 1:E:538:GLN:NE2 | 2.03 | 0.56 |
| 1:E:645:GLU:N | 1:E:649:LYS:HZ2 | 2.01 | 0.56 |
| 1:E:761:GLU:OE1 | 1:E:761:GLU:N | 2.39 | 0.56 |
| 1:F:360:GLU:OE1 | 1:F:367:ILE:HD12 | 2.06 | 0.56 |
| 1:F:558:VAL:HA | 1:F:561:LEU:O | 2.04 | 0.56 |
| 1:A:274:GLU:HB3 | 1:A:276:LYS:NZ | 2.21 | 0.56 |
| 1:A:796:GLU:OE2 | 1:A:800:LYS:N | 2.39 | 0.56 |
| 1:B:228:ARG:HH22 | 1:B:233:ASP:HB2 | 1.71 | 0.56 |
| 1:B:610:PHE:HB2 | 1:B:724:ILE:HG13 | 1.87 | 0.56 |
| 1:B:617:GLY:H | 1:B:620:LYS:HZ2 | 1.54 | 0.56 |
| 1:B:681:SER:HB3 | 1:B:722:ILE:N | 2.20 | 0.56 |
| 1:B:764:ASN:C | 1:B:765:ARG:HH11 | 2.13 | 0.56 |
| 1:B:777:ARG:HG3 | 1:B:778:LYS:H | 1.69 | 0.56 |
| 1:C:48:VAL:CA | 1:C:53:ASN:H | 2.18 | 0.56 |
| 1:C:168:SER:C | 1:C:264:ARG:NH2 | 2.63 | 0.56 |
| 1:C:186:VAL:HG22 | 2:C:1001:AGS:C2 | 2.35 | 0.56 |
| 1:C:189:ARG:NH1 | 1:C:341:ALA:N | 2.51 | 0.56 |
| 1:C:236:THR:O | 1:C:239:GLN:N | 2.33 | 0.56 |
| 1:C:266:LYS:HA | 1:C:269:LEU:HG | 1.87 | 0.56 |
| 1:C:330:ALA:O | 1:C:333:ARG:N | 2.39 | 0.56 |
| 1:C:334:ARG:O | 1:C:336:GLN:NE2 | 2.39 | 0.56 |
| 1:C:356:GLN:HG2 | 1:C:357:PRO:CD | 2.35 | 0.56 |
| 1:C:747:LYS:O | 1:C:750:VAL:HB | 2.06 | 0.56 |
| 1:C:762:PHE:CZ | 1:C:766:ILE:HD11 | 2.40 | 0.56 |
| 1:C:808:GLN:OE1 | 1:C:811:LYS:HB2 | 2.06 | 0.56 |
| 1:C:839:LYS:NZ | 1:C:880:LEU:C | 2.64 | 0.56 |
| 1:D:425:GLN:CD | 1:D:456:GLN:HE22 | 2.14 | 0.56 |
| 1:D:466:TYR:HE1 | 1:D:538:GLN:NE2 | 2.00 | 0.56 |
| 1:D:490:ALA:O | 1:D:494:GLU:HG2 | 2.06 | 0.56 |
| 1:E:243:LEU:HD12 | 1:E:244:PHE:HA | 1.88 | 0.56 |
| 1:E:246:LEU:HB3 | 1:E:281:LEU:HD21 | 1.87 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:304:ALA:HA | 1:E:307:ARG:HB2 | 1.87 | 0.56 |
| 1:E:467:ASN:HA | 1:E:470:LYS:HB3 | 1.87 | 0.56 |
| 1:E:612:PHE:CA | 1:E:771:ILE:HA | 2.35 | 0.56 |
| 1:F:696:LEU:O | 1:F:703:LEU:HD21 | 2.06 | 0.56 |
| 1:A:223:GLU:OE2 | 1:A:284:ASP:OD2 | 2.24 | 0.56 |
| 1:A:381:ARG:CG | 1:A:382:TYR:HD1 | 2.18 | 0.56 |
| 1:A:782:LYS:O | 1:A:785:ASP:HB3 | 2.05 | 0.56 |
| 1:B:252:THR:HB | 1:B:254:GLY:H | 1.71 | 0.56 |
| 1:B:353:ARG:CZ | 1:B:372:LEU:HB2 | 2.35 | 0.56 |
| 1:B:398:ILE:HA | 1:B:401:ALA:HB3 | 1.88 | 0.56 |
| 1:B:637:MET:O | 1:B:637:MET:HG3 | 2.06 | 0.56 |
| 1:C:194:ARG:O | 1:C:197:ILE:N | 2.38 | 0.56 |
| 1:C:196:THR:O | 1:C:200:LEU:HG | 2.05 | 0.56 |
| 1:C:282:PHE:CB | 1:C:313:ILE:H | 2.19 | 0.56 |
| 1:C:366:ARG:HD3 | 1:C:476:LEU:HD21 | 1.86 | 0.56 |
| 1:C:815:ALA:C | 1:C:819:TYR:H | 2.13 | 0.56 |
| 1:C:839:LYS:HD3 | 1:C:842:LEU:HD13 | 1.87 | 0.56 |
| 1:D:186:VAL:HB | 2:D:1001:AGS:N3 | 2.21 | 0.56 |
| 1:D:198:ARG:HH12 | 1:E:406:ALA:H | 1.53 | 0.56 |
| 1:D:203:ARG:NH1 | 1:E:363:HIS:ND1 | 2.53 | 0.56 |
| 1:D:609:SER:O | 1:D:768:SER:OG | 2.20 | 0.56 |
| 1:D:641:VAL:HG12 | 1:D:642:ASP:N | 2.21 | 0.56 |
| 1:D:674:GLN:O | 1:D:677:TYR:N | 2.38 | 0.56 |
| 1:D:730:GLY:O | 1:D:734:ILE:HD12 | 2.06 | 0.56 |
| 1:D:811:LYS:O | 1:D:814:LEU:HB2 | 2.06 | 0.56 |
| 1:E:213:GLU:C | 1:E:387:ARG:NH1 | 2.64 | 0.56 |
| 1:E:463:ARG:HA | 1:E:466:TYR:HD2 | 1.71 | 0.56 |
| 1:E:687:GLU:HA | 1:E:727:SER:HA | 1.86 | 0.56 |
| 1:E:754:VAL:CA | 1:E:757:HIS:HD2 | 2.17 | 0.56 |
| 1:F:281:LEU:O | 1:F:312:VAL:HA | 2.05 | 0.56 |
| 1:F:344:SER:OG | 1:F:345:VAL:N | 2.29 | 0.56 |
| 1:F:621:THR:HB | 2:F:1002:AGS:O5' | 2.05 | 0.56 |
| 1:F:701:GLN:OE1 | 1:F:709:THR:HG21 | 2.06 | 0.56 |
| 1:F:819:TYR:HD1 | 1:F:824:GLY:O | 1.89 | 0.56 |
| 1:F:832:ILE:O | 1:F:836:ILE:HG12 | 2.06 | 0.56 |
| 1:A:229:ILE:HA | 1:A:233:ASP:CB | 2.21 | 0.56 |
| 1:A:248:LEU:N | 1:A:288:MET:SD | 2.79 | 0.56 |
| 1:A:639:ILE:C | 1:A:683:LEU:HD12 | 2.31 | 0.56 |
| 1:A:822:ASP:CG | 1:F:307:ARG:NH1 | 2.64 | 0.56 |
| 1:B:290:MET:HB2 | 1:B:324:ILE:HD11 | 1.88 | 0.56 |
| 1:C:216:ILE:O | 2:C:1001:AGS:O2' | 2.20 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:265:PHE:HZ | 1:C:301:LEU:HD11 | 1.71 | 0.56 |
| 1:C:274:GLU:N | 1:C:276:LYS:NZ | 2.53 | 0.56 |
| 1:C:349:VAL:HA | 1:C:352:LEU:CD1 | 2.35 | 0.56 |
| 1:C:366:ARG:NE | 1:C:539:ASN:HB3 | 2.21 | 0.56 |
| 1:C:428:ILE:CG2 | 1:C:449:ARG:HH12 | 2.18 | 0.56 |
| 1:C:638:MET:HA | 1:C:681:SER:OG | 2.06 | 0.56 |
| 1:C:785:ASP:CG | 1:C:811:LYS:NZ | 2.64 | 0.56 |
| 1:D:218:LYS:CA | 1:D:221:ILE:HB | 2.36 | 0.56 |
| 1:D:673:ASN:HA | 1:D:676:GLN:CD | 2.31 | 0.56 |
| 1:D:686:ASP:OD2 | 1:D:727:SER:HA | 2.06 | 0.56 |
| 1:D:703:LEU:O | 1:D:706:GLY:N | 2.39 | 0.56 |
| 1:D:791:ILE:O | 1:D:793:GLU:N | 2.39 | 0.56 |
| 1:D:818:GLY:HA2 | 1:D:828:LEU:HD11 | 1.88 | 0.56 |
| 1:D:835:GLU:OE1 | 1:D:836:ILE:HD13 | 2.05 | 0.56 |
| 1:E:207:ASN:HA | 1:E:311:LYS:NZ | 2.21 | 0.56 |
| 1:E:296:ASP:OD1 | 1:E:299:ASN:ND2 | 2.39 | 0.56 |
| 1:E:358:LYS:HZ1 | 1:E:359:TYR:CB | 2.19 | 0.56 |
| 1:E:654:LYS:NZ | 1:E:694:ASP:CG | 2.61 | 0.56 |
| 1:E:732:GLU:HG2 | 1:E:733:PHE:N | 2.21 | 0.56 |
| 1:E:737:GLN:HE21 | 1:E:739:GLY:H | 1.54 | 0.56 |
| 1:E:740:SER:HA | 1:E:774:LYS:O | 2.06 | 0.56 |
| 1:E:805:ASN:HA | 1:E:855:VAL:HG23 | 1.88 | 0.56 |
| 1:E:826:ARG:NE | 2:E:1002:AGS:H1' | 2.20 | 0.56 |
| 1:F:217:GLY:H | 2:F:1001:AGS:PB | 2.29 | 0.56 |
| 1:F:353:ARG:HG3 | 1:F:354:GLY:N | 2.20 | 0.56 |
| 1:F:563:GLU:OE2 | 1:F:571:HIS:HB2 | 2.05 | 0.56 |
| 1:F:622:GLU:OE1 | 2:F:1002:AGS:H8 | 2.06 | 0.56 |
| 1:A:565:GLU:HA | 1:A:568:LYS:HD3 | 1.86 | 0.56 |
| 1:A:591:SER:O | 1:A:595:ARG:N | 2.27 | 0.56 |
| 1:B:246:LEU:HD23 | 1:B:249:ALA:C | 2.31 | 0.56 |
| 1:B:252:THR:C | 1:B:264:ARG:HH21 | 2.14 | 0.56 |
| 1:B:329:GLY:O | 1:B:333:ARG:N | 2.30 | 0.56 |
| 1:B:344:SER:CA | 1:B:347:GLN:HE22 | 2.19 | 0.56 |
| 1:B:695:VAL:O | 1:B:699:MET:HG3 | 2.06 | 0.56 |
| 1:B:737:GLN:H | 1:B:774:LYS:NZ | 2.04 | 0.56 |
| 1:B:840:LEU:O | 1:B:843:ARG:N | 2.39 | 0.56 |
| 1:C:410:LYS:HD3 | 1:C:470:LYS:HZ3 | 1.70 | 0.56 |
| 1:C:620:LYS:H | 1:C:772:PHE:HE1 | 1.54 | 0.56 |
| 1:C:621:THR:O | 1:C:625:LYS:N | 2.29 | 0.56 |
| 1:C:828:LEU:O | 1:C:832:ILE:HG13 | 2.05 | 0.56 |
| 1:D:198:ARG:NH1 | 1:E:402:GLY:C | 2.64 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:206:SER:OG | 1:D:207:ASN:N | 2.34 | 0.56 |
| 1:D:216:ILE:HB | 2:D:1001:AGS:PA | 2.46 | 0.56 |
| 1:D:284:ASP:O | 1:D:315:ALA:N | 2.26 | 0.56 |
| 1:D:570:ILE:CB | 1:D:595:ARG:HH12 | 2.18 | 0.56 |
| 1:D:637:MET:SD | 1:D:678:LYS:HD3 | 2.46 | 0.56 |
| 1:E:186:VAL:HG22 | 2:E:1001:AGS:C5 | 2.35 | 0.56 |
| 1:E:191:GLU:HG2 | 1:E:192:GLU:N | 2.19 | 0.56 |
| 1:E:202:ARG:HD3 | 1:E:205:LYS:O | 2.06 | 0.56 |
| 1:E:407:ARG:HA | 1:E:536:MET:HE1 | 1.88 | 0.56 |
| 1:E:694:ASP:HA | 1:E:697:THR:OG1 | 2.05 | 0.56 |
| 1:E:785:ASP:OD1 | 1:E:785:ASP:N | 2.38 | 0.56 |
| 1:A:278:LEU:HA | 1:A:309:GLN:HG2 | 1.88 | 0.55 |
| 1:B:336:GLN:HE21 | 1:B:337:LYS:HA | 1.71 | 0.55 |
| 1:B:573:GLU:H | 1:B:595:ARG:HH22 | 1.53 | 0.55 |
| 1:B:593:ALA:HA | 1:B:596:LEU:HB2 | 1.88 | 0.55 |
| 1:B:643:CYS:O | 1:B:645:GLU:N | 2.40 | 0.55 |
| 1:C:190:GLU:CG | 1:C:191:GLU:H | 2.14 | 0.55 |
| 1:C:196:THR:O | 1:C:199:VAL:N | 2.39 | 0.55 |
| 1:C:622:GLU:N | 1:C:826:ARG:HH12 | 1.97 | 0.55 |
| 1:C:643:CYS:SG | 1:C:690:LYS:N | 2.79 | 0.55 |
| 1:C:707:ARG:HG3 | 1:C:707:ARG:O | 2.07 | 0.55 |
| 1:D:262:GLU:CB | 1:D:298:ALA:HB2 | 2.31 | 0.55 |
| 1:D:265:PHE:CD2 | 1:D:298:ALA:HB1 | 2.40 | 0.55 |
| 1:D:330:ALA:HA | 1:D:333:ARG:HG3 | 1.88 | 0.55 |
| 1:D:468:GLU:HA | 1:D:471:HIS:HB3 | 1.88 | 0.55 |
| 1:D:592:ASN:O | 1:D:596:LEU:HG | 2.06 | 0.55 |
| 1:D:740:SER:OG | 1:D:741:LYS:N | 2.39 | 0.55 |
| 1:E:434:ASP:OD2 | 1:E:436:ASP:OD2 | 2.24 | 0.55 |
| 1:E:611:LEU:HD12 | 1:E:612:PHE:H | 1.71 | 0.55 |
| 1:E:668:GLY:HA3 | 1:E:672:THR:OG1 | 2.07 | 0.55 |
| 1:E:671:LEU:HD23 | 1:E:672:THR:N | 2.20 | 0.55 |
| 1:E:701:GLN:HA | 1:E:704:ASP:HB3 | 1.87 | 0.55 |
| 1:F:202:ARG:NH1 | 1:F:208:PRO:CD | 2.62 | 0.55 |
| 1:F:219:THR:HG23 | 1:F:222:ILE:HB | 1.87 | 0.55 |
| 1:F:392:ALA:O | 1:F:396:VAL:HG23 | 2.05 | 0.55 |
| 1:F:785:ASP:O | 1:F:789:LYS:NZ | 2.36 | 0.55 |
| 1:A:282:PHE:HB2 | 1:A:313:ILE:HB | 1.88 | 0.55 |
| 1:A:302:LYS:N | 1:A:303:PRO:HD2 | 2.22 | 0.55 |
| 1:A:570:ILE:O | 1:A:573:GLU:OE2 | 2.24 | 0.55 |
| 1:A:874:GLU:OE2 | 1:F:203:ARG:HG3 | 2.07 | 0.55 |
| 1:B:186:VAL:HG11 | 1:B:216:ILE:HD11 | 1.87 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:543:SER:HA | 1:B:546:ILE:HB | 1.87 | 0.55 |
| 1:B:617:GLY:HA2 | 1:B:620:LYS:HZ1 | 1.68 | 0.55 |
| 1:B:646:LEU:HD13 | 1:B:687:GLU:C | 2.30 | 0.55 |
| 1:B:696:LEU:HD22 | 1:B:762:PHE:CZ | 2.41 | 0.55 |
| 1:B:751:MET:C | 1:B:755:ARG:NH1 | 2.64 | 0.55 |
| 1:B:792:GLU:O | 1:B:798:ASN:ND2 | 2.37 | 0.55 |
| 1:B:839:LYS:HB3 | 1:B:878:GLU:OE1 | 2.06 | 0.55 |
| 1:C:226:ALA:O | 1:C:229:ILE:HB | 2.05 | 0.55 |
| 1:C:268:VAL:O | 1:C:271:GLU:HB2 | 2.07 | 0.55 |
| 1:C:333:ARG:O | 1:C:335:PHE:N | 2.39 | 0.55 |
| 1:C:350:ALA:CA | 1:C:353:ARG:HH11 | 2.19 | 0.55 |
| 1:C:493:ALA:C | 1:C:495:ARG:H | 2.14 | 0.55 |
| 1:C:639:ILE:HG13 | 1:C:678:LYS:HZ3 | 1.71 | 0.55 |
| 1:C:738:GLN:OE1 | 1:C:743:GLN:HG2 | 2.06 | 0.55 |
| 1:D:166:TYR:HB2 | 1:D:264:ARG:NE | 2.21 | 0.55 |
| 1:D:369:ASP:C | 1:D:372:LEU:HB3 | 2.31 | 0.55 |
| 1:D:557:PRO:O | 1:D:559:LYS:HG2 | 2.05 | 0.55 |
| 1:D:719:SER:HA | 1:D:722:ILE:HD13 | 1.88 | 0.55 |
| 1:E:203:ARG:HG3 | 1:F:397:ASP:OD1 | 2.06 | 0.55 |
| 1:E:692:HIS:CD2 | 1:E:693:PRO:HD2 | 2.41 | 0.55 |
| 1:F:166:TYR:CE2 | 1:F:264:ARG:HA | 2.41 | 0.55 |
| 1:F:591:SER:C | 1:F:595:ARG:HH12 | 2.11 | 0.55 |
| 1:B:251:LEU:N | 1:B:264:ARG:NH1 | 2.46 | 0.55 |
| 1:B:344:SER:H | 1:B:347:GLN:NE2 | 2.05 | 0.55 |
| 1:B:634:ASP:OD1 | 1:B:634:ASP:C | 2.48 | 0.55 |
| 1:B:674:GLN:HA | 1:B:678:LYS:CE | 2.36 | 0.55 |
| 1:C:221:ILE:O | 1:C:223:GLU:N | 2.39 | 0.55 |
| 1:C:268:VAL:O | 1:C:272:ILE:HG12 | 2.06 | 0.55 |
| 1:C:280:VAL:HA | 1:C:311:LYS:CD | 2.36 | 0.55 |
| 1:C:628:ALA:HA | 1:C:631:LEU:HD13 | 1.87 | 0.55 |
| 1:C:699:MET:C | 1:C:703:LEU:HD13 | 2.32 | 0.55 |
| 1:C:743:GLN:HB2 | 1:C:746:THR:OG1 | 2.05 | 0.55 |
| 1:C:751:MET:HA | 1:C:755:ARG:HH12 | 1.70 | 0.55 |
| 1:D:175:THR:HG23 | 1:D:227:GLN:OE1 | 2.06 | 0.55 |
| 1:D:203:ARG:CZ | 1:E:362:HIS:C | 2.80 | 0.55 |
| 1:D:214:PRO:HG2 | 1:D:387:ARG:HE | 1.71 | 0.55 |
| 1:D:265:PHE:CD2 | 1:D:266:LYS:N | 2.75 | 0.55 |
| 1:D:280:VAL:HG12 | 1:D:281:LEU:H | 1.69 | 0.55 |
| 1:D:281:LEU:H | 1:D:312:VAL:HA | 1.70 | 0.55 |
| 1:D:290:MET:HB3 | 1:D:294:LYS:HG2 | 1.87 | 0.55 |
| 1:D:569:LEU:HD12 | 1:D:570:ILE:HA | 1.89 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:650:TYR:CD1 | 1:D:650:TYR:N | 2.74 | 0.55 |
| 1:E:366:ARG:HB3 | 1:E:539:ASN:HB2 | 1.88 | 0.55 |
| 1:E:464:GLN:OE1 | 1:E:464:GLN:N | 2.33 | 0.55 |
| 1:E:485:GLU:C | 1:E:489:LYS:NZ | 2.64 | 0.55 |
| 1:E:512:ASP:O | 1:E:515:LYS:N | 2.38 | 0.55 |
| 1:E:644:SER:H | 1:E:690:LYS:HE3 | 1.71 | 0.55 |
| 1:E:732:GLU:OE2 | 1:E:733:PHE:CE2 | 2.60 | 0.55 |
| 1:E:814:LEU:HD21 | 1:E:878:GLU:OE2 | 2.06 | 0.55 |
| 1:E:819:TYR:HA | 1:E:824:GLY:HA2 | 1.87 | 0.55 |
| 1:F:290:MET:HE3 | 1:F:293:GLY:HA2 | 1.88 | 0.55 |
| 1:F:607:PRO:HD3 | 1:F:706:GLY:HA2 | 1.88 | 0.55 |
| 1:F:737:GLN:HG2 | 1:F:742:ILE:CD1 | 2.33 | 0.55 |
| 1:A:300:ILE:HG12 | 1:B:253:ALA:HB3 | 1.89 | 0.55 |
| 1:A:592:ASN:HB3 | 1:A:595:ARG:HH21 | 1.71 | 0.55 |
| 1:A:595:ARG:NH1 | 1:B:842:LEU:H | 2.03 | 0.55 |
| 1:A:768:SER:OG | 1:A:769:ILE:N | 2.40 | 0.55 |
| 1:B:302:LYS:O | 1:B:305:LEU:N | 2.37 | 0.55 |
| 1:B:548:GLU:O | 1:B:551:ALA:HB3 | 2.07 | 0.55 |
| 1:B:616:SER:HA | 1:B:620:LYS:HB3 | 1.87 | 0.55 |
| 1:B:650:TYR:H | 1:B:692:HIS:CE1 | 2.20 | 0.55 |
| 1:C:236:THR:C | 1:C:239:GLN:H | 2.15 | 0.55 |
| 1:C:246:LEU:H | 1:C:283:ILE:HA | 1.72 | 0.55 |
| 1:D:179:ARG:HH22 | 1:D:230:ILE:CG2 | 2.20 | 0.55 |
| 1:D:198:ARG:HH22 | 1:E:406:ALA:H | 1.54 | 0.55 |
| 1:E:186:VAL:HG13 | 2:E:1001:AGS:N3 | 2.20 | 0.55 |
| 1:E:351:ILE:HD13 | 2:E:1001:AGS:C2 | 2.36 | 0.55 |
| 1:E:366:ARG:O | 1:E:367:ILE:HG13 | 2.06 | 0.55 |
| 1:E:701:GLN:HE22 | 1:E:709:THR:N | 2.04 | 0.55 |
| 1:E:799:ASP:CG | 1:E:800:LYS:H | 2.14 | 0.55 |
| 1:F:318:ASN:CG | 1:F:337:LYS:HZ2 | 2.13 | 0.55 |
| 1:A:377:GLN:H | 1:A:377:GLN:CD | 2.11 | 0.55 |
| 1:B:242:LYS:HA | 1:B:243:LEU:HD23 | 1.87 | 0.55 |
| 1:B:265:PHE:C | 1:B:269:LEU:HD13 | 2.31 | 0.55 |
| 1:B:290:MET:HG2 | 1:B:294:LYS:HA | 1.89 | 0.55 |
| 1:B:320:GLU:HA | 1:B:323:SER:HB2 | 1.87 | 0.55 |
| 1:B:329:GLY:O | 1:B:332:GLU:N | 2.40 | 0.55 |
| 1:B:359:TYR:CE1 | 1:B:362:HIS:CD2 | 2.95 | 0.55 |
| 1:B:592:ASN:O | 1:B:595:ARG:N | 2.40 | 0.55 |
| 1:B:708:ILE:HG12 | 1:B:717:ASP:N | 2.21 | 0.55 |
| 1:B:732:GLU:C | 1:B:735:ASN:H | 2.14 | 0.55 |
| 1:B:761:GLU:O | 1:B:765:ARG:HG2 | 2.07 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:427:GLU:OE2 | 1:C:448:ALA:HB1 | 2.07 | 0.55 |
| 1:C:757:HIS:ND1 | 1:C:757:HIS:O | 2.40 | 0.55 |
| 1:C:785:ASP:CB | 1:C:789:LYS:HZ2 | 2.19 | 0.55 |
| 1:C:823:MET:HB3 | 1:C:827:PRO:HG3 | 1.89 | 0.55 |
| 1:D:346:ARG:HA | 1:D:349:VAL:HB | 1.88 | 0.55 |
| 1:D:809:GLU:HG2 | 1:D:810:ALA:H | 1.71 | 0.55 |
| 1:E:554:THR:OG1 | 1:E:555:GLY:N | 2.40 | 0.55 |
| 1:E:575:ASP:O | 1:E:579:GLU:OE2 | 2.24 | 0.55 |
| 1:E:621:THR:HG22 | 1:E:625:LYS:HD2 | 1.89 | 0.55 |
| 1:E:772:PHE:HE1 | 1:E:775:LEU:HD12 | 1.71 | 0.55 |
| 1:F:194:ARG:HG2 | 1:F:228:ARG:HH22 | 1.71 | 0.55 |
| 1:F:229:ILE:O | 1:F:232:ASP:N | 2.33 | 0.55 |
| 1:F:612:PHE:CE1 | 1:F:770:VAL:HG11 | 2.41 | 0.55 |
| 1:F:671:LEU:HD23 | 1:F:674:GLN:HB2 | 1.89 | 0.55 |
| 1:F:700:LEU:CD2 | 1:F:703:LEU:HD23 | 2.22 | 0.55 |
| 1:F:827:PRO:O | 1:F:831:LEU:N | 2.38 | 0.55 |
| 1:F:828:LEU:HB3 | 1:F:832:ILE:CD1 | 2.36 | 0.55 |
| 1:A:646:LEU:HG | 1:A:691:ALA:HB1 | 1.89 | 0.55 |
| 1:A:689:GLU:H | 1:A:689:GLU:CD | 2.14 | 0.55 |
| 1:A:733:PHE:HD2 | 1:A:750:VAL:HG22 | 1.71 | 0.55 |
| 1:A:777:ARG:NH1 | 1:A:816:LYS:HG3 | 2.21 | 0.55 |
| 1:A:806:LEU:HD23 | 1:A:855:VAL:HB | 1.88 | 0.55 |
| 1:B:211:ILE:H | 1:B:339:GLU:CD | 2.15 | 0.55 |
| 1:B:251:LEU:HD12 | 1:B:252:THR:H | 1.71 | 0.55 |
| 1:B:281:LEU:C | 1:B:312:VAL:HA | 2.32 | 0.55 |
| 1:B:570:ILE:O | 1:B:573:GLU:OE2 | 2.25 | 0.55 |
| 1:B:685:PHE:HZ | 1:B:727:SER:HB2 | 1.70 | 0.55 |
| 1:B:803:LYS:H | 1:B:853:GLU:CB | 2.19 | 0.55 |
| 1:C:174:MET:H | 1:C:242:LYS:CE | 2.20 | 0.55 |
| 1:C:191:GLU:O | 1:C:194:ARG:N | 2.40 | 0.55 |
| 1:C:259:GLY:HA3 | 1:C:262:GLU:CD | 2.31 | 0.55 |
| 1:C:569:LEU:O | 1:C:573:GLU:HB3 | 2.07 | 0.55 |
| 1:C:718:CYS:C | 1:C:720:ASN:H | 2.15 | 0.55 |
| 1:D:175:THR:N | 1:D:223:GLU:OE2 | 2.39 | 0.55 |
| 1:D:344:SER:HB2 | 1:D:345:VAL:HG23 | 1.87 | 0.55 |
| 1:E:173:ASP:HA | 1:E:243:LEU:HD12 | 1.89 | 0.55 |
| 1:E:176:GLU:O | 1:E:179:ARG:HB3 | 2.07 | 0.55 |
| 1:E:394:ASP:O | 1:E:397:ASP:HB3 | 2.06 | 0.55 |
| 1:E:652:VAL:CG1 | 1:E:669:GLY:HA3 | 2.37 | 0.55 |
| 1:E:692:HIS:CG | 1:E:693:PRO:HD2 | 2.41 | 0.55 |
| 1:E:703:LEU:O | 1:E:703:LEU:HD23 | 2.06 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:173:ASP:HA | 1:F:244:PHE:CD2 | 2.42 | 0.55 |
| 1:F:268:VAL:O | 1:F:272:ILE:HG12 | 2.05 | 0.55 |
| 1:F:280:VAL:HG22 | 1:F:311:LYS:N | 2.19 | 0.55 |
| 1:F:702:MET:HB3 | 1:F:708:ILE:CA | 2.35 | 0.55 |
| 1:F:843:ARG:NH1 | 1:F:881:PRO:C | 2.65 | 0.55 |
| 1:A:610:PHE:C | 1:A:724:ILE:HG21 | 2.31 | 0.55 |
| 1:A:612:PHE:N | 1:A:770:VAL:H | 2.03 | 0.55 |
| 1:A:613:LEU:HD13 | 1:A:727:SER:H | 1.72 | 0.55 |
| 1:B:192:GLU:C | 1:B:195:SER:HG | 2.05 | 0.55 |
| 1:B:198:ARG:C | 1:B:200:LEU:N | 2.64 | 0.55 |
| 1:B:685:PHE:CZ | 1:B:727:SER:HB2 | 2.42 | 0.55 |
| 1:B:704:ASP:CG | 1:B:707:ARG:HH11 | 2.14 | 0.55 |
| 1:B:857:VAL:CG1 | 1:B:878:GLU:H | 2.18 | 0.55 |
| 1:C:168:SER:OG | 1:C:268:VAL:HG22 | 2.06 | 0.55 |
| 1:C:178:ALA:O | 1:C:181:GLY:N | 2.28 | 0.55 |
| 1:C:219:THR:O | 1:C:223:GLU:OE1 | 2.25 | 0.55 |
| 1:C:259:GLY:O | 1:C:262:GLU:HG2 | 2.07 | 0.55 |
| 1:C:488:ASN:ND2 | 1:C:489:LYS:NZ | 2.55 | 0.55 |
| 1:C:710:SER:HA | 1:C:716:ILE:HD11 | 1.88 | 0.55 |
| 1:C:834:ASN:HA | 1:C:837:LEU:HD21 | 1.87 | 0.55 |
| 1:D:218:LYS:HD3 | 1:D:221:ILE:CD1 | 2.36 | 0.55 |
| 1:D:295:ASP:C | 1:D:297:ALA:N | 2.63 | 0.55 |
| 1:D:345:VAL:O | 1:D:349:VAL:HG23 | 2.06 | 0.55 |
| 1:D:383:LEU:HB3 | 1:D:385:TYR:CE2 | 2.42 | 0.55 |
| 1:D:810:ALA:O | 1:D:813:PHE:N | 2.40 | 0.55 |
| 1:E:169:LYS:HZ1 | 1:E:267:GLY:CA | 2.16 | 0.55 |
| 1:E:169:LYS:HE2 | 1:E:264:ARG:NE | 2.22 | 0.55 |
| 1:E:214:PRO:C | 1:E:218:LYS:NZ | 2.50 | 0.55 |
| 1:E:460:GLU:CD | 1:E:463:ARG:HH12 | 2.10 | 0.55 |
| 1:E:473:HIS:HA | 1:E:521:GLU:CD | 2.32 | 0.55 |
| 1:E:705:ASP:H | 1:E:765:ARG:HH12 | 1.55 | 0.55 |
| 1:E:795:PHE:CD2 | 1:E:801:HIS:ND1 | 2.74 | 0.55 |
| 1:F:770:VAL:HG12 | 1:F:772:PHE:CE1 | 2.41 | 0.55 |
| 1:F:783:ILE:HD13 | 2:F:1002:AGS:N6 | 2.22 | 0.55 |
| 1:F:785:ASP:HA | 1:F:788:LEU:HB3 | 1.88 | 0.55 |
| 1:A:234:VAL:HA | 1:A:238:LEU:HD12 | 1.88 | 0.55 |
| 1:A:242:LYS:O | 1:A:279:ILE:HG12 | 2.07 | 0.55 |
| 1:A:776:SER:HB3 | 1:A:779:ALA:H | 1.71 | 0.55 |
| 1:B:250:ALA:HB3 | 1:B:264:ARG:NH1 | 2.22 | 0.55 |
| 1:B:639:ILE:O | 1:B:684:LEU:N | 2.30 | 0.55 |
| 1:C:6:GLN:O | 1:C:112:ALA:N | 2.39 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:173:ASP:HA | 1:C:244:PHE:HE1 | 1.70 | 0.55 |
| 1:C:302:LYS:NZ | 1:C:310:LEU:O | 2.39 | 0.55 |
| 1:C:342:GLU:HG2 | 1:C:343:PRO:HD2 | 1.88 | 0.55 |
| 1:C:366:ARG:NH1 | 1:C:473:HIS:CD2 | 2.75 | 0.55 |
| 1:D:281:LEU:HB2 | 1:D:312:VAL:HG12 | 1.89 | 0.55 |
| 1:D:282:PHE:O | 1:D:283:ILE:HD13 | 2.07 | 0.55 |
| 1:D:336:GLN:NE2 | 1:D:337:LYS:H | 2.04 | 0.55 |
| 1:D:357:PRO:HD2 | 1:D:358:LYS:HZ2 | 1.72 | 0.55 |
| 1:D:580:VAL:HG22 | 1:D:626:LYS:HE2 | 1.89 | 0.55 |
| 1:D:651:ALA:HA | 1:D:657:GLY:HA2 | 1.89 | 0.55 |
| 1:D:762:PHE:HB3 | 1:D:763:LEU:HD12 | 1.88 | 0.55 |
| 1:D:799:ASP:OD1 | 1:D:800:LYS:N | 2.36 | 0.55 |
| 1:D:872:GLU:N | 1:D:877:LEU:HD13 | 2.22 | 0.55 |
| 1:E:174:MET:O | 1:E:176:GLU:N | 2.39 | 0.55 |
| 1:E:190:GLU:C | 1:E:194:ARG:HG3 | 2.32 | 0.55 |
| 1:E:776:SER:OG | 1:E:777:ARG:HG2 | 2.07 | 0.55 |
| 1:F:694:ASP:O | 1:F:697:THR:OG1 | 2.23 | 0.55 |
| 1:A:541:VAL:N | 1:A:545:THR:OG1 | 2.38 | 0.55 |
| 1:A:595:ARG:HH11 | 1:B:841:ALA:CB | 2.19 | 0.55 |
| 1:A:785:ASP:CG | 1:A:789:LYS:HZ2 | 2.14 | 0.55 |
| 1:B:167:LEU:CD2 | 1:B:271:GLU:HA | 2.33 | 0.55 |
| 1:B:234:VAL:CG1 | 1:B:239:GLN:HG3 | 2.36 | 0.55 |
| 1:B:548:GLU:H | 1:B:560:LYS:NZ | 2.03 | 0.55 |
| 1:B:759:ARG:O | 1:B:763:LEU:N | 2.29 | 0.55 |
| 1:B:782:LYS:HA | 1:B:785:ASP:OD2 | 2.07 | 0.55 |
| 1:B:843:ARG:HA | 1:B:846:LYS:CB | 2.31 | 0.55 |
| 1:C:14:ILE:N | 1:C:160:THR:N | 2.52 | 0.55 |
| 1:C:174:MET:HE3 | 1:C:243:LEU:HB2 | 1.88 | 0.55 |
| 1:C:281:LEU:HG | 1:C:311:LYS:O | 2.07 | 0.55 |
| 1:C:325:VAL:HA | 1:C:331:PHE:HE2 | 1.71 | 0.55 |
| 1:C:638:MET:HG3 | 1:C:682:VAL:O | 2.06 | 0.55 |
| 1:D:140:ILE:O | 1:D:144:ALA:N | 2.40 | 0.55 |
| 1:D:179:ARG:NH1 | 1:D:227:GLN:OE1 | 2.37 | 0.55 |
| 1:D:198:ARG:HD3 | 1:E:401:ALA:O | 2.06 | 0.55 |
| 1:D:377:GLN:O | 1:D:381:ARG:N | 2.22 | 0.55 |
| 1:D:473:HIS:HA | 1:D:476:LEU:HD12 | 1.88 | 0.55 |
| 1:E:216:ILE:HG23 | 1:E:217:GLY:N | 2.20 | 0.55 |
| 1:E:256:LYS:HZ1 | 1:E:264:ARG:CD | 2.20 | 0.55 |
| 1:E:333:ARG:HH12 | 1:F:214:PRO:HG2 | 1.72 | 0.55 |
| 1:E:494:GLU:HG2 | 1:E:501:THR:HG22 | 1.88 | 0.55 |
| 1:E:576:LEU:HA | 1:E:579:GLU:CG | 2.29 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:627:VAL:O | 1:E:630:PHE:N | 2.40 | 0.55 |
| 1:E:668:GLY:O | 1:E:671:LEU:N | 2.39 | 0.55 |
| 1:F:605:ARG:HG2 | 1:F:707:ARG:N | 2.21 | 0.55 |
| 1:F:609:SER:HB3 | 1:F:722:ILE:CG2 | 2.36 | 0.55 |
| 1:F:837:LEU:HA | 1:F:840:LEU:HD22 | 1.88 | 0.55 |
| 1:A:822:ASP:OD2 | 1:F:333:ARG:NH1 | 2.39 | 0.55 |
| 1:B:197:ILE:HA | 1:B:200:LEU:HD12 | 1.88 | 0.55 |
| 1:C:180:GLN:N | 1:C:180:GLN:CD | 2.65 | 0.55 |
| 1:C:322:ARG:O | 1:C:326:GLU:HG3 | 2.07 | 0.55 |
| 1:C:411:PRO:HA | 1:C:414:LEU:HB2 | 1.89 | 0.55 |
| 1:C:417:LYS:NZ | 1:C:463:ARG:HG2 | 2.22 | 0.55 |
| 1:C:593:ALA:HA | 1:C:596:LEU:HB2 | 1.88 | 0.55 |
| 1:C:619:GLY:O | 1:C:622:GLU:HG2 | 2.07 | 0.55 |
| 1:C:652:VAL:C | 1:C:654:LYS:HZ2 | 2.12 | 0.55 |
| 1:D:210:LEU:HD11 | 1:D:338:ILE:HB | 1.88 | 0.55 |
| 1:D:296:ASP:O | 1:D:298:ALA:N | 2.40 | 0.55 |
| 1:D:530:ARG:NH2 | 1:D:538:GLN:H | 2.02 | 0.55 |
| 1:D:542:ASP:O | 1:D:546:ILE:N | 2.31 | 0.55 |
| 1:D:708:ILE:CD1 | 1:D:716:ILE:HB | 2.37 | 0.55 |
| 1:D:833:GLN:O | 1:D:834:ASN:C | 2.50 | 0.55 |
| 1:E:408:ASP:CB | 1:E:411:PRO:HG3 | 2.34 | 0.55 |
| 1:E:436:ASP:HB2 | 1:E:441:THR:OG1 | 2.07 | 0.55 |
| 1:E:654:LYS:HD3 | 1:E:698:VAL:HG11 | 1.89 | 0.55 |
| 1:F:563:GLU:CG | 1:F:568:LYS:HB3 | 2.36 | 0.55 |
| 1:F:611:LEU:HA | 1:F:724:ILE:HB | 1.89 | 0.55 |
| 1:F:841:ALA:O | 1:F:845:LEU:HG | 2.07 | 0.55 |
| 1:A:173:ASP:OD1 | 1:A:175:THR:N | 2.37 | 0.54 |
| 1:B:247:ASP:OD1 | 1:B:248:LEU:HG | 2.07 | 0.54 |
| 1:B:374:THR:HA | 1:B:377:GLN:OE1 | 2.07 | 0.54 |
| 1:B:381:ARG:NH2 | 1:B:559:LYS:HB3 | 2.22 | 0.54 |
| 1:B:590:VAL:HG13 | 1:B:610:PHE:HD2 | 1.72 | 0.54 |
| 1:C:211:ILE:HD13 | 1:C:316:THR:H | 1.71 | 0.54 |
| 1:C:332:GLU:O | 1:C:335:PHE:HB2 | 2.06 | 0.54 |
| 1:C:345:VAL:O | 1:C:348:THR:N | 2.40 | 0.54 |
| 1:C:372:LEU:HA | 1:C:542:ASP:CB | 2.37 | 0.54 |
| 1:C:639:ILE:O | 1:C:640:ARG:HD2 | 2.06 | 0.54 |
| 1:C:731:ALA:O | 1:C:734:ILE:HG22 | 2.07 | 0.54 |
| 1:D:351:ILE:O | 1:D:354:GLY:N | 2.40 | 0.54 |
| 1:D:556:ILE:C | 1:D:560:LYS:NZ | 2.61 | 0.54 |
| 1:D:737:GLN:H | 1:D:774:LYS:CE | 2.20 | 0.54 |
| 1:D:752:GLY:O | 1:D:756:GLN:HG2 | 2.07 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:876:CYS:O | 1:D:877:LEU:HB2 | 2.05 | 0.54 |
| 1:E:358:LYS:HZ2 | 1:E:359:TYR:CA | 2.19 | 0.54 |
| 1:E:581:VAL:HG12 | 1:E:582:GLY:N | 2.22 | 0.54 |
| 1:E:674:GLN:OE1 | 1:E:677:TYR:HB3 | 2.07 | 0.54 |
| 1:F:302:LYS:HE2 | 1:F:305:LEU:HD21 | 1.89 | 0.54 |
| 1:F:331:PHE:CB | 1:F:334:ARG:HG3 | 2.36 | 0.54 |
| 1:F:543:SER:OG | 1:F:546:ILE:HD12 | 2.07 | 0.54 |
| 1:F:783:ILE:HD11 | 1:F:787:ARG:NH1 | 2.22 | 0.54 |
| 1:F:879:VAL:HG12 | 1:F:880:LEU:N | 2.15 | 0.54 |
| 1:A:283:ILE:HG23 | 1:A:288:MET:HB2 | 1.89 | 0.54 |
| 1:A:873:ALA:HB3 | 1:F:201:ALA:O | 2.08 | 0.54 |
| 1:B:174:MET:HG2 | 1:B:244:PHE:HA | 1.89 | 0.54 |
| 1:B:177:GLN:O | 1:B:182:LYS:HB2 | 2.06 | 0.54 |
| 1:B:214:PRO:O | 1:B:218:LYS:N | 2.40 | 0.54 |
| 1:B:565:GLU:O | 1:B:568:LYS:NZ | 2.40 | 0.54 |
| 1:C:259:GLY:C | 1:C:263:GLU:OE2 | 2.49 | 0.54 |
| 1:C:568:LYS:NZ | 1:C:630:PHE:C | 2.63 | 0.54 |
| 1:C:709:THR:HG23 | 1:C:714:LYS:C | 2.32 | 0.54 |
| 1:D:651:ALA:CA | 1:D:654:LYS:HG2 | 2.37 | 0.54 |
| 1:E:202:ARG:NH1 | 1:E:336:GLN:NE2 | 2.54 | 0.54 |
| 1:E:218:LYS:HZ1 | 1:E:387:ARG:NH1 | 2.04 | 0.54 |
| 1:E:322:ARG:O | 1:E:326:GLU:N | 2.20 | 0.54 |
| 1:E:448:ALA:O | 1:E:451:LYS:HG2 | 2.07 | 0.54 |
| 1:F:179:ARG:HA | 1:F:230:ILE:HG21 | 1.88 | 0.54 |
| 1:F:199:VAL:HG13 | 1:F:206:SER:O | 2.07 | 0.54 |
| 1:F:382:TYR:CD2 | 1:F:560:LYS:HE3 | 2.43 | 0.54 |
| 1:F:569:LEU:O | 1:F:572:MET:HB3 | 2.07 | 0.54 |
| 1:F:835:GLU:OE1 | 1:F:835:GLU:N | 2.40 | 0.54 |
| 1:A:196:THR:HG23 | 1:A:199:VAL:HB | 1.89 | 0.54 |
| 1:A:213:GLU:C | 1:A:218:LYS:HZ3 | 2.16 | 0.54 |
| 1:A:282:PHE:HA | 1:A:312:VAL:HG23 | 1.89 | 0.54 |
| 1:B:303:PRO:O | 1:B:307:ARG:N | 2.32 | 0.54 |
| 1:B:337:LYS:HG3 | 1:B:338:ILE:O | 2.06 | 0.54 |
| 1:B:613:LEU:O | 1:B:772:PHE:N | 2.41 | 0.54 |
| 1:B:634:ASP:OD1 | 1:B:636:ASP:CG | 2.50 | 0.54 |
| 1:B:742:ILE:HG22 | 1:B:743:GLN:N | 2.23 | 0.54 |
| 1:B:764:ASN:ND2 | 1:B:765:ARG:NH1 | 2.55 | 0.54 |
| 1:C:14:ILE:C | 1:C:160:THR:N | 2.61 | 0.54 |
| 1:C:592:ASN:HA | 1:C:595:ARG:HH11 | 1.72 | 0.54 |
| 1:C:739:GLY:H | 1:C:774:LYS:HE3 | 1.72 | 0.54 |
| 1:C:746:THR:C | 1:C:748:ASN:H | 2.15 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:241:ALA:C | 1:D:278:LEU:HA | 2.32 | 0.54 |
| 1:D:285:GLU:HB3 | 1:D:288:MET:H | 1.73 | 0.54 |
| 1:D:591:SER:HA | 1:D:594:VAL:HB | 1.90 | 0.54 |
| 1:D:650:TYR:CD2 | 1:D:654:LYS:HD2 | 2.43 | 0.54 |
| 1:D:775:LEU:HB2 | 1:D:780:ILE:HD11 | 1.89 | 0.54 |
| 1:D:800:LYS:HZ3 | 1:D:801:HIS:CE1 | 2.25 | 0.54 |
| 1:E:304:ALA:O | 1:E:308:GLY:N | 2.26 | 0.54 |
| 1:E:322:ARG:HG3 | 1:E:323:SER:H | 1.71 | 0.54 |
| 1:E:637:MET:HG3 | 1:E:682:VAL:HG12 | 1.88 | 0.54 |
| 1:E:802:TYR:HB3 | 1:E:852:LYS:O | 2.07 | 0.54 |
| 1:F:206:SER:HG | 1:F:335:PHE:HE1 | 1.55 | 0.54 |
| 1:F:605:ARG:HD2 | 1:F:707:ARG:CB | 2.38 | 0.54 |
| 1:F:761:GLU:OE2 | 1:F:765:ARG:NH2 | 2.40 | 0.54 |
| 1:F:833:GLN:HG3 | 1:F:834:ASN:ND2 | 2.22 | 0.54 |
| 1:A:382:TYR:HD2 | 1:A:383:LEU:HB2 | 1.71 | 0.54 |
| 1:A:643:CYS:HB3 | 1:A:685:PHE:HB3 | 1.90 | 0.54 |
| 1:A:807:THR:O | 1:A:811:LYS:HG3 | 2.07 | 0.54 |
| 1:B:302:LYS:HD2 | 1:B:305:LEU:HB2 | 1.89 | 0.54 |
| 1:B:358:LYS:O | 1:B:362:HIS:N | 2.30 | 0.54 |
| 1:B:367:ILE:N | 1:B:539:ASN:HB2 | 2.22 | 0.54 |
| 1:B:392:ALA:O | 1:B:396:VAL:HG23 | 2.06 | 0.54 |
| 1:B:591:SER:O | 1:B:594:VAL:HB | 2.07 | 0.54 |
| 1:B:646:LEU:CD1 | 1:B:690:LYS:H | 2.17 | 0.54 |
| 1:B:835:GLU:HA | 1:B:838:ASN:ND2 | 2.23 | 0.54 |
| 1:C:14:ILE:C | 1:C:160:THR:CA | 2.81 | 0.54 |
| 1:C:176:GLU:HA | 1:C:179:ARG:HB2 | 1.88 | 0.54 |
| 1:C:202:ARG:O | 1:C:206:SER:HA | 2.07 | 0.54 |
| 1:C:262:GLU:HG2 | 1:C:263:GLU:CD | 2.32 | 0.54 |
| 1:C:333:ARG:HH11 | 1:C:334:ARG:HG2 | 1.73 | 0.54 |
| 1:C:404:ALA:O | 1:C:409:SER:N | 2.31 | 0.54 |
| 1:C:599:SER:C | 1:C:601:LEU:N | 2.62 | 0.54 |
| 1:C:613:LEU:HG | 1:C:772:PHE:N | 2.21 | 0.54 |
| 1:C:816:LYS:NZ | 1:C:817:TYR:CZ | 2.75 | 0.54 |
| 1:D:205:LYS:HE3 | 1:D:334:ARG:C | 2.33 | 0.54 |
| 1:D:391:SER:O | 1:D:394:ASP:HB2 | 2.07 | 0.54 |
| 1:D:826:ARG:N | 1:D:827:PRO:HD2 | 2.22 | 0.54 |
| 1:E:166:TYR:HB3 | 1:E:169:LYS:HG3 | 1.89 | 0.54 |
| 1:E:291:GLY:O | 1:E:292:ASN:ND2 | 2.41 | 0.54 |
| 1:E:366:ARG:NH1 | 1:E:368:LEU:N | 2.56 | 0.54 |
| 1:E:611:LEU:HB2 | 1:E:725:MET:CG | 2.37 | 0.54 |
| 1:B:224:GLY:O | 1:B:228:ARG:N | 2.30 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:332:GLU:HA | 1:B:335:PHE:CB | 2.37 | 0.54 |
| 1:B:656:LEU:HA | 1:B:668:GLY:C | 2.33 | 0.54 |
| 1:B:687:GLU:OE1 | 1:B:727:SER:OG | 2.20 | 0.54 |
| 1:B:814:LEU:O | 1:B:817:TYR:N | 2.40 | 0.54 |
| 1:B:858:VAL:O | 1:B:875:GLU:HG3 | 2.08 | 0.54 |
| 1:C:190:GLU:O | 1:C:194:ARG:HG3 | 2.06 | 0.54 |
| 1:C:259:GLY:O | 1:C:263:GLU:OE2 | 2.26 | 0.54 |
| 1:C:368:LEU:HD22 | 1:C:541:VAL:HA | 1.88 | 0.54 |
| 1:C:378:LEU:O | 1:C:381:ARG:HB3 | 2.08 | 0.54 |
| 1:C:634:ASP:OD2 | 1:C:637:MET:HE3 | 2.07 | 0.54 |
| 1:D:193:ILE:HG23 | 1:D:222:ILE:HG23 | 1.90 | 0.54 |
| 1:D:356:GLN:HG2 | 1:D:360:GLU:CD | 2.32 | 0.54 |
| 1:D:613:LEU:H | 1:D:770:VAL:C | 2.16 | 0.54 |
| 1:D:636:ASP:C | 1:D:638:MET:H | 2.16 | 0.54 |
| 1:D:686:ASP:C | 1:D:688:VAL:N | 2.66 | 0.54 |
| 1:D:699:MET:HE3 | 1:D:762:PHE:CE2 | 2.42 | 0.54 |
| 1:E:195:SER:N | 1:E:198:ARG:HH11 | 2.06 | 0.54 |
| 1:E:230:ILE:HG22 | 1:E:495:ARG:HE | 1.72 | 0.54 |
| 1:E:611:LEU:HD12 | 1:E:612:PHE:N | 2.23 | 0.54 |
| 1:E:644:SER:HA | 1:E:691:ALA:N | 2.23 | 0.54 |
| 1:E:708:ILE:HG23 | 1:E:716:ILE:O | 2.07 | 0.54 |
| 1:F:207:ASN:HB2 | 1:F:335:PHE:CD2 | 2.42 | 0.54 |
| 1:F:608:ALA:H | 1:F:722:ILE:HD12 | 1.73 | 0.54 |
| 1:F:761:GLU:CD | 1:F:765:ARG:HH22 | 2.15 | 0.54 |
| 1:A:345:VAL:O | 1:A:349:VAL:HG23 | 2.08 | 0.54 |
| 1:A:572:MET:O | 1:A:576:LEU:HG | 2.08 | 0.54 |
| 1:A:632:PHE:CD2 | 1:A:637:MET:HG2 | 2.43 | 0.54 |
| 1:A:820:SER:HG | 1:F:307:ARG:HH22 | 1.56 | 0.54 |
| 1:B:248:LEU:O | 1:B:264:ARG:NH2 | 2.41 | 0.54 |
| 1:B:612:PHE:HA | 1:B:770:VAL:C | 2.33 | 0.54 |
| 1:B:617:GLY:H | 1:B:620:LYS:CD | 2.21 | 0.54 |
| 1:B:618:SER:O | 1:B:826:ARG:NE | 2.41 | 0.54 |
| 1:B:645:GLU:O | 1:B:646:LEU:HD23 | 2.06 | 0.54 |
| 1:B:792:GLU:OE2 | 1:B:795:PHE:CD2 | 2.60 | 0.54 |
| 1:B:843:ARG:N | 1:B:846:LYS:HZ3 | 2.04 | 0.54 |
| 1:C:172:ILE:O | 1:C:244:PHE:HD1 | 1.90 | 0.54 |
| 1:C:189:ARG:NH2 | 1:C:342:GLU:HA | 2.16 | 0.54 |
| 1:C:201:ALA:HB2 | 1:C:238:LEU:HD11 | 1.88 | 0.54 |
| 1:C:366:ARG:HH12 | 1:C:538:GLN:CB | 2.17 | 0.54 |
| 1:C:534:ASN:HB3 | 1:C:537:ILE:CA | 2.38 | 0.54 |
| 1:C:685:PHE:C | 1:C:688:VAL:H | 2.16 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:776:SER:OG | 1:C:777:ARG:N | 2.40 | 0.54 |
| 1:C:797:GLN:H | 1:C:797:GLN:CD | 2.16 | 0.54 |
| 1:C:857:VAL:CG1 | 1:C:879:VAL:H | 2.20 | 0.54 |
| 1:D:352:LEU:HA | 1:D:355:LEU:HD21 | 1.90 | 0.54 |
| 1:D:396:VAL:O | 1:D:399:SER:HB2 | 2.08 | 0.54 |
| 1:D:401:ALA:O | 1:D:405:VAL:HG23 | 2.07 | 0.54 |
| 1:D:569:LEU:HD12 | 1:D:573:GLU:OE2 | 2.08 | 0.54 |
| 1:D:637:MET:C | 1:D:678:LYS:NZ | 2.64 | 0.54 |
| 1:D:834:ASN:CG | 1:D:835:GLU:N | 2.66 | 0.54 |
| 1:E:358:LYS:NZ | 1:E:359:TYR:CA | 2.70 | 0.54 |
| 1:E:392:ALA:O | 1:E:395:LEU:N | 2.41 | 0.54 |
| 1:E:473:HIS:HA | 1:E:521:GLU:OE2 | 2.08 | 0.54 |
| 1:E:616:SER:HA | 2:E:1002:AGS:O2B | 2.07 | 0.54 |
| 1:E:620:LYS:NZ | 2:E:1002:AGS:O3A | 2.41 | 0.54 |
| 1:E:759:ARG:HB3 | 1:E:761:GLU:OE2 | 2.08 | 0.54 |
| 1:E:837:LEU:HA | 1:E:840:LEU:HD13 | 1.90 | 0.54 |
| 1:E:856:ASN:ND2 | 1:E:880:LEU:O | 2.40 | 0.54 |
| 1:F:197:ILE:HG12 | 1:F:228:ARG:NH1 | 2.22 | 0.54 |
| 1:F:212:GLY:H | 1:F:218:LYS:HD3 | 1.72 | 0.54 |
| 1:F:368:LEU:O | 1:F:372:LEU:HD13 | 2.07 | 0.54 |
| 1:F:649:LYS:HA | 1:F:693:PRO:HD2 | 1.89 | 0.54 |
| 1:A:175:THR:HA | 1:A:243:LEU:HG | 1.88 | 0.54 |
| 1:A:563:GLU:HB3 | 1:A:568:LYS:HE3 | 1.89 | 0.54 |
| 1:A:601:LEU:HD11 | 1:B:841:ALA:HB2 | 1.88 | 0.54 |
| 1:A:751:MET:HG2 | 1:A:755:ARG:NH1 | 2.23 | 0.54 |
| 1:B:253:ALA:C | 1:B:260:ASP:OD2 | 2.51 | 0.54 |
| 1:B:374:THR:O | 1:B:378:LEU:HG | 2.08 | 0.54 |
| 1:B:650:TYR:CD1 | 1:B:652:VAL:HG22 | 2.43 | 0.54 |
| 1:C:171:ALA:HB1 | 1:C:244:PHE:CD1 | 2.43 | 0.54 |
| 1:C:190:GLU:HB2 | 1:C:194:ARG:NH1 | 2.23 | 0.54 |
| 1:C:197:ILE:O | 1:C:200:LEU:HB2 | 2.07 | 0.54 |
| 1:C:247:ASP:HB2 | 1:C:248:LEU:HD13 | 1.90 | 0.54 |
| 1:C:342:GLU:OE2 | 1:C:389:PRO:HD3 | 2.07 | 0.54 |
| 1:C:614:GLY:CA | 1:C:728:ALA:HA | 2.31 | 0.54 |
| 1:C:839:LYS:HZ1 | 1:C:880:LEU:N | 2.06 | 0.54 |
| 1:D:192:GLU:HG2 | 1:D:193:ILE:N | 2.22 | 0.54 |
| 1:D:333:ARG:HH22 | 2:E:1001:AGS:PB | 2.30 | 0.54 |
| 1:D:421:LEU:HD22 | 1:D:459:LEU:HD11 | 1.90 | 0.54 |
| 1:D:463:ARG:HB2 | 1:D:463:ARG:CZ | 2.38 | 0.54 |
| 1:D:586:ALA:O | 1:D:590:VAL:HG23 | 2.08 | 0.54 |
| 1:E:239:GLN:C | 1:E:241:ALA:H | 2.14 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:482:LYS:HA | 1:E:485:GLU:CD | 2.33 | 0.54 |
| 1:E:496:ARG:HG3 | 1:E:499:THR:OG1 | 2.07 | 0.54 |
| 1:E:634:ASP:HB3 | 1:E:637:MET:H | 1.73 | 0.54 |
| 1:E:703:LEU:HB3 | 1:E:765:ARG:HD2 | 1.90 | 0.54 |
| 1:F:859:LEU:HB2 | 1:F:876:CYS:HB3 | 1.88 | 0.54 |
| 1:A:349:VAL:O | 1:A:352:LEU:HD13 | 2.08 | 0.54 |
| 1:A:379:ALA:HA | 1:A:382:TYR:CE1 | 2.42 | 0.54 |
| 1:A:624:ALA:O | 1:A:628:ALA:N | 2.41 | 0.54 |
| 1:B:753:ALA:HA | 1:B:756:GLN:CD | 2.32 | 0.54 |
| 1:C:506:ARG:NE | 1:D:430:ALA:O | 2.40 | 0.54 |
| 1:C:565:GLU:CA | 1:C:568:LYS:HB3 | 2.35 | 0.54 |
| 1:C:618:SER:C | 1:C:826:ARG:NH1 | 2.65 | 0.54 |
| 1:C:650:TYR:CE1 | 1:C:654:LYS:NZ | 2.64 | 0.54 |
| 1:C:779:ALA:HB1 | 1:C:783:ILE:HD12 | 1.89 | 0.54 |
| 1:C:794:ARG:O | 1:C:795:PHE:C | 2.51 | 0.54 |
| 1:D:203:ARG:NH1 | 1:E:363:HIS:NE2 | 2.56 | 0.54 |
| 1:D:272:ILE:HA | 1:D:276:LYS:HZ2 | 1.73 | 0.54 |
| 1:D:362:HIS:CD2 | 1:D:363:HIS:CE1 | 2.96 | 0.54 |
| 1:D:364:GLY:HA2 | 1:D:473:HIS:HE2 | 1.72 | 0.54 |
| 1:D:424:ILE:O | 1:D:427:GLU:HB3 | 2.08 | 0.54 |
| 1:D:741:LYS:HA | 1:D:773:ASN:CG | 2.33 | 0.54 |
| 1:D:825:ALA:O | 1:D:828:LEU:HG | 2.08 | 0.54 |
| 1:E:366:ARG:O | 1:E:539:ASN:HA | 2.08 | 0.54 |
| 1:E:557:PRO:O | 1:E:560:LYS:N | 2.40 | 0.54 |
| 1:E:577:SER:OG | 1:E:578:SER:N | 2.37 | 0.54 |
| 1:E:637:MET:HE2 | 1:E:681:SER:HA | 1.90 | 0.54 |
| 1:F:332:GLU:OE1 | 1:F:332:GLU:HA | 2.08 | 0.54 |
| 1:F:669:GLY:O | 1:F:672:THR:HB | 2.08 | 0.54 |
| 1:A:170:TYR:CE1 | 1:A:264:ARG:HG3 | 2.43 | 0.54 |
| 1:A:259:GLY:N | 1:A:261:PHE:HB2 | 2.23 | 0.54 |
| 1:A:638:MET:C | 1:A:639:ILE:HG13 | 2.32 | 0.54 |
| 1:B:234:VAL:HG11 | 1:B:238:LEU:N | 2.22 | 0.54 |
| 1:B:348:THR:O | 1:B:349:VAL:C | 2.51 | 0.54 |
| 1:B:403:VAL:O | 1:B:407:ARG:N | 2.22 | 0.54 |
| 1:C:203:ARG:CG | 1:C:204:ILE:H | 2.19 | 0.54 |
| 1:C:209:CYS:HB2 | 1:C:335:PHE:HA | 1.90 | 0.54 |
| 1:C:237:ILE:HD13 | 1:D:362:HIS:NE2 | 2.22 | 0.54 |
| 1:C:505:LEU:HD12 | 1:C:508:PHE:HB2 | 1.88 | 0.54 |
| 1:D:378:LEU:O | 1:D:381:ARG:N | 2.41 | 0.54 |
| 1:D:390:ASP:HA | 1:D:393:LEU:HD13 | 1.90 | 0.54 |
| 1:D:689:GLU:CB | 1:D:729:LEU:HD12 | 2.38 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:820:SER:O | 1:D:822:ASP:N | 2.41 | 0.54 |
| 1:E:195:SER:O | 1:E:198:ARG:HB2 | 2.08 | 0.54 |
| 1:E:653:SER:OG | 1:E:654:LYS:N | 2.39 | 0.54 |
| 1:E:703:LEU:HD22 | 1:E:765:ARG:CD | 2.37 | 0.54 |
| 1:E:826:ARG:O | 1:E:829:ASN:HB2 | 2.08 | 0.54 |
| 1:F:210:LEU:HD11 | 1:F:340:VAL:HG22 | 1.88 | 0.54 |
| 1:F:279:ILE:C | 1:F:310:LEU:HD11 | 2.33 | 0.54 |
| 1:F:638:MET:N | 1:F:682:VAL:HG12 | 2.19 | 0.54 |
| 1:F:701:GLN:OE1 | 1:F:709:THR:CG2 | 2.55 | 0.54 |
| 1:F:781:HIS:O | 1:F:784:VAL:HG22 | 2.07 | 0.54 |
| 1:F:808:GLN:O | 1:F:811:LYS:N | 2.41 | 0.54 |
| 1:A:227:GLN:O | 1:A:231:ASP:N | 2.34 | 0.54 |
| 1:A:702:MET:SD | 1:A:708:ILE:HA | 2.48 | 0.54 |
| 1:B:207:ASN:HB2 | 1:B:335:PHE:CD1 | 2.43 | 0.54 |
| 1:B:365:VAL:HG13 | 1:B:407:ARG:CZ | 2.38 | 0.54 |
| 1:B:548:GLU:H | 1:B:560:LYS:HZ2 | 1.52 | 0.54 |
| 1:B:648:GLU:HA | 1:B:691:ALA:O | 2.08 | 0.54 |
| 1:B:654:LYS:NZ | 1:B:694:ASP:H | 2.05 | 0.54 |
| 1:B:826:ARG:HB2 | 1:B:827:PRO:HD3 | 1.89 | 0.54 |
| 1:B:849:ILE:HG13 | 1:B:882:ASN:HA | 1.89 | 0.54 |
| 1:C:194:ARG:O | 1:C:198:ARG:HG3 | 2.07 | 0.54 |
| 1:C:209:CYS:HB2 | 1:C:336:GLN:OE1 | 2.08 | 0.54 |
| 1:C:270:LYS:HA | 1:C:273:GLU:HB3 | 1.90 | 0.54 |
| 1:C:741:LYS:HG2 | 1:C:742:ILE:H | 1.72 | 0.54 |
| 1:C:846:LYS:HZ3 | 1:C:882:ASN:HD21 | 1.55 | 0.54 |
| 1:D:248:LEU:CA | 1:D:251:LEU:HG | 2.37 | 0.54 |
| 1:D:510:ILE:HD12 | 1:E:426:VAL:HG21 | 1.90 | 0.54 |
| 1:D:544:ASP:O | 1:D:547:SER:HB2 | 2.08 | 0.54 |
| 1:E:218:LYS:HE2 | 2:E:1001:AGS:S1G | 2.47 | 0.54 |
| 1:E:361:ILE:HD13 | 1:E:481:LYS:HA | 1.89 | 0.54 |
| 1:E:454:SER:HA | 1:E:457:GLU:OE1 | 2.08 | 0.54 |
| 1:E:491:LEU:HD22 | 1:E:494:GLU:OE2 | 2.07 | 0.54 |
| 1:E:702:MET:O | 1:E:707:ARG:NE | 2.40 | 0.54 |
| 1:F:839:LYS:CA | 1:F:842:LEU:HB3 | 2.32 | 0.54 |
| 1:A:383:LEU:N | 1:A:384:PRO:HD3 | 2.23 | 0.53 |
| 1:A:762:PHE:O | 1:A:766:ILE:HG13 | 2.08 | 0.53 |
| 1:A:776:SER:O | 1:A:780:ILE:HG23 | 2.08 | 0.53 |
| 1:B:337:LYS:CG | 1:B:338:ILE:H | 2.22 | 0.53 |
| 1:B:616:SER:HB3 | 1:B:620:LYS:HD3 | 1.90 | 0.53 |
| 1:B:759:ARG:HG3 | 1:B:761:GLU:OE1 | 2.09 | 0.53 |
| 1:C:208:PRO:O | 1:C:336:GLN:C | 2.51 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:693:PRO:O | 1:C:696:LEU:HB2 | 2.08 | 0.53 |
| 1:D:198:ARG:HH11 | 1:E:404:ALA:N | 2.05 | 0.53 |
| 1:D:262:GLU:HB2 | 1:D:298:ALA:CB | 2.34 | 0.53 |
| 1:D:272:ILE:O | 1:D:276:LYS:HB2 | 2.08 | 0.53 |
| 1:D:729:LEU:O | 1:D:729:LEU:HD23 | 2.08 | 0.53 |
| 1:E:175:THR:C | 1:E:179:ARG:H | 2.16 | 0.53 |
| 1:E:297:ALA:O | 1:E:300:ILE:HB | 2.07 | 0.53 |
| 1:E:322:ARG:O | 1:E:326:GLU:HG3 | 2.08 | 0.53 |
| 1:E:383:LEU:HD21 | 1:E:385:TYR:CD1 | 2.43 | 0.53 |
| 1:E:826:ARG:HH21 | 2:E:1002:AGS:H1' | 1.73 | 0.53 |
| 1:F:574:ARG:C | 1:F:577:SER:HG | 2.13 | 0.53 |
| 1:F:620:LYS:HD2 | 2:F:1002:AGS:H4' | 1.90 | 0.53 |
| 1:F:640:ARG:NH2 | 1:F:641:VAL:O | 2.41 | 0.53 |
| 1:F:714:LYS:O | 1:F:716:ILE:HG12 | 2.07 | 0.53 |
| 1:B:280:VAL:HG12 | 1:B:310:LEU:CA | 2.38 | 0.53 |
| 1:B:353:ARG:NH1 | 1:B:373:VAL:N | 2.56 | 0.53 |
| 1:B:843:ARG:N | 1:B:846:LYS:NZ | 2.57 | 0.53 |
| 1:C:175:THR:HA | 1:C:230:ILE:HD12 | 1.90 | 0.53 |
| 1:C:189:ARG:O | 1:C:192:GLU:HB2 | 2.08 | 0.53 |
| 1:C:249:ALA:HB3 | 1:C:251:LEU:HB3 | 1.91 | 0.53 |
| 1:C:266:LYS:HA | 1:C:269:LEU:CD1 | 2.37 | 0.53 |
| 1:C:286:ILE:C | 1:C:289:LEU:H | 2.16 | 0.53 |
| 1:C:349:VAL:HG12 | 1:C:353:ARG:HG3 | 1.89 | 0.53 |
| 1:C:360:GLU:C | 1:C:360:GLU:CD | 2.75 | 0.53 |
| 1:C:368:LEU:C | 1:C:372:LEU:HD11 | 2.34 | 0.53 |
| 1:C:504:ASP:OD1 | 1:D:433:ARG:NH2 | 2.38 | 0.53 |
| 1:C:564:SER:OG | 1:C:565:GLU:N | 2.39 | 0.53 |
| 1:D:422:GLN:O | 1:D:426:VAL:N | 2.39 | 0.53 |
| 1:D:595:ARG:HB2 | 1:E:838:ASN:OD1 | 2.07 | 0.53 |
| 1:D:736:SER:N | 1:D:774:LYS:HZ1 | 2.05 | 0.53 |
| 1:E:225:VAL:HG12 | 1:E:229:ILE:HD11 | 1.89 | 0.53 |
| 1:E:281:LEU:HD23 | 1:E:282:PHE:H | 1.70 | 0.53 |
| 1:E:372:LEU:O | 1:E:375:ALA:HB3 | 2.07 | 0.53 |
| 1:F:193:ILE:C | 1:F:228:ARG:HH12 | 2.16 | 0.53 |
| 1:F:615:LEU:HB2 | 1:F:772:PHE:CE1 | 2.43 | 0.53 |
| 1:F:700:LEU:HD21 | 1:F:762:PHE:CD1 | 2.43 | 0.53 |
| 1:B:751:MET:O | 1:B:755:ARG:NH1 | 2.41 | 0.53 |
| 1:C:17:LEU:O | 1:C:21:LEU:N | 2.36 | 0.53 |
| 1:C:208:PRO:HD3 | 1:C:313:ILE:HG12 | 1.91 | 0.53 |
| 1:C:599:SER:HB3 | 1:C:602:ALA:HB2 | 1.89 | 0.53 |
| 1:C:695:VAL:HA | 1:C:698:VAL:HB | 1.90 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:801:HIS:C | 1:C:853:GLU:OE2 | 2.51 | 0.53 |
| 1:C:837:LEU:HA | 1:C:840:LEU:CB | 2.38 | 0.53 |
| 1:D:328:ASP:OD2 | 1:D:330:ALA:HB3 | 2.08 | 0.53 |
| 1:D:482:LYS:O | 1:D:485:GLU:HB2 | 2.07 | 0.53 |
| 1:D:585:ASP:HA | 1:D:588:LYS:NZ | 2.23 | 0.53 |
| 2:D:1001:AGS:H8 | 2:D:1001:AGS:O1A | 2.08 | 0.53 |
| 1:E:169:LYS:CE | 1:E:264:ARG:HB3 | 2.37 | 0.53 |
| 1:E:408:ASP:OD2 | 1:E:411:PRO:HG3 | 2.07 | 0.53 |
| 1:E:641:VAL:N | 1:E:684:LEU:HD22 | 2.22 | 0.53 |
| 1:F:170:TYR:HD1 | 1:F:264:ARG:HH21 | 1.56 | 0.53 |
| 1:F:347:GLN:OE1 | 1:F:347:GLN:N | 2.41 | 0.53 |
| 1:F:612:PHE:HE2 | 1:F:614:GLY:HA2 | 1.72 | 0.53 |
| 1:F:808:GLN:HA | 1:F:811:LYS:NZ | 2.24 | 0.53 |
| 1:A:173:ASP:OD1 | 1:A:174:MET:N | 2.42 | 0.53 |
| 1:A:355:LEU:C | 1:A:357:PRO:HD3 | 2.33 | 0.53 |
| 1:A:642:ASP:OD2 | 1:A:645:GLU:HB3 | 2.08 | 0.53 |
| 1:B:391:SER:O | 1:B:395:LEU:HG | 2.08 | 0.53 |
| 1:B:630:PHE:CE2 | 1:B:631:LEU:HD23 | 2.43 | 0.53 |
| 1:B:645:GLU:C | 1:B:692:HIS:H | 2.16 | 0.53 |
| 1:B:680:TYR:HA | 1:B:721:CYS:SG | 2.48 | 0.53 |
| 1:B:693:PRO:O | 1:B:696:LEU:HG | 2.08 | 0.53 |
| 1:B:740:SER:CB | 1:B:773:ASN:HB2 | 2.39 | 0.53 |
| 1:B:829:ASN:O | 1:B:830:ARG:C | 2.52 | 0.53 |
| 1:B:843:ARG:NE | 1:B:846:LYS:HE2 | 2.24 | 0.53 |
| 1:C:169:LYS:NZ | 1:C:264:ARG:HB2 | 2.22 | 0.53 |
| 1:C:228:ARG:HA | 1:C:231:ASP:CG | 2.34 | 0.53 |
| 1:C:282:PHE:CE1 | 1:C:314:GLY:HA2 | 2.44 | 0.53 |
| 1:C:566:ASN:O | 1:C:570:ILE:HG12 | 2.08 | 0.53 |
| 1:C:716:ILE:HG22 | 1:C:717:ASP:N | 2.24 | 0.53 |
| 1:C:771:ILE:HB | 1:C:772:PHE:O | 2.09 | 0.53 |
| 1:C:788:LEU:O | 1:C:792:GLU:N | 2.38 | 0.53 |
| 1:D:189:ARG:C | 1:D:192:GLU:OE2 | 2.52 | 0.53 |
| 1:D:189:ARG:O | 1:D:192:GLU:OE2 | 2.26 | 0.53 |
| 1:D:218:LYS:HA | 1:D:221:ILE:HD12 | 1.90 | 0.53 |
| 1:D:260:ASP:C | 1:D:263:GLU:H | 2.15 | 0.53 |
| 1:D:634:ASP:CG | 1:D:636:ASP:HB3 | 2.33 | 0.53 |
| 1:D:824:GLY:O | 1:D:828:LEU:HD11 | 2.08 | 0.53 |
| 1:E:175:THR:HG22 | 1:E:230:ILE:HD11 | 1.89 | 0.53 |
| 1:E:247:ASP:OD2 | 1:E:249:ALA:HB3 | 2.09 | 0.53 |
| 1:E:602:ALA:O | 1:E:606:GLN:HB2 | 2.09 | 0.53 |
| 1:E:782:LYS:O | 1:E:784:VAL:N | 2.42 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:836:ILE:O | 1:E:839:LYS:HB2 | 2.08 | 0.53 |
| 1:F:200:LEU:HD22 | 1:F:238:LEU:HB2 | 1.91 | 0.53 |
| 1:F:218:LYS:HB2 | 2:F:1001:AGS:S1G | 2.47 | 0.53 |
| 1:F:548:GLU:CD | 1:F:552:ARG:HH12 | 2.13 | 0.53 |
| 1:F:620:LYS:NZ | 2:F:1002:AGS:PG | 2.82 | 0.53 |
| 1:F:704:ASP:CB | 1:F:765:ARG:NH1 | 2.42 | 0.53 |
| 1:F:777:ARG:HG3 | 1:F:778:LYS:N | 2.23 | 0.53 |
| 1:A:708:ILE:H | 1:A:717:ASP:N | 2.07 | 0.53 |
| 1:A:733:PHE:O | 1:A:736:SER:OG | 2.25 | 0.53 |
| 1:B:207:ASN:HA | 1:B:311:LYS:HD2 | 1.90 | 0.53 |
| 1:B:617:GLY:H | 1:B:620:LYS:NZ | 2.07 | 0.53 |
| 1:C:200:LEU:HD22 | 1:C:313:ILE:HD13 | 1.91 | 0.53 |
| 1:C:229:ILE:HA | 1:C:234:VAL:HG22 | 1.90 | 0.53 |
| 1:C:655:LEU:HA | 1:C:668:GLY:O | 2.09 | 0.53 |
| 1:C:796:GLU:OE2 | 1:C:797:GLN:HB2 | 2.09 | 0.53 |
| 1:D:208:PRO:HA | 1:D:336:GLN:C | 2.34 | 0.53 |
| 1:D:247:ASP:OD1 | 1:D:283:ILE:HA | 2.08 | 0.53 |
| 1:D:321:TYR:CD1 | 1:D:321:TYR:CA | 2.92 | 0.53 |
| 1:D:461:PRO:HB2 | 1:D:465:ARG:HH21 | 1.73 | 0.53 |
| 1:D:630:PHE:CE2 | 1:D:631:LEU:HA | 2.44 | 0.53 |
| 1:D:718:CYS:C | 1:D:720:ASN:N | 2.67 | 0.53 |
| 1:E:522:ASP:O | 1:E:526:GLU:HG2 | 2.08 | 0.53 |
| 1:E:808:GLN:CD | 1:E:809:GLU:H | 2.15 | 0.53 |
| 1:F:166:TYR:CE2 | 1:F:264:ARG:HD2 | 2.43 | 0.53 |
| 1:F:205:LYS:HZ2 | 1:F:334:ARG:C | 2.08 | 0.53 |
| 1:F:285:GLU:CB | 1:F:288:MET:H | 2.04 | 0.53 |
| 1:F:713:GLY:O | 1:F:714:LYS:CB | 2.55 | 0.53 |
| 1:F:761:GLU:OE2 | 1:F:765:ARG:NH1 | 2.41 | 0.53 |
| 1:A:205:LYS:HD3 | 1:B:397:ASP:OD2 | 2.09 | 0.53 |
| 1:A:252:THR:HA | 1:A:255:ALA:HB3 | 1.89 | 0.53 |
| 1:A:349:VAL:HA | 1:A:352:LEU:HD13 | 1.91 | 0.53 |
| 1:A:816:LYS:HA | 1:A:819:TYR:CE2 | 2.43 | 0.53 |
| 1:A:858:VAL:HG12 | 1:A:859:LEU:N | 2.24 | 0.53 |
| 1:B:185:PRO:HB3 | 1:B:227:GLN:OE1 | 2.08 | 0.53 |
| 1:B:689:GLU:OE2 | 1:B:729:LEU:HD13 | 2.08 | 0.53 |
| 1:C:387:ARG:HB2 | 1:C:390:ASP:CG | 2.33 | 0.53 |
| 1:C:545:THR:O | 1:C:548:GLU:OE2 | 2.26 | 0.53 |
| 1:C:838:ASN:OD1 | 1:C:839:LYS:HG2 | 2.08 | 0.53 |
| 1:D:177:GLN:HE21 | 1:D:182:LYS:C | 2.16 | 0.53 |
| 1:D:184:ASP:O | 1:D:186:VAL:N | 2.41 | 0.53 |
| 1:D:307:ARG:HG3 | 1:D:308:GLY:H | 1.74 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:321:TYR:CD1 | 1:D:321:TYR:CB | 2.79 | 0.53 |
| 1:D:393:LEU:HD21 | 2:D:1001:AGS:H1' | 1.90 | 0.53 |
| 1:D:516:GLN:O | 1:D:520:LEU:N | 2.22 | 0.53 |
| 1:D:606:GLN:CD | 1:D:704:ASP:HB3 | 2.34 | 0.53 |
| 1:D:828:LEU:O | 1:D:829:ASN:C | 2.52 | 0.53 |
| 1:D:879:VAL:O | 1:D:880:LEU:HG | 2.09 | 0.53 |
| 1:E:285:GLU:O | 1:E:285:GLU:HG2 | 2.07 | 0.53 |
| 1:E:381:ARG:HA | 1:E:680:TYR:OH | 2.09 | 0.53 |
| 1:E:597:SER:OG | 1:E:598:ARG:HG2 | 2.09 | 0.53 |
| 1:E:745:SER:N | 1:E:747:LYS:HZ1 | 2.06 | 0.53 |
| 1:F:352:LEU:O | 1:F:356:GLN:N | 2.41 | 0.53 |
| 1:F:844:ILE:HA | 1:F:847:ASN:OD1 | 2.08 | 0.53 |
| 1:A:302:LYS:NZ | 1:A:310:LEU:C | 2.67 | 0.53 |
| 1:A:759:ARG:O | 1:A:762:PHE:HB3 | 2.09 | 0.53 |
| 1:A:830:ARG:HH22 | 1:F:275:SER:N | 1.95 | 0.53 |
| 1:A:858:VAL:O | 1:A:877:LEU:N | 2.42 | 0.53 |
| 1:B:112:ALA:O | 1:B:116:ILE:N | 2.24 | 0.53 |
| 1:B:174:MET:SD | 1:B:244:PHE:HA | 2.49 | 0.53 |
| 1:C:345:VAL:O | 1:C:349:VAL:HG23 | 2.09 | 0.53 |
| 1:C:407:ARG:O | 1:C:410:LYS:N | 2.37 | 0.53 |
| 1:C:616:SER:OG | 1:C:617:GLY:N | 2.40 | 0.53 |
| 1:C:629:GLY:O | 1:C:633:ASN:ND2 | 2.41 | 0.53 |
| 1:D:150:ASN:C | 1:D:152:ARG:H | 2.16 | 0.53 |
| 1:D:186:VAL:HB | 2:D:1001:AGS:C5 | 2.38 | 0.53 |
| 1:D:198:ARG:NH2 | 1:E:406:ALA:N | 2.56 | 0.53 |
| 1:D:229:ILE:HG23 | 1:D:234:VAL:HB | 1.90 | 0.53 |
| 1:D:285:GLU:CD | 1:D:321:TYR:HE1 | 2.17 | 0.53 |
| 1:D:395:LEU:O | 1:D:399:SER:N | 2.26 | 0.53 |
| 1:D:483:LEU:HD11 | 1:D:487:GLU:HB2 | 1.90 | 0.53 |
| 1:D:570:ILE:CG1 | 1:D:595:ARG:HH12 | 2.21 | 0.53 |
| 1:D:619:GLY:O | 1:D:623:LEU:HD13 | 2.08 | 0.53 |
| 1:D:630:PHE:CD1 | 1:D:630:PHE:C | 2.84 | 0.53 |
| 1:D:847:ASN:HB3 | 1:D:850:LYS:CD | 2.39 | 0.53 |
| 1:E:249:ALA:HA | 1:E:252:THR:HG23 | 1.91 | 0.53 |
| 1:E:428:ILE:HG12 | 1:E:449:ARG:HG2 | 1.90 | 0.53 |
| 1:E:457:GLU:O | 1:E:460:GLU:N | 2.38 | 0.53 |
| 1:E:541:VAL:HG12 | 1:E:544:ASP:CB | 2.39 | 0.53 |
| 1:E:650:TYR:CE1 | 1:E:656:LEU:HD11 | 2.43 | 0.53 |
| 1:F:170:TYR:OH | 1:F:253:ALA:O | 2.27 | 0.53 |
| 1:F:286:ILE:HD13 | 1:F:322:ARG:HE | 1.70 | 0.53 |
| 1:F:637:MET:HB3 | 1:F:682:VAL:H | 1.72 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:810:ALA:O | 1:F:814:LEU:HG | 2.09 | 0.53 |
| 1:A:195:SER:O | 1:A:199:VAL:N | 2.42 | 0.53 |
| 1:A:208:PRO:HB3 | 1:A:338:ILE:HD12 | 1.91 | 0.53 |
| 1:A:682:VAL:HG12 | 1:A:683:LEU:N | 2.23 | 0.53 |
| 1:A:777:ARG:NH1 | 1:A:816:LYS:N | 2.52 | 0.53 |
| 1:B:183:LEU:HG | 1:B:184:ASP:N | 2.23 | 0.53 |
| 1:B:193:ILE:O | 1:B:196:THR:N | 2.42 | 0.53 |
| 1:B:259:GLY:HA2 | 1:B:261:PHE:CZ | 2.43 | 0.53 |
| 1:B:317:THR:O | 1:B:320:GLU:OE2 | 2.27 | 0.53 |
| 1:B:323:SER:HB3 | 1:B:327:LYS:NZ | 2.23 | 0.53 |
| 1:B:384:PRO:HD2 | 1:B:386:ARG:HG2 | 1.91 | 0.53 |
| 1:B:643:CYS:C | 1:B:645:GLU:N | 2.59 | 0.53 |
| 1:C:176:GLU:HA | 1:C:179:ARG:CB | 2.38 | 0.53 |
| 1:C:494:GLU:O | 1:C:497:TYR:N | 2.40 | 0.53 |
| 1:C:796:GLU:H | 1:C:802:TYR:HH | 1.45 | 0.53 |
| 1:C:841:ALA:HA | 1:C:844:ILE:HB | 1.90 | 0.53 |
| 1:D:202:ARG:HG3 | 1:D:206:SER:HA | 1.91 | 0.53 |
| 1:D:217:GLY:N | 2:D:1001:AGS:PB | 2.82 | 0.53 |
| 1:D:218:LYS:H | 2:D:1001:AGS:PB | 2.31 | 0.53 |
| 1:E:216:ILE:CD1 | 1:E:387:ARG:HB2 | 2.38 | 0.53 |
| 1:E:365:VAL:CG1 | 1:E:538:GLN:HB2 | 2.37 | 0.53 |
| 1:E:378:LEU:HB3 | 1:E:382:TYR:CD2 | 2.44 | 0.53 |
| 1:E:470:LYS:O | 1:E:473:HIS:HB2 | 2.08 | 0.53 |
| 1:E:544:ASP:O | 1:E:545:THR:C | 2.52 | 0.53 |
| 1:E:627:VAL:C | 1:E:631:LEU:HG | 2.34 | 0.53 |
| 1:F:176:GLU:HG2 | 1:F:177:GLN:N | 2.24 | 0.53 |
| 1:F:730:GLY:O | 1:F:733:PHE:N | 2.41 | 0.53 |
| 1:A:258:LYS:NZ | 1:A:295:ASP:HB3 | 2.22 | 0.53 |
| 1:A:296:ASP:O | 1:A:301:LEU:N | 2.41 | 0.53 |
| 1:A:587:ILE:HA | 1:A:590:VAL:HB | 1.91 | 0.53 |
| 1:A:660:ALA:HB2 | 1:A:667:GLU:OE2 | 2.08 | 0.53 |
| 1:A:805:ASN:HB3 | 1:A:854:THR:HB | 1.90 | 0.53 |
| 1:B:195:SER:CA | 1:B:198:ARG:NH1 | 2.72 | 0.53 |
| 1:B:573:GLU:OE1 | 1:B:595:ARG:NH1 | 2.41 | 0.53 |
| 1:B:580:VAL:HG22 | 1:B:622:GLU:HG2 | 1.91 | 0.53 |
| 1:B:583:GLN:HE21 | 1:B:773:ASN:HB3 | 1.74 | 0.53 |
| 1:B:731:ALA:C | 1:B:733:PHE:N | 2.65 | 0.53 |
| 1:C:303:PRO:C | 1:C:333:ARG:HH22 | 2.17 | 0.53 |
| 1:C:350:ALA:HA | 1:C:353:ARG:HH11 | 1.74 | 0.53 |
| 1:C:351:ILE:HD13 | 2:C:1001:AGS:N7 | 2.24 | 0.53 |
| 1:C:449:ARG:HA | 1:C:452:GLU:HB3 | 1.91 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:710:SER:OG | 1:C:713:GLY:N | 2.42 | 0.53 |
| 1:C:809:GLU:HA | 1:C:812:ASP:OD2 | 2.09 | 0.53 |
| 1:D:176:GLU:OE1 | 1:D:179:ARG:HG3 | 2.09 | 0.53 |
| 1:D:372:LEU:O | 1:D:375:ALA:HB3 | 2.09 | 0.53 |
| 1:D:616:SER:C | 1:D:618:SER:N | 2.66 | 0.53 |
| 1:D:785:ASP:O | 1:D:786:ILE:C | 2.52 | 0.53 |
| 1:E:260:ASP:HA | 1:E:263:GLU:HB2 | 1.91 | 0.53 |
| 1:E:359:TYR:HA | 1:E:362:HIS:NE2 | 2.24 | 0.53 |
| 1:E:383:LEU:HD11 | 1:E:385:TYR:OH | 2.09 | 0.53 |
| 1:E:575:ASP:O | 1:E:578:SER:N | 2.42 | 0.53 |
| 1:F:550:ALA:HB3 | 1:F:557:PRO:HB3 | 1.89 | 0.53 |
| 1:A:191:GLU:HG2 | 1:A:192:GLU:N | 2.24 | 0.53 |
| 1:A:279:ILE:H | 1:A:309:GLN:HG2 | 1.74 | 0.53 |
| 1:A:325:VAL:HA | 1:A:328:ASP:OD2 | 2.09 | 0.53 |
| 1:A:542:ASP:O | 1:A:546:ILE:HB | 2.09 | 0.53 |
| 1:A:654:LYS:HE2 | 1:A:657:GLY:O | 2.09 | 0.53 |
| 1:A:728:ALA:O | 1:A:731:ALA:N | 2.39 | 0.53 |
| 1:A:872:GLU:OE2 | 1:F:237:ILE:HB | 2.09 | 0.53 |
| 1:B:250:ALA:CA | 1:B:264:ARG:HH12 | 2.21 | 0.53 |
| 1:B:648:GLU:HB3 | 1:B:693:PRO:CD | 2.39 | 0.53 |
| 1:C:413:GLU:N | 1:C:413:GLU:OE1 | 2.40 | 0.53 |
| 1:C:421:LEU:HB2 | 1:C:456:GLN:HE21 | 1.73 | 0.53 |
| 1:C:607:PRO:HD3 | 1:C:719:SER:HA | 1.91 | 0.53 |
| 1:C:628:ALA:O | 1:C:633:ASN:N | 2.42 | 0.53 |
| 1:C:757:HIS:O | 1:C:758:PHE:CG | 2.62 | 0.53 |
| 1:C:850:LYS:HG3 | 1:C:851:ASP:CG | 2.34 | 0.53 |
| 1:D:276:LYS:HE2 | 1:D:279:ILE:HD11 | 1.90 | 0.53 |
| 1:D:330:ALA:HA | 1:D:333:ARG:CG | 2.39 | 0.53 |
| 1:D:872:GLU:HG3 | 1:D:877:LEU:HD21 | 1.89 | 0.53 |
| 1:E:637:MET:CE | 1:E:682:VAL:HG12 | 2.36 | 0.53 |
| 1:E:684:LEU:HD23 | 1:E:685:PHE:C | 2.33 | 0.53 |
| 1:A:249:ALA:O | 1:A:254:GLY:HA3 | 2.08 | 0.52 |
| 1:A:307:ARG:N | 1:A:310:LEU:HD12 | 2.12 | 0.52 |
| 1:A:643:CYS:SG | 1:A:686:ASP:N | 2.82 | 0.52 |
| 1:A:803:LYS:H | 1:A:853:GLU:H | 1.56 | 0.52 |
| 1:B:353:ARG:NH2 | 1:B:372:LEU:HD12 | 2.24 | 0.52 |
| 1:B:814:LEU:HD13 | 1:B:832:ILE:HG12 | 1.90 | 0.52 |
| 1:C:193:ILE:O | 1:C:194:ARG:C | 2.51 | 0.52 |
| 1:C:650:TYR:HE1 | 1:C:654:LYS:HZ1 | 1.49 | 0.52 |
| 1:C:839:LYS:HE2 | 1:C:879:VAL:HG13 | 1.91 | 0.52 |
| 1:D:286:ILE:HG22 | 1:D:290:MET:HE2 | 1.90 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:317:THR:CA | 1:D:321:TYR:CG | 2.92 | 0.52 |
| 1:D:549:THR:O | 1:D:553:LEU:HG | 2.09 | 0.52 |
| 1:D:655:LEU:HA | 1:D:671:LEU:HD11 | 1.91 | 0.52 |
| 1:D:670:PHE:CD2 | 1:D:671:LEU:N | 2.77 | 0.52 |
| 1:D:683:LEU:O | 1:D:724:ILE:N | 2.42 | 0.52 |
| 1:D:835:GLU:OE1 | 1:D:839:LYS:HE2 | 2.09 | 0.52 |
| 1:E:220:ALA:O | 1:E:224:GLY:N | 2.20 | 0.52 |
| 1:E:256:LYS:CE | 1:E:263:GLU:HG2 | 2.39 | 0.52 |
| 1:E:349:VAL:O | 1:E:352:LEU:N | 2.42 | 0.52 |
| 1:E:508:PHE:HE2 | 1:E:510:ILE:HD11 | 1.71 | 0.52 |
| 1:E:626:LYS:HZ2 | 1:E:635:GLU:CD | 2.15 | 0.52 |
| 1:E:658:THR:OG1 | 1:E:663:VAL:O | 2.15 | 0.52 |
| 1:E:804:LEU:HA | 1:E:854:THR:CA | 2.40 | 0.52 |
| 1:E:881:PRO:O | 1:E:882:ASN:ND2 | 2.42 | 0.52 |
| 1:F:806:LEU:CB | 1:F:811:LYS:HZ2 | 2.19 | 0.52 |
| 1:A:563:GLU:HB3 | 1:A:568:LYS:CE | 2.39 | 0.52 |
| 1:A:654:LYS:HG2 | 1:A:656:LEU:HB3 | 1.91 | 0.52 |
| 1:A:704:ASP:OD2 | 1:A:765:ARG:NE | 2.42 | 0.52 |
| 1:A:853:GLU:OE2 | 1:A:880:LEU:HD22 | 2.09 | 0.52 |
| 1:A:872:GLU:HB3 | 1:F:201:ALA:CB | 2.38 | 0.52 |
| 1:B:878:GLU:CG | 1:B:879:VAL:H | 2.23 | 0.52 |
| 1:C:15:LEU:N | 1:C:160:THR:N | 2.54 | 0.52 |
| 1:C:401:ALA:O | 1:C:404:ALA:N | 2.42 | 0.52 |
| 1:C:682:VAL:HA | 1:C:722:ILE:O | 2.10 | 0.52 |
| 1:C:751:MET:HB3 | 1:C:755:ARG:CZ | 2.38 | 0.52 |
| 1:C:784:VAL:HG22 | 1:C:811:LYS:HZ2 | 1.74 | 0.52 |
| 1:D:512:ASP:OD1 | 1:D:513:ILE:HG12 | 2.09 | 0.52 |
| 1:D:580:VAL:HA | 1:D:626:LYS:CE | 2.40 | 0.52 |
| 1:D:779:ALA:HA | 1:D:782:LYS:HZ2 | 1.74 | 0.52 |
| 1:D:791:ILE:HA | 1:D:794:ARG:HH12 | 1.74 | 0.52 |
| 1:D:847:ASN:HB3 | 1:D:850:LYS:HD3 | 1.90 | 0.52 |
| 1:E:189:ARG:CZ | 1:E:192:GLU:OE2 | 2.58 | 0.52 |
| 1:E:208:PRO:HB3 | 1:E:336:GLN:HB2 | 1.91 | 0.52 |
| 1:E:210:LEU:HG | 1:E:339:GLU:N | 2.24 | 0.52 |
| 1:E:311:LYS:NZ | 1:E:313:ILE:HD11 | 2.21 | 0.52 |
| 1:E:730:GLY:O | 1:E:733:PHE:N | 2.42 | 0.52 |
| 1:F:678:LYS:NZ | 1:F:679:PRO:C | 2.67 | 0.52 |
| 1:F:839:LYS:NZ | 1:F:879:VAL:HA | 2.25 | 0.52 |
| 1:A:221:ILE:O | 1:A:225:VAL:HG23 | 2.09 | 0.52 |
| 1:A:235:PRO:O | 1:A:236:THR:C | 2.53 | 0.52 |
| 1:A:727:SER:C | 1:A:729:LEU:H | 2.16 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:777:ARG:CA | 1:A:780:ILE:HG12 | 2.31 | 0.52 |
| 1:A:791:ILE:O | 1:A:794:ARG:HG2 | 2.09 | 0.52 |
| 1:A:809:GLU:OE1 | 1:A:857:VAL:HB | 2.09 | 0.52 |
| 1:B:323:SER:C | 1:B:327:LYS:HZ3 | 2.17 | 0.52 |
| 1:B:610:PHE:H | 1:B:724:ILE:CD1 | 2.20 | 0.52 |
| 1:B:625:LYS:O | 1:B:635:GLU:OE2 | 2.26 | 0.52 |
| 1:C:419:ARG:O | 1:C:423:LEU:N | 2.41 | 0.52 |
| 1:C:574:ARG:HG3 | 1:C:575:ASP:OD1 | 2.09 | 0.52 |
| 1:C:732:GLU:HA | 1:C:735:ASN:ND2 | 2.24 | 0.52 |
| 1:D:166:TYR:CE1 | 1:D:169:LYS:HD2 | 2.44 | 0.52 |
| 1:D:196:THR:O | 1:D:200:LEU:HG | 2.09 | 0.52 |
| 1:D:223:GLU:CA | 1:D:226:ALA:HB3 | 2.31 | 0.52 |
| 1:D:395:LEU:O | 1:D:398:ILE:N | 2.43 | 0.52 |
| 1:D:589:ALA:HA | 1:D:592:ASN:OD1 | 2.09 | 0.52 |
| 1:E:347:GLN:CD | 1:E:347:GLN:N | 2.67 | 0.52 |
| 1:E:746:THR:O | 1:E:750:VAL:HG23 | 2.08 | 0.52 |
| 1:E:812:ASP:OD1 | 1:E:816:LYS:HG3 | 2.09 | 0.52 |
| 1:F:398:ILE:O | 1:F:401:ALA:HB3 | 2.10 | 0.52 |
| 1:A:175:THR:HA | 1:A:243:LEU:CG | 2.39 | 0.52 |
| 1:A:356:GLN:HB2 | 1:A:360:GLU:CB | 2.33 | 0.52 |
| 1:A:733:PHE:CE2 | 1:A:750:VAL:HA | 2.45 | 0.52 |
| 1:A:872:GLU:N | 1:F:198:ARG:HA | 2.24 | 0.52 |
| 1:B:621:THR:O | 1:B:625:LYS:N | 2.43 | 0.52 |
| 1:C:15:LEU:H | 1:C:160:THR:H | 1.53 | 0.52 |
| 1:C:280:VAL:HA | 1:C:311:LYS:HD2 | 1.92 | 0.52 |
| 1:C:302:LYS:HD2 | 1:C:305:LEU:C | 2.34 | 0.52 |
| 1:C:350:ALA:O | 1:C:353:ARG:HB2 | 2.09 | 0.52 |
| 1:C:628:ALA:HA | 1:C:631:LEU:HB2 | 1.92 | 0.52 |
| 1:C:761:GLU:HA | 1:C:764:ASN:HD21 | 1.73 | 0.52 |
| 1:C:784:VAL:CG2 | 1:C:811:LYS:NZ | 2.71 | 0.52 |
| 1:D:328:ASP:OD1 | 1:D:330:ALA:N | 2.42 | 0.52 |
| 1:D:459:LEU:HB3 | 1:D:463:ARG:NH2 | 2.20 | 0.52 |
| 1:D:569:LEU:O | 1:D:573:GLU:OE2 | 2.27 | 0.52 |
| 1:D:639:ILE:N | 1:D:640:ARG:HH12 | 2.07 | 0.52 |
| 1:D:746:THR:OG1 | 1:D:747:LYS:N | 2.42 | 0.52 |
| 1:D:858:VAL:HG23 | 1:D:859:LEU:HG | 1.92 | 0.52 |
| 1:E:194:ARG:CB | 1:E:198:ARG:HH12 | 2.15 | 0.52 |
| 1:E:393:LEU:O | 1:E:396:VAL:HB | 2.09 | 0.52 |
| 1:E:399:SER:OG | 1:E:400:CYS:N | 2.43 | 0.52 |
| 1:E:580:VAL:HB | 1:E:581:VAL:HG23 | 1.92 | 0.52 |
| 1:E:606:GLN:CD | 1:F:794:ARG:NH1 | 2.67 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:655:LEU:HD21 | 1:E:709:THR:HB | 1.91 | 0.52 |
| 1:E:802:TYR:CZ | 1:E:850:LYS:O | 2.62 | 0.52 |
| 1:F:303:PRO:O | 1:F:306:SER:N | 2.42 | 0.52 |
| 1:F:373:VAL:O | 1:F:376:ALA:HB3 | 2.09 | 0.52 |
| 1:F:568:LYS:HA | 1:F:571:HIS:CD2 | 2.45 | 0.52 |
| 1:F:820:SER:N | 1:F:823:MET:O | 2.42 | 0.52 |
| 1:A:204:ILE:HD12 | 1:A:334:ARG:CZ | 2.39 | 0.52 |
| 1:A:543:SER:OG | 1:A:544:ASP:N | 2.42 | 0.52 |
| 1:A:573:GLU:HA | 1:A:576:LEU:HD12 | 1.91 | 0.52 |
| 1:A:803:LYS:N | 1:A:853:GLU:H | 2.06 | 0.52 |
| 1:B:324:ILE:O | 1:B:327:LYS:N | 2.43 | 0.52 |
| 1:B:541:VAL:O | 1:B:541:VAL:HG12 | 2.09 | 0.52 |
| 1:B:606:GLN:HB2 | 1:B:703:LEU:O | 2.09 | 0.52 |
| 1:C:222:ILE:N | 1:C:223:GLU:OE1 | 2.42 | 0.52 |
| 1:C:242:LYS:HB3 | 1:C:279:ILE:HG23 | 1.92 | 0.52 |
| 1:C:413:GLU:HB2 | 1:C:417:LYS:CE | 2.39 | 0.52 |
| 1:C:417:LYS:HD3 | 1:C:463:ARG:CZ | 2.40 | 0.52 |
| 1:C:622:GLU:O | 1:C:626:LYS:HG3 | 2.09 | 0.52 |
| 1:C:643:CYS:HB2 | 1:C:690:LYS:HE2 | 1.90 | 0.52 |
| 1:D:198:ARG:NH1 | 1:E:406:ALA:H | 2.08 | 0.52 |
| 1:D:286:ILE:HA | 1:D:289:LEU:CB | 2.39 | 0.52 |
| 1:D:307:ARG:HG3 | 1:D:308:GLY:N | 2.25 | 0.52 |
| 1:D:365:VAL:HG13 | 1:D:536:MET:O | 2.09 | 0.52 |
| 1:D:494:GLU:OE1 | 1:D:499:THR:HA | 2.10 | 0.52 |
| 1:D:710:SER:C | 1:D:713:GLY:H | 2.16 | 0.52 |
| 1:D:777:ARG:HA | 1:D:780:ILE:HD12 | 1.91 | 0.52 |
| 1:D:782:LYS:C | 1:D:784:VAL:N | 2.67 | 0.52 |
| 1:D:789:LYS:HZ2 | 1:D:790:GLU:CA | 2.21 | 0.52 |
| 1:E:168:SER:HG | 1:E:264:ARG:HH21 | 1.54 | 0.52 |
| 1:E:176:GLU:HG2 | 1:E:177:GLN:N | 2.21 | 0.52 |
| 1:E:542:ASP:OD1 | 1:E:543:SER:N | 2.39 | 0.52 |
| 1:F:198:ARG:CB | 1:F:202:ARG:HH21 | 2.22 | 0.52 |
| 1:F:205:LYS:NZ | 1:F:334:ARG:N | 2.57 | 0.52 |
| 1:F:209:CYS:N | 1:F:337:LYS:HA | 2.24 | 0.52 |
| 1:A:196:THR:HA | 1:A:199:VAL:CB | 2.38 | 0.52 |
| 1:A:210:LEU:HD22 | 1:A:339:GLU:CA | 2.25 | 0.52 |
| 1:A:211:ILE:H | 1:A:316:THR:H | 1.57 | 0.52 |
| 1:A:244:PHE:CD2 | 1:A:279:ILE:HG22 | 2.45 | 0.52 |
| 1:A:283:ILE:HD12 | 1:A:288:MET:HB3 | 1.91 | 0.52 |
| 1:A:346:ARG:HH11 | 1:A:349:VAL:HG11 | 1.75 | 0.52 |
| 1:A:404:ALA:O | 1:A:408:ASP:HB2 | 2.09 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:593:ALA:O | 1:A:597:SER:N | 2.35 | 0.52 |
| 1:A:684:LEU:HA | 1:A:723:VAL:CG2 | 2.40 | 0.52 |
| 1:A:787:ARG:C | 1:A:790:GLU:HB3 | 2.35 | 0.52 |
| 1:B:167:LEU:HD21 | 1:B:274:GLU:OE2 | 2.09 | 0.52 |
| 1:C:203:ARG:HA | 1:C:206:SER:OG | 2.10 | 0.52 |
| 1:C:592:ASN:N | 1:C:595:ARG:HH11 | 2.06 | 0.52 |
| 1:C:669:GLY:C | 1:C:672:THR:HG1 | 2.14 | 0.52 |
| 1:D:198:ARG:NH2 | 1:E:406:ALA:H | 2.08 | 0.52 |
| 1:D:216:ILE:HB | 2:D:1001:AGS:O5' | 2.09 | 0.52 |
| 1:D:218:LYS:HD3 | 1:D:221:ILE:HD12 | 1.91 | 0.52 |
| 1:D:620:LYS:NZ | 1:D:621:THR:HG23 | 2.25 | 0.52 |
| 1:D:622:GLU:HG3 | 1:D:826:ARG:CZ | 2.40 | 0.52 |
| 1:D:638:MET:C | 1:D:640:ARG:HH12 | 2.18 | 0.52 |
| 1:E:246:LEU:HD11 | 1:E:251:LEU:HD12 | 1.91 | 0.52 |
| 1:E:458:GLU:OE1 | 1:E:458:GLU:N | 2.33 | 0.52 |
| 1:E:592:ASN:O | 1:E:595:ARG:N | 2.43 | 0.52 |
| 1:E:746:THR:N | 1:E:747:LYS:NZ | 2.54 | 0.52 |
| 1:E:779:ALA:HB1 | 1:E:783:ILE:HD11 | 1.91 | 0.52 |
| 1:E:859:LEU:C | 1:E:877:LEU:HG | 2.35 | 0.52 |
| 1:F:269:LEU:HA | 1:F:272:ILE:HG12 | 1.91 | 0.52 |
| 1:F:859:LEU:N | 1:F:876:CYS:O | 2.28 | 0.52 |
| 1:A:209:CYS:HA | 1:A:314:GLY:O | 2.09 | 0.52 |
| 1:A:248:LEU:HD11 | 1:A:254:GLY:H | 1.75 | 0.52 |
| 1:A:261:PHE:HD2 | 1:A:263:GLU:HG2 | 1.74 | 0.52 |
| 1:A:269:LEU:HA | 1:A:272:ILE:HD12 | 1.90 | 0.52 |
| 1:A:298:ALA:N | 1:A:301:LEU:HB3 | 2.24 | 0.52 |
| 1:A:592:ASN:HA | 1:A:595:ARG:HE | 1.75 | 0.52 |
| 1:A:689:GLU:OE1 | 1:A:689:GLU:N | 2.28 | 0.52 |
| 1:A:747:LYS:HA | 1:A:750:VAL:HB | 1.92 | 0.52 |
| 1:B:265:PHE:O | 1:B:268:VAL:N | 2.42 | 0.52 |
| 1:C:245:SER:HA | 1:C:282:PHE:O | 2.09 | 0.52 |
| 1:C:545:THR:C | 1:C:548:GLU:OE2 | 2.53 | 0.52 |
| 1:C:630:PHE:HD1 | 1:C:631:LEU:HA | 1.74 | 0.52 |
| 1:C:642:ASP:HB2 | 1:C:645:GLU:CG | 2.25 | 0.52 |
| 1:C:682:VAL:HG23 | 1:C:723:VAL:CA | 2.33 | 0.52 |
| 1:C:857:VAL:HG13 | 1:C:879:VAL:HA | 1.90 | 0.52 |
| 1:D:207:ASN:ND2 | 1:D:312:VAL:HG22 | 2.24 | 0.52 |
| 1:D:610:PHE:HA | 1:D:768:SER:C | 2.35 | 0.52 |
| 1:D:645:GLU:OE1 | 1:D:645:GLU:N | 2.39 | 0.52 |
| 1:D:823:MET:C | 1:D:825:ALA:N | 2.63 | 0.52 |
| 1:E:175:THR:O | 1:E:179:ARG:N | 2.43 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:226:ALA:CA | 1:E:229:ILE:HD12 | 2.32 | 0.52 |
| 1:E:228:ARG:O | 1:E:231:ASP:HB2 | 2.09 | 0.52 |
| 1:E:303:PRO:O | 1:E:307:ARG:N | 2.32 | 0.52 |
| 1:E:318:ASN:HB3 | 1:E:322:ARG:HH22 | 1.74 | 0.52 |
| 1:E:389:PRO:C | 1:E:393:LEU:HG | 2.35 | 0.52 |
| 1:E:566:ASN:O | 1:E:569:LEU:N | 2.42 | 0.52 |
| 1:E:665:TYR:HE1 | 1:E:667:GLU:OE2 | 1.93 | 0.52 |
| 1:E:786:ILE:HA | 1:E:789:LYS:NZ | 2.25 | 0.52 |
| 1:F:569:LEU:CD2 | 1:F:598:ARG:HH21 | 2.22 | 0.52 |
| 1:F:639:ILE:O | 1:F:684:LEU:HB3 | 2.10 | 0.52 |
| 2:F:1002:AGS:O3A | 2:F:1002:AGS:O2G | 2.27 | 0.52 |
| 1:A:800:LYS:HE3 | 1:A:851:ASP:CB | 2.39 | 0.52 |
| 1:B:349:VAL:O | 1:B:353:ARG:HG2 | 2.10 | 0.52 |
| 1:B:367:ILE:HG23 | 1:B:540:VAL:HG21 | 1.92 | 0.52 |
| 1:B:672:THR:OG1 | 1:B:673:ASN:N | 2.41 | 0.52 |
| 1:B:820:SER:HB3 | 1:B:824:GLY:N | 2.13 | 0.52 |
| 1:B:839:LYS:C | 1:B:842:LEU:HD13 | 2.34 | 0.52 |
| 1:C:171:ALA:HB1 | 1:C:244:PHE:CG | 2.45 | 0.52 |
| 1:C:189:ARG:HH22 | 1:C:341:ALA:C | 2.18 | 0.52 |
| 1:C:333:ARG:NH1 | 1:C:334:ARG:CG | 2.73 | 0.52 |
| 1:C:472:GLY:HA2 | 1:C:475:GLU:OE2 | 2.10 | 0.52 |
| 1:C:803:LYS:HZ1 | 1:C:854:THR:N | 2.08 | 0.52 |
| 1:D:656:LEU:HG | 1:D:710:SER:C | 2.34 | 0.52 |
| 1:D:785:ASP:OD1 | 1:D:785:ASP:O | 2.28 | 0.52 |
| 1:D:847:ASN:CG | 1:D:850:LYS:HZ3 | 2.18 | 0.52 |
| 1:E:193:ILE:CG2 | 1:E:225:VAL:HG22 | 2.40 | 0.52 |
| 1:E:216:ILE:O | 2:E:1001:AGS:PB | 2.68 | 0.52 |
| 1:E:222:ILE:HG21 | 1:E:282:PHE:CZ | 2.45 | 0.52 |
| 1:E:652:VAL:HG13 | 1:E:669:GLY:HA3 | 1.91 | 0.52 |
| 1:F:211:ILE:N | 1:F:339:GLU:HG2 | 2.21 | 0.52 |
| 1:F:568:LYS:HA | 1:F:571:HIS:HB2 | 1.92 | 0.52 |
| 1:F:614:GLY:O | 1:F:615:LEU:HG | 2.08 | 0.52 |
| 1:F:818:GLY:HA3 | 1:F:828:LEU:HD11 | 1.92 | 0.52 |
| 1:A:751:MET:CG | 1:A:755:ARG:HH12 | 2.23 | 0.52 |
| 1:A:823:MET:SD | 1:A:826:ARG:HD3 | 2.49 | 0.52 |
| 1:B:262:GLU:O | 1:B:265:PHE:N | 2.43 | 0.52 |
| 1:B:541:VAL:HG12 | 1:B:544:ASP:OD2 | 2.10 | 0.52 |
| 1:B:580:VAL:HG21 | 1:B:622:GLU:O | 2.09 | 0.52 |
| 1:B:609:SER:HA | 1:B:724:ILE:HD12 | 1.91 | 0.52 |
| 1:B:645:GLU:C | 1:B:646:LEU:HD23 | 2.34 | 0.52 |
| 1:B:846:LYS:HE3 | 1:B:879:VAL:HA | 1.91 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:186:VAL:HA | 2:C:1001:AGS:N6 | 2.25 | 0.52 |
| 1:C:190:GLU:CG | 1:C:191:GLU:N | 2.72 | 0.52 |
| 1:C:621:THR:CB | 1:C:826:ARG:NH1 | 2.69 | 0.52 |
| 1:C:738:GLN:NE2 | 1:C:746:THR:HG1 | 2.03 | 0.52 |
| 1:D:231:ASP:C | 1:D:495:ARG:HE | 2.14 | 0.52 |
| 1:D:260:ASP:O | 1:D:264:ARG:N | 2.37 | 0.52 |
| 1:D:609:SER:CA | 1:D:724:ILE:HG13 | 2.26 | 0.52 |
| 1:D:639:ILE:HD11 | 1:D:682:VAL:O | 2.09 | 0.52 |
| 1:D:692:HIS:O | 1:D:696:LEU:HG | 2.09 | 0.52 |
| 1:D:732:GLU:OE2 | 1:D:750:VAL:HG23 | 2.10 | 0.52 |
| 1:E:216:ILE:O | 1:E:218:LYS:N | 2.43 | 0.52 |
| 1:E:476:LEU:HD23 | 1:E:521:GLU:HG3 | 1.90 | 0.52 |
| 1:F:250:ALA:HA | 1:F:253:ALA:HB3 | 1.91 | 0.52 |
| 1:F:285:GLU:CG | 1:F:288:MET:HG2 | 2.40 | 0.52 |
| 1:F:352:LEU:HA | 1:F:355:LEU:HB2 | 1.90 | 0.52 |
| 1:F:375:ALA:HB2 | 1:F:546:ILE:HD13 | 1.92 | 0.52 |
| 1:F:549:THR:HA | 1:F:552:ARG:HH11 | 1.75 | 0.52 |
| 1:F:651:ALA:N | 1:F:654:LYS:HZ1 | 2.08 | 0.52 |
| 1:A:213:GLU:HB3 | 1:A:214:PRO:HD2 | 1.92 | 0.52 |
| 1:A:673:ASN:HB3 | 1:A:676:GLN:HB3 | 1.91 | 0.52 |
| 1:A:824:GLY:O | 1:A:827:PRO:HD2 | 2.10 | 0.52 |
| 1:A:879:VAL:O | 1:A:880:LEU:HD23 | 2.10 | 0.52 |
| 1:B:202:ARG:CZ | 1:B:204:ILE:O | 2.58 | 0.52 |
| 1:B:237:ILE:O | 1:B:240:GLY:N | 2.42 | 0.52 |
| 1:B:307:ARG:O | 1:B:309:GLN:NE2 | 2.43 | 0.52 |
| 1:B:633:ASN:CG | 1:B:636:ASP:OD2 | 2.53 | 0.52 |
| 1:B:781:HIS:O | 1:B:784:VAL:HB | 2.08 | 0.52 |
| 1:C:165:GLU:H | 1:C:165:GLU:CD | 2.12 | 0.52 |
| 1:C:174:MET:HG2 | 1:C:243:LEU:O | 2.09 | 0.52 |
| 1:C:212:GLY:O | 1:C:317:THR:HA | 2.10 | 0.52 |
| 1:C:544:ASP:O | 1:C:547:SER:N | 2.36 | 0.52 |
| 1:C:596:LEU:C | 1:C:599:SER:H | 2.17 | 0.52 |
| 1:C:615:LEU:HD22 | 1:C:734:ILE:HD13 | 1.91 | 0.52 |
| 1:D:198:ARG:NH1 | 1:E:403:VAL:C | 2.67 | 0.52 |
| 1:D:265:PHE:O | 1:D:269:LEU:N | 2.38 | 0.52 |
| 1:D:357:PRO:HD2 | 1:D:358:LYS:NZ | 2.25 | 0.52 |
| 1:D:369:ASP:CG | 1:D:372:LEU:HD22 | 2.34 | 0.52 |
| 1:D:681:SER:OG | 1:D:721:CYS:SG | 2.30 | 0.52 |
| 1:D:708:ILE:N | 1:D:716:ILE:HG22 | 2.25 | 0.52 |
| 1:D:762:PHE:CD1 | 1:D:763:LEU:HD12 | 2.44 | 0.52 |
| 1:D:843:ARG:NH1 | 1:D:881:PRO:C | 2.51 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:544:ASP:N | 1:E:547:SER:OG | 2.43 | 0.52 |
| 1:E:620:LYS:O | 1:E:623:LEU:HB3 | 2.09 | 0.52 |
| 1:F:211:ILE:HB | 1:F:339:GLU:OE2 | 2.08 | 0.52 |
| 1:F:615:LEU:HD21 | 1:F:734:ILE:HG21 | 1.90 | 0.52 |
| 1:F:678:LYS:HG2 | 1:F:679:PRO:O | 2.10 | 0.52 |
| 1:A:210:LEU:HD22 | 1:A:339:GLU:HG3 | 1.92 | 0.51 |
| 1:A:274:GLU:CA | 1:A:276:LYS:HZ2 | 2.23 | 0.51 |
| 1:A:375:ALA:HA | 1:A:378:LEU:HD12 | 1.91 | 0.51 |
| 1:A:389:PRO:O | 1:A:393:LEU:HG | 2.09 | 0.51 |
| 1:A:568:LYS:O | 1:A:572:MET:HB3 | 2.11 | 0.51 |
| 1:A:606:GLN:HG2 | 1:A:608:ALA:N | 2.25 | 0.51 |
| 1:A:751:MET:O | 1:A:754:VAL:HB | 2.10 | 0.51 |
| 1:B:242:LYS:O | 1:B:279:ILE:HA | 2.10 | 0.51 |
| 1:B:548:GLU:CG | 1:B:560:LYS:HZ3 | 2.08 | 0.51 |
| 1:B:549:THR:O | 1:B:552:ARG:NH1 | 2.40 | 0.51 |
| 1:B:787:ARG:CA | 1:B:790:GLU:HB3 | 2.36 | 0.51 |
| 1:B:789:LYS:HG3 | 1:B:790:GLU:N | 2.24 | 0.51 |
| 1:C:417:LYS:NZ | 1:C:463:ARG:CG | 2.71 | 0.51 |
| 1:C:460:GLU:O | 1:C:464:GLN:HG2 | 2.11 | 0.51 |
| 1:C:639:ILE:C | 1:C:640:ARG:HD2 | 2.35 | 0.51 |
| 1:C:697:THR:HG1 | 1:C:698:VAL:H | 1.57 | 0.51 |
| 1:C:700:LEU:HD22 | 1:C:762:PHE:HD1 | 1.74 | 0.51 |
| 1:E:385:TYR:HD1 | 1:E:386:ARG:HH12 | 1.55 | 0.51 |
| 1:E:451:LYS:O | 1:E:455:LEU:HB2 | 2.10 | 0.51 |
| 1:E:529:ARG:NH1 | 1:E:535:SER:HB3 | 2.25 | 0.51 |
| 1:E:571:HIS:HB3 | 1:E:574:ARG:HD3 | 1.91 | 0.51 |
| 1:E:698:VAL:O | 1:E:702:MET:HG2 | 2.09 | 0.51 |
| 1:F:283:ILE:HG12 | 1:F:312:VAL:CG2 | 2.37 | 0.51 |
| 1:F:307:ARG:HH11 | 1:F:333:ARG:NH1 | 2.04 | 0.51 |
| 1:F:787:ARG:HD3 | 1:F:790:GLU:OE1 | 2.10 | 0.51 |
| 1:A:321:TYR:O | 1:A:325:VAL:HG23 | 2.10 | 0.51 |
| 1:A:348:THR:HA | 1:A:351:ILE:HG13 | 1.93 | 0.51 |
| 1:A:740:SER:HB3 | 1:A:774:LYS:HE2 | 1.93 | 0.51 |
| 1:A:857:VAL:HA | 1:A:878:GLU:H | 1.75 | 0.51 |
| 1:B:195:SER:HA | 1:B:198:ARG:NH1 | 2.26 | 0.51 |
| 1:B:375:ALA:HA | 1:B:378:LEU:HD12 | 1.91 | 0.51 |
| 1:B:573:GLU:C | 1:B:575:ASP:H | 2.18 | 0.51 |
| 1:B:612:PHE:CG | 1:B:613:LEU:N | 2.78 | 0.51 |
| 1:B:779:ALA:O | 1:B:782:LYS:N | 2.44 | 0.51 |
| 1:C:174:MET:H | 1:C:242:LYS:HZ3 | 1.44 | 0.51 |
| 1:C:373:VAL:O | 1:C:376:ALA:HB3 | 2.09 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:579:GLU:CD | 1:C:579:GLU:H | 2.18 | 0.51 |
| 1:C:655:LEU:HB2 | 1:C:671:LEU:HD21 | 1.91 | 0.51 |
| 1:C:708:ILE:C | 1:C:716:ILE:H | 2.16 | 0.51 |
| 1:D:166:TYR:HB2 | 1:D:264:ARG:HE | 1.75 | 0.51 |
| 1:D:233:ASP:HB2 | 1:D:234:VAL:HG23 | 1.91 | 0.51 |
| 1:D:563:GLU:HA | 1:D:568:LYS:CE | 2.40 | 0.51 |
| 1:D:590:VAL:O | 1:D:594:VAL:N | 2.22 | 0.51 |
| 1:D:596:LEU:C | 1:D:599:SER:HG | 2.11 | 0.51 |
| 1:D:619:GLY:H | 1:D:772:PHE:HE2 | 1.55 | 0.51 |
| 1:D:655:LEU:O | 1:D:657:GLY:N | 2.43 | 0.51 |
| 1:D:746:THR:O | 1:D:748:ASN:N | 2.42 | 0.51 |
| 1:D:771:ILE:HG22 | 1:D:772:PHE:N | 2.26 | 0.51 |
| 1:D:790:GLU:HA | 1:D:793:GLU:OE2 | 2.08 | 0.51 |
| 1:D:807:THR:OG1 | 1:D:856:ASN:ND2 | 2.42 | 0.51 |
| 1:D:849:ILE:HD13 | 1:D:852:LYS:HG3 | 1.91 | 0.51 |
| 1:E:235:PRO:HD2 | 1:E:238:LEU:HD12 | 1.93 | 0.51 |
| 1:E:356:GLN:CG | 1:E:360:GLU:HB2 | 2.40 | 0.51 |
| 1:E:484:ASP:HA | 1:E:487:GLU:HB3 | 1.92 | 0.51 |
| 1:E:651:ALA:HA | 1:E:656:LEU:CB | 2.27 | 0.51 |
| 1:E:802:TYR:HB2 | 1:E:804:LEU:CD1 | 2.39 | 0.51 |
| 1:F:317:THR:C | 1:F:321:TYR:HH | 2.17 | 0.51 |
| 1:F:697:THR:HA | 1:F:700:LEU:HB2 | 1.91 | 0.51 |
| 1:F:700:LEU:HD23 | 1:F:703:LEU:CG | 2.23 | 0.51 |
| 1:F:701:GLN:CD | 1:F:709:THR:HG1 | 2.09 | 0.51 |
| 1:F:702:MET:CB | 1:F:708:ILE:CG2 | 2.79 | 0.51 |
| 1:A:249:ALA:O | 1:A:264:ARG:NH1 | 2.43 | 0.51 |
| 1:B:329:GLY:O | 1:B:333:ARG:HG2 | 2.11 | 0.51 |
| 1:B:344:SER:O | 1:B:347:GLN:NE2 | 2.43 | 0.51 |
| 1:B:688:VAL:HG13 | 1:B:727:SER:CB | 2.41 | 0.51 |
| 1:C:270:LYS:HA | 1:C:273:GLU:CB | 2.39 | 0.51 |
| 1:C:505:LEU:HA | 1:C:508:PHE:HB2 | 1.91 | 0.51 |
| 1:C:542:ASP:O | 1:C:543:SER:C | 2.54 | 0.51 |
| 1:C:803:LYS:HD2 | 1:C:853:GLU:C | 2.36 | 0.51 |
| 1:C:812:ASP:O | 1:C:813:PHE:C | 2.53 | 0.51 |
| 1:D:228:ARG:O | 1:D:231:ASP:HB2 | 2.10 | 0.51 |
| 1:D:483:LEU:CD1 | 1:D:487:GLU:HB2 | 2.40 | 0.51 |
| 1:D:535:SER:HB3 | 1:D:538:GLN:HA | 1.93 | 0.51 |
| 1:D:541:VAL:HB | 1:D:544:ASP:OD2 | 2.10 | 0.51 |
| 1:D:684:LEU:CA | 1:D:725:MET:HG2 | 2.40 | 0.51 |
| 1:D:765:ARG:NH2 | 1:E:640:ARG:HH12 | 2.08 | 0.51 |
| 1:E:246:LEU:HG | 1:E:247:ASP:C | 2.35 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:302:LYS:HB3 | 1:E:303:PRO:HD3 | 1.92 | 0.51 |
| 1:E:316:THR:HG23 | 1:E:317:THR:O | 2.10 | 0.51 |
| 1:E:597:SER:C | 1:E:599:SER:H | 2.16 | 0.51 |
| 1:E:772:PHE:CE1 | 1:E:775:LEU:HD12 | 2.44 | 0.51 |
| 1:E:794:ARG:HH22 | 1:E:796:GLU:HA | 1.76 | 0.51 |
| 1:F:191:GLU:O | 1:F:195:SER:N | 2.37 | 0.51 |
| 1:F:192:GLU:OE2 | 1:F:339:GLU:C | 2.53 | 0.51 |
| 1:F:199:VAL:O | 1:F:200:LEU:C | 2.53 | 0.51 |
| 1:F:322:ARG:HH12 | 1:F:326:GLU:HA | 1.75 | 0.51 |
| 1:F:609:SER:HB2 | 1:F:724:ILE:CG2 | 2.40 | 0.51 |
| 1:F:637:MET:HE3 | 1:F:681:SER:C | 2.36 | 0.51 |
| 1:F:684:LEU:HD12 | 1:F:684:LEU:O | 2.09 | 0.51 |
| 1:A:692:HIS:CD2 | 1:A:693:PRO:HD2 | 2.45 | 0.51 |
| 1:A:808:GLN:OE1 | 1:A:811:LYS:HD2 | 2.10 | 0.51 |
| 1:B:189:ARG:CZ | 1:B:343:PRO:HD3 | 2.40 | 0.51 |
| 1:B:244:PHE:CE2 | 1:B:312:VAL:HG12 | 2.46 | 0.51 |
| 1:B:343:PRO:O | 1:B:388:LEU:HD22 | 2.11 | 0.51 |
| 1:B:348:THR:O | 1:B:351:ILE:HG22 | 2.10 | 0.51 |
| 1:B:356:GLN:HB3 | 1:B:357:PRO:HD3 | 1.92 | 0.51 |
| 1:B:367:ILE:CA | 1:B:539:ASN:HB2 | 2.41 | 0.51 |
| 1:B:663:VAL:H | 1:B:667:GLU:HG2 | 1.76 | 0.51 |
| 1:B:747:LYS:O | 1:B:751:MET:HG3 | 2.11 | 0.51 |
| 1:C:168:SER:O | 1:C:169:LYS:C | 2.53 | 0.51 |
| 1:C:217:GLY:CA | 2:C:1001:AGS:H4' | 2.40 | 0.51 |
| 1:C:488:ASN:ND2 | 1:C:489:LYS:HZ2 | 2.08 | 0.51 |
| 1:C:542:ASP:OD1 | 1:C:542:ASP:N | 2.43 | 0.51 |
| 1:C:640:ARG:HH21 | 1:C:684:LEU:HD13 | 1.75 | 0.51 |
| 1:C:650:TYR:HE2 | 1:C:657:GLY:N | 2.08 | 0.51 |
| 1:C:692:HIS:O | 1:C:695:VAL:HB | 2.11 | 0.51 |
| 1:C:776:SER:C | 1:C:780:ILE:HG12 | 2.36 | 0.51 |
| 1:C:853:GLU:O | 1:C:854:THR:OG1 | 2.27 | 0.51 |
| 1:D:210:LEU:HB3 | 1:D:340:VAL:HG23 | 1.92 | 0.51 |
| 1:D:351:ILE:O | 1:D:355:LEU:N | 2.37 | 0.51 |
| 1:D:615:LEU:HD12 | 1:D:616:SER:H | 1.76 | 0.51 |
| 1:D:847:ASN:CG | 1:D:850:LYS:NZ | 2.68 | 0.51 |
| 1:E:202:ARG:NH1 | 1:E:205:LYS:CB | 2.73 | 0.51 |
| 1:E:468:GLU:O | 1:E:471:HIS:HB2 | 2.09 | 0.51 |
| 1:E:602:ALA:HB1 | 1:E:606:GLN:HB3 | 1.92 | 0.51 |
| 1:E:734:ILE:HA | 1:E:774:LYS:HD2 | 1.92 | 0.51 |
| 1:E:744:GLU:C | 1:E:746:THR:H | 2.18 | 0.51 |
| 1:E:745:SER:HA | 1:E:748:ASN:CG | 2.35 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:812:ASP:CG | 1:E:816:LYS:HE3 | 2.36 | 0.51 |
| 1:E:827:PRO:O | 1:E:830:ARG:N | 2.43 | 0.51 |
| 1:F:286:ILE:HG13 | 1:F:287:HIS:CD2 | 2.46 | 0.51 |
| 1:F:403:VAL:O | 1:F:406:ALA:N | 2.44 | 0.51 |
| 1:F:618:SER:O | 1:F:620:LYS:HG2 | 2.10 | 0.51 |
| 1:F:628:ALA:HA | 1:F:631:LEU:HG | 1.92 | 0.51 |
| 1:A:233:ASP:O | 1:A:234:VAL:HG13 | 2.11 | 0.51 |
| 1:A:356:GLN:O | 1:A:358:LYS:N | 2.43 | 0.51 |
| 1:A:542:ASP:C | 1:A:546:ILE:HB | 2.36 | 0.51 |
| 1:A:569:LEU:HA | 1:A:572:MET:SD | 2.51 | 0.51 |
| 1:A:796:GLU:CG | 1:A:800:LYS:H | 2.22 | 0.51 |
| 1:B:189:ARG:HH22 | 1:B:342:GLU:C | 2.19 | 0.51 |
| 1:B:281:LEU:HD12 | 1:B:282:PHE:H | 1.75 | 0.51 |
| 1:B:337:LYS:HG3 | 1:B:338:ILE:N | 2.25 | 0.51 |
| 1:B:579:GLU:CD | 1:B:626:LYS:HE2 | 2.34 | 0.51 |
| 1:B:610:PHE:HD1 | 1:B:767:SER:HB2 | 1.75 | 0.51 |
| 1:B:759:ARG:HG3 | 1:B:761:GLU:CD | 2.36 | 0.51 |
| 1:B:770:VAL:HG12 | 1:B:771:ILE:N | 2.24 | 0.51 |
| 1:B:780:ILE:HA | 1:B:783:ILE:HD12 | 1.92 | 0.51 |
| 1:B:812:ASP:O | 1:B:815:ALA:N | 2.44 | 0.51 |
| 1:C:322:ARG:HA | 1:C:325:VAL:HG23 | 1.93 | 0.51 |
| 1:C:357:PRO:O | 1:C:360:GLU:N | 2.44 | 0.51 |
| 1:C:646:LEU:HB2 | 1:C:692:HIS:H | 1.75 | 0.51 |
| 1:D:210:LEU:HG | 1:D:338:ILE:O | 2.11 | 0.51 |
| 1:D:611:LEU:O | 1:D:612:PHE:C | 2.54 | 0.51 |
| 1:D:672:THR:O | 1:D:675:LEU:N | 2.43 | 0.51 |
| 1:D:679:PRO:HB2 | 1:D:680:TYR:CD2 | 2.45 | 0.51 |
| 1:D:704:ASP:OD1 | 1:D:704:ASP:O | 2.28 | 0.51 |
| 1:D:728:ALA:O | 1:D:730:GLY:N | 2.41 | 0.51 |
| 1:D:783:ILE:HA | 1:D:786:ILE:CD1 | 2.28 | 0.51 |
| 1:D:787:ARG:HA | 1:D:790:GLU:OE1 | 2.11 | 0.51 |
| 1:D:789:LYS:HZ2 | 1:D:790:GLU:N | 2.08 | 0.51 |
| 1:E:227:GLN:O | 1:E:230:ILE:N | 2.43 | 0.51 |
| 1:E:428:ILE:HG12 | 1:E:449:ARG:CD | 2.41 | 0.51 |
| 1:E:446:LYS:HA | 1:E:449:ARG:NH2 | 2.26 | 0.51 |
| 1:E:656:LEU:O | 1:E:659:THR:OG1 | 2.28 | 0.51 |
| 1:F:625:LYS:CE | 1:F:637:MET:HB2 | 2.39 | 0.51 |
| 1:F:827:PRO:O | 1:F:828:LEU:C | 2.52 | 0.51 |
| 1:A:244:PHE:CD2 | 1:A:281:LEU:HG | 2.45 | 0.51 |
| 1:A:285:GLU:HG3 | 1:A:288:MET:N | 2.26 | 0.51 |
| 1:A:379:ALA:HA | 1:A:382:TYR:OH | 2.11 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:403:VAL:O | 1:A:407:ARG:N | 2.44 | 0.51 |
| 1:A:698:VAL:HA | 1:A:701:GLN:HB2 | 1.92 | 0.51 |
| 1:A:837:LEU:HA | 1:A:840:LEU:HB2 | 1.93 | 0.51 |
| 1:B:203:ARG:HG3 | 1:B:204:ILE:HG13 | 1.93 | 0.51 |
| 1:B:224:GLY:O | 1:B:227:GLN:HB3 | 2.10 | 0.51 |
| 1:B:374:THR:OG1 | 1:B:375:ALA:N | 2.44 | 0.51 |
| 1:C:180:GLN:CD | 1:C:180:GLN:H | 2.14 | 0.51 |
| 1:C:187:ILE:HD12 | 1:C:351:ILE:CG1 | 2.41 | 0.51 |
| 1:C:229:ILE:O | 1:C:232:ASP:N | 2.42 | 0.51 |
| 1:C:247:ASP:O | 1:C:248:LEU:HD12 | 2.11 | 0.51 |
| 1:C:324:ILE:HB | 1:C:331:PHE:CE1 | 2.45 | 0.51 |
| 1:C:331:PHE:O | 1:C:335:PHE:CD2 | 2.63 | 0.51 |
| 1:C:387:ARG:HB3 | 1:C:389:PRO:HD2 | 1.93 | 0.51 |
| 1:C:571:HIS:CA | 1:C:574:ARG:HG2 | 2.36 | 0.51 |
| 1:C:709:THR:HA | 1:C:716:ILE:N | 2.25 | 0.51 |
| 1:D:213:GLU:HA | 1:D:387:ARG:CZ | 2.40 | 0.51 |
| 1:D:543:SER:HA | 1:D:546:ILE:HD12 | 1.92 | 0.51 |
| 1:D:573:GLU:CD | 1:D:595:ARG:NH2 | 2.69 | 0.51 |
| 1:D:740:SER:CB | 1:D:774:LYS:HB2 | 2.40 | 0.51 |
| 1:E:219:THR:HG23 | 1:E:222:ILE:HD12 | 1.92 | 0.51 |
| 1:E:639:ILE:HD13 | 1:E:683:LEU:HD13 | 1.91 | 0.51 |
| 1:E:643:CYS:C | 1:E:649:LYS:HZ2 | 2.18 | 0.51 |
| 1:E:701:GLN:O | 1:E:704:ASP:N | 2.44 | 0.51 |
| 1:E:806:LEU:HD13 | 1:E:809:GLU:OE2 | 2.10 | 0.51 |
| 1:F:205:LYS:HG3 | 1:F:334:ARG:HA | 1.92 | 0.51 |
| 1:F:282:PHE:HA | 1:F:313:ILE:H | 1.75 | 0.51 |
| 1:F:317:THR:O | 1:F:321:TYR:OH | 2.21 | 0.51 |
| 1:F:363:HIS:HE2 | 1:F:397:ASP:CA | 2.19 | 0.51 |
| 1:F:829:ASN:CG | 1:F:830:ARG:N | 2.68 | 0.51 |
| 1:A:282:PHE:HA | 1:A:312:VAL:HA | 1.92 | 0.51 |
| 1:A:542:ASP:O | 1:A:547:SER:N | 2.41 | 0.51 |
| 1:A:632:PHE:HD2 | 1:A:637:MET:HG2 | 1.76 | 0.51 |
| 1:A:647:SER:HA | 1:A:692:HIS:CB | 2.40 | 0.51 |
| 1:A:828:LEU:HD11 | 1:A:831:LEU:HD22 | 1.92 | 0.51 |
| 1:B:215:GLY:N | 1:B:218:LYS:HG2 | 2.26 | 0.51 |
| 1:B:333:ARG:CZ | 1:B:334:ARG:HE | 2.24 | 0.51 |
| 1:B:336:GLN:O | 1:B:337:LYS:HB2 | 2.11 | 0.51 |
| 1:B:338:ILE:HD12 | 1:B:339:GLU:N | 2.26 | 0.51 |
| 1:B:631:LEU:CD1 | 1:B:632:PHE:HB2 | 2.41 | 0.51 |
| 1:C:188:GLY:H | 1:C:351:ILE:HD11 | 1.74 | 0.51 |
| 1:C:226:ALA:O | 1:C:230:ILE:HG12 | 2.11 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:744:GLU:HA | 1:C:747:LYS:CE | 2.41 | 0.51 |
| 1:C:805:ASN:OD1 | 1:C:856:ASN:ND2 | 2.43 | 0.51 |
| 1:D:585:ASP:HA | 1:D:588:LYS:HB2 | 1.92 | 0.51 |
| 1:D:874:GLU:HB3 | 1:D:876:CYS:HB2 | 1.93 | 0.51 |
| 1:E:202:ARG:HH12 | 1:E:205:LYS:CB | 2.24 | 0.51 |
| 1:E:208:PRO:HA | 1:E:336:GLN:C | 2.36 | 0.51 |
| 1:E:215:GLY:HA2 | 2:E:1001:AGS:O3G | 2.10 | 0.51 |
| 1:E:245:SER:CA | 1:E:281:LEU:HG | 2.41 | 0.51 |
| 1:E:276:LYS:HE2 | 1:E:279:ILE:HB | 1.93 | 0.51 |
| 1:E:350:ALA:HA | 1:E:353:ARG:CZ | 2.41 | 0.51 |
| 1:E:356:GLN:HG3 | 1:E:360:GLU:HB2 | 1.93 | 0.51 |
| 1:E:366:ARG:HB3 | 1:E:539:ASN:CB | 2.41 | 0.51 |
| 1:E:603:ASN:HB3 | 1:F:795:PHE:CD1 | 2.45 | 0.51 |
| 1:E:620:LYS:CA | 1:E:623:LEU:HB3 | 2.40 | 0.51 |
| 1:E:668:GLY:C | 1:E:671:LEU:H | 2.19 | 0.51 |
| 1:E:857:VAL:HA | 1:E:878:GLU:CA | 2.28 | 0.51 |
| 1:F:170:TYR:CD1 | 1:F:250:ALA:HB2 | 2.46 | 0.51 |
| 1:F:560:LYS:O | 1:F:562:SER:OG | 2.21 | 0.51 |
| 1:F:612:PHE:HA | 1:F:770:VAL:CG2 | 2.41 | 0.51 |
| 1:F:704:ASP:CA | 1:F:765:ARG:NH1 | 2.73 | 0.51 |
| 1:F:787:ARG:HD3 | 1:F:790:GLU:CD | 2.36 | 0.51 |
| 1:A:204:ILE:HG13 | 1:A:205:LYS:N | 2.26 | 0.51 |
| 1:A:213:GLU:O | 1:A:218:LYS:HD2 | 2.10 | 0.51 |
| 1:A:246:LEU:HB2 | 1:A:281:LEU:HD22 | 1.93 | 0.51 |
| 1:A:709:THR:HG22 | 1:A:710:SER:H | 1.75 | 0.51 |
| 1:A:823:MET:HB2 | 1:F:307:ARG:CZ | 2.41 | 0.51 |
| 1:B:180:GLN:HG2 | 1:B:182:LYS:HZ3 | 1.76 | 0.51 |
| 1:B:190:GLU:O | 1:B:193:ILE:N | 2.44 | 0.51 |
| 1:B:208:PRO:CG | 1:B:313:ILE:HG23 | 2.41 | 0.51 |
| 1:B:728:ALA:HB1 | 1:B:732:GLU:OE1 | 2.11 | 0.51 |
| 1:B:784:VAL:HB | 1:B:811:LYS:NZ | 2.25 | 0.51 |
| 1:C:140:ILE:O | 1:C:144:ALA:N | 2.32 | 0.51 |
| 1:C:189:ARG:NH2 | 1:C:343:PRO:HD3 | 2.26 | 0.51 |
| 1:C:265:PHE:CE2 | 1:C:269:LEU:HD11 | 2.45 | 0.51 |
| 1:C:265:PHE:CZ | 1:C:301:LEU:HD11 | 2.46 | 0.51 |
| 1:C:467:ASN:O | 1:C:471:HIS:N | 2.40 | 0.51 |
| 1:C:558:VAL:O | 1:C:561:LEU:HB2 | 2.10 | 0.51 |
| 1:C:637:MET:SD | 1:C:681:SER:HA | 2.51 | 0.51 |
| 1:C:820:SER:HB3 | 1:C:824:GLY:N | 2.25 | 0.51 |
| 1:D:165:GLU:HB2 | 1:D:170:TYR:OH | 2.11 | 0.51 |
| 1:D:388:LEU:O | 1:D:391:SER:OG | 2.25 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:545:THR:OG1 | 1:D:546:ILE:N | 2.42 | 0.51 |
| 1:D:585:ASP:CA | 1:D:588:LYS:NZ | 2.74 | 0.51 |
| 1:D:650:TYR:HB2 | 1:D:654:LYS:H | 1.74 | 0.51 |
| 1:D:733:PHE:O | 1:D:774:LYS:NZ | 2.43 | 0.51 |
| 1:D:811:LYS:H | 1:D:811:LYS:CD | 2.16 | 0.51 |
| 1:E:218:LYS:O | 1:E:221:ILE:HB | 2.11 | 0.51 |
| 1:E:228:ARG:NH1 | 1:E:232:ASP:O | 2.43 | 0.51 |
| 1:E:319:ASN:CA | 1:E:322:ARG:NH1 | 2.65 | 0.51 |
| 1:E:362:HIS:H | 1:E:362:HIS:CD2 | 2.28 | 0.51 |
| 1:E:378:LEU:HD23 | 1:E:382:TYR:CZ | 2.45 | 0.51 |
| 1:E:546:ILE:O | 1:E:550:ALA:N | 2.40 | 0.51 |
| 1:E:610:PHE:H | 1:E:724:ILE:CA | 2.14 | 0.51 |
| 1:E:619:GLY:O | 1:E:622:GLU:HB3 | 2.11 | 0.51 |
| 1:E:777:ARG:HG3 | 1:E:778:LYS:N | 2.24 | 0.51 |
| 1:F:175:THR:HG1 | 1:F:244:PHE:HZ | 1.58 | 0.51 |
| 1:F:834:ASN:O | 1:F:837:LEU:N | 2.43 | 0.51 |
| 1:A:210:LEU:HD12 | 1:A:337:LYS:HB3 | 1.92 | 0.51 |
| 1:A:611:LEU:C | 1:A:770:VAL:H | 2.19 | 0.51 |
| 1:A:658:THR:H | 1:A:667:GLU:C | 2.18 | 0.51 |
| 1:A:780:ILE:O | 1:A:783:ILE:N | 2.44 | 0.51 |
| 1:B:285:GLU:OE1 | 1:B:287:HIS:N | 2.44 | 0.51 |
| 1:B:594:VAL:CG2 | 1:B:610:PHE:HE2 | 2.24 | 0.51 |
| 1:B:620:LYS:NZ | 1:B:826:ARG:HH11 | 2.05 | 0.51 |
| 1:B:764:ASN:CG | 1:B:765:ARG:HH12 | 2.19 | 0.51 |
| 1:C:174:MET:H | 1:C:242:LYS:HE2 | 1.74 | 0.51 |
| 1:C:243:LEU:CD2 | 1:C:282:PHE:HB3 | 2.35 | 0.51 |
| 1:C:304:ALA:O | 1:C:307:ARG:N | 2.42 | 0.51 |
| 1:C:621:THR:CB | 1:C:826:ARG:HH11 | 2.23 | 0.51 |
| 1:D:180:GLN:OE1 | 1:D:182:LYS:HD2 | 2.11 | 0.51 |
| 1:D:248:LEU:HG | 1:D:249:ALA:HA | 1.93 | 0.51 |
| 1:D:286:ILE:HA | 1:D:289:LEU:HD12 | 1.93 | 0.51 |
| 1:D:321:TYR:CD1 | 1:D:321:TYR:HA | 2.46 | 0.51 |
| 1:D:684:LEU:HG | 1:D:726:THR:H | 1.75 | 0.51 |
| 1:D:686:ASP:CG | 1:D:687:GLU:H | 2.18 | 0.51 |
| 1:D:804:LEU:CD1 | 1:D:855:VAL:H | 2.13 | 0.51 |
| 1:E:180:GLN:O | 1:E:488:ASN:ND2 | 2.44 | 0.51 |
| 1:E:290:MET:SD | 1:E:327:LYS:HE3 | 2.51 | 0.51 |
| 1:E:486:LEU:N | 1:E:489:LYS:NZ | 2.57 | 0.51 |
| 1:E:698:VAL:O | 1:E:701:GLN:N | 2.44 | 0.51 |
| 1:E:787:ARG:O | 1:E:790:GLU:HB3 | 2.10 | 0.51 |
| 1:E:806:LEU:O | 1:E:809:GLU:HB3 | 2.11 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:290:MET:HA | 1:F:298:ALA:HB3 | 1.93 | 0.51 |
| 1:F:620:LYS:HZ2 | 2:F:1002:AGS:PG | 2.34 | 0.51 |
| 1:F:623:LEU:HD12 | 1:F:626:LYS:CB | 2.39 | 0.51 |
| 1:A:391:SER:O | 1:A:394:ASP:HB3 | 2.11 | 0.51 |
| 1:A:762:PHE:CG | 1:A:766:ILE:HD11 | 2.46 | 0.51 |
| 1:A:788:LEU:HD12 | 1:A:789:LYS:N | 2.26 | 0.51 |
| 1:B:195:SER:HB2 | 1:B:198:ARG:CZ | 2.40 | 0.51 |
| 1:B:206:SER:O | 1:B:311:LYS:HE3 | 2.10 | 0.51 |
| 1:B:222:ILE:HD12 | 1:B:222:ILE:H | 1.75 | 0.51 |
| 1:B:337:LYS:HE2 | 1:B:338:ILE:O | 2.11 | 0.51 |
| 1:B:346:ARG:HG3 | 1:B:347:GLN:N | 2.26 | 0.51 |
| 1:B:594:VAL:C | 1:B:597:SER:HG | 2.10 | 0.51 |
| 1:B:633:ASN:O | 1:B:634:ASP:OD1 | 2.29 | 0.51 |
| 1:B:640:ARG:HA | 1:B:684:LEU:CB | 2.41 | 0.51 |
| 1:B:672:THR:O | 1:B:675:LEU:N | 2.43 | 0.51 |
| 1:C:190:GLU:CG | 1:C:194:ARG:HH12 | 2.24 | 0.51 |
| 1:C:226:ALA:HA | 1:C:229:ILE:HB | 1.93 | 0.51 |
| 1:C:285:GLU:OE1 | 1:C:287:HIS:CE1 | 2.64 | 0.51 |
| 1:C:593:ALA:O | 1:C:596:LEU:HB2 | 2.11 | 0.51 |
| 1:C:643:CYS:SG | 1:C:691:ALA:N | 2.83 | 0.51 |
| 1:C:681:SER:HG | 1:C:682:VAL:N | 2.09 | 0.51 |
| 1:D:265:PHE:O | 1:D:268:VAL:N | 2.44 | 0.51 |
| 1:D:355:LEU:HA | 1:D:358:LYS:HD3 | 1.93 | 0.51 |
| 1:D:421:LEU:HG | 1:D:452:GLU:HG3 | 1.92 | 0.51 |
| 1:D:503:ALA:HB1 | 1:D:507:TYR:CZ | 2.46 | 0.51 |
| 1:D:656:LEU:HD21 | 1:D:709:THR:CG2 | 2.41 | 0.51 |
| 1:D:763:LEU:HD12 | 1:D:763:LEU:N | 2.26 | 0.51 |
| 1:D:829:ASN:HA | 1:D:832:ILE:HD12 | 1.93 | 0.51 |
| 1:E:351:ILE:O | 1:E:355:LEU:HG | 2.10 | 0.51 |
| 1:E:383:LEU:HD23 | 1:E:383:LEU:C | 2.36 | 0.51 |
| 1:E:546:ILE:O | 1:E:549:THR:HB | 2.11 | 0.51 |
| 1:E:746:THR:O | 1:E:749:LEU:HB2 | 2.11 | 0.51 |
| 1:F:192:GLU:HA | 1:F:195:SER:HB2 | 1.92 | 0.51 |
| 1:F:318:ASN:O | 1:F:319:ASN:O | 2.29 | 0.51 |
| 1:F:389:PRO:O | 1:F:393:LEU:HG | 2.11 | 0.51 |
| 1:F:810:ALA:HA | 1:F:813:PHE:HB3 | 1.93 | 0.51 |
| 1:A:317:THR:HB | 1:A:319:ASN:H | 1.77 | 0.50 |
| 1:B:167:LEU:HA | 1:B:170:TYR:CE1 | 2.47 | 0.50 |
| 1:B:187:ILE:HD12 | 1:B:188:GLY:N | 2.26 | 0.50 |
| 1:B:262:GLU:C | 1:B:262:GLU:CD | 2.79 | 0.50 |
| 1:B:646:LEU:CD1 | 1:B:690:LYS:NZ | 2.72 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:704:ASP:HB2 | 1:B:707:ARG:HH11 | 1.76 | 0.50 |
| 1:B:859:LEU:HD21 | 1:B:873:ALA:HB1 | 1.93 | 0.50 |
| 1:C:195:SER:O | 1:C:199:VAL:HG23 | 2.12 | 0.50 |
| 1:C:217:GLY:O | 1:C:220:ALA:N | 2.45 | 0.50 |
| 1:C:218:LYS:N | 2:C:1001:AGS:O1B | 2.45 | 0.50 |
| 1:C:363:HIS:HD2 | 1:C:404:ALA:HB2 | 1.76 | 0.50 |
| 1:C:659:THR:HA | 1:C:712:GLN:HE22 | 1.75 | 0.50 |
| 1:D:320:GLU:O | 1:D:323:SER:N | 2.44 | 0.50 |
| 1:D:558:VAL:HA | 1:D:561:LEU:HD13 | 1.91 | 0.50 |
| 1:D:646:LEU:O | 1:D:692:HIS:HD2 | 1.94 | 0.50 |
| 1:D:744:GLU:C | 1:D:746:THR:N | 2.68 | 0.50 |
| 1:D:830:ARG:HA | 1:D:833:GLN:HG2 | 1.93 | 0.50 |
| 1:E:210:LEU:CD1 | 1:E:338:ILE:HB | 2.39 | 0.50 |
| 1:E:210:LEU:HA | 1:E:338:ILE:O | 2.11 | 0.50 |
| 1:E:329:GLY:O | 1:E:331:PHE:N | 2.44 | 0.50 |
| 1:E:530:ARG:HG3 | 1:E:531:ALA:H | 1.76 | 0.50 |
| 1:E:804:LEU:HD23 | 1:E:854:THR:N | 2.26 | 0.50 |
| 1:E:833:GLN:HG2 | 1:E:837:LEU:CD1 | 2.39 | 0.50 |
| 1:F:356:GLN:O | 1:F:360:GLU:N | 2.36 | 0.50 |
| 1:F:593:ALA:HB1 | 1:F:608:ALA:HB1 | 1.92 | 0.50 |
| 1:F:830:ARG:O | 1:F:833:GLN:NE2 | 2.44 | 0.50 |
| 1:A:575:ASP:HB2 | 1:A:630:PHE:HZ | 1.75 | 0.50 |
| 1:B:385:TYR:CE1 | 1:B:386:ARG:NH1 | 2.79 | 0.50 |
| 1:B:607:PRO:CG | 1:B:703:LEU:HA | 2.41 | 0.50 |
| 1:B:618:SER:N | 1:B:826:ARG:NH1 | 2.60 | 0.50 |
| 1:B:632:PHE:CD2 | 1:B:680:TYR:HB3 | 2.46 | 0.50 |
| 1:C:234:VAL:N | 1:D:409:SER:OG | 2.45 | 0.50 |
| 1:C:291:GLY:N | 1:C:294:LYS:HG2 | 2.26 | 0.50 |
| 1:C:348:THR:OG1 | 1:C:388:LEU:HD21 | 2.11 | 0.50 |
| 1:C:370:SER:C | 1:C:372:LEU:N | 2.67 | 0.50 |
| 1:C:782:LYS:O | 1:C:784:VAL:HG22 | 2.10 | 0.50 |
| 1:D:197:ILE:O | 1:D:200:LEU:N | 2.45 | 0.50 |
| 1:D:261:PHE:HB3 | 1:D:262:GLU:OE1 | 2.11 | 0.50 |
| 1:D:302:LYS:O | 1:D:305:LEU:N | 2.44 | 0.50 |
| 1:D:480:LYS:HA | 1:D:483:LEU:HB3 | 1.93 | 0.50 |
| 1:D:530:ARG:NH2 | 1:D:538:GLN:N | 2.57 | 0.50 |
| 1:D:542:ASP:O | 1:D:543:SER:C | 2.55 | 0.50 |
| 1:D:728:ALA:HB1 | 1:D:734:ILE:CD1 | 2.41 | 0.50 |
| 1:D:742:ILE:C | 1:D:747:LYS:HZ2 | 2.15 | 0.50 |
| 1:E:200:LEU:HD23 | 1:E:208:PRO:HD2 | 1.91 | 0.50 |
| 1:E:276:LYS:NZ | 1:E:279:ILE:HB | 2.25 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:278:LEU:O | 1:E:280:VAL:HG23 | 2.12 | 0.50 |
| 1:E:283:ILE:HB | 1:E:286:ILE:CG2 | 2.40 | 0.50 |
| 1:E:391:SER:O | 1:E:394:ASP:HB2 | 2.11 | 0.50 |
| 1:E:459:LEU:HB3 | 1:E:463:ARG:HH21 | 1.76 | 0.50 |
| 1:E:613:LEU:HD11 | 1:E:729:LEU:H | 1.76 | 0.50 |
| 1:E:711:GLY:C | 1:E:713:GLY:H | 2.18 | 0.50 |
| 1:E:794:ARG:NH2 | 1:E:797:GLN:CD | 2.70 | 0.50 |
| 1:F:345:VAL:HA | 1:F:380:LYS:CE | 2.42 | 0.50 |
| 1:F:798:ASN:O | 1:F:799:ASP:C | 2.54 | 0.50 |
| 1:F:810:ALA:C | 1:F:814:LEU:HG | 2.35 | 0.50 |
| 1:A:572:MET:HE1 | 1:A:631:LEU:HD13 | 1.94 | 0.50 |
| 1:A:675:LEU:O | 1:A:678:LYS:N | 2.44 | 0.50 |
| 1:A:843:ARG:HH11 | 1:A:846:LYS:HD2 | 1.76 | 0.50 |
| 1:A:855:VAL:HG12 | 1:A:857:VAL:HG23 | 1.94 | 0.50 |
| 1:B:324:ILE:N | 1:B:327:LYS:NZ | 2.58 | 0.50 |
| 1:B:628:ALA:HA | 1:B:631:LEU:HD11 | 1.93 | 0.50 |
| 1:B:743:GLN:HB3 | 1:B:745:SER:OG | 2.10 | 0.50 |
| 1:C:190:GLU:N | 1:C:190:GLU:CD | 2.69 | 0.50 |
| 1:C:368:LEU:HD13 | 1:C:540:VAL:N | 2.26 | 0.50 |
| 1:C:407:ARG:CD | 1:C:538:GLN:HA | 2.29 | 0.50 |
| 1:C:417:LYS:HE3 | 1:C:459:LEU:HD22 | 1.93 | 0.50 |
| 1:C:514:LYS:HA | 1:C:517:ILE:HB | 1.94 | 0.50 |
| 1:C:557:PRO:HA | 1:C:560:LYS:HE2 | 1.93 | 0.50 |
| 1:C:583:GLN:NE2 | 1:C:773:ASN:N | 2.58 | 0.50 |
| 1:C:605:ARG:HG3 | 1:C:606:GLN:H | 1.76 | 0.50 |
| 1:C:619:GLY:HA2 | 1:C:826:ARG:HH22 | 1.75 | 0.50 |
| 1:D:191:GLU:HA | 1:D:194:ARG:HD2 | 1.94 | 0.50 |
| 1:D:194:ARG:O | 1:D:197:ILE:HB | 2.11 | 0.50 |
| 1:D:461:PRO:HB2 | 1:D:465:ARG:NE | 2.26 | 0.50 |
| 1:D:464:GLN:HA | 1:D:467:ASN:HB2 | 1.93 | 0.50 |
| 1:D:596:LEU:O | 1:D:600:GLY:N | 2.43 | 0.50 |
| 1:D:804:LEU:HG | 1:D:805:ASN:OD1 | 2.10 | 0.50 |
| 1:E:203:ARG:CG | 1:F:363:HIS:ND1 | 2.74 | 0.50 |
| 1:E:216:ILE:HD11 | 1:E:389:PRO:HD2 | 1.93 | 0.50 |
| 1:E:359:TYR:CZ | 1:E:396:VAL:HG12 | 2.47 | 0.50 |
| 1:E:392:ALA:O | 1:E:393:LEU:C | 2.52 | 0.50 |
| 1:E:479:ALA:HA | 1:E:482:LYS:HB3 | 1.93 | 0.50 |
| 1:E:485:GLU:O | 1:E:488:ASN:HB3 | 2.11 | 0.50 |
| 1:E:842:LEU:O | 1:E:848:GLU:OE2 | 2.30 | 0.50 |
| 1:F:207:ASN:HD21 | 1:F:311:LYS:CE | 2.19 | 0.50 |
| 1:F:222:ILE:O | 1:F:225:VAL:HB | 2.11 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:565:GLU:HB3 | 1:F:598:ARG:NH2 | 2.26 | 0.50 |
| 1:F:793:GLU:HA | 1:F:797:GLN:HG3 | 1.93 | 0.50 |
| 1:A:172:ILE:O | 1:A:245:SER:HB3 | 2.11 | 0.50 |
| 1:A:193:ILE:O | 1:A:196:THR:N | 2.45 | 0.50 |
| 1:A:213:GLU:CD | 1:A:318:ASN:H | 2.19 | 0.50 |
| 1:A:261:PHE:CG | 1:A:262:GLU:N | 2.79 | 0.50 |
| 1:A:286:ILE:C | 1:A:290:MET:HE3 | 2.36 | 0.50 |
| 1:A:347:GLN:O | 1:A:350:ALA:HB3 | 2.11 | 0.50 |
| 1:A:351:ILE:HG22 | 1:A:355:LEU:CD1 | 2.42 | 0.50 |
| 1:A:395:LEU:HD12 | 1:A:398:ILE:HB | 1.94 | 0.50 |
| 1:A:639:ILE:O | 1:A:683:LEU:HD12 | 2.11 | 0.50 |
| 1:B:172:ILE:HD12 | 1:B:174:MET:N | 2.24 | 0.50 |
| 1:B:368:LEU:O | 1:B:540:VAL:HG21 | 2.11 | 0.50 |
| 1:B:583:GLN:NE2 | 1:B:773:ASN:HB3 | 2.27 | 0.50 |
| 1:B:623:LEU:HD12 | 1:B:627:VAL:HG11 | 1.94 | 0.50 |
| 1:C:317:THR:HB | 1:C:320:GLU:CB | 2.42 | 0.50 |
| 1:C:625:LYS:HZ1 | 1:C:635:GLU:HB2 | 1.75 | 0.50 |
| 1:C:654:LYS:O | 1:C:670:PHE:HB3 | 2.12 | 0.50 |
| 1:C:655:LEU:HG | 1:C:656:LEU:H | 1.76 | 0.50 |
| 1:C:782:LYS:HG3 | 1:C:783:ILE:N | 2.26 | 0.50 |
| 1:D:411:PRO:HB3 | 1:D:538:GLN:HG2 | 1.92 | 0.50 |
| 1:D:557:PRO:O | 1:D:559:LYS:N | 2.38 | 0.50 |
| 1:E:215:GLY:N | 1:E:218:LYS:NZ | 2.59 | 0.50 |
| 1:E:285:GLU:OE2 | 1:E:288:MET:SD | 2.69 | 0.50 |
| 1:E:510:ILE:HG12 | 1:E:513:ILE:HB | 1.93 | 0.50 |
| 1:E:513:ILE:O | 1:E:517:ILE:HG13 | 2.11 | 0.50 |
| 1:E:551:ALA:O | 1:E:554:THR:N | 2.45 | 0.50 |
| 1:E:603:ASN:CG | 1:F:794:ARG:NH1 | 2.70 | 0.50 |
| 1:E:637:MET:HA | 1:E:678:LYS:HZ3 | 1.72 | 0.50 |
| 1:E:654:LYS:CE | 1:E:694:ASP:OD2 | 2.59 | 0.50 |
| 1:E:688:VAL:HG22 | 1:E:689:GLU:OE1 | 2.11 | 0.50 |
| 1:F:225:VAL:O | 1:F:229:ILE:N | 2.44 | 0.50 |
| 1:F:403:VAL:HA | 1:F:406:ALA:HB3 | 1.92 | 0.50 |
| 1:F:583:GLN:NE2 | 1:F:773:ASN:OD1 | 2.44 | 0.50 |
| 1:F:638:MET:HE3 | 1:F:681:SER:OG | 2.11 | 0.50 |
| 1:F:683:LEU:HD23 | 1:F:684:LEU:N | 2.22 | 0.50 |
| 1:F:700:LEU:HD22 | 1:F:761:GLU:CG | 2.41 | 0.50 |
| 1:F:707:ARG:HG3 | 1:F:715:THR:CB | 2.40 | 0.50 |
| 1:F:723:VAL:HG12 | 1:F:724:ILE:H | 1.76 | 0.50 |
| 1:A:637:MET:HG3 | 1:A:681:SER:CB | 2.41 | 0.50 |
| 1:B:242:LYS:C | 1:B:279:ILE:HA | 2.36 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:266:LYS:O | 1:B:269:LEU:HB2 | 2.12 | 0.50 |
| 1:B:285:GLU:C | 1:B:285:GLU:CD | 2.80 | 0.50 |
| 1:B:337:LYS:CD | 1:B:338:ILE:H | 2.24 | 0.50 |
| 1:B:350:ALA:HA | 1:B:353:ARG:HB2 | 1.93 | 0.50 |
| 1:B:367:ILE:HA | 1:B:539:ASN:HB2 | 1.93 | 0.50 |
| 1:C:198:ARG:HD2 | 1:D:405:VAL:HA | 1.93 | 0.50 |
| 1:C:219:THR:O | 1:C:221:ILE:N | 2.43 | 0.50 |
| 1:C:223:GLU:O | 1:C:226:ALA:N | 2.45 | 0.50 |
| 1:C:287:HIS:O | 1:C:324:ILE:HD11 | 2.11 | 0.50 |
| 1:C:288:MET:HA | 1:C:320:GLU:OE2 | 2.11 | 0.50 |
| 1:C:331:PHE:HA | 1:C:335:PHE:CE2 | 2.46 | 0.50 |
| 1:C:625:LYS:C | 1:C:627:VAL:H | 2.17 | 0.50 |
| 1:C:640:ARG:HE | 1:C:684:LEU:HD13 | 1.76 | 0.50 |
| 1:C:828:LEU:O | 1:C:831:LEU:N | 2.45 | 0.50 |
| 1:D:14:ILE:N | 1:D:116:ILE:O | 2.36 | 0.50 |
| 1:D:232:ASP:C | 1:D:495:ARG:HH21 | 2.20 | 0.50 |
| 1:D:348:THR:HA | 1:D:351:ILE:HD12 | 1.94 | 0.50 |
| 1:D:367:ILE:HD11 | 1:D:540:VAL:HG13 | 1.92 | 0.50 |
| 1:D:404:ALA:HA | 1:D:407:ARG:HE | 1.76 | 0.50 |
| 1:D:736:SER:N | 1:D:774:LYS:NZ | 2.59 | 0.50 |
| 1:D:781:HIS:O | 1:D:784:VAL:HG12 | 2.11 | 0.50 |
| 1:E:400:CYS:HA | 1:E:403:VAL:HB | 1.94 | 0.50 |
| 1:E:457:GLU:HA | 1:E:460:GLU:CB | 2.42 | 0.50 |
| 1:F:236:THR:HB | 1:F:239:GLN:CD | 2.37 | 0.50 |
| 1:F:351:ILE:O | 1:F:355:LEU:HD13 | 2.12 | 0.50 |
| 1:F:352:LEU:HA | 1:F:355:LEU:HD22 | 1.93 | 0.50 |
| 1:F:367:ILE:CD1 | 1:F:372:LEU:HD11 | 2.41 | 0.50 |
| 1:F:391:SER:O | 1:F:395:LEU:HG | 2.11 | 0.50 |
| 1:F:543:SER:OG | 1:F:543:SER:O | 2.24 | 0.50 |
| 1:F:570:ILE:HD12 | 1:F:595:ARG:HH21 | 1.76 | 0.50 |
| 1:F:612:PHE:HB3 | 1:F:725:MET:O | 2.10 | 0.50 |
| 1:F:819:TYR:CE1 | 1:F:827:PRO:HD2 | 2.46 | 0.50 |
| 1:A:266:LYS:HA | 1:A:269:LEU:HB3 | 1.93 | 0.50 |
| 1:A:541:VAL:HB | 1:A:545:THR:HG23 | 1.93 | 0.50 |
| 1:A:709:THR:HA | 1:A:715:THR:HA | 1.92 | 0.50 |
| 1:A:788:LEU:O | 1:A:791:ILE:N | 2.45 | 0.50 |
| 1:B:173:ASP:O | 1:B:174:MET:HB2 | 2.12 | 0.50 |
| 1:B:556:ILE:HB | 1:B:557:PRO:HD2 | 1.93 | 0.50 |
| 1:B:623:LEU:O | 1:B:625:LYS:N | 2.44 | 0.50 |
| 1:B:693:PRO:O | 1:B:695:VAL:N | 2.45 | 0.50 |
| 1:B:755:ARG:NH1 | 1:B:755:ARG:HG3 | 2.27 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:225:VAL:O | 1:C:226:ALA:C | 2.54 | 0.50 |
| 1:C:488:ASN:HD21 | 1:C:489:LYS:HZ2 | 1.60 | 0.50 |
| 1:C:642:ASP:O | 1:C:645:GLU:N | 2.45 | 0.50 |
| 1:C:759:ARG:HG3 | 1:C:761:GLU:N | 2.26 | 0.50 |
| 1:C:788:LEU:HD21 | 1:C:804:LEU:HD21 | 1.92 | 0.50 |
| 1:C:810:ALA:HA | 1:C:878:GLU:OE2 | 2.11 | 0.50 |
| 1:D:203:ARG:NH1 | 1:E:362:HIS:CB | 2.74 | 0.50 |
| 1:D:205:LYS:HZ1 | 1:D:332:GLU:C | 2.17 | 0.50 |
| 1:D:243:LEU:C | 1:D:244:PHE:CG | 2.89 | 0.50 |
| 1:D:248:LEU:O | 1:D:250:ALA:N | 2.44 | 0.50 |
| 1:D:625:LYS:HA | 1:D:628:ALA:HB3 | 1.93 | 0.50 |
| 1:D:762:PHE:CE1 | 1:D:766:ILE:HD13 | 2.47 | 0.50 |
| 1:E:569:LEU:HG | 1:E:595:ARG:CZ | 2.42 | 0.50 |
| 1:E:599:SER:C | 1:E:601:LEU:HD12 | 2.36 | 0.50 |
| 1:F:269:LEU:HA | 1:F:272:ILE:CG1 | 2.42 | 0.50 |
| 1:F:605:ARG:NH1 | 1:F:705:ASP:CB | 2.58 | 0.50 |
| 1:F:689:GLU:OE1 | 1:F:689:GLU:N | 2.31 | 0.50 |
| 1:A:331:PHE:HZ | 1:A:335:PHE:HE2 | 1.58 | 0.50 |
| 1:A:643:CYS:SG | 1:A:686:ASP:C | 2.95 | 0.50 |
| 1:A:808:GLN:CD | 1:A:811:LYS:HD2 | 2.36 | 0.50 |
| 1:B:353:ARG:HH12 | 1:B:372:LEU:CB | 2.15 | 0.50 |
| 1:B:387:ARG:HB3 | 1:B:389:PRO:HD2 | 1.94 | 0.50 |
| 1:B:700:LEU:O | 1:B:704:ASP:N | 2.45 | 0.50 |
| 1:B:778:LYS:CA | 1:B:781:HIS:HB3 | 2.41 | 0.50 |
| 1:B:797:GLN:HB3 | 1:B:799:ASP:OD1 | 2.10 | 0.50 |
| 1:C:193:ILE:C | 1:C:197:ILE:HG12 | 2.37 | 0.50 |
| 1:C:218:LYS:H | 1:C:218:LYS:HZ3 | 1.58 | 0.50 |
| 1:C:242:LYS:O | 1:C:280:VAL:O | 2.30 | 0.50 |
| 1:C:264:ARG:O | 1:C:268:VAL:N | 2.35 | 0.50 |
| 1:C:317:THR:O | 1:C:320:GLU:HB3 | 2.12 | 0.50 |
| 1:C:374:THR:O | 1:C:375:ALA:C | 2.52 | 0.50 |
| 1:C:569:LEU:HD11 | 1:C:595:ARG:CZ | 2.42 | 0.50 |
| 1:C:638:MET:HG2 | 1:C:639:ILE:O | 2.11 | 0.50 |
| 1:D:195:SER:O | 1:D:199:VAL:HG23 | 2.12 | 0.50 |
| 1:D:214:PRO:CG | 1:D:387:ARG:HE | 2.25 | 0.50 |
| 1:D:643:CYS:C | 1:D:645:GLU:N | 2.67 | 0.50 |
| 1:D:828:LEU:O | 1:D:831:LEU:N | 2.44 | 0.50 |
| 1:E:415:ASP:O | 1:E:419:ARG:HG3 | 2.11 | 0.50 |
| 1:E:513:ILE:O | 1:E:516:GLN:HB2 | 2.12 | 0.50 |
| 1:E:619:GLY:H | 2:E:1002:AGS:C4' | 2.24 | 0.50 |
| 1:F:552:ARG:HB2 | 1:F:552:ARG:HH11 | 1.74 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:575:ASP:O | 1:F:578:SER:HB2 | 2.12 | 0.50 |
| 1:F:658:THR:HG22 | 1:F:666:ASP:HA | 1.94 | 0.50 |
| 1:F:825:ALA:HB3 | 2:F:1002:AGS:S1G | 2.52 | 0.50 |
| 1:F:836:ILE:C | 1:F:840:LEU:HD13 | 2.37 | 0.50 |
| 1:A:169:LYS:O | 1:A:264:ARG:NH2 | 2.45 | 0.50 |
| 1:A:872:GLU:CB | 1:F:201:ALA:H | 2.24 | 0.50 |
| 1:B:688:VAL:HG13 | 1:B:727:SER:HB3 | 1.94 | 0.50 |
| 1:B:746:THR:HA | 1:B:749:LEU:HD12 | 1.93 | 0.50 |
| 1:C:193:ILE:HG23 | 1:C:197:ILE:HD11 | 1.94 | 0.50 |
| 1:C:207:ASN:H | 1:C:336:GLN:NE2 | 2.09 | 0.50 |
| 1:C:280:VAL:HG22 | 1:C:311:LYS:HD3 | 1.93 | 0.50 |
| 1:C:390:ASP:O | 1:C:391:SER:C | 2.53 | 0.50 |
| 1:C:594:VAL:HA | 1:C:597:SER:CB | 2.42 | 0.50 |
| 1:C:744:GLU:HA | 1:C:747:LYS:HE2 | 1.93 | 0.50 |
| 1:D:243:LEU:HD12 | 1:D:280:VAL:HG12 | 1.94 | 0.50 |
| 1:D:473:HIS:HA | 1:D:476:LEU:CG | 2.42 | 0.50 |
| 1:D:515:LYS:O | 1:D:519:LYS:N | 2.25 | 0.50 |
| 1:D:616:SER:O | 1:D:823:MET:HE2 | 2.12 | 0.50 |
| 1:E:179:ARG:NH1 | 1:E:495:ARG:HB3 | 2.27 | 0.50 |
| 1:E:274:GLU:C | 1:E:276:LYS:N | 2.68 | 0.50 |
| 1:E:318:ASN:O | 1:E:322:ARG:NH1 | 2.45 | 0.50 |
| 1:E:502:ALA:HA | 1:E:505:LEU:HB3 | 1.94 | 0.50 |
| 1:E:534:ASN:O | 1:E:537:ILE:HD13 | 2.12 | 0.50 |
| 1:E:639:ILE:HD12 | 1:E:682:VAL:O | 2.10 | 0.50 |
| 1:E:650:TYR:HA | 1:E:653:SER:OG | 2.12 | 0.50 |
| 1:E:682:VAL:HG22 | 1:E:683:LEU:N | 2.26 | 0.50 |
| 1:E:732:GLU:O | 1:E:736:SER:N | 2.21 | 0.50 |
| 1:E:820:SER:OG | 1:E:822:ASP:OD1 | 2.27 | 0.50 |
| 1:E:835:GLU:O | 1:E:839:LYS:HE2 | 2.11 | 0.50 |
| 1:E:846:LYS:O | 1:E:848:GLU:HG3 | 2.11 | 0.50 |
| 1:F:652:VAL:HG22 | 1:F:667:GLU:OE2 | 2.12 | 0.50 |
| 1:F:752:GLY:O | 1:F:755:ARG:N | 2.45 | 0.50 |
| 1:F:810:ALA:O | 1:F:813:PHE:N | 2.45 | 0.50 |
| 1:A:190:GLU:O | 1:A:193:ILE:N | 2.45 | 0.50 |
| 1:A:210:LEU:HB2 | 1:A:338:ILE:N | 2.27 | 0.50 |
| 1:A:837:LEU:HA | 1:A:840:LEU:HD12 | 1.93 | 0.50 |
| 1:B:263:GLU:CA | 1:B:266:LYS:NZ | 2.63 | 0.50 |
| 1:B:282:PHE:CD2 | 1:B:284:ASP:HA | 2.47 | 0.50 |
| 1:B:397:ASP:O | 1:B:400:CYS:HB2 | 2.12 | 0.50 |
| 1:B:803:LYS:NZ | 1:B:854:THR:HG23 | 2.17 | 0.50 |
| 1:B:809:GLU:O | 1:B:812:ASP:N | 2.37 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:174:MET:HG2 | 1:C:242:LYS:HZ2 | 1.75 | 0.50 |
| 1:C:222:ILE:HA | 1:C:225:VAL:HB | 1.92 | 0.50 |
| 1:C:302:LYS:HE2 | 1:C:310:LEU:CB | 2.42 | 0.50 |
| 1:C:583:GLN:NE2 | 1:C:775:LEU:HD21 | 2.27 | 0.50 |
| 1:C:708:ILE:H | 1:C:717:ASP:HB2 | 1.76 | 0.50 |
| 1:C:786:ILE:HD12 | 1:C:789:LYS:NZ | 2.27 | 0.50 |
| 1:D:212:GLY:O | 1:D:318:ASN:OD1 | 2.30 | 0.50 |
| 1:D:332:GLU:O | 1:D:334:ARG:N | 2.45 | 0.50 |
| 1:D:508:PHE:CA | 1:D:511:PRO:HD2 | 2.41 | 0.50 |
| 1:D:586:ALA:O | 1:D:587:ILE:C | 2.54 | 0.50 |
| 1:D:613:LEU:N | 1:D:771:ILE:HA | 2.26 | 0.50 |
| 1:D:650:TYR:O | 1:D:654:LYS:HD2 | 2.12 | 0.50 |
| 1:D:825:ALA:C | 1:D:827:PRO:HD2 | 2.37 | 0.50 |
| 1:D:842:LEU:HG | 1:D:846:LYS:NZ | 2.27 | 0.50 |
| 1:E:805:ASN:HB2 | 1:E:807:THR:CG2 | 2.42 | 0.50 |
| 1:F:174:MET:HE2 | 1:F:183:LEU:HD22 | 1.94 | 0.50 |
| 1:F:186:VAL:HB | 2:F:1001:AGS:C5 | 2.41 | 0.50 |
| 1:F:260:ASP:HA | 1:F:263:GLU:HB3 | 1.94 | 0.50 |
| 1:F:802:TYR:N | 1:F:802:TYR:CD1 | 2.79 | 0.50 |
| 1:F:805:ASN:CG | 1:F:856:ASN:HB2 | 2.37 | 0.50 |
| 1:F:819:TYR:CD1 | 1:F:824:GLY:O | 2.64 | 0.50 |
| 1:F:843:ARG:NH2 | 1:F:849:ILE:HG21 | 2.17 | 0.50 |
| 1:A:228:ARG:HA | 1:A:231:ASP:HB2 | 1.93 | 0.49 |
| 1:A:262:GLU:HA | 1:A:265:PHE:CB | 2.42 | 0.49 |
| 1:A:597:SER:HG | 1:A:598:ARG:H | 1.59 | 0.49 |
| 1:A:764:ASN:ND2 | 1:A:765:ARG:CZ | 2.75 | 0.49 |
| 1:B:189:ARG:HH22 | 1:B:342:GLU:N | 2.09 | 0.49 |
| 1:B:195:SER:CA | 1:B:198:ARG:HH12 | 2.26 | 0.49 |
| 1:B:205:LYS:NZ | 1:B:334:ARG:HG2 | 2.27 | 0.49 |
| 1:B:329:GLY:HA2 | 1:B:332:GLU:OE1 | 2.11 | 0.49 |
| 1:B:348:THR:HA | 1:B:351:ILE:HG22 | 1.94 | 0.49 |
| 1:B:611:LEU:HG | 1:B:768:SER:O | 2.11 | 0.49 |
| 1:B:793:GLU:N | 1:B:802:TYR:OH | 2.45 | 0.49 |
| 1:C:205:LYS:HD3 | 1:C:335:PHE:N | 2.27 | 0.49 |
| 1:C:294:LYS:HZ3 | 1:C:327:LYS:HE2 | 1.77 | 0.49 |
| 1:C:568:LYS:NZ | 1:C:630:PHE:CA | 2.75 | 0.49 |
| 1:C:576:LEU:HD12 | 1:C:587:ILE:CG2 | 2.42 | 0.49 |
| 1:C:592:ASN:O | 1:C:596:LEU:HG | 2.11 | 0.49 |
| 1:C:692:HIS:HE1 | 1:C:694:ASP:OD2 | 1.95 | 0.49 |
| 1:C:810:ALA:O | 1:C:811:LYS:C | 2.54 | 0.49 |
| 1:C:823:MET:CB | 1:C:827:PRO:HG3 | 2.42 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:185:PRO:O | 1:D:187:ILE:HG23 | 2.11 | 0.49 |
| 1:D:355:LEU:O | 1:D:356:GLN:C | 2.53 | 0.49 |
| 1:D:498:ASP:OD1 | 1:D:499:THR:N | 2.44 | 0.49 |
| 1:D:596:LEU:HD11 | 1:E:838:ASN:HD21 | 1.76 | 0.49 |
| 1:E:306:SER:OG | 1:E:334:ARG:NH2 | 2.45 | 0.49 |
| 1:E:319:ASN:C | 1:E:322:ARG:NH1 | 2.69 | 0.49 |
| 1:E:478:GLN:O | 1:E:481:LYS:HB3 | 2.12 | 0.49 |
| 1:E:529:ARG:HG3 | 1:E:530:ARG:N | 2.18 | 0.49 |
| 1:E:557:PRO:O | 1:E:561:LEU:HG | 2.12 | 0.49 |
| 1:E:645:GLU:CB | 1:E:649:LYS:HZ1 | 2.25 | 0.49 |
| 1:E:685:PHE:H | 1:E:726:THR:H | 1.59 | 0.49 |
| 1:F:700:LEU:CB | 1:F:703:LEU:HD21 | 2.08 | 0.49 |
| 1:F:793:GLU:HB3 | 1:F:797:GLN:HE21 | 1.77 | 0.49 |
| 1:A:560:LYS:NZ | 1:A:633:ASN:HB2 | 2.27 | 0.49 |
| 1:A:625:LYS:NZ | 1:A:635:GLU:O | 2.45 | 0.49 |
| 1:B:407:ARG:HH21 | 1:B:538:GLN:C | 2.16 | 0.49 |
| 1:B:590:VAL:O | 1:B:594:VAL:HG23 | 2.13 | 0.49 |
| 1:B:621:THR:O | 1:B:624:ALA:N | 2.45 | 0.49 |
| 1:B:628:ALA:HB3 | 1:B:635:GLU:HG3 | 1.93 | 0.49 |
| 1:B:704:ASP:N | 1:B:704:ASP:OD1 | 2.38 | 0.49 |
| 1:C:198:ARG:HD2 | 1:D:405:VAL:HG22 | 1.93 | 0.49 |
| 1:C:228:ARG:HG2 | 1:C:233:ASP:O | 2.12 | 0.49 |
| 1:C:281:LEU:HD21 | 1:C:311:LYS:H | 1.77 | 0.49 |
| 1:C:404:ALA:O | 1:C:408:ASP:N | 2.45 | 0.49 |
| 1:C:476:LEU:O | 1:C:520:LEU:HD13 | 2.12 | 0.49 |
| 1:C:591:SER:O | 1:C:594:VAL:HB | 2.11 | 0.49 |
| 1:C:613:LEU:HD21 | 1:C:772:PHE:CD2 | 2.47 | 0.49 |
| 1:C:810:ALA:O | 1:C:814:LEU:HG | 2.12 | 0.49 |
| 1:C:836:ILE:O | 1:C:840:LEU:N | 2.45 | 0.49 |
| 1:D:262:GLU:O | 1:D:265:PHE:CD2 | 2.63 | 0.49 |
| 1:D:272:ILE:HG22 | 1:D:276:LYS:HZ3 | 1.77 | 0.49 |
| 1:D:414:LEU:O | 1:D:417:LYS:N | 2.44 | 0.49 |
| 1:D:543:SER:HA | 1:D:546:ILE:HB | 1.93 | 0.49 |
| 1:D:584:MET:HA | 1:D:587:ILE:HD13 | 1.95 | 0.49 |
| 1:D:623:LEU:O | 1:D:627:VAL:HG23 | 2.11 | 0.49 |
| 1:D:695:VAL:HA | 1:D:698:VAL:HB | 1.94 | 0.49 |
| 1:D:771:ILE:HG22 | 1:D:772:PHE:O | 2.12 | 0.49 |
| 1:E:219:THR:HA | 1:E:222:ILE:HD12 | 1.94 | 0.49 |
| 1:E:221:ILE:O | 1:E:222:ILE:C | 2.55 | 0.49 |
| 1:E:270:LYS:HZ2 | 1:E:274:GLU:HB3 | 1.77 | 0.49 |
| 1:E:535:SER:C | 1:E:537:ILE:HG12 | 2.36 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:620:LYS:C | 1:E:623:LEU:HB3 | 2.37 | 0.49 |
| 1:E:723:VAL:HG22 | 1:E:725:MET:HA | 1.93 | 0.49 |
| 1:E:794:ARG:HH22 | 1:E:796:GLU:CA | 2.26 | 0.49 |
| 1:E:794:ARG:HG3 | 1:E:795:PHE:O | 2.12 | 0.49 |
| 1:E:813:PHE:CD1 | 1:E:813:PHE:N | 2.76 | 0.49 |
| 1:F:202:ARG:HD2 | 1:F:206:SER:O | 2.12 | 0.49 |
| 1:F:294:LYS:HA | 1:F:300:ILE:HD11 | 1.94 | 0.49 |
| 1:F:391:SER:O | 1:F:394:ASP:HB2 | 2.12 | 0.49 |
| 1:F:817:TYR:OH | 1:F:874:GLU:HG2 | 2.11 | 0.49 |
| 1:A:618:SER:OG | 1:A:772:PHE:HB3 | 2.11 | 0.49 |
| 1:A:839:LYS:O | 1:A:842:LEU:HB2 | 2.11 | 0.49 |
| 1:B:205:LYS:CE | 1:B:334:ARG:HA | 2.31 | 0.49 |
| 1:B:245:SER:HB3 | 1:B:282:PHE:O | 2.11 | 0.49 |
| 1:B:261:PHE:HB2 | 1:B:265:PHE:CZ | 2.47 | 0.49 |
| 1:B:590:VAL:HA | 1:B:593:ALA:HB3 | 1.95 | 0.49 |
| 1:B:594:VAL:O | 1:B:597:SER:OG | 2.12 | 0.49 |
| 1:B:744:GLU:CA | 1:B:747:LYS:HB2 | 2.38 | 0.49 |
| 1:B:764:ASN:HB3 | 1:B:765:ARG:NH1 | 2.21 | 0.49 |
| 1:B:803:LYS:NZ | 1:B:854:THR:HA | 2.28 | 0.49 |
| 1:C:186:VAL:HG12 | 1:C:187:ILE:N | 2.27 | 0.49 |
| 1:C:421:LEU:HB2 | 1:C:456:GLN:NE2 | 2.27 | 0.49 |
| 1:C:558:VAL:HG13 | 1:C:561:LEU:HD12 | 1.93 | 0.49 |
| 1:C:654:LYS:CG | 1:C:655:LEU:H | 1.88 | 0.49 |
| 1:C:656:LEU:HD13 | 1:C:711:GLY:HA3 | 1.94 | 0.49 |
| 1:C:826:ARG:N | 1:C:827:PRO:HD2 | 2.27 | 0.49 |
| 1:D:202:ARG:HH12 | 1:D:205:LYS:HB3 | 1.77 | 0.49 |
| 1:D:273:GLU:HB3 | 1:D:310:LEU:HD11 | 1.94 | 0.49 |
| 1:D:342:GLU:HG2 | 1:D:388:LEU:HD12 | 1.94 | 0.49 |
| 1:D:584:MET:O | 1:D:588:LYS:HG3 | 2.11 | 0.49 |
| 1:E:287:HIS:CE1 | 1:E:315:ALA:C | 2.90 | 0.49 |
| 1:E:592:ASN:HA | 1:E:595:ARG:HB2 | 1.93 | 0.49 |
| 1:E:613:LEU:HG | 1:E:728:ALA:CA | 2.42 | 0.49 |
| 1:E:641:VAL:HG23 | 1:E:684:LEU:HB3 | 1.94 | 0.49 |
| 1:E:644:SER:N | 1:E:690:LYS:HB3 | 2.27 | 0.49 |
| 1:E:689:GLU:OE2 | 1:E:754:VAL:HG13 | 2.12 | 0.49 |
| 1:E:703:LEU:HD22 | 1:E:765:ARG:HD3 | 1.94 | 0.49 |
| 1:F:198:ARG:HB2 | 1:F:202:ARG:NH2 | 2.25 | 0.49 |
| 1:F:201:ALA:O | 1:F:203:ARG:HG2 | 2.12 | 0.49 |
| 1:F:349:VAL:O | 1:F:352:LEU:N | 2.45 | 0.49 |
| 1:F:563:GLU:HB3 | 1:F:568:LYS:CB | 2.40 | 0.49 |
| 1:F:567:GLU:O | 1:F:571:HIS:N | 2.34 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:781:HIS:CE1 | 1:F:782:LYS:HZ2 | 2.30 | 0.49 |
| 1:F:802:TYR:C | 1:F:804:LEU:H | 2.17 | 0.49 |
| 1:F:845:LEU:O | 1:F:847:ASN:ND2 | 2.46 | 0.49 |
| 1:A:248:LEU:HD12 | 1:A:250:ALA:H | 1.76 | 0.49 |
| 1:A:595:ARG:CZ | 1:B:842:LEU:HD12 | 2.42 | 0.49 |
| 1:B:174:MET:HB3 | 1:B:243:LEU:CD1 | 2.39 | 0.49 |
| 1:B:218:LYS:O | 1:B:221:ILE:HD12 | 2.12 | 0.49 |
| 1:B:224:GLY:HA2 | 1:B:227:GLN:HB3 | 1.94 | 0.49 |
| 1:B:234:VAL:HB | 1:B:238:LEU:HD23 | 1.95 | 0.49 |
| 1:B:573:GLU:H | 1:B:595:ARG:NH2 | 2.10 | 0.49 |
| 1:B:592:ASN:O | 1:B:593:ALA:C | 2.55 | 0.49 |
| 1:B:740:SER:O | 1:B:742:ILE:HD12 | 2.12 | 0.49 |
| 1:B:837:LEU:HA | 1:B:840:LEU:CD1 | 2.42 | 0.49 |
| 1:C:191:GLU:HA | 1:C:194:ARG:CB | 2.37 | 0.49 |
| 1:C:381:ARG:HG3 | 1:C:382:TYR:CE1 | 2.48 | 0.49 |
| 1:C:567:GLU:CD | 1:C:567:GLU:N | 2.67 | 0.49 |
| 1:C:584:MET:HA | 1:C:587:ILE:HD12 | 1.95 | 0.49 |
| 1:C:640:ARG:N | 1:C:683:LEU:HD12 | 2.28 | 0.49 |
| 1:C:671:LEU:O | 1:C:672:THR:C | 2.55 | 0.49 |
| 1:C:787:ARG:HH12 | 1:C:826:ARG:HE | 1.59 | 0.49 |
| 1:C:803:LYS:HZ2 | 1:C:853:GLU:CA | 2.26 | 0.49 |
| 1:D:206:SER:O | 1:D:335:PHE:HA | 2.13 | 0.49 |
| 1:D:280:VAL:HG12 | 1:D:281:LEU:N | 2.27 | 0.49 |
| 1:D:286:ILE:O | 1:D:290:MET:HE2 | 2.11 | 0.49 |
| 1:D:378:LEU:HB3 | 1:D:382:TYR:CE2 | 2.47 | 0.49 |
| 1:D:792:GLU:HA | 1:D:795:PHE:CD2 | 2.47 | 0.49 |
| 1:E:362:HIS:CD2 | 1:E:362:HIS:N | 2.80 | 0.49 |
| 1:E:787:ARG:HD2 | 1:E:790:GLU:OE1 | 2.12 | 0.49 |
| 1:E:855:VAL:HG12 | 1:E:856:ASN:O | 2.11 | 0.49 |
| 1:F:685:PHE:CB | 1:F:726:THR:H | 2.25 | 0.49 |
| 1:F:708:ILE:N | 1:F:708:ILE:CD1 | 2.73 | 0.49 |
| 1:F:808:GLN:HA | 1:F:811:LYS:HE2 | 1.93 | 0.49 |
| 1:A:216:ILE:O | 1:A:217:GLY:C | 2.56 | 0.49 |
| 1:A:376:ALA:HA | 1:A:379:ALA:HB3 | 1.94 | 0.49 |
| 1:A:815:ALA:O | 1:A:819:TYR:HD2 | 1.96 | 0.49 |
| 1:B:166:TYR:CA | 1:B:169:LYS:HG2 | 2.37 | 0.49 |
| 1:B:195:SER:HA | 1:B:198:ARG:HH12 | 1.77 | 0.49 |
| 1:B:244:PHE:C | 1:B:281:LEU:HD23 | 2.37 | 0.49 |
| 1:B:549:THR:O | 1:B:552:ARG:HG2 | 2.12 | 0.49 |
| 1:B:781:HIS:CE1 | 1:B:811:LYS:HE3 | 2.47 | 0.49 |
| 1:C:158:ALA:C | 1:C:159:ASP:O | 2.53 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:221:ILE:O | 1:C:222:ILE:C | 2.55 | 0.49 |
| 1:C:466:TYR:CE1 | 1:C:535:SER:HB2 | 2.47 | 0.49 |
| 1:C:471:HIS:HA | 1:C:474:GLU:CB | 2.36 | 0.49 |
| 1:C:691:ALA:HB3 | 1:C:696:LEU:CD2 | 2.43 | 0.49 |
| 1:C:813:PHE:HB3 | 1:C:878:GLU:OE2 | 2.13 | 0.49 |
| 1:C:837:LEU:O | 1:C:840:LEU:N | 2.46 | 0.49 |
| 1:D:201:ALA:HB2 | 1:D:238:LEU:HD11 | 1.95 | 0.49 |
| 1:D:290:MET:C | 1:D:294:LYS:HA | 2.38 | 0.49 |
| 1:D:321:TYR:O | 1:D:324:ILE:HB | 2.12 | 0.49 |
| 1:D:351:ILE:HG12 | 2:D:1001:AGS:C2 | 2.43 | 0.49 |
| 1:D:395:LEU:HA | 1:D:398:ILE:HB | 1.95 | 0.49 |
| 1:D:517:ILE:O | 1:D:521:GLU:N | 2.31 | 0.49 |
| 1:D:733:PHE:CZ | 1:D:746:THR:O | 2.65 | 0.49 |
| 1:D:733:PHE:CD2 | 1:D:750:VAL:HB | 2.47 | 0.49 |
| 1:D:782:LYS:O | 1:D:786:ILE:HG13 | 2.12 | 0.49 |
| 1:E:232:ASP:HA | 1:E:239:GLN:OE1 | 2.13 | 0.49 |
| 1:E:331:PHE:CE1 | 1:E:335:PHE:HE2 | 2.30 | 0.49 |
| 1:E:625:LYS:HE2 | 1:E:626:LYS:HZ1 | 1.78 | 0.49 |
| 1:E:825:ALA:O | 1:E:828:LEU:N | 2.45 | 0.49 |
| 1:E:828:LEU:O | 1:E:829:ASN:C | 2.54 | 0.49 |
| 1:F:576:LEU:O | 1:F:579:GLU:HB2 | 2.12 | 0.49 |
| 1:F:618:SER:OG | 1:F:619:GLY:N | 2.44 | 0.49 |
| 1:F:620:LYS:NZ | 2:F:1002:AGS:O2G | 2.41 | 0.49 |
| 1:F:708:ILE:O | 1:F:715:THR:OG1 | 2.20 | 0.49 |
| 1:F:819:TYR:CZ | 1:F:828:LEU:HB2 | 2.48 | 0.49 |
| 1:F:836:ILE:O | 1:F:839:LYS:N | 2.46 | 0.49 |
| 1:A:209:CYS:C | 1:A:315:ALA:HA | 2.38 | 0.49 |
| 1:A:573:GLU:HA | 1:A:576:LEU:HB2 | 1.94 | 0.49 |
| 1:A:607:PRO:HD3 | 1:A:706:GLY:HA3 | 1.94 | 0.49 |
| 1:A:613:LEU:HD11 | 1:A:726:THR:HA | 1.95 | 0.49 |
| 1:A:872:GLU:HB3 | 1:F:201:ALA:H | 1.77 | 0.49 |
| 1:B:217:GLY:O | 1:B:221:ILE:HD11 | 2.12 | 0.49 |
| 1:B:301:LEU:CD1 | 1:B:305:LEU:HD11 | 2.42 | 0.49 |
| 1:B:361:ILE:C | 1:B:364:GLY:H | 2.20 | 0.49 |
| 1:B:857:VAL:HG12 | 1:B:878:GLU:N | 2.21 | 0.49 |
| 1:C:174:MET:N | 1:C:242:LYS:NZ | 2.53 | 0.49 |
| 1:C:186:VAL:HG13 | 2:C:1001:AGS:N7 | 2.28 | 0.49 |
| 1:C:191:GLU:HB2 | 1:C:194:ARG:HH21 | 1.74 | 0.49 |
| 1:C:344:SER:O | 1:C:348:THR:OG1 | 2.20 | 0.49 |
| 1:C:377:GLN:HA | 1:C:380:LYS:HB3 | 1.94 | 0.49 |
| 1:C:542:ASP:O | 1:C:545:THR:N | 2.45 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:567:GLU:HB3 | 1:C:571:HIS:NE2 | 2.28 | 0.49 |
| 1:C:837:LEU:C | 1:C:840:LEU:H | 2.20 | 0.49 |
| 1:D:391:SER:O | 1:D:394:ASP:N | 2.45 | 0.49 |
| 1:D:460:GLU:HA | 1:D:463:ARG:NH1 | 2.25 | 0.49 |
| 1:D:607:PRO:HB3 | 1:D:719:SER:HA | 1.93 | 0.49 |
| 1:D:607:PRO:HB3 | 1:D:722:ILE:HD13 | 1.94 | 0.49 |
| 1:E:246:LEU:HB2 | 1:E:281:LEU:HD11 | 1.94 | 0.49 |
| 1:E:379:ALA:O | 1:E:383:LEU:N | 2.39 | 0.49 |
| 1:E:476:LEU:HD23 | 1:E:521:GLU:CG | 2.43 | 0.49 |
| 1:E:618:SER:C | 2:E:1002:AGS:N3 | 2.71 | 0.49 |
| 1:E:644:SER:HA | 1:E:691:ALA:HB2 | 1.94 | 0.49 |
| 1:E:709:THR:N | 1:E:716:ILE:N | 2.54 | 0.49 |
| 1:E:846:LYS:C | 1:E:848:GLU:HG3 | 2.38 | 0.49 |
| 1:E:858:VAL:HG12 | 1:E:859:LEU:N | 2.28 | 0.49 |
| 1:F:399:SER:HA | 1:F:545:THR:OG1 | 2.13 | 0.49 |
| 1:F:682:VAL:HG22 | 1:F:683:LEU:H | 1.77 | 0.49 |
| 1:A:200:LEU:HD12 | 1:A:201:ALA:CA | 2.38 | 0.49 |
| 1:A:740:SER:HB3 | 1:A:774:LYS:CE | 2.42 | 0.49 |
| 1:B:337:LYS:HG3 | 1:B:338:ILE:H | 1.77 | 0.49 |
| 1:B:353:ARG:HH12 | 1:B:373:VAL:H | 1.59 | 0.49 |
| 1:B:355:LEU:O | 1:B:358:LYS:HG2 | 2.13 | 0.49 |
| 1:B:391:SER:HA | 1:B:394:ASP:CG | 2.37 | 0.49 |
| 1:B:566:ASN:HA | 1:B:569:LEU:HD12 | 1.95 | 0.49 |
| 1:B:585:ASP:HA | 1:B:588:LYS:CD | 2.37 | 0.49 |
| 1:B:780:ILE:O | 1:B:784:VAL:HG23 | 2.13 | 0.49 |
| 1:C:193:ILE:O | 1:C:197:ILE:HG12 | 2.13 | 0.49 |
| 1:C:261:PHE:O | 1:C:262:GLU:C | 2.55 | 0.49 |
| 1:C:372:LEU:HA | 1:C:542:ASP:HB3 | 1.94 | 0.49 |
| 1:C:397:ASP:O | 1:C:398:ILE:C | 2.55 | 0.49 |
| 1:C:557:PRO:CA | 1:C:560:LYS:HB2 | 2.43 | 0.49 |
| 1:C:837:LEU:HA | 1:C:840:LEU:HB3 | 1.95 | 0.49 |
| 1:D:232:ASP:O | 1:D:495:ARG:NH2 | 2.45 | 0.49 |
| 1:D:357:PRO:HG2 | 1:D:358:LYS:NZ | 2.25 | 0.49 |
| 1:D:365:VAL:HA | 1:D:536:MET:O | 2.12 | 0.49 |
| 1:D:461:PRO:HB2 | 1:D:465:ARG:NH2 | 2.27 | 0.49 |
| 1:D:557:PRO:HG2 | 1:D:558:VAL:HG23 | 1.93 | 0.49 |
| 1:D:733:PHE:CD1 | 1:D:733:PHE:N | 2.74 | 0.49 |
| 1:D:736:SER:H | 1:D:774:LYS:HZ1 | 1.60 | 0.49 |
| 1:D:762:PHE:O | 1:D:765:ARG:HB2 | 2.12 | 0.49 |
| 1:D:808:GLN:C | 1:D:811:LYS:HD3 | 2.37 | 0.49 |
| 1:D:825:ALA:N | 1:D:827:PRO:HD2 | 2.28 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:232:ASP:O | 1:E:234:VAL:HG13 | 2.13 | 0.49 |
| 1:E:283:ILE:O | 1:E:314:GLY:HA2 | 2.12 | 0.49 |
| 1:E:365:VAL:HB | 1:E:538:GLN:C | 2.38 | 0.49 |
| 1:E:794:ARG:NH2 | 1:E:796:GLU:HA | 2.28 | 0.49 |
| 1:F:194:ARG:O | 1:F:198:ARG:HG3 | 2.13 | 0.49 |
| 1:F:198:ARG:C | 1:F:202:ARG:HH21 | 2.20 | 0.49 |
| 1:F:218:LYS:NZ | 2:F:1001:AGS:O3G | 2.46 | 0.49 |
| 1:A:221:ILE:O | 1:A:222:ILE:C | 2.55 | 0.49 |
| 1:A:262:GLU:O | 1:A:267:GLY:N | 2.41 | 0.49 |
| 1:A:302:LYS:O | 1:A:305:LEU:N | 2.45 | 0.49 |
| 1:A:654:LYS:HE3 | 1:A:657:GLY:N | 2.27 | 0.49 |
| 1:B:387:ARG:HB2 | 1:B:390:ASP:HB2 | 1.94 | 0.49 |
| 1:C:208:PRO:CD | 1:C:313:ILE:HG23 | 2.42 | 0.49 |
| 1:C:316:THR:OG1 | 1:C:317:THR:N | 2.46 | 0.49 |
| 1:C:383:LEU:HB3 | 1:C:385:TYR:CE1 | 2.48 | 0.49 |
| 1:D:558:VAL:HA | 1:D:561:LEU:CB | 2.38 | 0.49 |
| 1:D:609:SER:H | 1:D:767:SER:CB | 2.21 | 0.49 |
| 1:E:590:VAL:O | 1:E:591:SER:C | 2.55 | 0.49 |
| 1:E:611:LEU:HB3 | 1:E:769:ILE:HG12 | 1.95 | 0.49 |
| 1:F:261:PHE:O | 1:F:264:ARG:HB3 | 2.13 | 0.49 |
| 1:F:287:HIS:CE1 | 1:F:321:TYR:HD2 | 2.31 | 0.49 |
| 1:F:331:PHE:CG | 1:F:334:ARG:HG3 | 2.48 | 0.49 |
| 1:A:194:ARG:HA | 1:A:197:ILE:HD12 | 1.93 | 0.49 |
| 1:A:211:ILE:O | 1:A:213:GLU:HG2 | 2.13 | 0.49 |
| 1:A:283:ILE:CG2 | 1:A:288:MET:HB2 | 2.43 | 0.49 |
| 1:A:343:PRO:HG2 | 1:A:388:LEU:HB2 | 1.95 | 0.49 |
| 1:A:380:LYS:O | 1:A:382:TYR:N | 2.46 | 0.49 |
| 1:A:396:VAL:O | 1:A:400:CYS:N | 2.45 | 0.49 |
| 1:A:810:ALA:HA | 1:A:813:PHE:CE1 | 2.47 | 0.49 |
| 1:B:176:GLU:C | 1:B:178:ALA:H | 2.21 | 0.49 |
| 1:B:387:ARG:O | 1:B:390:ASP:HB3 | 2.12 | 0.49 |
| 1:B:631:LEU:O | 1:B:633:ASN:N | 2.46 | 0.49 |
| 1:B:656:LEU:HD12 | 1:B:656:LEU:O | 2.12 | 0.49 |
| 1:B:820:SER:H | 1:B:828:LEU:HD11 | 1.78 | 0.49 |
| 1:C:168:SER:C | 1:C:264:ARG:CZ | 2.85 | 0.49 |
| 1:C:173:ASP:C | 1:C:177:GLN:HB2 | 2.38 | 0.49 |
| 1:C:207:ASN:HB2 | 1:C:313:ILE:HG12 | 1.95 | 0.49 |
| 1:C:298:ALA:O | 1:C:303:PRO:HD2 | 2.12 | 0.49 |
| 1:C:374:THR:HA | 1:C:377:GLN:CD | 2.38 | 0.49 |
| 1:C:618:SER:O | 1:C:621:THR:N | 2.25 | 0.49 |
| 1:C:796:GLU:OE1 | 1:C:799:ASP:HB3 | 2.13 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:824:GLY:O | 1:C:828:LEU:HD12 | 2.13 | 0.49 |
| 1:C:875:GLU:HG2 | 1:C:876:CYS:N | 2.21 | 0.49 |
| 1:D:260:ASP:CG | 1:D:264:ARG:HB2 | 2.38 | 0.49 |
| 1:D:298:ALA:O | 1:D:301:LEU:HD11 | 2.13 | 0.49 |
| 1:D:564:SER:HB3 | 1:D:567:GLU:HB3 | 1.94 | 0.49 |
| 1:D:606:GLN:CG | 1:D:704:ASP:HB3 | 2.43 | 0.49 |
| 1:D:616:SER:C | 1:D:618:SER:H | 2.21 | 0.49 |
| 1:D:780:ILE:O | 1:D:781:HIS:C | 2.56 | 0.49 |
| 1:E:209:CYS:C | 1:E:210:LEU:HD12 | 2.38 | 0.49 |
| 1:E:247:ASP:HB3 | 1:E:249:ALA:HB3 | 1.95 | 0.49 |
| 1:E:285:GLU:HA | 1:E:287:HIS:HE1 | 1.75 | 0.49 |
| 1:E:548:GLU:HA | 1:E:551:ALA:HB3 | 1.95 | 0.49 |
| 1:E:606:GLN:CD | 1:F:794:ARG:CZ | 2.85 | 0.49 |
| 1:E:877:LEU:O | 1:E:879:VAL:HG23 | 2.13 | 0.49 |
| 1:F:548:GLU:OE2 | 1:F:552:ARG:NH2 | 2.46 | 0.49 |
| 1:F:585:ASP:HA | 1:F:588:LYS:HB2 | 1.94 | 0.49 |
| 1:F:592:ASN:O | 1:F:595:ARG:HG2 | 2.13 | 0.49 |
| 1:F:612:PHE:CG | 1:F:726:THR:HG22 | 2.48 | 0.49 |
| 1:F:619:GLY:O | 1:F:623:LEU:N | 2.41 | 0.49 |
| 1:A:197:ILE:HA | 1:A:200:LEU:HD21 | 1.95 | 0.49 |
| 1:A:321:TYR:O | 1:A:325:VAL:N | 2.44 | 0.49 |
| 1:A:351:ILE:HG23 | 1:A:393:LEU:HD11 | 1.94 | 0.49 |
| 1:A:707:ARG:HG3 | 1:A:717:ASP:HB2 | 1.94 | 0.49 |
| 1:B:167:LEU:O | 1:B:171:ALA:HB2 | 2.13 | 0.49 |
| 1:B:210:LEU:CB | 1:B:339:GLU:HB3 | 2.42 | 0.49 |
| 1:B:265:PHE:CE2 | 1:B:297:ALA:HA | 2.46 | 0.49 |
| 1:B:710:SER:C | 1:B:713:GLY:H | 2.21 | 0.49 |
| 1:B:750:VAL:HG12 | 1:B:754:VAL:HG23 | 1.95 | 0.49 |
| 1:C:190:GLU:HB2 | 1:C:194:ARG:HH12 | 1.77 | 0.49 |
| 1:C:243:LEU:HA | 1:C:280:VAL:O | 2.13 | 0.49 |
| 1:C:371:ALA:C | 1:C:542:ASP:OD2 | 2.56 | 0.49 |
| 1:C:594:VAL:HA | 1:C:597:SER:OG | 2.13 | 0.49 |
| 1:C:612:PHE:CB | 1:C:727:SER:H | 2.26 | 0.49 |
| 1:D:227:GLN:NE2 | 1:D:227:GLN:O | 2.46 | 0.49 |
| 1:D:283:ILE:O | 1:D:313:ILE:HD12 | 2.12 | 0.49 |
| 1:D:507:TYR:C | 1:D:509:ALA:H | 2.20 | 0.49 |
| 1:D:616:SER:HA | 1:D:620:LYS:HE3 | 1.95 | 0.49 |
| 1:D:619:GLY:HA2 | 1:D:622:GLU:OE1 | 2.13 | 0.49 |
| 1:D:622:GLU:O | 1:D:623:LEU:C | 2.56 | 0.49 |
| 1:E:219:THR:H | 2:E:1001:AGS:PB | 2.36 | 0.49 |
| 1:E:228:ARG:HA | 1:E:231:ASP:HB2 | 1.94 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:242:LYS:H | 1:E:279:ILE:CA | 2.22 | 0.49 |
| 1:E:349:VAL:HA | 1:E:352:LEU:HB2 | 1.95 | 0.49 |
| 1:E:447:LEU:O | 1:E:450:GLN:HB3 | 2.13 | 0.49 |
| 1:E:514:LYS:HG2 | 1:E:517:ILE:HD12 | 1.95 | 0.49 |
| 1:E:707:ARG:O | 1:E:708:ILE:HD13 | 2.12 | 0.49 |
| 1:E:787:ARG:HA | 1:E:790:GLU:OE1 | 2.12 | 0.49 |
| 1:E:791:ILE:O | 1:E:792:GLU:C | 2.56 | 0.49 |
| 1:E:820:SER:OG | 1:E:820:SER:O | 2.27 | 0.49 |
| 1:E:853:GLU:CD | 1:E:881:PRO:HB2 | 2.38 | 0.49 |
| 1:F:605:ARG:HG2 | 1:F:605:ARG:HH11 | 1.78 | 0.49 |
| 1:F:682:VAL:C | 1:F:723:VAL:HG21 | 2.38 | 0.49 |
| 1:F:827:PRO:O | 1:F:831:LEU:HG | 2.12 | 0.49 |
| 1:A:343:PRO:HG3 | 1:A:389:PRO:HD3 | 1.95 | 0.48 |
| 1:A:375:ALA:HA | 1:A:378:LEU:HB2 | 1.94 | 0.48 |
| 1:A:598:ARG:NH2 | 1:A:720:ASN:HA | 2.28 | 0.48 |
| 1:A:603:ASN:HB3 | 1:A:605:ARG:HE | 1.77 | 0.48 |
| 1:A:660:ALA:HA | 1:A:665:TYR:HE1 | 1.78 | 0.48 |
| 1:A:675:LEU:HD13 | 1:A:716:ILE:HG13 | 1.94 | 0.48 |
| 1:A:698:VAL:HG12 | 1:A:702:MET:HG2 | 1.94 | 0.48 |
| 1:A:809:GLU:OE2 | 1:A:813:PHE:HB3 | 2.13 | 0.48 |
| 1:B:214:PRO:HD3 | 1:B:317:THR:CG2 | 2.42 | 0.48 |
| 1:B:292:ASN:HB3 | 1:B:295:ASP:CG | 2.37 | 0.48 |
| 1:B:651:ALA:O | 1:B:654:LYS:HG2 | 2.13 | 0.48 |
| 1:B:841:ALA:O | 1:B:844:ILE:HB | 2.13 | 0.48 |
| 1:C:169:LYS:NZ | 1:C:264:ARG:CB | 2.75 | 0.48 |
| 1:C:318:ASN:N | 1:C:318:ASN:OD1 | 2.47 | 0.48 |
| 1:C:557:PRO:O | 1:C:559:LYS:N | 2.46 | 0.48 |
| 1:C:628:ALA:HB1 | 1:C:632:PHE:H | 1.78 | 0.48 |
| 1:C:658:THR:H | 1:C:667:GLU:HB3 | 1.77 | 0.48 |
| 1:C:743:GLN:O | 1:C:746:THR:HB | 2.13 | 0.48 |
| 1:C:843:ARG:HA | 1:C:846:LYS:N | 2.28 | 0.48 |
| 1:D:220:ALA:HA | 1:D:223:GLU:HB3 | 1.94 | 0.48 |
| 1:D:319:ASN:HD21 | 1:D:714:LYS:N | 2.10 | 0.48 |
| 1:D:441:THR:HG22 | 1:D:442:LYS:N | 2.27 | 0.48 |
| 1:D:464:GLN:HA | 1:D:468:GLU:H | 1.78 | 0.48 |
| 1:D:579:GLU:CB | 1:D:626:LYS:NZ | 2.76 | 0.48 |
| 1:D:683:LEU:N | 1:D:723:VAL:HA | 2.26 | 0.48 |
| 1:D:721:CYS:O | 1:D:722:ILE:HD13 | 2.12 | 0.48 |
| 1:D:781:HIS:O | 1:D:783:ILE:N | 2.46 | 0.48 |
| 1:E:194:ARG:O | 1:E:198:ARG:HG3 | 2.13 | 0.48 |
| 1:E:267:GLY:O | 1:E:268:VAL:C | 2.56 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:481:LYS:O | 1:E:485:GLU:HG3 | 2.13 | 0.48 |
| 1:E:564:SER:O | 1:E:565:GLU:C | 2.55 | 0.48 |
| 1:E:588:LYS:HG3 | 1:E:592:ASN:ND2 | 2.27 | 0.48 |
| 1:E:624:ALA:O | 1:E:627:VAL:N | 2.46 | 0.48 |
| 1:E:668:GLY:HA3 | 1:E:672:THR:CB | 2.43 | 0.48 |
| 1:E:682:VAL:O | 1:E:683:LEU:HB2 | 2.13 | 0.48 |
| 1:E:686:ASP:OD1 | 1:E:686:ASP:N | 2.43 | 0.48 |
| 1:E:791:ILE:HD13 | 1:E:791:ILE:HA | 1.66 | 0.48 |
| 1:E:839:LYS:CD | 1:E:879:VAL:HG13 | 2.43 | 0.48 |
| 1:E:858:VAL:CB | 1:E:877:LEU:HD12 | 2.43 | 0.48 |
| 1:F:190:GLU:O | 1:F:228:ARG:NH2 | 2.37 | 0.48 |
| 1:F:640:ARG:NH1 | 1:F:686:ASP:OD2 | 2.45 | 0.48 |
| 1:A:296:ASP:OD1 | 1:A:300:ILE:HB | 2.13 | 0.48 |
| 1:A:788:LEU:HD22 | 1:A:804:LEU:HD21 | 1.95 | 0.48 |
| 1:B:211:ILE:HA | 1:B:316:THR:O | 2.12 | 0.48 |
| 1:B:296:ASP:HB2 | 1:B:300:ILE:HD12 | 1.95 | 0.48 |
| 1:B:391:SER:HA | 1:B:394:ASP:CB | 2.40 | 0.48 |
| 1:B:555:GLY:C | 1:B:556:ILE:HG23 | 2.37 | 0.48 |
| 1:B:569:LEU:C | 1:B:595:ARG:HE | 2.21 | 0.48 |
| 1:B:801:HIS:HD1 | 1:B:851:ASP:CG | 2.20 | 0.48 |
| 1:B:827:PRO:O | 1:B:830:ARG:HB3 | 2.12 | 0.48 |
| 1:B:843:ARG:NE | 1:B:880:LEU:O | 2.46 | 0.48 |
| 1:C:129:ILE:C | 1:C:131:LYS:H | 2.21 | 0.48 |
| 1:C:410:LYS:N | 1:C:411:PRO:HD3 | 2.28 | 0.48 |
| 1:C:499:THR:HA | 1:C:502:ALA:HB3 | 1.94 | 0.48 |
| 1:D:242:LYS:HG2 | 1:D:278:LEU:C | 2.38 | 0.48 |
| 1:D:272:ILE:HA | 1:D:276:LYS:CE | 2.43 | 0.48 |
| 1:D:273:GLU:HA | 1:D:310:LEU:HD21 | 1.93 | 0.48 |
| 1:D:388:LEU:C | 1:D:391:SER:HG | 2.20 | 0.48 |
| 1:D:566:ASN:O | 1:D:567:GLU:C | 2.53 | 0.48 |
| 1:D:611:LEU:CB | 1:D:769:ILE:HA | 2.43 | 0.48 |
| 1:D:615:LEU:HD21 | 1:D:822:ASP:O | 2.13 | 0.48 |
| 1:E:276:LYS:HZ3 | 1:E:279:ILE:HB | 1.78 | 0.48 |
| 1:E:346:ARG:HB3 | 1:E:347:GLN:CD | 2.38 | 0.48 |
| 1:E:350:ALA:O | 1:E:354:GLY:N | 2.31 | 0.48 |
| 1:E:368:LEU:HB3 | 1:E:540:VAL:HB | 1.95 | 0.48 |
| 1:E:371:ALA:HB3 | 1:E:540:VAL:HG11 | 1.94 | 0.48 |
| 1:E:385:TYR:CD1 | 1:E:386:ARG:CZ | 2.96 | 0.48 |
| 1:E:528:GLU:H | 1:E:528:GLU:CD | 2.20 | 0.48 |
| 1:E:583:GLN:CD | 1:E:772:PHE:HD1 | 2.21 | 0.48 |
| 1:E:588:LYS:C | 1:E:592:ASN:HD22 | 2.21 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:241:ALA:HA | 1:F:279:ILE:CB | 2.30 | 0.48 |
| 1:F:563:GLU:OE2 | 1:F:572:MET:N | 2.46 | 0.48 |
| 1:F:685:PHE:O | 1:F:686:ASP:OD1 | 2.30 | 0.48 |
| 1:F:751:MET:O | 1:F:755:ARG:HG2 | 2.13 | 0.48 |
| 1:A:199:VAL:HG21 | 1:A:208:PRO:HB3 | 1.95 | 0.48 |
| 1:A:226:ALA:O | 1:A:230:ILE:HG12 | 2.13 | 0.48 |
| 1:A:541:VAL:HG12 | 1:A:543:SER:N | 2.26 | 0.48 |
| 1:B:191:GLU:CA | 1:B:194:ARG:HB2 | 2.39 | 0.48 |
| 1:B:193:ILE:HG13 | 1:B:194:ARG:N | 2.29 | 0.48 |
| 1:B:209:CYS:N | 1:B:335:PHE:HZ | 2.11 | 0.48 |
| 1:B:285:GLU:CD | 1:B:286:ILE:N | 2.71 | 0.48 |
| 1:B:651:ALA:N | 1:B:692:HIS:CE1 | 2.73 | 0.48 |
| 1:B:777:ARG:O | 1:B:778:LYS:C | 2.56 | 0.48 |
| 1:B:837:LEU:HD12 | 1:B:840:LEU:HD12 | 1.95 | 0.48 |
| 1:C:207:ASN:OD1 | 1:C:209:CYS:SG | 2.71 | 0.48 |
| 1:C:214:PRO:HD3 | 1:C:317:THR:OG1 | 2.12 | 0.48 |
| 1:C:268:VAL:HA | 1:C:271:GLU:CG | 2.43 | 0.48 |
| 1:C:278:LEU:O | 1:C:279:ILE:HG13 | 2.13 | 0.48 |
| 1:C:642:ASP:HB3 | 1:C:644:SER:OG | 2.14 | 0.48 |
| 1:C:643:CYS:SG | 1:C:686:ASP:HB2 | 2.53 | 0.48 |
| 1:C:643:CYS:CB | 1:C:690:LYS:HB2 | 2.43 | 0.48 |
| 1:C:836:ILE:HG22 | 1:C:840:LEU:HB2 | 1.96 | 0.48 |
| 1:D:234:VAL:HG13 | 1:D:235:PRO:HD2 | 1.96 | 0.48 |
| 1:D:356:GLN:NE2 | 1:D:367:ILE:H | 2.11 | 0.48 |
| 1:D:618:SER:HA | 1:D:826:ARG:CG | 2.42 | 0.48 |
| 1:D:680:TYR:HD1 | 1:D:720:ASN:C | 2.21 | 0.48 |
| 1:D:684:LEU:HD23 | 1:D:685:PHE:CA | 2.44 | 0.48 |
| 1:D:805:ASN:CG | 1:D:856:ASN:HA | 2.38 | 0.48 |
| 2:D:1001:AGS:O2A | 2:D:1001:AGS:PG | 2.71 | 0.48 |
| 1:E:213:GLU:HB3 | 1:E:387:ARG:HD2 | 1.95 | 0.48 |
| 1:E:222:ILE:HG21 | 1:E:282:PHE:CE2 | 2.49 | 0.48 |
| 1:E:268:VAL:CA | 1:E:271:GLU:HB2 | 2.42 | 0.48 |
| 1:E:365:VAL:CG1 | 1:E:407:ARG:HH11 | 2.23 | 0.48 |
| 1:E:544:ASP:N | 1:E:544:ASP:OD1 | 2.39 | 0.48 |
| 1:E:572:MET:H | 1:E:595:ARG:HH22 | 1.61 | 0.48 |
| 1:E:598:ARG:C | 1:E:601:LEU:HG | 2.38 | 0.48 |
| 1:E:608:ALA:HB3 | 1:E:721:CYS:O | 2.13 | 0.48 |
| 1:E:620:LYS:NZ | 2:E:1002:AGS:O2A | 2.38 | 0.48 |
| 1:E:667:GLU:O | 1:E:672:THR:HB | 2.12 | 0.48 |
| 1:E:803:LYS:NZ | 1:E:854:THR:HG23 | 2.28 | 0.48 |
| 1:F:594:VAL:N | 1:F:610:PHE:HZ | 2.11 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:614:GLY:H | 1:F:727:SER:C | 2.21 | 0.48 |
| 1:F:687:GLU:C | 1:F:727:SER:HG | 2.21 | 0.48 |
| 1:F:700:LEU:HD23 | 1:F:703:LEU:HD22 | 0.49 | 0.48 |
| 1:F:704:ASP:N | 1:F:765:ARG:NH1 | 2.62 | 0.48 |
| 1:F:804:LEU:O | 1:F:854:THR:HA | 2.12 | 0.48 |
| 1:A:197:ILE:HG23 | 1:A:235:PRO:CG | 2.44 | 0.48 |
| 1:A:563:GLU:HA | 1:A:568:LYS:CB | 2.44 | 0.48 |
| 1:A:575:ASP:HB2 | 1:A:630:PHE:CZ | 2.48 | 0.48 |
| 1:A:598:ARG:HH22 | 1:A:720:ASN:HA | 1.76 | 0.48 |
| 1:A:658:THR:HG22 | 1:A:659:THR:N | 2.27 | 0.48 |
| 1:A:831:LEU:O | 1:A:832:ILE:C | 2.55 | 0.48 |
| 1:A:843:ARG:HB3 | 1:A:849:ILE:HG21 | 1.95 | 0.48 |
| 1:B:169:LYS:HG3 | 1:B:170:TYR:H | 1.78 | 0.48 |
| 1:B:214:PRO:CA | 1:B:218:LYS:HB3 | 2.32 | 0.48 |
| 1:B:344:SER:OG | 1:B:347:GLN:NE2 | 2.46 | 0.48 |
| 1:B:353:ARG:HH22 | 1:B:372:LEU:CB | 2.26 | 0.48 |
| 1:B:544:ASP:O | 1:B:545:THR:C | 2.56 | 0.48 |
| 1:B:735:ASN:CG | 1:B:774:LYS:HE3 | 2.39 | 0.48 |
| 1:B:752:GLY:O | 1:B:755:ARG:N | 2.45 | 0.48 |
| 1:B:778:LYS:O | 1:B:781:HIS:HB3 | 2.13 | 0.48 |
| 1:C:189:ARG:HB2 | 1:C:193:ILE:HG13 | 1.96 | 0.48 |
| 1:C:507:TYR:HB2 | 1:D:433:ARG:HB3 | 1.95 | 0.48 |
| 1:C:626:LYS:HA | 1:C:635:GLU:OE1 | 2.13 | 0.48 |
| 1:C:730:GLY:O | 1:C:732:GLU:N | 2.47 | 0.48 |
| 1:C:758:PHE:CD1 | 1:C:762:PHE:CE2 | 3.01 | 0.48 |
| 1:C:787:ARG:NH1 | 1:C:826:ARG:HE | 2.12 | 0.48 |
| 1:C:843:ARG:HH21 | 1:C:882:ASN:HA | 1.79 | 0.48 |
| 1:D:352:LEU:CD1 | 1:D:373:VAL:HG13 | 2.42 | 0.48 |
| 1:D:759:ARG:NE | 1:D:763:LEU:HD11 | 2.29 | 0.48 |
| 1:D:763:LEU:CD1 | 1:D:763:LEU:H | 2.26 | 0.48 |
| 1:D:789:LYS:HZ2 | 1:D:790:GLU:HA | 1.77 | 0.48 |
| 1:D:791:ILE:O | 1:D:792:GLU:C | 2.55 | 0.48 |
| 1:E:283:ILE:HG22 | 1:E:284:ASP:H | 1.79 | 0.48 |
| 1:E:288:MET:HE3 | 1:E:289:LEU:O | 2.14 | 0.48 |
| 1:E:518:GLU:O | 1:E:522:ASP:HB2 | 2.13 | 0.48 |
| 1:E:573:GLU:OE1 | 1:E:573:GLU:N | 2.46 | 0.48 |
| 1:E:696:LEU:HA | 1:E:699:MET:SD | 2.53 | 0.48 |
| 1:E:771:ILE:CG2 | 1:E:772:PHE:N | 2.77 | 0.48 |
| 1:E:780:ILE:HA | 1:E:783:ILE:HD12 | 1.95 | 0.48 |
| 1:E:837:LEU:O | 1:E:838:ASN:C | 2.56 | 0.48 |
| 1:F:374:THR:O | 1:F:378:LEU:HD13 | 2.14 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:580:VAL:HG12 | 1:F:581:VAL:O | 2.14 | 0.48 |
| 1:F:632:PHE:C | 1:F:634:ASP:H | 2.19 | 0.48 |
| 1:F:786:ILE:O | 1:F:790:GLU:N | 2.38 | 0.48 |
| 1:F:831:LEU:O | 1:F:834:ASN:N | 2.25 | 0.48 |
| 1:A:195:SER:HA | 1:A:198:ARG:CZ | 2.43 | 0.48 |
| 1:A:780:ILE:HG22 | 1:A:783:ILE:HD12 | 1.95 | 0.48 |
| 1:A:826:ARG:HH12 | 1:F:304:ALA:CB | 2.27 | 0.48 |
| 1:B:198:ARG:HB3 | 1:C:405:VAL:CG2 | 2.44 | 0.48 |
| 1:B:263:GLU:C | 1:B:266:LYS:HZ1 | 2.22 | 0.48 |
| 1:B:384:PRO:CG | 1:B:386:ARG:HE | 2.27 | 0.48 |
| 1:B:545:THR:CA | 1:B:548:GLU:HB2 | 2.41 | 0.48 |
| 1:B:617:GLY:HA2 | 1:B:826:ARG:HH11 | 1.78 | 0.48 |
| 1:B:728:ALA:HB1 | 1:B:732:GLU:CD | 2.39 | 0.48 |
| 1:B:815:ALA:HA | 1:B:818:GLY:HA3 | 1.95 | 0.48 |
| 1:B:839:LYS:HZ3 | 1:B:877:LEU:CA | 2.15 | 0.48 |
| 1:C:14:ILE:CA | 1:C:160:THR:CA | 2.91 | 0.48 |
| 1:C:167:LEU:C | 1:C:167:LEU:CD1 | 2.85 | 0.48 |
| 1:C:222:ILE:CA | 1:C:225:VAL:HB | 2.43 | 0.48 |
| 1:C:351:ILE:HG23 | 2:C:1001:AGS:C6 | 2.44 | 0.48 |
| 1:C:514:LYS:HA | 1:C:517:ILE:HD12 | 1.94 | 0.48 |
| 1:C:546:ILE:HA | 1:C:549:THR:HB | 1.94 | 0.48 |
| 1:D:579:GLU:HB2 | 1:D:626:LYS:HZ2 | 1.77 | 0.48 |
| 1:D:603:ASN:OD1 | 1:D:605:ARG:N | 2.26 | 0.48 |
| 1:D:605:ARG:NH1 | 1:D:717:ASP:CG | 2.70 | 0.48 |
| 1:D:651:ALA:CA | 1:D:657:GLY:HA2 | 2.43 | 0.48 |
| 1:D:654:LYS:HG3 | 1:D:657:GLY:H | 1.78 | 0.48 |
| 1:E:395:LEU:O | 1:E:398:ILE:N | 2.47 | 0.48 |
| 1:E:424:ILE:HD13 | 1:E:448:ALA:O | 2.13 | 0.48 |
| 1:E:478:GLN:CA | 1:E:481:LYS:HB3 | 2.41 | 0.48 |
| 1:E:580:VAL:HG12 | 2:E:1002:AGS:C6 | 2.44 | 0.48 |
| 1:E:583:GLN:NE2 | 1:E:772:PHE:HA | 2.29 | 0.48 |
| 1:E:806:LEU:HG | 1:E:855:VAL:HB | 1.96 | 0.48 |
| 1:E:833:GLN:CD | 1:E:834:ASN:H | 2.21 | 0.48 |
| 1:E:839:LYS:HZ2 | 1:E:879:VAL:HG13 | 1.79 | 0.48 |
| 1:F:220:ALA:O | 1:F:224:GLY:N | 2.26 | 0.48 |
| 1:F:245:SER:HA | 1:F:283:ILE:CD1 | 2.43 | 0.48 |
| 1:F:285:GLU:CD | 1:F:288:MET:HG2 | 2.39 | 0.48 |
| 1:A:196:THR:HA | 1:A:199:VAL:CG2 | 2.43 | 0.48 |
| 1:A:331:PHE:CG | 1:A:332:GLU:N | 2.81 | 0.48 |
| 1:A:343:PRO:HG2 | 1:A:388:LEU:HD12 | 1.95 | 0.48 |
| 1:A:592:ASN:O | 1:A:596:LEU:N | 2.40 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:814:LEU:HA | 1:A:817:TYR:CD2 | 2.48 | 0.48 |
| 1:B:173:ASP:CB | 1:B:177:GLN:HG3 | 2.43 | 0.48 |
| 1:B:189:ARG:NH2 | 1:B:342:GLU:C | 2.72 | 0.48 |
| 1:B:246:LEU:HB3 | 1:B:249:ALA:HB3 | 1.96 | 0.48 |
| 1:B:334:ARG:CZ | 1:B:334:ARG:HB2 | 2.43 | 0.48 |
| 1:B:403:VAL:O | 1:B:407:ARG:HG2 | 2.13 | 0.48 |
| 1:B:583:GLN:O | 1:B:584:MET:C | 2.56 | 0.48 |
| 1:B:671:LEU:HD12 | 1:B:672:THR:H | 1.77 | 0.48 |
| 1:B:748:ASN:O | 1:B:751:MET:N | 2.45 | 0.48 |
| 1:B:814:LEU:O | 1:B:818:GLY:N | 2.47 | 0.48 |
| 1:C:291:GLY:N | 1:C:294:LYS:NZ | 2.60 | 0.48 |
| 1:C:417:LYS:HG2 | 1:C:456:GLN:NE2 | 2.25 | 0.48 |
| 1:C:534:ASN:CB | 1:C:537:ILE:HA | 2.43 | 0.48 |
| 1:C:571:HIS:HA | 1:C:574:ARG:CG | 2.40 | 0.48 |
| 1:C:586:ALA:O | 1:C:587:ILE:C | 2.56 | 0.48 |
| 1:C:682:VAL:HB | 1:C:722:ILE:HG23 | 1.96 | 0.48 |
| 1:C:705:ASP:O | 1:C:717:ASP:OD2 | 2.32 | 0.48 |
| 1:C:825:ALA:CA | 1:C:828:LEU:HB2 | 2.44 | 0.48 |
| 1:C:839:LYS:NZ | 1:C:881:PRO:N | 2.62 | 0.48 |
| 1:D:193:ILE:HG12 | 1:D:222:ILE:HD12 | 1.96 | 0.48 |
| 1:D:362:HIS:CD2 | 1:D:363:HIS:ND1 | 2.82 | 0.48 |
| 1:D:452:GLU:HA | 1:D:455:LEU:HD12 | 1.94 | 0.48 |
| 1:D:566:ASN:O | 1:D:570:ILE:HG13 | 2.14 | 0.48 |
| 1:D:640:ARG:HG2 | 1:D:640:ARG:HH11 | 1.79 | 0.48 |
| 1:D:708:ILE:CG1 | 1:D:716:ILE:HB | 2.44 | 0.48 |
| 1:D:845:LEU:HG | 1:D:846:LYS:HG3 | 1.95 | 0.48 |
| 1:E:376:ALA:HA | 1:E:395:LEU:HD11 | 1.96 | 0.48 |
| 1:E:541:VAL:HB | 1:E:545:THR:HG1 | 1.77 | 0.48 |
| 1:E:584:MET:HA | 1:E:587:ILE:HD12 | 1.94 | 0.48 |
| 1:E:612:PHE:HA | 1:E:771:ILE:HG13 | 1.94 | 0.48 |
| 1:E:622:GLU:CA | 1:E:625:LYS:HD3 | 2.43 | 0.48 |
| 1:E:723:VAL:HG13 | 1:E:724:ILE:O | 2.13 | 0.48 |
| 1:E:775:LEU:HD23 | 1:E:775:LEU:HA | 1.54 | 0.48 |
| 1:E:823:MET:O | 1:E:826:ARG:HG2 | 2.13 | 0.48 |
| 1:F:193:ILE:CG2 | 1:F:225:VAL:HG22 | 2.44 | 0.48 |
| 1:F:286:ILE:HG22 | 1:F:289:LEU:HD12 | 1.96 | 0.48 |
| 1:F:287:HIS:HD2 | 1:F:316:THR:HG21 | 1.78 | 0.48 |
| 1:F:348:THR:C | 1:F:351:ILE:HB | 2.38 | 0.48 |
| 1:F:637:MET:HB3 | 1:F:682:VAL:N | 2.28 | 0.48 |
| 1:F:702:MET:HE3 | 1:F:708:ILE:HG12 | 1.94 | 0.48 |
| 1:A:194:ARG:HA | 1:A:197:ILE:HB | 1.95 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:213:GLU:HB2 | 1:A:218:LYS:HZ1 | 1.75 | 0.48 |
| 1:A:234:VAL:CG1 | 1:A:238:LEU:HB2 | 2.44 | 0.48 |
| 1:A:258:LYS:NZ | 1:A:295:ASP:CG | 2.72 | 0.48 |
| 1:A:262:GLU:HB3 | 1:A:266:LYS:CB | 2.43 | 0.48 |
| 1:A:344:SER:OG | 1:A:345:VAL:N | 2.47 | 0.48 |
| 1:A:373:VAL:O | 1:A:376:ALA:N | 2.38 | 0.48 |
| 1:A:563:GLU:HA | 1:A:568:LYS:HB3 | 1.95 | 0.48 |
| 1:A:641:VAL:HG21 | 1:A:683:LEU:HD21 | 1.96 | 0.48 |
| 1:A:659:THR:HA | 1:A:667:GLU:HB3 | 1.96 | 0.48 |
| 1:B:199:VAL:HG12 | 1:B:206:SER:O | 2.13 | 0.48 |
| 1:B:285:GLU:CD | 1:B:287:HIS:ND1 | 2.71 | 0.48 |
| 1:B:394:ASP:O | 1:B:398:ILE:HB | 2.14 | 0.48 |
| 1:B:646:LEU:H | 1:B:691:ALA:CA | 2.27 | 0.48 |
| 1:B:704:ASP:O | 1:B:707:ARG:HG2 | 2.13 | 0.48 |
| 1:B:831:LEU:O | 1:B:834:ASN:N | 2.47 | 0.48 |
| 1:C:60:TYR:H | 1:C:136:ASP:N | 2.12 | 0.48 |
| 1:C:288:MET:HE2 | 1:C:288:MET:HB3 | 1.71 | 0.48 |
| 1:C:568:LYS:O | 1:C:569:LEU:C | 2.57 | 0.48 |
| 1:C:577:SER:O | 1:C:581:VAL:HG23 | 2.13 | 0.48 |
| 1:C:834:ASN:HA | 1:C:837:LEU:CD2 | 2.43 | 0.48 |
| 1:D:177:GLN:CD | 1:D:183:LEU:HG | 2.38 | 0.48 |
| 1:D:192:GLU:CG | 1:D:193:ILE:N | 2.76 | 0.48 |
| 1:D:213:GLU:HB3 | 1:D:387:ARG:HD2 | 1.96 | 0.48 |
| 1:D:395:LEU:HA | 1:D:398:ILE:HD12 | 1.95 | 0.48 |
| 1:D:419:ARG:O | 1:D:423:LEU:HD12 | 2.14 | 0.48 |
| 1:D:611:LEU:H | 1:D:769:ILE:CA | 2.25 | 0.48 |
| 1:D:833:GLN:O | 1:D:836:ILE:N | 2.47 | 0.48 |
| 1:D:834:ASN:O | 1:D:835:GLU:C | 2.54 | 0.48 |
| 1:E:202:ARG:NH1 | 1:E:336:GLN:HE21 | 2.11 | 0.48 |
| 1:E:347:GLN:N | 1:E:347:GLN:OE1 | 2.24 | 0.48 |
| 1:F:211:ILE:HG13 | 1:F:337:LYS:HD2 | 1.96 | 0.48 |
| 1:F:581:VAL:HG12 | 1:F:582:GLY:N | 2.23 | 0.48 |
| 1:F:638:MET:HB2 | 1:F:681:SER:HB2 | 1.95 | 0.48 |
| 1:F:760:PRO:O | 1:F:763:LEU:N | 2.47 | 0.48 |
| 1:F:802:TYR:C | 1:F:803:LYS:HG2 | 2.39 | 0.48 |
| 1:A:247:ASP:OD2 | 1:A:284:ASP:HB2 | 2.13 | 0.48 |
| 1:A:549:THR:HA | 1:A:552:ARG:HH12 | 1.76 | 0.48 |
| 1:A:655:LEU:O | 1:A:672:THR:OG1 | 2.31 | 0.48 |
| 1:A:659:THR:HG22 | 1:A:660:ALA:N | 2.27 | 0.48 |
| 1:B:187:ILE:H | 1:B:351:ILE:CD1 | 2.26 | 0.48 |
| 1:B:214:PRO:C | 1:B:218:LYS:H | 2.22 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:244:PHE:CE2 | 1:B:281:LEU:O | 2.67 | 0.48 |
| 1:B:607:PRO:HB3 | 1:B:722:ILE:HG12 | 1.95 | 0.48 |
| 1:B:610:PHE:C | 1:B:724:ILE:HG21 | 2.39 | 0.48 |
| 1:B:646:LEU:CD1 | 1:B:690:LYS:HZ3 | 2.26 | 0.48 |
| 1:B:674:GLN:O | 1:B:675:LEU:C | 2.57 | 0.48 |
| 1:B:761:GLU:CD | 1:B:762:PHE:H | 2.22 | 0.48 |
| 1:B:775:LEU:HB3 | 1:B:779:ALA:HB3 | 1.95 | 0.48 |
| 1:B:785:ASP:HA | 1:B:788:LEU:HD11 | 1.94 | 0.48 |
| 1:B:805:ASN:ND2 | 1:B:855:VAL:O | 2.47 | 0.48 |
| 1:C:211:ILE:CG2 | 1:C:316:THR:H | 2.26 | 0.48 |
| 1:C:228:ARG:HH22 | 1:D:409:SER:CB | 2.26 | 0.48 |
| 1:C:345:VAL:C | 1:C:348:THR:H | 2.22 | 0.48 |
| 1:C:397:ASP:O | 1:C:400:CYS:N | 2.46 | 0.48 |
| 1:C:400:CYS:O | 1:C:403:VAL:HB | 2.13 | 0.48 |
| 1:C:570:ILE:O | 1:C:573:GLU:HB3 | 2.13 | 0.48 |
| 1:C:652:VAL:HG12 | 1:C:654:LYS:HG2 | 1.94 | 0.48 |
| 1:C:739:GLY:C | 1:C:774:LYS:HD2 | 2.39 | 0.48 |
| 1:C:767:SER:CA | 1:D:830:ARG:NH1 | 2.72 | 0.48 |
| 1:C:786:ILE:CA | 1:C:789:LYS:HZ3 | 2.26 | 0.48 |
| 1:C:809:GLU:HG2 | 1:C:810:ALA:N | 2.29 | 0.48 |
| 1:D:245:SER:HA | 1:D:282:PHE:HB3 | 1.95 | 0.48 |
| 1:D:317:THR:CG2 | 1:D:321:TYR:CZ | 2.93 | 0.48 |
| 1:D:367:ILE:HG22 | 1:D:369:ASP:N | 2.29 | 0.48 |
| 1:D:530:ARG:HH12 | 1:D:537:ILE:CA | 2.26 | 0.48 |
| 1:D:577:SER:O | 1:D:580:VAL:HB | 2.14 | 0.48 |
| 1:E:285:GLU:HG2 | 1:E:288:MET:HB3 | 1.96 | 0.48 |
| 1:E:585:ASP:O | 1:E:588:LYS:N | 2.46 | 0.48 |
| 1:E:695:VAL:O | 1:E:698:VAL:N | 2.47 | 0.48 |
| 1:E:785:ASP:CG | 1:E:789:LYS:HZ1 | 2.22 | 0.48 |
| 1:E:800:LYS:HE2 | 1:E:850:LYS:HB3 | 1.95 | 0.48 |
| 1:E:837:LEU:O | 1:E:840:LEU:HB2 | 2.14 | 0.48 |
| 1:F:261:PHE:CD2 | 1:F:297:ALA:HA | 2.49 | 0.48 |
| 1:F:569:LEU:HD23 | 1:F:594:VAL:HG12 | 1.96 | 0.48 |
| 1:F:674:GLN:HA | 1:F:677:TYR:HD2 | 1.78 | 0.48 |
| 1:F:778:LYS:HG3 | 1:F:779:ALA:N | 2.29 | 0.48 |
| 1:A:213:GLU:O | 1:A:215:GLY:N | 2.44 | 0.48 |
| 1:A:274:GLU:CA | 1:A:276:LYS:NZ | 2.77 | 0.48 |
| 1:A:294:LYS:HA | 1:A:299:ASN:ND2 | 2.29 | 0.48 |
| 1:A:613:LEU:HD22 | 1:A:728:ALA:N | 2.29 | 0.48 |
| 1:A:639:ILE:CD1 | 1:A:674:GLN:HB3 | 2.43 | 0.48 |
| 1:A:831:LEU:HD23 | 1:A:831:LEU:C | 2.38 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:247:ASP:OD1 | 1:B:288:MET:HE3 | 2.14 | 0.48 |
| 1:B:331:PHE:HD1 | 1:B:334:ARG:NH2 | 2.11 | 0.48 |
| 1:B:563:GLU:OE2 | 1:B:564:SER:O | 2.31 | 0.48 |
| 1:B:613:LEU:HD11 | 1:B:771:ILE:HG23 | 1.96 | 0.48 |
| 1:B:654:LYS:HZ3 | 1:B:692:HIS:HB3 | 1.78 | 0.48 |
| 1:B:789:LYS:O | 1:B:793:GLU:OE2 | 2.31 | 0.48 |
| 1:C:175:THR:N | 1:C:242:LYS:HE2 | 2.26 | 0.48 |
| 1:C:217:GLY:HA2 | 2:C:1001:AGS:O3A | 2.14 | 0.48 |
| 1:C:395:LEU:O | 1:C:396:VAL:C | 2.56 | 0.48 |
| 1:C:410:LYS:HD3 | 1:C:470:LYS:HZ2 | 1.79 | 0.48 |
| 1:C:548:GLU:N | 1:C:548:GLU:CD | 2.71 | 0.48 |
| 1:C:696:LEU:CA | 1:C:699:MET:HG2 | 2.43 | 0.48 |
| 1:C:839:LYS:HZ1 | 1:C:880:LEU:CA | 2.27 | 0.48 |
| 1:D:183:LEU:HA | 1:D:183:LEU:HD23 | 1.73 | 0.48 |
| 1:D:285:GLU:OE1 | 1:D:321:TYR:HE1 | 1.97 | 0.48 |
| 1:D:285:GLU:OE2 | 1:D:315:ALA:HB3 | 2.13 | 0.48 |
| 1:D:684:LEU:HA | 1:D:725:MET:CG | 2.43 | 0.48 |
| 1:D:728:ALA:HB1 | 1:D:734:ILE:HD13 | 1.94 | 0.48 |
| 1:D:855:VAL:HG23 | 1:D:880:LEU:HD13 | 1.94 | 0.48 |
| 1:D:859:LEU:C | 1:D:878:GLU:H | 2.19 | 0.48 |
| 1:E:428:ILE:O | 1:E:445:LEU:HD11 | 2.14 | 0.48 |
| 1:E:522:ASP:C | 1:E:526:GLU:HG2 | 2.39 | 0.48 |
| 1:E:543:SER:O | 1:E:546:ILE:HG12 | 2.14 | 0.48 |
| 1:E:551:ALA:HA | 1:E:555:GLY:N | 2.29 | 0.48 |
| 1:E:622:GLU:O | 1:E:625:LYS:HB2 | 2.14 | 0.48 |
| 1:E:745:SER:N | 1:E:747:LYS:NZ | 2.62 | 0.48 |
| 1:E:758:PHE:O | 1:E:762:PHE:HB3 | 2.13 | 0.48 |
| 1:F:202:ARG:HD2 | 1:F:206:SER:C | 2.39 | 0.48 |
| 1:F:205:LYS:HZ3 | 1:F:333:ARG:C | 2.21 | 0.48 |
| 1:F:265:PHE:HZ | 1:F:305:LEU:HD22 | 1.79 | 0.48 |
| 1:F:294:LYS:HG3 | 1:F:325:VAL:CG1 | 2.44 | 0.48 |
| 1:F:839:LYS:HZ2 | 1:F:879:VAL:HA | 1.78 | 0.48 |
| 1:A:173:ASP:HA | 1:A:244:PHE:C | 2.39 | 0.48 |
| 1:A:283:ILE:N | 1:A:312:VAL:HG23 | 2.22 | 0.48 |
| 1:A:316:THR:OG1 | 1:A:317:THR:N | 2.47 | 0.48 |
| 1:A:549:THR:CA | 1:A:552:ARG:NH1 | 2.72 | 0.48 |
| 1:A:610:PHE:HB3 | 1:A:767:SER:OG | 2.14 | 0.48 |
| 1:A:625:LYS:C | 1:A:628:ALA:H | 2.21 | 0.48 |
| 1:A:685:PHE:HB2 | 1:A:725:MET:CG | 2.39 | 0.48 |
| 1:A:693:PRO:C | 1:A:696:LEU:HD11 | 2.39 | 0.48 |
| 1:A:751:MET:HG2 | 1:A:751:MET:O | 2.14 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:173:ASP:OD1 | 1:B:173:ASP:O | 2.31 | 0.48 |
| 1:B:298:ALA:O | 1:B:302:LYS:HB2 | 2.14 | 0.48 |
| 1:B:319:ASN:O | 1:B:322:ARG:N | 2.46 | 0.48 |
| 1:B:704:ASP:CB | 1:B:707:ARG:HH11 | 2.27 | 0.48 |
| 1:C:183:LEU:HA | 1:C:183:LEU:HD23 | 1.65 | 0.48 |
| 1:C:193:ILE:O | 1:C:196:THR:N | 2.47 | 0.48 |
| 1:C:211:ILE:HG13 | 1:C:340:VAL:CG1 | 2.44 | 0.48 |
| 1:C:281:LEU:CD2 | 1:C:311:LYS:H | 2.27 | 0.48 |
| 1:C:321:TYR:CE1 | 1:C:331:PHE:CZ | 3.01 | 0.48 |
| 1:C:500:ALA:O | 1:C:504:ASP:HB2 | 2.14 | 0.48 |
| 1:C:698:VAL:O | 1:C:701:GLN:HB3 | 2.14 | 0.48 |
| 1:C:751:MET:HA | 1:C:755:ARG:NH1 | 2.28 | 0.48 |
| 1:D:172:ILE:N | 1:D:245:SER:H | 2.11 | 0.48 |
| 1:D:179:ARG:NH2 | 1:D:230:ILE:HG21 | 2.26 | 0.48 |
| 1:D:195:SER:O | 1:D:196:THR:C | 2.56 | 0.48 |
| 1:D:196:THR:HA | 1:D:199:VAL:HB | 1.96 | 0.48 |
| 1:D:213:GLU:HG2 | 1:D:387:ARG:CZ | 2.44 | 0.48 |
| 1:D:235:PRO:HG3 | 1:E:408:ASP:CA | 2.44 | 0.48 |
| 1:D:333:ARG:NH2 | 2:E:1001:AGS:O1B | 2.47 | 0.48 |
| 1:D:403:VAL:O | 1:D:406:ALA:N | 2.47 | 0.48 |
| 1:D:507:TYR:HE1 | 1:E:425:GLN:O | 1.97 | 0.48 |
| 1:D:752:GLY:HA2 | 1:D:755:ARG:NE | 2.29 | 0.48 |
| 1:D:853:GLU:HG2 | 1:D:854:THR:OG1 | 2.13 | 0.48 |
| 1:E:206:SER:C | 1:E:311:LYS:NZ | 2.66 | 0.48 |
| 1:E:282:PHE:HB2 | 1:E:313:ILE:O | 2.14 | 0.48 |
| 1:E:285:GLU:O | 1:E:286:ILE:C | 2.56 | 0.48 |
| 1:E:318:ASN:C | 1:E:322:ARG:HH12 | 2.22 | 0.48 |
| 1:E:332:GLU:CD | 1:E:337:LYS:HG3 | 2.38 | 0.48 |
| 1:E:394:ASP:O | 1:E:395:LEU:C | 2.55 | 0.48 |
| 1:E:409:SER:HA | 1:E:470:LYS:NZ | 2.29 | 0.48 |
| 1:E:612:PHE:O | 1:E:613:LEU:HB2 | 2.14 | 0.48 |
| 1:E:613:LEU:CG | 1:E:728:ALA:HA | 2.43 | 0.48 |
| 1:E:668:GLY:CA | 1:E:672:THR:H | 2.27 | 0.48 |
| 1:E:786:ILE:HG13 | 1:E:789:LYS:HZ3 | 1.78 | 0.48 |
| 1:E:802:TYR:HD1 | 1:E:852:LYS:HG2 | 1.78 | 0.48 |
| 1:E:826:ARG:NH2 | 2:E:1002:AGS:H1' | 2.28 | 0.48 |
| 1:F:403:VAL:O | 1:F:407:ARG:N | 2.33 | 0.48 |
| 1:F:645:GLU:OE1 | 1:F:645:GLU:N | 2.37 | 0.48 |
| 1:A:166:TYR:CZ | 1:A:170:TYR:CE2 | 3.02 | 0.47 |
| 1:A:287:HIS:CG | 1:A:290:MET:HB2 | 2.49 | 0.47 |
| 1:A:346:ARG:HH11 | 1:A:349:VAL:CG1 | 2.27 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:621:THR:OG1 | 1:A:622:GLU:N | 2.46 | 0.47 |
| 1:A:709:THR:HG22 | 1:A:710:SER:N | 2.28 | 0.47 |
| 1:A:828:LEU:CD1 | 1:A:831:LEU:HD22 | 2.44 | 0.47 |
| 1:A:835:GLU:OE1 | 1:A:835:GLU:N | 2.36 | 0.47 |
| 1:B:209:CYS:CB | 1:B:315:ALA:HB2 | 2.35 | 0.47 |
| 1:B:255:ALA:O | 1:B:256:LYS:C | 2.57 | 0.47 |
| 1:B:265:PHE:CA | 1:B:268:VAL:HB | 2.40 | 0.47 |
| 1:B:543:SER:O | 1:B:544:ASP:HB3 | 2.13 | 0.47 |
| 1:B:571:HIS:O | 1:B:574:ARG:HB2 | 2.13 | 0.47 |
| 1:B:606:GLN:HA | 1:B:705:ASP:O | 2.14 | 0.47 |
| 1:C:342:GLU:OE2 | 1:C:389:PRO:CD | 2.62 | 0.47 |
| 1:C:465:ARG:HA | 1:C:468:GLU:HB3 | 1.96 | 0.47 |
| 1:C:606:GLN:HE22 | 1:C:704:ASP:CA | 2.26 | 0.47 |
| 1:C:801:HIS:ND1 | 1:C:851:ASP:CG | 2.72 | 0.47 |
| 1:C:813:PHE:HA | 1:C:816:LYS:HB3 | 1.96 | 0.47 |
| 1:C:833:GLN:CA | 1:C:836:ILE:HG12 | 2.42 | 0.47 |
| 1:D:190:GLU:CG | 1:D:191:GLU:N | 2.77 | 0.47 |
| 1:D:333:ARG:CZ | 2:E:1001:AGS:O3G | 2.61 | 0.47 |
| 1:D:349:VAL:HG12 | 1:D:353:ARG:HG2 | 1.96 | 0.47 |
| 1:D:752:GLY:HA2 | 1:D:755:ARG:HE | 1.79 | 0.47 |
| 1:D:769:ILE:C | 1:D:770:VAL:HG23 | 2.39 | 0.47 |
| 1:D:800:LYS:NZ | 1:D:801:HIS:CE1 | 2.82 | 0.47 |
| 1:D:828:LEU:O | 1:D:832:ILE:HG13 | 2.14 | 0.47 |
| 1:D:836:ILE:O | 1:D:840:LEU:HG | 2.14 | 0.47 |
| 1:E:230:ILE:CG2 | 1:E:495:ARG:HE | 2.27 | 0.47 |
| 1:E:284:ASP:CA | 1:E:315:ALA:H | 2.27 | 0.47 |
| 1:E:369:ASP:C | 1:E:369:ASP:OD1 | 2.56 | 0.47 |
| 1:E:377:GLN:O | 1:E:380:LYS:HB3 | 2.13 | 0.47 |
| 1:E:420:GLN:HA | 1:E:423:LEU:HD12 | 1.94 | 0.47 |
| 1:E:566:ASN:O | 1:E:570:ILE:HG23 | 2.14 | 0.47 |
| 1:F:242:LYS:HZ3 | 1:F:277:THR:CG2 | 2.23 | 0.47 |
| 1:F:285:GLU:HA | 1:F:315:ALA:H | 1.79 | 0.47 |
| 1:F:378:LEU:O | 1:F:381:ARG:O | 2.31 | 0.47 |
| 1:F:382:TYR:CD2 | 1:F:383:LEU:HG | 2.49 | 0.47 |
| 1:F:670:PHE:O | 1:F:673:ASN:N | 2.47 | 0.47 |
| 1:F:785:ASP:C | 1:F:789:LYS:HZ3 | 2.22 | 0.47 |
| 1:F:831:LEU:HA | 1:F:834:ASN:OD1 | 2.12 | 0.47 |
| 1:F:878:GLU:H | 1:F:878:GLU:CD | 2.16 | 0.47 |
| 1:A:625:LYS:O | 1:A:629:GLY:N | 2.47 | 0.47 |
| 1:A:640:ARG:HA | 1:A:684:LEU:CG | 2.37 | 0.47 |
| 1:A:793:GLU:OE1 | 1:A:793:GLU:N | 2.47 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:236:THR:OG1 | 1:B:237:ILE:HG23 | 2.14 | 0.47 |
| 1:B:286:ILE:HG13 | 1:B:320:GLU:CG | 2.44 | 0.47 |
| 1:B:323:SER:CB | 1:B:327:LYS:NZ | 2.77 | 0.47 |
| 1:B:361:ILE:O | 1:B:364:GLY:N | 2.47 | 0.47 |
| 1:B:583:GLN:HE21 | 1:B:773:ASN:N | 2.12 | 0.47 |
| 1:B:618:SER:OG | 1:B:619:GLY:N | 2.40 | 0.47 |
| 1:B:785:ASP:OD1 | 1:B:785:ASP:N | 2.43 | 0.47 |
| 1:B:804:LEU:HA | 1:B:855:VAL:CG2 | 2.40 | 0.47 |
| 1:C:168:SER:CA | 1:C:271:GLU:CD | 2.77 | 0.47 |
| 1:C:276:LYS:HB2 | 1:C:276:LYS:HE2 | 1.55 | 0.47 |
| 1:C:385:TYR:HE2 | 1:C:386:ARG:CZ | 2.27 | 0.47 |
| 1:C:681:SER:OG | 1:C:682:VAL:O | 2.28 | 0.47 |
| 1:C:843:ARG:HA | 1:C:846:LYS:H | 1.79 | 0.47 |
| 1:D:208:PRO:HA | 1:D:336:GLN:O | 2.13 | 0.47 |
| 1:D:592:ASN:O | 1:D:593:ALA:C | 2.57 | 0.47 |
| 1:D:645:GLU:O | 1:D:646:LEU:HB3 | 2.13 | 0.47 |
| 1:D:692:HIS:HE1 | 1:D:694:ASP:HB2 | 1.79 | 0.47 |
| 1:D:710:SER:HB3 | 1:D:714:LYS:HB3 | 1.96 | 0.47 |
| 1:D:795:PHE:N | 1:D:795:PHE:CD1 | 2.82 | 0.47 |
| 1:D:810:ALA:O | 1:D:811:LYS:C | 2.57 | 0.47 |
| 1:D:835:GLU:CD | 1:D:839:LYS:HE2 | 2.39 | 0.47 |
| 1:E:172:ILE:HB | 1:E:245:SER:HB3 | 1.96 | 0.47 |
| 1:E:173:ASP:O | 1:E:173:ASP:CG | 2.58 | 0.47 |
| 1:E:440:THR:HA | 1:E:443:ASP:HB2 | 1.97 | 0.47 |
| 1:E:484:ASP:O | 1:E:488:ASN:N | 2.33 | 0.47 |
| 1:E:486:LEU:HD23 | 1:E:489:LYS:CE | 2.44 | 0.47 |
| 1:E:676:GLN:CG | 1:E:677:TYR:N | 2.77 | 0.47 |
| 1:E:680:TYR:HA | 1:E:720:ASN:CB | 2.44 | 0.47 |
| 1:E:872:GLU:N | 1:E:875:GLU:HB3 | 2.28 | 0.47 |
| 1:F:785:ASP:O | 1:F:789:LYS:N | 2.26 | 0.47 |
| 1:A:563:GLU:HB3 | 1:A:568:LYS:NZ | 2.30 | 0.47 |
| 1:A:612:PHE:HB2 | 1:A:771:ILE:CA | 2.44 | 0.47 |
| 1:B:180:GLN:HG3 | 1:B:182:LYS:HZ2 | 1.78 | 0.47 |
| 1:B:245:SER:C | 1:B:246:LEU:HD12 | 2.38 | 0.47 |
| 1:B:254:GLY:N | 1:B:260:ASP:OD2 | 2.47 | 0.47 |
| 1:B:321:TYR:CZ | 1:B:325:VAL:HG21 | 2.49 | 0.47 |
| 1:B:354:GLY:O | 1:B:357:PRO:HD2 | 2.13 | 0.47 |
| 1:B:544:ASP:CA | 1:B:560:LYS:HZ1 | 2.27 | 0.47 |
| 1:B:607:PRO:HA | 1:B:722:ILE:HD11 | 1.97 | 0.47 |
| 1:B:713:GLY:O | 1:B:715:THR:HG23 | 2.14 | 0.47 |
| 1:B:744:GLU:N | 1:B:747:LYS:HE3 | 2.28 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:177:GLN:O | 1:C:182:LYS:HD2 | 2.14 | 0.47 |
| 1:C:207:ASN:OD1 | 1:C:207:ASN:C | 2.57 | 0.47 |
| 1:C:220:ALA:C | 1:C:223:GLU:OE1 | 2.57 | 0.47 |
| 1:C:255:ALA:CB | 1:C:256:LYS:HZ3 | 2.26 | 0.47 |
| 1:C:286:ILE:O | 1:C:290:MET:HE2 | 2.14 | 0.47 |
| 1:C:370:SER:OG | 1:C:371:ALA:N | 2.47 | 0.47 |
| 1:C:459:LEU:HA | 1:C:462:LEU:HB2 | 1.96 | 0.47 |
| 1:C:542:ASP:CG | 1:C:543:SER:N | 2.70 | 0.47 |
| 1:C:588:LYS:O | 1:C:589:ALA:C | 2.55 | 0.47 |
| 1:C:603:ASN:CG | 1:C:605:ARG:HG2 | 2.38 | 0.47 |
| 1:C:828:LEU:O | 1:C:829:ASN:C | 2.55 | 0.47 |
| 1:D:369:ASP:OD1 | 1:D:369:ASP:C | 2.58 | 0.47 |
| 1:D:406:ALA:O | 1:D:412:GLU:HB2 | 2.14 | 0.47 |
| 1:D:469:GLU:OE1 | 1:D:535:SER:N | 2.48 | 0.47 |
| 1:E:265:PHE:O | 1:E:268:VAL:HB | 2.15 | 0.47 |
| 1:E:269:LEU:O | 1:E:272:ILE:HB | 2.15 | 0.47 |
| 1:E:403:VAL:O | 1:E:406:ALA:HB3 | 2.14 | 0.47 |
| 1:E:671:LEU:O | 1:E:675:LEU:HB2 | 2.14 | 0.47 |
| 1:E:701:GLN:HE21 | 1:E:708:ILE:N | 2.11 | 0.47 |
| 1:E:740:SER:OG | 1:E:741:LYS:N | 2.47 | 0.47 |
| 1:E:786:ILE:CA | 1:E:789:LYS:NZ | 2.77 | 0.47 |
| 1:E:859:LEU:C | 1:E:877:LEU:H | 2.22 | 0.47 |
| 1:F:175:THR:HB | 1:F:230:ILE:HD11 | 1.94 | 0.47 |
| 1:F:285:GLU:HA | 1:F:315:ALA:C | 2.38 | 0.47 |
| 1:F:294:LYS:HG3 | 1:F:325:VAL:HG12 | 1.95 | 0.47 |
| 1:F:360:GLU:OE1 | 1:F:367:ILE:CG2 | 2.62 | 0.47 |
| 1:F:812:ASP:CB | 1:F:816:LYS:NZ | 2.76 | 0.47 |
| 1:A:205:LYS:CE | 1:B:398:ILE:HG13 | 2.45 | 0.47 |
| 1:A:262:GLU:CG | 1:A:301:LEU:HD13 | 2.44 | 0.47 |
| 1:B:189:ARG:C | 1:B:192:GLU:OE1 | 2.58 | 0.47 |
| 1:B:272:ILE:HG12 | 1:B:279:ILE:O | 2.14 | 0.47 |
| 1:B:610:PHE:CD1 | 1:B:767:SER:HB2 | 2.49 | 0.47 |
| 1:B:640:ARG:HA | 1:B:684:LEU:HD13 | 1.97 | 0.47 |
| 1:B:693:PRO:CD | 1:B:694:ASP:N | 2.78 | 0.47 |
| 1:B:709:THR:CA | 1:B:715:THR:HG22 | 2.45 | 0.47 |
| 1:B:843:ARG:CZ | 1:B:848:GLU:OE2 | 2.57 | 0.47 |
| 1:C:168:SER:CB | 1:C:264:ARG:HE | 2.27 | 0.47 |
| 1:C:281:LEU:N | 1:C:311:LYS:O | 2.42 | 0.47 |
| 1:C:300:ILE:HG23 | 1:D:248:LEU:HD11 | 1.97 | 0.47 |
| 1:C:417:LYS:CE | 1:C:459:LEU:HB3 | 2.45 | 0.47 |
| 1:C:472:GLY:O | 1:C:475:GLU:HG2 | 2.14 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:610:PHE:HA | 1:C:768:SER:HB3 | 1.96 | 0.47 |
| 1:D:162:THR:O | 1:D:165:GLU:OE2 | 2.33 | 0.47 |
| 1:D:228:ARG:HA | 1:D:231:ASP:HB2 | 1.95 | 0.47 |
| 1:D:241:ALA:C | 1:D:278:LEU:HD23 | 2.39 | 0.47 |
| 1:D:357:PRO:O | 1:D:360:GLU:HB2 | 2.13 | 0.47 |
| 1:D:537:ILE:HA | 1:D:540:VAL:HG12 | 1.97 | 0.47 |
| 1:D:829:ASN:O | 1:D:832:ILE:HB | 2.14 | 0.47 |
| 1:E:303:PRO:HB2 | 1:E:307:ARG:NH2 | 2.29 | 0.47 |
| 1:E:424:ILE:HG21 | 1:E:448:ALA:C | 2.39 | 0.47 |
| 1:E:614:GLY:H | 1:E:728:ALA:HB1 | 1.78 | 0.47 |
| 1:E:634:ASP:OD1 | 1:E:636:ASP:OD2 | 2.32 | 0.47 |
| 1:E:785:ASP:CG | 1:E:789:LYS:NZ | 2.72 | 0.47 |
| 1:E:848:GLU:O | 1:E:849:ILE:HD13 | 2.15 | 0.47 |
| 1:F:166:TYR:CZ | 1:F:263:GLU:OE2 | 2.67 | 0.47 |
| 1:F:202:ARG:HH12 | 1:F:208:PRO:CG | 2.28 | 0.47 |
| 1:F:236:THR:O | 1:F:239:GLN:HB2 | 2.14 | 0.47 |
| 1:F:859:LEU:HB2 | 1:F:876:CYS:CB | 2.44 | 0.47 |
| 1:A:236:THR:O | 1:A:239:GLN:CD | 2.57 | 0.47 |
| 1:A:286:ILE:CD1 | 1:A:321:TYR:HD2 | 2.27 | 0.47 |
| 1:A:544:ASP:HA | 1:A:548:GLU:CG | 2.44 | 0.47 |
| 1:A:579:GLU:OE2 | 1:A:580:VAL:HG23 | 2.14 | 0.47 |
| 1:A:597:SER:OG | 1:A:598:ARG:N | 2.46 | 0.47 |
| 1:A:785:ASP:CG | 1:A:789:LYS:NZ | 2.72 | 0.47 |
| 1:B:174:MET:H | 1:B:177:GLN:NE2 | 2.13 | 0.47 |
| 1:B:185:PRO:HB3 | 1:B:227:GLN:HE22 | 1.80 | 0.47 |
| 1:B:204:ILE:HG22 | 1:B:205:LYS:H | 1.80 | 0.47 |
| 1:B:344:SER:N | 1:B:347:GLN:HE22 | 2.13 | 0.47 |
| 1:B:353:ARG:NE | 1:B:369:ASP:HB2 | 2.30 | 0.47 |
| 1:B:647:SER:H | 1:B:690:LYS:C | 2.22 | 0.47 |
| 1:B:759:ARG:HG3 | 1:B:761:GLU:OE2 | 2.14 | 0.47 |
| 1:C:46:GLY:O | 1:C:50:TYR:N | 2.48 | 0.47 |
| 1:C:217:GLY:HA2 | 2:C:1001:AGS:H4' | 1.95 | 0.47 |
| 1:C:229:ILE:C | 1:C:232:ASP:H | 2.22 | 0.47 |
| 1:C:247:ASP:CG | 1:C:248:LEU:HB2 | 2.39 | 0.47 |
| 1:C:286:ILE:HA | 1:C:289:LEU:CB | 2.42 | 0.47 |
| 1:C:479:ALA:HB1 | 1:C:516:GLN:HE21 | 1.79 | 0.47 |
| 1:C:650:TYR:CZ | 1:C:652:VAL:O | 2.68 | 0.47 |
| 1:C:656:LEU:O | 1:C:668:GLY:HA3 | 2.14 | 0.47 |
| 1:C:787:ARG:HH12 | 1:C:826:ARG:HH21 | 1.58 | 0.47 |
| 1:D:190:GLU:HG2 | 1:D:194:ARG:NE | 2.28 | 0.47 |
| 1:D:191:GLU:OE2 | 1:D:194:ARG:CZ | 2.56 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:343:PRO:HA | 1:D:347:GLN:NE2 | 2.30 | 0.47 |
| 1:D:350:ALA:O | 1:D:353:ARG:HB2 | 2.15 | 0.47 |
| 1:D:393:LEU:O | 1:D:394:ASP:C | 2.57 | 0.47 |
| 1:D:456:GLN:HG3 | 1:D:459:LEU:CD1 | 2.41 | 0.47 |
| 1:D:580:VAL:N | 1:D:626:LYS:NZ | 2.63 | 0.47 |
| 1:D:748:ASN:HA | 1:D:751:MET:CE | 2.43 | 0.47 |
| 1:D:839:LYS:O | 1:D:842:LEU:HB3 | 2.15 | 0.47 |
| 1:E:166:TYR:HB3 | 1:E:169:LYS:CG | 2.44 | 0.47 |
| 1:E:189:ARG:HB2 | 1:E:193:ILE:HD11 | 1.95 | 0.47 |
| 1:E:190:GLU:O | 1:E:193:ILE:N | 2.48 | 0.47 |
| 1:E:193:ILE:O | 1:E:194:ARG:C | 2.58 | 0.47 |
| 1:E:222:ILE:O | 1:E:226:ALA:N | 2.22 | 0.47 |
| 1:E:228:ARG:HH12 | 1:E:231:ASP:C | 2.22 | 0.47 |
| 1:E:256:LYS:HZ1 | 1:E:264:ARG:CG | 2.28 | 0.47 |
| 1:E:301:LEU:O | 1:E:302:LYS:C | 2.56 | 0.47 |
| 1:E:543:SER:O | 1:E:544:ASP:C | 2.58 | 0.47 |
| 1:E:628:ALA:HA | 1:E:631:LEU:HD12 | 1.97 | 0.47 |
| 1:F:363:HIS:CE1 | 1:F:397:ASP:N | 2.82 | 0.47 |
| 1:F:642:ASP:O | 1:F:645:GLU:OE2 | 2.31 | 0.47 |
| 1:F:702:MET:CE | 1:F:708:ILE:HG12 | 2.44 | 0.47 |
| 1:F:832:ILE:HA | 1:F:835:GLU:CD | 2.37 | 0.47 |
| 1:A:227:GLN:HG3 | 1:A:228:ARG:N | 2.27 | 0.47 |
| 1:A:643:CYS:SG | 1:A:688:VAL:HB | 2.54 | 0.47 |
| 1:A:675:LEU:HB3 | 1:A:716:ILE:HG21 | 1.96 | 0.47 |
| 1:A:872:GLU:OE2 | 1:F:237:ILE:HD13 | 2.14 | 0.47 |
| 1:B:211:ILE:HG23 | 1:B:318:ASN:HA | 1.97 | 0.47 |
| 1:B:583:GLN:O | 1:B:587:ILE:HD12 | 2.15 | 0.47 |
| 1:B:645:GLU:CA | 1:B:691:ALA:HB3 | 2.18 | 0.47 |
| 1:B:663:VAL:HG13 | 1:B:665:TYR:O | 2.15 | 0.47 |
| 1:B:695:VAL:O | 1:B:698:VAL:N | 2.48 | 0.47 |
| 1:B:746:THR:O | 1:B:750:VAL:HG23 | 2.14 | 0.47 |
| 1:B:777:ARG:O | 1:B:780:ILE:N | 2.47 | 0.47 |
| 1:B:807:THR:OG1 | 1:B:809:GLU:N | 2.45 | 0.47 |
| 1:B:824:GLY:O | 1:B:828:LEU:HG | 2.14 | 0.47 |
| 1:B:843:ARG:NH1 | 1:B:848:GLU:HG2 | 2.29 | 0.47 |
| 1:C:217:GLY:N | 2:C:1001:AGS:PB | 2.86 | 0.47 |
| 1:C:370:SER:O | 1:C:372:LEU:N | 2.47 | 0.47 |
| 1:C:673:ASN:HA | 1:C:676:GLN:OE1 | 2.14 | 0.47 |
| 1:C:738:GLN:CD | 1:C:743:GLN:HG2 | 2.39 | 0.47 |
| 1:D:210:LEU:CA | 1:D:316:THR:HG22 | 2.44 | 0.47 |
| 1:D:218:LYS:C | 1:D:221:ILE:HB | 2.40 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:283:ILE:N | 1:D:313:ILE:O | 2.47 | 0.47 |
| 1:D:345:VAL:HG12 | 1:D:346:ARG:N | 2.29 | 0.47 |
| 1:D:672:THR:O | 1:D:673:ASN:C | 2.58 | 0.47 |
| 1:D:799:ASP:OD2 | 1:D:850:LYS:HE3 | 2.15 | 0.47 |
| 1:D:827:PRO:O | 1:D:828:LEU:C | 2.57 | 0.47 |
| 1:E:176:GLU:O | 1:E:180:GLN:N | 2.36 | 0.47 |
| 1:E:187:ILE:HG22 | 1:E:188:GLY:N | 2.29 | 0.47 |
| 1:E:270:LYS:O | 1:E:274:GLU:HG2 | 2.14 | 0.47 |
| 1:E:805:ASN:H | 1:E:854:THR:HA | 1.78 | 0.47 |
| 1:E:851:ASP:CG | 1:E:852:LYS:H | 2.22 | 0.47 |
| 1:F:544:ASP:HA | 1:F:547:SER:HB3 | 1.96 | 0.47 |
| 1:F:629:GLY:HA2 | 1:F:634:ASP:O | 2.14 | 0.47 |
| 1:F:685:PHE:CD1 | 1:F:725:MET:HG3 | 2.48 | 0.47 |
| 1:F:799:ASP:O | 1:F:800:LYS:HD3 | 2.15 | 0.47 |
| 1:A:196:THR:O | 1:A:199:VAL:N | 2.48 | 0.47 |
| 1:A:211:ILE:O | 1:A:211:ILE:HG22 | 2.15 | 0.47 |
| 1:A:211:ILE:HG23 | 1:A:318:ASN:HA | 1.96 | 0.47 |
| 1:A:222:ILE:O | 1:A:225:VAL:HB | 2.14 | 0.47 |
| 1:A:248:LEU:CD1 | 1:A:254:GLY:H | 2.27 | 0.47 |
| 1:A:260:ASP:OD1 | 1:A:264:ARG:HB2 | 2.14 | 0.47 |
| 1:A:324:ILE:HG22 | 1:A:328:ASP:OD1 | 2.15 | 0.47 |
| 1:A:599:SER:HB2 | 1:A:601:LEU:CD1 | 2.45 | 0.47 |
| 1:A:702:MET:SD | 1:A:709:THR:N | 2.86 | 0.47 |
| 1:A:751:MET:HG2 | 1:A:755:ARG:HH12 | 1.78 | 0.47 |
| 1:A:828:LEU:HG | 1:A:832:ILE:HG13 | 1.96 | 0.47 |
| 1:B:174:MET:CG | 1:B:244:PHE:HA | 2.45 | 0.47 |
| 1:B:176:GLU:C | 1:B:178:ALA:N | 2.71 | 0.47 |
| 1:B:195:SER:CB | 1:B:198:ARG:NH1 | 2.77 | 0.47 |
| 1:B:210:LEU:HA | 1:B:339:GLU:HB3 | 1.97 | 0.47 |
| 1:B:211:ILE:C | 1:B:316:THR:O | 2.58 | 0.47 |
| 1:B:296:ASP:OD1 | 1:B:296:ASP:O | 2.32 | 0.47 |
| 1:B:393:LEU:HA | 1:B:396:VAL:CB | 2.40 | 0.47 |
| 1:B:625:LYS:HA | 1:B:635:GLU:HG2 | 1.97 | 0.47 |
| 1:B:654:LYS:HD2 | 1:B:695:VAL:HG23 | 1.97 | 0.47 |
| 1:C:191:GLU:O | 1:C:192:GLU:C | 2.57 | 0.47 |
| 1:C:210:LEU:O | 1:C:338:ILE:HG13 | 2.14 | 0.47 |
| 1:C:243:LEU:HD12 | 1:C:280:VAL:HB | 1.96 | 0.47 |
| 1:C:244:PHE:HB2 | 1:C:246:LEU:HD11 | 1.97 | 0.47 |
| 1:C:275:SER:C | 1:C:276:LYS:HZ3 | 2.23 | 0.47 |
| 1:C:338:ILE:HD12 | 1:C:339:GLU:O | 2.14 | 0.47 |
| 1:C:379:ALA:O | 1:C:380:LYS:C | 2.56 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:515:LYS:O | 1:C:519:LYS:HG2 | 2.15 | 0.47 |
| 1:C:563:GLU:OE2 | 1:C:565:GLU:CD | 2.58 | 0.47 |
| 1:C:611:LEU:HB3 | 1:C:769:ILE:C | 2.39 | 0.47 |
| 1:C:626:LYS:HE3 | 1:C:626:LYS:HB3 | 1.65 | 0.47 |
| 1:C:743:GLN:HB3 | 1:C:745:SER:N | 2.30 | 0.47 |
| 1:C:790:GLU:O | 1:C:791:ILE:C | 2.57 | 0.47 |
| 1:C:799:ASP:N | 1:C:799:ASP:OD1 | 2.46 | 0.47 |
| 1:C:819:TYR:OH | 1:C:821:ASP:HA | 2.15 | 0.47 |
| 1:C:843:ARG:NH1 | 1:C:846:LYS:HE3 | 2.29 | 0.47 |
| 1:D:102:ILE:N | 1:D:110:PHE:O | 2.48 | 0.47 |
| 1:D:213:GLU:CG | 1:D:387:ARG:HD2 | 2.45 | 0.47 |
| 1:D:321:TYR:O | 1:D:325:VAL:N | 2.47 | 0.47 |
| 1:D:357:PRO:HB2 | 1:D:358:LYS:HD2 | 1.97 | 0.47 |
| 1:D:429:LYS:HE3 | 1:D:449:ARG:HH21 | 1.79 | 0.47 |
| 1:D:487:GLU:O | 1:D:490:ALA:HB3 | 2.13 | 0.47 |
| 1:D:537:ILE:HG13 | 1:D:540:VAL:HG12 | 1.97 | 0.47 |
| 1:D:550:ALA:C | 1:D:553:LEU:H | 2.22 | 0.47 |
| 1:D:572:MET:HA | 1:D:575:ASP:CB | 2.41 | 0.47 |
| 1:D:619:GLY:CA | 1:D:622:GLU:HB2 | 2.44 | 0.47 |
| 1:D:637:MET:CA | 1:D:678:LYS:HZ3 | 2.27 | 0.47 |
| 1:D:684:LEU:HD11 | 1:D:726:THR:OG1 | 2.14 | 0.47 |
| 1:D:785:ASP:OD2 | 1:D:806:LEU:HD22 | 2.14 | 0.47 |
| 1:D:806:LEU:O | 1:D:807:THR:OG1 | 2.23 | 0.47 |
| 1:D:809:GLU:HG2 | 1:D:810:ALA:N | 2.29 | 0.47 |
| 1:D:810:ALA:O | 1:D:812:ASP:N | 2.48 | 0.47 |
| 1:D:839:LYS:HZ3 | 1:D:879:VAL:H | 1.59 | 0.47 |
| 1:D:842:LEU:CD1 | 1:D:846:LYS:HZ2 | 2.27 | 0.47 |
| 1:D:848:GLU:O | 1:D:849:ILE:HG13 | 2.14 | 0.47 |
| 1:E:166:TYR:HD2 | 1:E:168:SER:OG | 1.97 | 0.47 |
| 1:E:172:ILE:HG12 | 1:E:246:LEU:HA | 1.96 | 0.47 |
| 1:E:216:ILE:HD12 | 1:E:390:ASP:HB2 | 1.97 | 0.47 |
| 1:E:244:PHE:H | 1:E:281:LEU:HA | 1.78 | 0.47 |
| 1:E:262:GLU:HA | 1:E:265:PHE:CD2 | 2.50 | 0.47 |
| 1:E:477:THR:O | 1:E:480:LYS:HB2 | 2.15 | 0.47 |
| 1:E:543:SER:O | 1:E:545:THR:N | 2.47 | 0.47 |
| 1:E:611:LEU:HD21 | 1:E:727:SER:OG | 2.14 | 0.47 |
| 1:E:643:CYS:CA | 1:E:649:LYS:HZ3 | 2.28 | 0.47 |
| 1:E:791:ILE:HG22 | 1:E:795:PHE:HB2 | 1.97 | 0.47 |
| 1:E:807:THR:HB | 1:E:811:LYS:HZ2 | 1.80 | 0.47 |
| 1:E:815:ALA:O | 1:E:818:GLY:N | 2.48 | 0.47 |
| 1:E:825:ALA:O | 1:E:826:ARG:C | 2.57 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:210:LEU:HA | 1:F:338:ILE:O | 2.15 | 0.47 |
| 1:F:343:PRO:HG3 | 1:F:388:LEU:HD23 | 1.96 | 0.47 |
| 1:F:360:GLU:OE1 | 1:F:367:ILE:HG21 | 2.15 | 0.47 |
| 1:F:556:ILE:HG12 | 1:F:559:LYS:HG3 | 1.96 | 0.47 |
| 1:F:649:LYS:HA | 1:F:692:HIS:HA | 1.95 | 0.47 |
| 1:F:693:PRO:HA | 1:F:696:LEU:HD12 | 1.97 | 0.47 |
| 1:F:774:LYS:HG2 | 1:F:775:LEU:N | 2.29 | 0.47 |
| 1:F:810:ALA:O | 1:F:811:LYS:C | 2.57 | 0.47 |
| 1:F:818:GLY:HA3 | 1:F:828:LEU:CD2 | 2.40 | 0.47 |
| 2:F:1001:AGS:O2A | 2:F:1001:AGS:H4' | 2.13 | 0.47 |
| 1:A:189:ARG:O | 1:A:192:GLU:OE2 | 2.33 | 0.47 |
| 1:A:194:ARG:CB | 1:A:198:ARG:HH12 | 2.26 | 0.47 |
| 1:A:612:PHE:CD2 | 1:A:771:ILE:HG13 | 2.50 | 0.47 |
| 1:A:629:GLY:HA3 | 1:A:635:GLU:HG2 | 1.97 | 0.47 |
| 1:A:638:MET:HE2 | 1:A:684:LEU:HD23 | 1.97 | 0.47 |
| 1:A:806:LEU:O | 1:A:810:ALA:HB3 | 2.15 | 0.47 |
| 1:A:842:LEU:HB3 | 1:A:846:LYS:HZ3 | 1.78 | 0.47 |
| 1:B:300:ILE:HG23 | 1:C:248:LEU:HD23 | 1.96 | 0.47 |
| 1:B:331:PHE:CE2 | 1:B:335:PHE:HB2 | 2.49 | 0.47 |
| 1:B:611:LEU:HD21 | 1:B:769:ILE:HG12 | 1.97 | 0.47 |
| 1:B:649:LYS:H | 1:B:692:HIS:CE1 | 2.32 | 0.47 |
| 1:B:803:LYS:HE3 | 1:B:854:THR:HA | 1.96 | 0.47 |
| 1:C:208:PRO:HD2 | 1:C:314:GLY:H | 1.79 | 0.47 |
| 1:C:305:LEU:HD23 | 1:C:305:LEU:HA | 1.51 | 0.47 |
| 1:C:324:ILE:O | 1:C:328:ASP:N | 2.32 | 0.47 |
| 1:C:399:SER:HB3 | 1:C:545:THR:HG21 | 1.97 | 0.47 |
| 1:C:511:PRO:HG3 | 1:D:435:GLU:HA | 1.96 | 0.47 |
| 1:C:627:VAL:C | 1:C:635:GLU:OE2 | 2.58 | 0.47 |
| 1:C:839:LYS:HZ1 | 1:C:880:LEU:C | 2.21 | 0.47 |
| 1:D:124:SER:C | 1:D:126:ILE:N | 2.68 | 0.47 |
| 1:D:235:PRO:HD3 | 1:E:408:ASP:CB | 2.43 | 0.47 |
| 1:D:349:VAL:HA | 1:D:352:LEU:HB2 | 1.95 | 0.47 |
| 1:D:376:ALA:O | 1:D:379:ALA:N | 2.48 | 0.47 |
| 1:D:403:VAL:HG12 | 1:D:407:ARG:NE | 2.30 | 0.47 |
| 1:D:487:GLU:HA | 1:D:490:ALA:HB3 | 1.97 | 0.47 |
| 1:D:569:LEU:CD1 | 1:D:595:ARG:HG2 | 2.45 | 0.47 |
| 1:D:580:VAL:HA | 1:D:626:LYS:NZ | 2.30 | 0.47 |
| 1:E:372:LEU:HD21 | 1:E:540:VAL:CG2 | 2.44 | 0.47 |
| 1:E:397:ASP:OD2 | 1:E:398:ILE:HG13 | 2.15 | 0.47 |
| 1:E:514:LYS:O | 1:E:517:ILE:N | 2.48 | 0.47 |
| 1:E:603:ASN:ND2 | 1:F:794:ARG:CZ | 2.78 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:610:PHE:HB2 | 1:E:724:ILE:HG23 | 1.96 | 0.47 |
| 1:E:617:GLY:HA2 | 2:E:1002:AGS:O3' | 2.15 | 0.47 |
| 1:E:683:LEU:HB3 | 1:E:723:VAL:HA | 1.96 | 0.47 |
| 1:F:166:TYR:CE2 | 1:F:263:GLU:OE2 | 2.68 | 0.47 |
| 1:F:167:LEU:HB2 | 1:F:271:GLU:OE1 | 2.14 | 0.47 |
| 1:F:174:MET:HE3 | 1:F:178:ALA:N | 2.30 | 0.47 |
| 1:F:210:LEU:CD1 | 1:F:340:VAL:H | 2.28 | 0.47 |
| 1:F:685:PHE:CD1 | 1:F:725:MET:HA | 2.50 | 0.47 |
| 1:F:715:THR:C | 1:F:717:ASP:H | 2.21 | 0.47 |
| 1:A:227:GLN:O | 1:A:230:ILE:N | 2.47 | 0.47 |
| 1:A:355:LEU:HG | 1:A:393:LEU:CD2 | 2.44 | 0.47 |
| 1:A:378:LEU:O | 1:A:379:ALA:C | 2.57 | 0.47 |
| 1:A:595:ARG:NH1 | 1:B:842:LEU:N | 2.63 | 0.47 |
| 1:A:700:LEU:HA | 1:A:703:LEU:HB3 | 1.96 | 0.47 |
| 1:A:801:HIS:CE1 | 1:A:851:ASP:OD2 | 2.68 | 0.47 |
| 1:B:203:ARG:HA | 1:C:362:HIS:CE1 | 2.49 | 0.47 |
| 1:B:301:LEU:HD12 | 1:B:305:LEU:HD11 | 1.96 | 0.47 |
| 1:B:540:VAL:HG12 | 1:B:542:ASP:N | 2.23 | 0.47 |
| 1:B:652:VAL:HG23 | 1:B:653:SER:H | 1.80 | 0.47 |
| 1:B:708:ILE:C | 1:B:715:THR:HB | 2.40 | 0.47 |
| 1:B:839:LYS:HD3 | 1:B:878:GLU:HB3 | 1.96 | 0.47 |
| 1:C:248:LEU:CG | 1:C:251:LEU:HD21 | 2.36 | 0.47 |
| 1:C:530:ARG:HD2 | 1:C:537:ILE:HD11 | 1.97 | 0.47 |
| 1:C:547:SER:HB2 | 1:C:548:GLU:OE1 | 2.15 | 0.47 |
| 1:C:842:LEU:HD21 | 1:C:881:PRO:CB | 2.45 | 0.47 |
| 1:D:173:ASP:HB2 | 1:D:244:PHE:HD1 | 1.75 | 0.47 |
| 1:D:198:ARG:NH1 | 1:E:405:VAL:H | 2.11 | 0.47 |
| 1:D:285:GLU:CB | 1:D:287:HIS:HB3 | 2.34 | 0.47 |
| 1:D:302:LYS:HD2 | 1:D:305:LEU:C | 2.39 | 0.47 |
| 1:D:520:LEU:HA | 1:D:523:GLN:OE1 | 2.14 | 0.47 |
| 1:D:592:ASN:O | 1:D:596:LEU:N | 2.40 | 0.47 |
| 1:D:770:VAL:HG12 | 1:D:771:ILE:N | 2.30 | 0.47 |
| 1:D:818:GLY:HA2 | 1:D:828:LEU:CD1 | 2.45 | 0.47 |
| 1:E:611:LEU:CD1 | 1:E:726:THR:HA | 2.44 | 0.47 |
| 1:E:613:LEU:CB | 1:E:771:ILE:HG12 | 2.44 | 0.47 |
| 1:E:836:ILE:HA | 1:E:839:LYS:HE3 | 1.95 | 0.47 |
| 1:E:872:GLU:HB2 | 1:E:875:GLU:HB3 | 1.97 | 0.47 |
| 1:F:201:ALA:C | 1:F:203:ARG:NH1 | 2.73 | 0.47 |
| 1:F:274:GLU:HA | 1:F:309:GLN:HG2 | 1.97 | 0.47 |
| 1:F:395:LEU:CA | 1:F:398:ILE:HB | 2.37 | 0.47 |
| 1:F:620:LYS:HD2 | 2:F:1002:AGS:O4' | 2.15 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:638:MET:HG2 | 1:F:639:ILE:N | 2.30 | 0.47 |
| 1:F:819:TYR:CG | 1:F:825:ALA:HA | 2.49 | 0.47 |
| 1:A:195:SER:O | 1:A:198:ARG:HB2 | 2.15 | 0.47 |
| 1:A:237:ILE:HA | 1:A:239:GLN:NE2 | 2.29 | 0.47 |
| 1:A:266:LYS:O | 1:A:270:LYS:HG3 | 2.14 | 0.47 |
| 1:A:322:ARG:HA | 1:A:325:VAL:CG2 | 2.45 | 0.47 |
| 1:A:332:GLU:OE2 | 1:A:334:ARG:N | 2.48 | 0.47 |
| 1:A:355:LEU:HG | 1:A:393:LEU:HD22 | 1.97 | 0.47 |
| 1:A:558:VAL:HG23 | 1:A:559:LYS:H | 1.79 | 0.47 |
| 1:A:609:SER:HB3 | 1:A:724:ILE:CG1 | 2.39 | 0.47 |
| 1:A:647:SER:HA | 1:A:692:HIS:N | 2.29 | 0.47 |
| 1:A:768:SER:C | 1:A:769:ILE:HG13 | 2.40 | 0.47 |
| 1:A:828:LEU:HG | 1:A:832:ILE:HD11 | 1.97 | 0.47 |
| 1:A:872:GLU:CG | 1:F:200:LEU:HB2 | 2.30 | 0.47 |
| 1:B:193:ILE:HA | 1:B:196:THR:HB | 1.97 | 0.47 |
| 1:B:211:ILE:CG2 | 1:B:318:ASN:HA | 2.45 | 0.47 |
| 1:B:300:ILE:O | 1:B:303:PRO:HD2 | 2.15 | 0.47 |
| 1:B:302:LYS:HZ1 | 1:B:306:SER:N | 2.13 | 0.47 |
| 1:B:333:ARG:HH12 | 1:B:334:ARG:HD3 | 1.79 | 0.47 |
| 1:B:337:LYS:CG | 1:B:338:ILE:N | 2.77 | 0.47 |
| 1:B:559:LYS:NZ | 1:B:630:PHE:O | 2.36 | 0.47 |
| 1:B:654:LYS:NZ | 1:B:694:ASP:HB2 | 2.29 | 0.47 |
| 1:B:707:ARG:HA | 1:B:708:ILE:HD12 | 1.96 | 0.47 |
| 1:C:546:ILE:O | 1:C:547:SER:C | 2.56 | 0.47 |
| 1:C:576:LEU:O | 1:C:579:GLU:HG2 | 2.15 | 0.47 |
| 1:D:190:GLU:O | 1:D:193:ILE:HB | 2.15 | 0.47 |
| 1:D:192:GLU:CD | 1:D:193:ILE:H | 2.23 | 0.47 |
| 1:D:242:LYS:N | 1:D:278:LEU:HA | 2.30 | 0.47 |
| 1:D:385:TYR:CD1 | 1:D:386:ARG:N | 2.83 | 0.47 |
| 1:D:421:LEU:O | 1:D:425:GLN:N | 2.45 | 0.47 |
| 1:D:515:LYS:HG3 | 1:D:519:LYS:HE3 | 1.96 | 0.47 |
| 1:D:567:GLU:HA | 1:D:570:ILE:HB | 1.96 | 0.47 |
| 1:D:735:ASN:O | 1:D:737:GLN:HG3 | 2.15 | 0.47 |
| 1:D:763:LEU:HA | 1:D:766:ILE:CG1 | 2.44 | 0.47 |
| 1:D:819:TYR:CD1 | 1:D:823:MET:O | 2.67 | 0.47 |
| 1:D:840:LEU:O | 1:D:841:ALA:C | 2.58 | 0.47 |
| 1:E:175:THR:CA | 1:E:178:ALA:HB3 | 2.40 | 0.47 |
| 1:E:179:ARG:HH12 | 1:E:495:ARG:HB3 | 1.80 | 0.47 |
| 1:E:242:LYS:N | 1:E:279:ILE:HA | 2.26 | 0.47 |
| 1:E:460:GLU:HB3 | 1:E:461:PRO:HD3 | 1.96 | 0.47 |
| 1:E:552:ARG:NH1 | 1:E:552:ARG:HG3 | 2.30 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:176:GLU:CG | 1:F:177:GLN:N | 2.78 | 0.47 |
| 1:F:375:ALA:O | 1:F:378:LEU:N | 2.47 | 0.47 |
| 1:F:623:LEU:O | 1:F:627:VAL:HG22 | 2.15 | 0.47 |
| 1:F:654:LYS:HB2 | 1:F:657:GLY:N | 2.28 | 0.47 |
| 1:F:808:GLN:HA | 1:F:811:LYS:CE | 2.45 | 0.47 |
| 1:A:234:VAL:HB | 1:A:235:PRO:O | 2.15 | 0.46 |
| 1:A:268:VAL:O | 1:A:271:GLU:HB3 | 2.16 | 0.46 |
| 1:A:290:MET:CB | 1:A:293:GLY:H | 2.28 | 0.46 |
| 1:A:326:GLU:CD | 1:A:326:GLU:N | 2.69 | 0.46 |
| 1:A:609:SER:C | 1:A:767:SER:HG | 2.22 | 0.46 |
| 1:A:879:VAL:HG12 | 1:A:880:LEU:N | 2.30 | 0.46 |
| 1:B:199:VAL:O | 1:B:202:ARG:HG2 | 2.15 | 0.46 |
| 1:B:323:SER:O | 1:B:327:LYS:N | 2.27 | 0.46 |
| 1:B:343:PRO:HG2 | 1:B:388:LEU:CD2 | 2.45 | 0.46 |
| 1:B:360:GLU:CG | 1:B:367:ILE:HD12 | 2.45 | 0.46 |
| 1:B:393:LEU:O | 1:B:396:VAL:N | 2.48 | 0.46 |
| 1:B:393:LEU:HG | 1:B:397:ASP:H | 1.80 | 0.46 |
| 1:B:646:LEU:HD13 | 1:B:687:GLU:O | 2.15 | 0.46 |
| 1:B:656:LEU:HA | 1:B:669:GLY:N | 2.30 | 0.46 |
| 1:C:173:ASP:HB3 | 1:C:177:GLN:OE1 | 2.15 | 0.46 |
| 1:C:174:MET:O | 1:C:177:GLN:HB3 | 2.15 | 0.46 |
| 1:C:210:LEU:C | 1:C:211:ILE:HG22 | 2.39 | 0.46 |
| 1:C:332:GLU:C | 1:C:332:GLU:CD | 2.82 | 0.46 |
| 1:C:395:LEU:HD12 | 1:C:396:VAL:N | 2.30 | 0.46 |
| 1:C:412:GLU:HB3 | 1:C:536:MET:HE1 | 1.96 | 0.46 |
| 1:C:478:GLN:O | 1:C:481:LYS:HG2 | 2.15 | 0.46 |
| 1:C:765:ARG:C | 1:D:830:ARG:HH22 | 2.23 | 0.46 |
| 1:D:175:THR:HG21 | 1:D:230:ILE:HG13 | 1.96 | 0.46 |
| 1:D:214:PRO:HD2 | 1:D:387:ARG:CZ | 2.44 | 0.46 |
| 1:D:263:GLU:O | 1:D:267:GLY:N | 2.42 | 0.46 |
| 1:D:284:ASP:OD1 | 1:D:284:ASP:C | 2.57 | 0.46 |
| 1:D:650:TYR:HD2 | 1:D:654:LYS:HD2 | 1.80 | 0.46 |
| 1:D:708:ILE:HG22 | 1:D:714:LYS:C | 2.41 | 0.46 |
| 1:D:753:ALA:O | 1:D:757:HIS:N | 2.19 | 0.46 |
| 1:D:788:LEU:HA | 1:D:791:ILE:CG1 | 2.38 | 0.46 |
| 1:D:792:GLU:OE2 | 1:D:800:LYS:HE2 | 2.15 | 0.46 |
| 1:D:817:TYR:OH | 1:D:874:GLU:OE2 | 2.14 | 0.46 |
| 1:D:857:VAL:HG22 | 1:D:880:LEU:HG | 1.97 | 0.46 |
| 1:E:196:THR:O | 1:E:199:VAL:HB | 2.15 | 0.46 |
| 1:E:202:ARG:CZ | 1:E:204:ILE:HB | 2.44 | 0.46 |
| 1:E:398:ILE:O | 1:E:401:ALA:HB3 | 2.15 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:585:ASP:CG | 1:E:586:ALA:H | 2.23 | 0.46 |
| 1:E:701:GLN:O | 1:E:707:ARG:NE | 2.41 | 0.46 |
| 1:E:802:TYR:CB | 1:E:804:LEU:HG | 2.45 | 0.46 |
| 1:F:639:ILE:HG22 | 1:F:640:ARG:N | 2.26 | 0.46 |
| 1:F:674:GLN:HA | 1:F:677:TYR:CD2 | 2.49 | 0.46 |
| 1:F:701:GLN:CD | 1:F:709:THR:OG1 | 2.51 | 0.46 |
| 1:F:802:TYR:C | 1:F:853:GLU:H | 2.17 | 0.46 |
| 1:F:807:THR:O | 1:F:808:GLN:C | 2.58 | 0.46 |
| 1:A:403:VAL:CG1 | 1:A:407:ARG:NH1 | 2.77 | 0.46 |
| 1:A:625:LYS:C | 1:A:635:GLU:OE2 | 2.58 | 0.46 |
| 1:A:637:MET:HG3 | 1:A:681:SER:HB3 | 1.95 | 0.46 |
| 1:A:685:PHE:CD2 | 1:A:723:VAL:HG21 | 2.49 | 0.46 |
| 1:A:688:VAL:O | 1:A:691:ALA:HB3 | 2.15 | 0.46 |
| 1:B:234:VAL:HG11 | 1:B:239:GLN:H | 1.81 | 0.46 |
| 1:B:367:ILE:HA | 1:B:540:VAL:HG23 | 1.97 | 0.46 |
| 1:B:378:LEU:CA | 1:B:381:ARG:HG2 | 2.45 | 0.46 |
| 1:B:550:ALA:N | 1:B:552:ARG:HH12 | 2.12 | 0.46 |
| 1:B:571:HIS:ND1 | 1:B:574:ARG:HG3 | 2.30 | 0.46 |
| 1:C:180:GLN:CG | 1:C:182:LYS:HE3 | 2.45 | 0.46 |
| 1:C:211:ILE:CG2 | 1:C:316:THR:N | 2.78 | 0.46 |
| 1:C:366:ARG:CZ | 1:C:537:ILE:O | 2.60 | 0.46 |
| 1:C:558:VAL:C | 1:C:561:LEU:H | 2.23 | 0.46 |
| 1:C:609:SER:HB2 | 1:C:766:ILE:HA | 1.97 | 0.46 |
| 1:C:777:ARG:O | 1:C:778:LYS:C | 2.58 | 0.46 |
| 1:C:782:LYS:HG3 | 1:C:783:ILE:HG13 | 1.96 | 0.46 |
| 1:D:321:TYR:HA | 1:D:324:ILE:HD13 | 1.97 | 0.46 |
| 1:D:399:SER:O | 1:D:403:VAL:N | 2.45 | 0.46 |
| 1:D:475:GLU:HA | 1:D:478:GLN:OE1 | 2.15 | 0.46 |
| 1:D:792:GLU:CD | 1:D:801:HIS:HA | 2.39 | 0.46 |
| 1:E:170:TYR:HB2 | 1:E:246:LEU:CD1 | 2.44 | 0.46 |
| 1:E:256:LYS:HE3 | 1:E:263:GLU:HG2 | 1.96 | 0.46 |
| 1:E:343:PRO:HG2 | 1:E:388:LEU:CD2 | 2.40 | 0.46 |
| 1:E:552:ARG:HG3 | 1:E:552:ARG:HH11 | 1.80 | 0.46 |
| 1:E:571:HIS:O | 1:E:572:MET:C | 2.58 | 0.46 |
| 1:E:609:SER:C | 1:E:610:PHE:CD2 | 2.94 | 0.46 |
| 1:F:187:ILE:O | 1:F:187:ILE:HG13 | 2.15 | 0.46 |
| 1:F:250:ALA:HB1 | 1:F:264:ARG:CG | 2.45 | 0.46 |
| 1:F:625:LYS:NZ | 1:F:636:ASP:C | 2.74 | 0.46 |
| 1:F:682:VAL:HG13 | 1:F:683:LEU:N | 2.30 | 0.46 |
| 1:F:786:ILE:O | 1:F:789:LYS:N | 2.48 | 0.46 |
| 1:A:274:GLU:HG3 | 1:A:275:SER:O | 2.14 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:580:VAL:HG12 | 1:A:581:VAL:N | 2.31 | 0.46 |
| 1:A:813:PHE:HB2 | 1:A:817:TYR:CE2 | 2.48 | 0.46 |
| 1:B:282:PHE:CD2 | 1:B:283:ILE:C | 2.94 | 0.46 |
| 1:B:382:TYR:CE2 | 1:B:384:PRO:HD3 | 2.50 | 0.46 |
| 1:B:573:GLU:O | 1:B:577:SER:HB3 | 2.14 | 0.46 |
| 1:B:621:THR:HA | 1:B:624:ALA:CB | 2.43 | 0.46 |
| 1:B:708:ILE:HB | 1:B:715:THR:CA | 2.45 | 0.46 |
| 1:B:745:SER:O | 1:B:749:LEU:HG | 2.14 | 0.46 |
| 1:B:803:LYS:HZ2 | 1:B:854:THR:HA | 1.80 | 0.46 |
| 1:B:843:ARG:NH1 | 1:B:848:GLU:CG | 2.78 | 0.46 |
| 1:C:178:ALA:HA | 1:C:182:LYS:N | 2.30 | 0.46 |
| 1:C:349:VAL:HG13 | 1:C:373:VAL:HG21 | 1.96 | 0.46 |
| 1:C:410:LYS:HB2 | 1:C:536:MET:HE3 | 1.97 | 0.46 |
| 1:C:594:VAL:HA | 1:C:597:SER:HB2 | 1.96 | 0.46 |
| 1:C:740:SER:OG | 1:C:741:LYS:N | 2.47 | 0.46 |
| 1:C:757:HIS:C | 1:C:758:PHE:CG | 2.94 | 0.46 |
| 1:C:770:VAL:HA | 1:C:771:ILE:HD12 | 1.97 | 0.46 |
| 1:C:839:LYS:NZ | 1:C:881:PRO:HD3 | 2.31 | 0.46 |
| 1:D:210:LEU:C | 1:D:211:ILE:HG12 | 2.40 | 0.46 |
| 1:D:241:ALA:CA | 1:D:278:LEU:HA | 2.46 | 0.46 |
| 1:D:332:GLU:C | 1:D:332:GLU:CD | 2.82 | 0.46 |
| 1:D:360:GLU:HA | 1:D:364:GLY:H | 1.80 | 0.46 |
| 1:D:381:ARG:HG3 | 1:D:382:TYR:CE1 | 2.51 | 0.46 |
| 1:D:545:THR:HA | 1:D:548:GLU:HB2 | 1.98 | 0.46 |
| 1:D:553:LEU:C | 1:D:555:GLY:H | 2.23 | 0.46 |
| 1:D:560:LYS:CA | 1:D:563:GLU:OE2 | 2.61 | 0.46 |
| 1:D:614:GLY:HA2 | 1:D:772:PHE:CD2 | 2.51 | 0.46 |
| 1:D:710:SER:HG | 1:D:714:LYS:H | 1.55 | 0.46 |
| 1:E:296:ASP:HA | 1:E:299:ASN:CB | 2.37 | 0.46 |
| 1:E:303:PRO:HB2 | 1:E:307:ARG:HH12 | 1.75 | 0.46 |
| 1:E:332:GLU:HA | 1:E:335:PHE:CB | 2.28 | 0.46 |
| 1:E:431:LEU:HB3 | 1:E:441:THR:HG22 | 1.97 | 0.46 |
| 1:E:445:LEU:HD23 | 1:E:449:ARG:NH2 | 2.31 | 0.46 |
| 1:E:470:LYS:HG2 | 1:E:474:GLU:CD | 2.40 | 0.46 |
| 1:E:510:ILE:HG21 | 1:E:514:LYS:NZ | 2.30 | 0.46 |
| 1:E:583:GLN:CD | 1:E:772:PHE:CD1 | 2.93 | 0.46 |
| 1:E:688:VAL:HG22 | 1:E:689:GLU:H | 1.81 | 0.46 |
| 1:E:747:LYS:HB3 | 1:E:751:MET:HE2 | 1.97 | 0.46 |
| 1:E:802:TYR:HA | 1:E:852:LYS:CG | 2.39 | 0.46 |
| 1:F:556:ILE:O | 1:F:559:LYS:HB2 | 2.16 | 0.46 |
| 1:F:841:ALA:O | 1:F:845:LEU:N | 2.48 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:657:GLY:HA3 | 1:A:668:GLY:HA2 | 1.97 | 0.46 |
| 1:A:668:GLY:C | 1:A:670:PHE:H | 2.23 | 0.46 |
| 1:B:227:GLN:O | 1:B:230:ILE:HG13 | 2.16 | 0.46 |
| 1:B:611:LEU:CD2 | 1:B:769:ILE:HA | 2.46 | 0.46 |
| 1:B:654:LYS:HZ1 | 1:B:694:ASP:HB2 | 1.79 | 0.46 |
| 1:B:693:PRO:CD | 1:B:694:ASP:H | 2.21 | 0.46 |
| 1:B:764:ASN:CB | 1:B:765:ARG:NH1 | 2.76 | 0.46 |
| 1:C:265:PHE:O | 1:C:268:VAL:HB | 2.16 | 0.46 |
| 1:C:299:ASN:OD1 | 1:C:299:ASN:C | 2.58 | 0.46 |
| 1:C:306:SER:HG | 1:C:334:ARG:HH21 | 1.62 | 0.46 |
| 1:C:395:LEU:HA | 1:C:398:ILE:HB | 1.96 | 0.46 |
| 1:C:417:LYS:HA | 1:C:456:GLN:HE22 | 1.80 | 0.46 |
| 1:C:609:SER:CB | 1:C:766:ILE:HA | 2.45 | 0.46 |
| 1:C:699:MET:HG3 | 1:C:700:LEU:N | 2.30 | 0.46 |
| 1:C:732:GLU:O | 1:C:735:ASN:HB2 | 2.15 | 0.46 |
| 1:C:839:LYS:NZ | 1:C:879:VAL:C | 2.71 | 0.46 |
| 1:C:842:LEU:HA | 1:C:845:LEU:HD12 | 1.98 | 0.46 |
| 1:D:172:ILE:HB | 1:D:245:SER:HB3 | 1.97 | 0.46 |
| 1:D:218:LYS:O | 1:D:219:THR:C | 2.57 | 0.46 |
| 1:D:281:LEU:HB2 | 1:D:312:VAL:HA | 1.98 | 0.46 |
| 1:D:367:ILE:HG12 | 1:D:537:ILE:HD12 | 1.98 | 0.46 |
| 1:D:369:ASP:O | 1:D:373:VAL:HG23 | 2.15 | 0.46 |
| 1:D:707:ARG:HA | 1:D:716:ILE:CG2 | 2.45 | 0.46 |
| 1:D:742:ILE:HG22 | 1:D:743:GLN:O | 2.15 | 0.46 |
| 1:D:794:ARG:HG2 | 1:D:795:PHE:CD1 | 2.50 | 0.46 |
| 1:E:190:GLU:O | 1:E:191:GLU:C | 2.59 | 0.46 |
| 1:E:287:HIS:HE1 | 1:E:315:ALA:C | 2.23 | 0.46 |
| 1:E:294:LYS:HE2 | 1:E:327:LYS:HB3 | 1.98 | 0.46 |
| 1:E:304:ALA:HA | 1:E:307:ARG:CG | 2.45 | 0.46 |
| 1:E:322:ARG:HG3 | 1:E:323:SER:N | 2.30 | 0.46 |
| 1:E:383:LEU:HD21 | 1:E:385:TYR:CZ | 2.50 | 0.46 |
| 1:E:434:ASP:HB3 | 1:E:441:THR:HG21 | 1.97 | 0.46 |
| 1:E:537:ILE:HG22 | 1:E:537:ILE:O | 2.15 | 0.46 |
| 1:E:652:VAL:C | 1:E:669:GLY:H | 2.22 | 0.46 |
| 1:E:704:ASP:O | 1:E:707:ARG:CZ | 2.64 | 0.46 |
| 1:E:858:VAL:HB | 1:E:877:LEU:CB | 2.44 | 0.46 |
| 1:F:316:THR:HG23 | 1:F:317:THR:O | 2.15 | 0.46 |
| 1:F:788:LEU:HD23 | 1:F:789:LYS:HZ2 | 1.80 | 0.46 |
| 1:A:270:LYS:C | 1:A:273:GLU:H | 2.22 | 0.46 |
| 1:A:322:ARG:NH2 | 1:A:337:LYS:HD3 | 2.25 | 0.46 |
| 1:A:325:VAL:O | 1:A:328:ASP:HB2 | 2.15 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:329:GLY:HA2 | 1:A:331:PHE:CE1 | 2.50 | 0.46 |
| 1:A:828:LEU:HG | 1:A:832:ILE:CG1 | 2.45 | 0.46 |
| 1:B:220:ALA:C | 1:B:223:GLU:OE1 | 2.59 | 0.46 |
| 1:B:302:LYS:CE | 1:B:305:LEU:HB2 | 2.45 | 0.46 |
| 1:B:632:PHE:CG | 1:B:680:TYR:HB3 | 2.50 | 0.46 |
| 1:B:647:SER:HA | 1:B:693:PRO:N | 2.30 | 0.46 |
| 1:B:684:LEU:HD23 | 1:B:685:PHE:N | 2.30 | 0.46 |
| 1:B:840:LEU:C | 1:B:842:LEU:N | 2.70 | 0.46 |
| 1:C:167:LEU:O | 1:C:167:LEU:HD12 | 2.15 | 0.46 |
| 1:C:211:ILE:HB | 1:C:338:ILE:HD11 | 1.98 | 0.46 |
| 1:C:251:LEU:HA | 1:C:260:ASP:CG | 2.41 | 0.46 |
| 1:C:640:ARG:NH2 | 1:C:684:LEU:HD13 | 2.31 | 0.46 |
| 1:C:753:ALA:HA | 1:C:756:GLN:OE1 | 2.15 | 0.46 |
| 1:C:757:HIS:O | 1:C:758:PHE:CD1 | 2.68 | 0.46 |
| 1:C:790:GLU:O | 1:C:793:GLU:N | 2.48 | 0.46 |
| 1:D:357:PRO:O | 1:D:361:ILE:HG13 | 2.15 | 0.46 |
| 1:D:377:GLN:O | 1:D:380:LYS:HE3 | 2.16 | 0.46 |
| 1:D:462:LEU:CD2 | 1:D:465:ARG:NH1 | 2.78 | 0.46 |
| 1:D:556:ILE:HB | 1:D:560:LYS:HZ1 | 1.80 | 0.46 |
| 1:D:571:HIS:HB2 | 1:D:575:ASP:OD2 | 2.15 | 0.46 |
| 1:D:572:MET:HE2 | 1:D:576:LEU:HD11 | 1.97 | 0.46 |
| 1:D:603:ASN:HD21 | 1:D:605:ARG:HB3 | 1.81 | 0.46 |
| 1:D:618:SER:C | 1:D:826:ARG:NH1 | 2.57 | 0.46 |
| 1:D:699:MET:O | 1:D:700:LEU:C | 2.57 | 0.46 |
| 1:D:702:MET:HA | 1:D:706:GLY:CA | 2.44 | 0.46 |
| 1:E:260:ASP:CA | 1:E:263:GLU:HB2 | 2.46 | 0.46 |
| 1:E:296:ASP:O | 1:E:300:ILE:HG12 | 2.14 | 0.46 |
| 1:E:350:ALA:O | 1:E:353:ARG:HB2 | 2.16 | 0.46 |
| 1:E:394:ASP:O | 1:E:398:ILE:HG13 | 2.16 | 0.46 |
| 1:E:410:LYS:O | 1:E:413:GLU:N | 2.48 | 0.46 |
| 1:E:597:SER:HG | 1:E:598:ARG:H | 1.64 | 0.46 |
| 1:E:624:ALA:O | 1:E:625:LYS:C | 2.56 | 0.46 |
| 1:E:636:ASP:OD1 | 1:E:636:ASP:N | 2.45 | 0.46 |
| 1:E:645:GLU:CD | 1:E:649:LYS:HZ1 | 2.19 | 0.46 |
| 1:E:695:VAL:O | 1:E:696:LEU:C | 2.57 | 0.46 |
| 1:F:166:TYR:CD1 | 1:F:264:ARG:NH1 | 2.83 | 0.46 |
| 1:F:194:ARG:HG2 | 1:F:228:ARG:NH2 | 2.31 | 0.46 |
| 1:F:299:ASN:CB | 1:F:302:LYS:HE3 | 2.34 | 0.46 |
| 1:F:649:LYS:HE2 | 1:F:649:LYS:HB3 | 1.78 | 0.46 |
| 1:F:781:HIS:CD2 | 1:F:782:LYS:NZ | 2.84 | 0.46 |
| 1:A:317:THR:HG1 | 1:A:322:ARG:H | 1.55 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:319:ASN:HD21 | 1:A:712:GLN:CB | 2.29 | 0.46 |
| 1:A:403:VAL:HG11 | 1:A:407:ARG:NH1 | 2.30 | 0.46 |
| 1:A:619:GLY:C | 1:A:623:LEU:HB3 | 2.40 | 0.46 |
| 1:A:628:ALA:O | 1:A:630:PHE:N | 2.48 | 0.46 |
| 1:A:654:LYS:CD | 1:A:656:LEU:HB3 | 2.46 | 0.46 |
| 1:A:669:GLY:C | 1:A:672:THR:H | 2.23 | 0.46 |
| 1:A:786:ILE:CA | 1:A:789:LYS:NZ | 2.74 | 0.46 |
| 1:B:166:TYR:O | 1:B:169:LYS:N | 2.49 | 0.46 |
| 1:B:169:LYS:CG | 1:B:170:TYR:H | 2.29 | 0.46 |
| 1:B:189:ARG:HG2 | 1:B:192:GLU:OE2 | 2.14 | 0.46 |
| 1:B:261:PHE:O | 1:B:265:PHE:N | 2.48 | 0.46 |
| 1:B:332:GLU:C | 1:B:335:PHE:H | 2.24 | 0.46 |
| 1:B:365:VAL:HG13 | 1:B:407:ARG:NH1 | 2.30 | 0.46 |
| 1:B:379:ALA:O | 1:B:382:TYR:N | 2.48 | 0.46 |
| 1:B:548:GLU:CD | 1:B:560:LYS:HD3 | 2.40 | 0.46 |
| 1:B:825:ALA:O | 1:B:826:ARG:C | 2.58 | 0.46 |
| 1:C:219:THR:HA | 1:C:222:ILE:HD12 | 1.98 | 0.46 |
| 1:C:282:PHE:HB2 | 1:C:313:ILE:N | 2.25 | 0.46 |
| 1:C:286:ILE:O | 1:C:289:LEU:N | 2.47 | 0.46 |
| 1:C:391:SER:O | 1:C:395:LEU:N | 2.42 | 0.46 |
| 1:C:770:VAL:CG2 | 1:C:771:ILE:H | 2.25 | 0.46 |
| 1:D:203:ARG:NH1 | 1:E:363:HIS:N | 2.63 | 0.46 |
| 1:D:398:ILE:O | 1:D:401:ALA:HB3 | 2.16 | 0.46 |
| 1:D:503:ALA:HB2 | 1:E:425:GLN:HE21 | 1.80 | 0.46 |
| 1:E:243:LEU:N | 1:E:279:ILE:HG23 | 2.30 | 0.46 |
| 1:E:341:ALA:O | 1:E:342:GLU:HB3 | 2.16 | 0.46 |
| 1:E:351:ILE:HG22 | 1:E:352:LEU:HD23 | 1.97 | 0.46 |
| 1:E:378:LEU:HD23 | 1:E:382:TYR:CE2 | 2.50 | 0.46 |
| 1:E:603:ASN:OD1 | 1:E:605:ARG:HB2 | 2.15 | 0.46 |
| 1:E:701:GLN:O | 1:E:707:ARG:HB3 | 2.16 | 0.46 |
| 1:E:745:SER:O | 1:E:749:LEU:N | 2.37 | 0.46 |
| 1:F:612:PHE:HB2 | 1:F:724:ILE:CG1 | 2.43 | 0.46 |
| 1:F:640:ARG:HA | 1:F:684:LEU:HB2 | 1.94 | 0.46 |
| 1:F:649:LYS:HE2 | 1:F:693:PRO:HG2 | 1.96 | 0.46 |
| 1:F:836:ILE:HD13 | 1:F:839:LYS:NZ | 2.31 | 0.46 |
| 1:A:374:THR:HA | 1:A:377:GLN:OE1 | 2.15 | 0.46 |
| 1:A:612:PHE:HB2 | 1:A:770:VAL:C | 2.41 | 0.46 |
| 1:A:758:PHE:CZ | 1:A:760:PRO:HA | 2.51 | 0.46 |
| 1:B:329:GLY:CA | 1:B:332:GLU:HB2 | 2.45 | 0.46 |
| 1:B:587:ILE:O | 1:B:591:SER:OG | 2.31 | 0.46 |
| 1:B:617:GLY:N | 1:B:620:LYS:NZ | 2.64 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:638:MET:HA | 1:B:682:VAL:HG12 | 1.97 | 0.46 |
| 1:B:654:LYS:NZ | 1:B:694:ASP:N | 2.64 | 0.46 |
| 1:B:704:ASP:OD2 | 1:B:707:ARG:HD2 | 2.16 | 0.46 |
| 1:B:798:ASN:C | 1:B:800:LYS:N | 2.72 | 0.46 |
| 1:B:848:GLU:CD | 1:B:882:ASN:H | 2.22 | 0.46 |
| 1:C:187:ILE:HD12 | 1:C:351:ILE:HG12 | 1.98 | 0.46 |
| 1:C:208:PRO:CG | 1:C:313:ILE:HG23 | 2.45 | 0.46 |
| 1:C:350:ALA:O | 1:C:354:GLY:N | 2.40 | 0.46 |
| 1:C:513:ILE:CD1 | 1:C:514:LYS:HG3 | 2.44 | 0.46 |
| 1:C:786:ILE:O | 1:C:787:ARG:C | 2.58 | 0.46 |
| 1:C:803:LYS:HZ2 | 1:C:853:GLU:HB2 | 1.81 | 0.46 |
| 1:D:173:ASP:OD2 | 1:D:176:GLU:HG2 | 2.16 | 0.46 |
| 1:D:203:ARG:HH12 | 1:E:363:HIS:N | 2.14 | 0.46 |
| 1:D:301:LEU:O | 1:D:304:ALA:HB3 | 2.16 | 0.46 |
| 1:D:394:ASP:O | 1:D:398:ILE:HG13 | 2.15 | 0.46 |
| 1:D:459:LEU:CB | 1:D:463:ARG:HH12 | 2.28 | 0.46 |
| 1:D:549:THR:O | 1:D:552:ARG:N | 2.49 | 0.46 |
| 1:D:556:ILE:C | 1:D:559:LYS:NZ | 2.66 | 0.46 |
| 1:D:693:PRO:O | 1:D:696:LEU:HB2 | 2.15 | 0.46 |
| 1:D:714:LYS:CD | 1:D:715:THR:H | 2.26 | 0.46 |
| 1:D:788:LEU:CA | 1:D:791:ILE:HG12 | 2.37 | 0.46 |
| 1:D:799:ASP:CG | 1:D:800:LYS:N | 2.74 | 0.46 |
| 1:E:215:GLY:C | 2:E:1001:AGS:O1B | 2.58 | 0.46 |
| 1:E:223:GLU:HA | 1:E:226:ALA:HB3 | 1.97 | 0.46 |
| 1:E:349:VAL:O | 1:E:350:ALA:C | 2.58 | 0.46 |
| 1:E:794:ARG:NH2 | 1:E:797:GLN:OE1 | 2.49 | 0.46 |
| 1:E:806:LEU:HD13 | 1:E:809:GLU:CD | 2.41 | 0.46 |
| 1:F:356:GLN:NE2 | 1:F:367:ILE:CG2 | 2.71 | 0.46 |
| 1:F:576:LEU:HD23 | 1:F:576:LEU:HA | 1.59 | 0.46 |
| 1:F:686:ASP:O | 1:F:727:SER:HB2 | 2.16 | 0.46 |
| 1:F:742:ILE:HG22 | 1:F:743:GLN:O | 2.16 | 0.46 |
| 1:F:803:LYS:NZ | 1:F:852:LYS:O | 2.48 | 0.46 |
| 1:A:320:GLU:HA | 1:A:323:SER:CB | 2.46 | 0.46 |
| 1:A:567:GLU:OE1 | 1:A:567:GLU:N | 2.42 | 0.46 |
| 1:A:682:VAL:HG12 | 1:A:683:LEU:O | 2.15 | 0.46 |
| 1:A:791:ILE:HG23 | 1:A:794:ARG:HG3 | 1.98 | 0.46 |
| 1:B:234:VAL:HG22 | 1:B:236:THR:N | 2.24 | 0.46 |
| 1:B:263:GLU:CA | 1:B:266:LYS:HZ1 | 2.27 | 0.46 |
| 1:B:324:ILE:O | 1:B:325:VAL:C | 2.58 | 0.46 |
| 1:B:580:VAL:CG2 | 1:B:622:GLU:HG2 | 2.46 | 0.46 |
| 1:B:662:TYR:HB3 | 1:B:663:VAL:HG23 | 1.97 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:728:ALA:HB1 | 1:B:732:GLU:OE2 | 2.16 | 0.46 |
| 1:B:753:ALA:HA | 1:B:756:GLN:NE2 | 2.31 | 0.46 |
| 1:B:849:ILE:CG1 | 1:B:882:ASN:HA | 2.46 | 0.46 |
| 1:C:178:ALA:HA | 1:C:182:LYS:H | 1.81 | 0.46 |
| 1:C:279:ILE:C | 1:C:311:LYS:HD2 | 2.41 | 0.46 |
| 1:C:375:ALA:HB1 | 1:C:546:ILE:HD12 | 1.98 | 0.46 |
| 1:C:377:GLN:O | 1:C:378:LEU:C | 2.58 | 0.46 |
| 1:C:417:LYS:HG2 | 1:C:459:LEU:HD13 | 1.98 | 0.46 |
| 1:C:417:LYS:CG | 1:C:459:LEU:HD13 | 2.45 | 0.46 |
| 1:C:655:LEU:HD13 | 1:C:671:LEU:HD11 | 1.96 | 0.46 |
| 1:C:842:LEU:HD21 | 1:C:881:PRO:HB3 | 1.98 | 0.46 |
| 1:D:199:VAL:CG1 | 1:D:336:GLN:HG2 | 2.46 | 0.46 |
| 1:D:459:LEU:HA | 1:D:462:LEU:HB2 | 1.98 | 0.46 |
| 1:D:530:ARG:HH12 | 1:D:538:GLN:N | 2.10 | 0.46 |
| 1:D:537:ILE:HG12 | 1:D:540:VAL:H | 1.81 | 0.46 |
| 1:D:553:LEU:C | 1:D:554:THR:HG1 | 2.18 | 0.46 |
| 1:D:568:LYS:O | 1:D:572:MET:HB2 | 2.15 | 0.46 |
| 1:D:623:LEU:O | 1:D:624:ALA:C | 2.59 | 0.46 |
| 1:D:845:LEU:HG | 1:D:846:LYS:N | 2.30 | 0.46 |
| 1:E:276:LYS:CE | 1:E:279:ILE:HB | 2.45 | 0.46 |
| 1:E:303:PRO:HA | 1:E:334:ARG:NH2 | 2.28 | 0.46 |
| 1:E:352:LEU:HG | 1:E:352:LEU:H | 1.47 | 0.46 |
| 1:E:371:ALA:O | 1:E:372:LEU:C | 2.58 | 0.46 |
| 1:E:416:SER:HA | 1:E:419:ARG:HE | 1.80 | 0.46 |
| 1:E:794:ARG:HH22 | 1:E:796:GLU:C | 2.23 | 0.46 |
| 1:E:880:LEU:HD23 | 1:E:880:LEU:HA | 1.65 | 0.46 |
| 1:F:185:PRO:HB3 | 1:F:227:GLN:OE1 | 2.16 | 0.46 |
| 1:F:212:GLY:HA3 | 1:F:216:ILE:HD13 | 1.98 | 0.46 |
| 1:F:238:LEU:HB3 | 1:F:279:ILE:HD13 | 1.98 | 0.46 |
| 1:F:701:GLN:CB | 1:F:709:THR:OG1 | 2.64 | 0.46 |
| 1:F:755:ARG:CZ | 1:F:763:LEU:HB3 | 2.46 | 0.46 |
| 1:F:788:LEU:HG | 1:F:789:LYS:N | 2.29 | 0.46 |
| 1:F:802:TYR:CE2 | 1:F:851:ASP:N | 2.80 | 0.46 |
| 1:A:302:LYS:HE2 | 1:A:306:SER:HA | 1.97 | 0.46 |
| 1:A:352:LEU:O | 1:A:360:GLU:OE2 | 2.34 | 0.46 |
| 1:A:654:LYS:CG | 1:A:656:LEU:HB3 | 2.46 | 0.46 |
| 1:A:823:MET:HE1 | 1:F:304:ALA:HA | 1.97 | 0.46 |
| 1:B:171:ALA:N | 1:B:250:ALA:HA | 2.31 | 0.46 |
| 1:B:196:THR:O | 1:B:200:LEU:HG | 2.16 | 0.46 |
| 1:B:296:ASP:O | 1:B:297:ALA:C | 2.58 | 0.46 |
| 1:B:366:ARG:HG2 | 1:B:407:ARG:HH22 | 1.81 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:583:GLN:HG3 | 1:B:771:ILE:O | 2.16 | 0.46 |
| 1:B:652:VAL:HG23 | 1:B:653:SER:N | 2.31 | 0.46 |
| 1:B:698:VAL:HG22 | 1:B:701:GLN:OE1 | 2.16 | 0.46 |
| 1:B:744:GLU:HG3 | 1:B:748:ASN:ND2 | 2.31 | 0.46 |
| 1:B:757:HIS:ND1 | 1:B:758:PHE:HD1 | 2.14 | 0.46 |
| 1:B:806:LEU:HD23 | 1:B:810:ALA:HB3 | 1.98 | 0.46 |
| 1:B:814:LEU:HD13 | 1:B:832:ILE:HG23 | 1.98 | 0.46 |
| 1:B:859:LEU:C | 1:B:875:GLU:OE2 | 2.58 | 0.46 |
| 1:C:392:ALA:O | 1:C:395:LEU:N | 2.49 | 0.46 |
| 1:C:474:GLU:O | 1:C:478:GLN:N | 2.46 | 0.46 |
| 1:C:564:SER:C | 1:C:566:ASN:N | 2.71 | 0.46 |
| 1:C:575:ASP:O | 1:C:576:LEU:C | 2.57 | 0.46 |
| 1:C:808:GLN:O | 1:C:811:LYS:N | 2.48 | 0.46 |
| 1:D:242:LYS:HE2 | 1:D:278:LEU:HB3 | 1.97 | 0.46 |
| 1:D:258:LYS:NZ | 1:D:262:GLU:H | 2.12 | 0.46 |
| 1:D:265:PHE:CE2 | 1:D:269:LEU:HD11 | 2.50 | 0.46 |
| 1:D:272:ILE:HB | 1:D:279:ILE:HD13 | 1.98 | 0.46 |
| 1:D:642:ASP:C | 1:D:644:SER:H | 2.23 | 0.46 |
| 1:D:740:SER:N | 1:D:743:GLN:OE1 | 2.48 | 0.46 |
| 1:E:231:ASP:HA | 1:E:495:ARG:HH22 | 1.81 | 0.46 |
| 1:E:277:THR:C | 1:E:279:ILE:H | 2.23 | 0.46 |
| 1:E:549:THR:HG22 | 1:E:553:LEU:HD11 | 1.98 | 0.46 |
| 1:E:565:GLU:HB2 | 1:E:566:ASN:CB | 2.46 | 0.46 |
| 1:E:607:PRO:CG | 1:E:707:ARG:NH1 | 2.78 | 0.46 |
| 1:E:674:GLN:O | 1:E:675:LEU:C | 2.59 | 0.46 |
| 1:E:701:GLN:HG2 | 1:E:707:ARG:CB | 2.40 | 0.46 |
| 1:E:762:PHE:HA | 1:E:765:ARG:CB | 2.39 | 0.46 |
| 1:E:807:THR:O | 1:E:810:ALA:N | 2.49 | 0.46 |
| 1:F:166:TYR:CE1 | 1:F:264:ARG:NH1 | 2.84 | 0.46 |
| 1:F:192:GLU:HG2 | 1:F:338:ILE:HG22 | 1.98 | 0.46 |
| 1:F:295:ASP:O | 1:F:300:ILE:HB | 2.16 | 0.46 |
| 1:F:626:LYS:HA | 1:F:626:LYS:HD2 | 1.74 | 0.46 |
| 1:F:697:THR:O | 1:F:700:LEU:N | 2.49 | 0.46 |
| 1:A:299:ASN:CG | 1:A:300:ILE:HD12 | 2.40 | 0.46 |
| 1:A:654:LYS:HG2 | 1:A:656:LEU:N | 2.29 | 0.46 |
| 1:A:809:GLU:O | 1:A:812:ASP:N | 2.49 | 0.46 |
| 1:B:184:ASP:CG | 1:B:358:LYS:HZ2 | 2.24 | 0.46 |
| 1:B:251:LEU:HD21 | 1:B:264:ARG:HA | 1.98 | 0.46 |
| 1:B:252:THR:N | 1:B:264:ARG:NH2 | 2.64 | 0.46 |
| 1:B:544:ASP:CG | 1:B:545:THR:N | 2.74 | 0.46 |
| 1:B:603:ASN:OD1 | 1:B:605:ARG:HG2 | 2.16 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:669:GLY:O | 1:B:671:LEU:HG | 2.16 | 0.46 |
| 1:B:737:GLN:N | 1:B:774:LYS:NZ | 2.63 | 0.46 |
| 1:C:218:LYS:HA | 1:C:221:ILE:CD1 | 2.39 | 0.46 |
| 1:C:286:ILE:HD12 | 1:C:297:ALA:HB3 | 1.98 | 0.46 |
| 1:C:322:ARG:HA | 1:C:325:VAL:CG2 | 2.45 | 0.46 |
| 1:C:643:CYS:HB3 | 1:C:690:LYS:HB2 | 1.96 | 0.46 |
| 1:C:759:ARG:CG | 1:C:761:GLU:HB3 | 2.46 | 0.46 |
| 1:D:166:TYR:HB2 | 1:D:264:ARG:NH2 | 2.31 | 0.46 |
| 1:D:248:LEU:HD12 | 1:D:251:LEU:CB | 2.45 | 0.46 |
| 1:D:264:ARG:O | 1:D:268:VAL:HG23 | 2.15 | 0.46 |
| 1:D:369:ASP:CA | 1:D:372:LEU:HB3 | 2.46 | 0.46 |
| 1:D:372:LEU:HB2 | 1:D:542:ASP:CB | 2.45 | 0.46 |
| 1:D:570:ILE:C | 1:D:595:ARG:HH22 | 2.17 | 0.46 |
| 1:D:708:ILE:HG13 | 1:D:716:ILE:HB | 1.98 | 0.46 |
| 1:D:802:TYR:N | 1:D:802:TYR:CD1 | 2.82 | 0.46 |
| 1:E:173:ASP:C | 1:E:175:THR:H | 2.17 | 0.46 |
| 1:E:174:MET:C | 1:E:176:GLU:N | 2.74 | 0.46 |
| 1:E:385:TYR:HD1 | 1:E:386:ARG:CZ | 2.29 | 0.46 |
| 1:E:610:PHE:O | 1:E:724:ILE:HG22 | 2.16 | 0.46 |
| 1:F:351:ILE:C | 1:F:355:LEU:HD13 | 2.41 | 0.46 |
| 1:F:605:ARG:HH11 | 1:F:706:GLY:N | 2.14 | 0.46 |
| 1:F:803:LYS:HZ2 | 1:F:853:GLU:N | 2.14 | 0.46 |
| 1:F:853:GLU:OE2 | 1:F:880:LEU:HD11 | 2.15 | 0.46 |
| 1:A:605:ARG:HG3 | 1:A:606:GLN:N | 2.31 | 0.45 |
| 1:A:610:PHE:H | 1:A:724:ILE:CG1 | 2.08 | 0.45 |
| 1:A:625:LYS:CE | 1:A:635:GLU:HB3 | 2.39 | 0.45 |
| 1:A:729:LEU:HG | 1:A:753:ALA:HB1 | 1.97 | 0.45 |
| 1:B:198:ARG:O | 1:B:201:ALA:N | 2.49 | 0.45 |
| 1:B:204:ILE:HG22 | 1:B:205:LYS:N | 2.30 | 0.45 |
| 1:B:205:LYS:HZ1 | 1:B:334:ARG:HG2 | 1.82 | 0.45 |
| 1:B:207:ASN:CG | 1:B:335:PHE:HA | 2.41 | 0.45 |
| 1:B:237:ILE:O | 1:B:241:ALA:N | 2.49 | 0.45 |
| 1:B:285:GLU:CD | 1:B:287:HIS:CE1 | 2.94 | 0.45 |
| 1:B:299:ASN:O | 1:B:302:LYS:N | 2.45 | 0.45 |
| 1:B:324:ILE:HG12 | 1:B:327:LYS:HE2 | 1.98 | 0.45 |
| 1:B:331:PHE:HE2 | 1:B:335:PHE:HD1 | 1.63 | 0.45 |
| 1:B:620:LYS:CG | 1:B:621:THR:H | 2.18 | 0.45 |
| 1:B:784:VAL:HB | 1:B:811:LYS:HZ3 | 1.81 | 0.45 |
| 1:B:801:HIS:CE1 | 1:B:851:ASP:OD2 | 2.69 | 0.45 |
| 1:B:829:ASN:O | 1:B:832:ILE:N | 2.50 | 0.45 |
| 1:B:842:LEU:C | 1:B:846:LYS:HZ3 | 2.23 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:17:LEU:CA | 1:C:36:LEU:H | 2.29 | 0.45 |
| 1:C:199:VAL:HA | 1:C:202:ARG:CB | 2.46 | 0.45 |
| 1:C:265:PHE:HA | 1:C:268:VAL:HB | 1.98 | 0.45 |
| 1:C:356:GLN:CG | 1:C:357:PRO:HD3 | 2.43 | 0.45 |
| 1:C:564:SER:O | 1:C:566:ASN:ND2 | 2.49 | 0.45 |
| 1:C:611:LEU:HD22 | 1:C:770:VAL:HB | 1.98 | 0.45 |
| 1:C:639:ILE:HG22 | 1:C:640:ARG:N | 2.27 | 0.45 |
| 1:C:700:LEU:O | 1:C:701:GLN:C | 2.59 | 0.45 |
| 1:D:285:GLU:CB | 1:D:288:MET:HG2 | 2.38 | 0.45 |
| 1:D:302:LYS:NZ | 1:D:306:SER:CA | 2.66 | 0.45 |
| 1:D:338:ILE:CG2 | 1:D:339:GLU:H | 2.27 | 0.45 |
| 1:D:380:LYS:O | 1:D:382:TYR:N | 2.48 | 0.45 |
| 1:D:460:GLU:HB2 | 1:D:461:PRO:HD3 | 1.98 | 0.45 |
| 1:D:537:ILE:HG13 | 1:D:540:VAL:HG13 | 1.98 | 0.45 |
| 1:D:595:ARG:O | 1:D:599:SER:HB3 | 2.16 | 0.45 |
| 1:D:730:GLY:C | 1:D:734:ILE:HD12 | 2.41 | 0.45 |
| 1:D:851:ASP:O | 1:D:852:LYS:HB2 | 2.16 | 0.45 |
| 1:E:265:PHE:O | 1:E:268:VAL:N | 2.49 | 0.45 |
| 1:E:266:LYS:HA | 1:E:269:LEU:HG | 1.98 | 0.45 |
| 1:E:544:ASP:O | 1:E:547:SER:N | 2.49 | 0.45 |
| 1:E:666:ASP:O | 1:E:667:GLU:HB3 | 2.16 | 0.45 |
| 1:F:192:GLU:CD | 1:F:338:ILE:HG22 | 2.41 | 0.45 |
| 1:F:389:PRO:O | 1:F:390:ASP:C | 2.59 | 0.45 |
| 1:F:666:ASP:CG | 1:F:672:THR:HG1 | 2.11 | 0.45 |
| 1:F:685:PHE:CD2 | 1:F:725:MET:HA | 2.52 | 0.45 |
| 1:F:698:VAL:O | 1:F:699:MET:HE2 | 2.15 | 0.45 |
| 1:F:784:VAL:HG23 | 1:F:785:ASP:N | 2.30 | 0.45 |
| 1:F:789:LYS:HA | 1:F:792:GLU:CD | 2.41 | 0.45 |
| 1:F:843:ARG:NH2 | 1:F:849:ILE:HD13 | 2.31 | 0.45 |
| 1:A:394:ASP:O | 1:A:397:ASP:HB3 | 2.16 | 0.45 |
| 1:A:651:ALA:O | 1:A:654:LYS:HB3 | 2.16 | 0.45 |
| 1:A:695:VAL:O | 1:A:698:VAL:N | 2.49 | 0.45 |
| 1:A:710:SER:OG | 1:A:713:GLY:N | 2.49 | 0.45 |
| 1:B:221:ILE:O | 1:B:225:VAL:HG23 | 2.15 | 0.45 |
| 1:B:374:THR:O | 1:B:377:GLN:N | 2.50 | 0.45 |
| 1:B:380:LYS:HA | 1:B:383:LEU:CD2 | 2.45 | 0.45 |
| 1:B:391:SER:O | 1:B:392:ALA:C | 2.59 | 0.45 |
| 1:B:719:SER:O | 1:B:722:ILE:HG13 | 2.16 | 0.45 |
| 1:B:779:ALA:O | 1:B:783:ILE:N | 2.40 | 0.45 |
| 1:C:209:CYS:CB | 1:C:335:PHE:HA | 2.45 | 0.45 |
| 1:C:268:VAL:O | 1:C:269:LEU:C | 2.59 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:383:LEU:HD11 | 1:C:553:LEU:HB3 | 1.98 | 0.45 |
| 1:C:576:LEU:CA | 1:C:579:GLU:OE2 | 2.63 | 0.45 |
| 1:C:738:GLN:N | 1:C:774:LYS:HE3 | 2.30 | 0.45 |
| 1:C:759:ARG:HG3 | 1:C:761:GLU:HB3 | 1.98 | 0.45 |
| 1:C:792:GLU:O | 1:C:795:PHE:N | 2.37 | 0.45 |
| 1:D:94:LYS:O | 1:D:98:ASP:N | 2.49 | 0.45 |
| 1:D:266:LYS:O | 1:D:269:LEU:HB2 | 2.15 | 0.45 |
| 1:D:294:LYS:NZ | 1:D:327:LYS:HD2 | 2.29 | 0.45 |
| 1:D:399:SER:H | 1:D:399:SER:HG | 1.33 | 0.45 |
| 1:D:631:LEU:HB3 | 1:D:632:PHE:CD2 | 2.52 | 0.45 |
| 1:D:708:ILE:HG22 | 1:D:714:LYS:O | 2.17 | 0.45 |
| 1:E:200:LEU:CD2 | 1:E:208:PRO:HD2 | 2.46 | 0.45 |
| 1:E:208:PRO:HA | 1:E:336:GLN:O | 2.16 | 0.45 |
| 1:E:216:ILE:HD12 | 1:E:387:ARG:HB2 | 1.97 | 0.45 |
| 1:E:218:LYS:O | 1:E:221:ILE:N | 2.48 | 0.45 |
| 1:E:316:THR:OG1 | 1:E:317:THR:N | 2.50 | 0.45 |
| 1:E:344:SER:HG | 1:E:347:GLN:HB2 | 1.80 | 0.45 |
| 1:E:392:ALA:O | 1:E:396:VAL:N | 2.39 | 0.45 |
| 1:E:608:ALA:H | 1:E:721:CYS:HB2 | 1.81 | 0.45 |
| 1:F:194:ARG:HD2 | 1:F:228:ARG:NH1 | 2.31 | 0.45 |
| 1:F:274:GLU:HA | 1:F:309:GLN:CG | 2.46 | 0.45 |
| 1:F:548:GLU:CD | 1:F:552:ARG:NH1 | 2.71 | 0.45 |
| 1:F:607:PRO:HD3 | 1:F:705:ASP:O | 2.16 | 0.45 |
| 1:F:701:GLN:HB2 | 1:F:709:THR:HG1 | 1.81 | 0.45 |
| 1:F:801:HIS:N | 1:F:802:TYR:HD1 | 2.14 | 0.45 |
| 1:F:840:LEU:O | 1:F:841:ALA:C | 2.59 | 0.45 |
| 1:A:174:MET:HE3 | 1:A:182:LYS:HE3 | 1.98 | 0.45 |
| 1:A:213:GLU:CG | 1:A:387:ARG:HH21 | 2.30 | 0.45 |
| 1:A:228:ARG:HA | 1:A:231:ASP:CG | 2.41 | 0.45 |
| 1:A:262:GLU:HG3 | 1:A:301:LEU:HD13 | 1.98 | 0.45 |
| 1:A:285:GLU:HG3 | 1:A:288:MET:H | 1.81 | 0.45 |
| 1:A:407:ARG:HD3 | 1:A:538:GLN:HB3 | 1.99 | 0.45 |
| 1:A:646:LEU:CD1 | 1:A:691:ALA:HB1 | 2.46 | 0.45 |
| 1:B:205:LYS:HA | 1:B:207:ASN:HD21 | 1.82 | 0.45 |
| 1:B:323:SER:O | 1:B:327:LYS:HG3 | 2.17 | 0.45 |
| 1:B:550:ALA:N | 1:B:552:ARG:NH1 | 2.63 | 0.45 |
| 1:B:590:VAL:O | 1:B:591:SER:C | 2.58 | 0.45 |
| 1:B:803:LYS:CE | 1:B:854:THR:HA | 2.47 | 0.45 |
| 1:B:812:ASP:O | 1:B:813:PHE:C | 2.60 | 0.45 |
| 1:C:170:TYR:HE1 | 1:C:249:ALA:CB | 2.26 | 0.45 |
| 1:C:194:ARG:HA | 1:C:197:ILE:HG12 | 1.97 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:349:VAL:CB | 1:C:353:ARG:NH1 | 2.79 | 0.45 |
| 1:C:355:LEU:HB3 | 1:C:358:LYS:HB3 | 1.98 | 0.45 |
| 1:C:502:ALA:C | 1:C:506:ARG:HD3 | 2.42 | 0.45 |
| 1:C:567:GLU:HA | 1:C:570:ILE:HG12 | 1.98 | 0.45 |
| 1:C:596:LEU:O | 1:C:597:SER:C | 2.58 | 0.45 |
| 1:C:785:ASP:CG | 1:C:789:LYS:HZ2 | 2.23 | 0.45 |
| 1:D:234:VAL:CG1 | 1:D:238:LEU:HB2 | 2.37 | 0.45 |
| 1:D:374:THR:O | 1:D:377:GLN:OE1 | 2.33 | 0.45 |
| 1:D:397:ASP:O | 1:D:398:ILE:C | 2.59 | 0.45 |
| 1:D:573:GLU:OE2 | 1:D:595:ARG:CZ | 2.64 | 0.45 |
| 1:D:626:LYS:HE3 | 1:D:626:LYS:HB3 | 1.63 | 0.45 |
| 1:D:753:ALA:O | 1:D:754:VAL:C | 2.58 | 0.45 |
| 1:D:830:ARG:HA | 1:D:833:GLN:CD | 2.41 | 0.45 |
| 1:E:216:ILE:HG22 | 1:E:387:ARG:NH1 | 2.31 | 0.45 |
| 1:E:241:ALA:CB | 1:E:278:LEU:HB3 | 2.45 | 0.45 |
| 1:E:374:THR:O | 1:E:377:GLN:HB2 | 2.16 | 0.45 |
| 1:E:462:LEU:HA | 1:E:465:ARG:HG2 | 1.96 | 0.45 |
| 1:E:487:GLU:O | 1:E:491:LEU:HG | 2.17 | 0.45 |
| 1:E:639:ILE:O | 1:E:640:ARG:HD3 | 2.16 | 0.45 |
| 1:E:649:LYS:C | 1:E:650:TYR:CG | 2.94 | 0.45 |
| 1:E:772:PHE:CD2 | 1:E:773:ASN:O | 2.70 | 0.45 |
| 1:F:170:TYR:CD2 | 1:F:248:LEU:HD12 | 2.51 | 0.45 |
| 1:F:261:PHE:HD2 | 1:F:297:ALA:HA | 1.82 | 0.45 |
| 1:A:210:LEU:CD2 | 1:A:339:GLU:HG3 | 2.46 | 0.45 |
| 1:A:260:ASP:OD1 | 1:A:264:ARG:HD2 | 2.15 | 0.45 |
| 1:A:374:THR:HA | 1:A:377:GLN:CD | 2.42 | 0.45 |
| 1:A:382:TYR:HD2 | 1:A:383:LEU:HD13 | 1.80 | 0.45 |
| 1:A:590:VAL:O | 1:A:594:VAL:HG23 | 2.16 | 0.45 |
| 1:A:611:LEU:HG | 1:A:612:PHE:O | 2.15 | 0.45 |
| 1:A:790:GLU:CG | 1:A:791:ILE:HG13 | 2.47 | 0.45 |
| 1:A:858:VAL:HG12 | 1:A:859:LEU:H | 1.81 | 0.45 |
| 1:B:167:LEU:HB3 | 1:B:267:GLY:HA3 | 1.98 | 0.45 |
| 1:B:265:PHE:HA | 1:B:268:VAL:CB | 2.43 | 0.45 |
| 1:B:544:ASP:C | 1:B:560:LYS:NZ | 2.74 | 0.45 |
| 1:B:685:PHE:CZ | 1:B:687:GLU:HA | 2.52 | 0.45 |
| 1:B:813:PHE:HA | 1:B:816:LYS:HG2 | 1.98 | 0.45 |
| 1:C:200:LEU:O | 1:C:206:SER:HB3 | 2.16 | 0.45 |
| 1:C:283:ILE:HG22 | 1:C:284:ASP:H | 1.81 | 0.45 |
| 1:C:291:GLY:N | 1:C:294:LYS:HZ2 | 2.12 | 0.45 |
| 1:C:298:ALA:HA | 1:C:301:LEU:CG | 2.45 | 0.45 |
| 1:C:368:LEU:HD11 | 1:C:539:ASN:ND2 | 2.31 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:424:ILE:HG23 | 1:C:425:GLN:N | 2.31 | 0.45 |
| 1:C:694:ASP:O | 1:C:698:VAL:HG23 | 2.17 | 0.45 |
| 1:C:751:MET:CA | 1:C:755:ARG:NH1 | 2.79 | 0.45 |
| 1:D:218:LYS:C | 1:D:222:ILE:HG12 | 2.41 | 0.45 |
| 1:D:226:ALA:HA | 1:D:229:ILE:HB | 1.97 | 0.45 |
| 1:D:266:LYS:O | 1:D:270:LYS:NZ | 2.49 | 0.45 |
| 1:D:296:ASP:CG | 1:D:300:ILE:HD12 | 2.41 | 0.45 |
| 1:D:583:GLN:NE2 | 1:D:771:ILE:O | 2.49 | 0.45 |
| 1:D:598:ARG:HH22 | 1:D:632:PHE:HZ | 1.64 | 0.45 |
| 1:D:616:SER:O | 1:D:618:SER:N | 2.50 | 0.45 |
| 1:D:673:ASN:O | 1:D:677:TYR:CG | 2.69 | 0.45 |
| 1:D:732:GLU:HG3 | 1:D:733:PHE:N | 2.30 | 0.45 |
| 1:D:842:LEU:C | 1:D:845:LEU:HB3 | 2.41 | 0.45 |
| 1:E:205:LYS:HZ2 | 1:E:334:ARG:CA | 2.29 | 0.45 |
| 1:E:227:GLN:O | 1:E:228:ARG:C | 2.60 | 0.45 |
| 1:E:246:LEU:HD12 | 1:E:247:ASP:H | 1.81 | 0.45 |
| 1:E:346:ARG:HG2 | 1:E:347:GLN:N | 2.32 | 0.45 |
| 1:E:351:ILE:C | 1:E:355:LEU:HG | 2.41 | 0.45 |
| 1:E:609:SER:C | 1:E:610:PHE:CG | 2.94 | 0.45 |
| 1:E:687:GLU:CD | 1:E:728:ALA:HB3 | 2.41 | 0.45 |
| 1:E:809:GLU:HA | 1:E:813:PHE:CZ | 2.52 | 0.45 |
| 1:F:263:GLU:O | 1:F:266:LYS:N | 2.49 | 0.45 |
| 1:F:369:ASP:OD1 | 1:F:370:SER:N | 2.50 | 0.45 |
| 1:F:386:ARG:HH21 | 1:F:391:SER:N | 2.15 | 0.45 |
| 1:A:571:HIS:CD2 | 1:A:574:ARG:NH1 | 2.85 | 0.45 |
| 1:A:810:ALA:HA | 1:A:813:PHE:HD1 | 1.73 | 0.45 |
| 1:A:812:ASP:O | 1:A:813:PHE:C | 2.59 | 0.45 |
| 1:A:814:LEU:CD2 | 1:A:828:LEU:HD11 | 2.47 | 0.45 |
| 1:B:202:ARG:NH1 | 1:B:205:LYS:CB | 2.69 | 0.45 |
| 1:B:298:ALA:H | 1:B:301:LEU:HD21 | 1.82 | 0.45 |
| 1:B:563:GLU:CD | 1:B:568:LYS:NZ | 2.73 | 0.45 |
| 1:B:617:GLY:C | 1:B:826:ARG:NH1 | 2.75 | 0.45 |
| 1:B:672:THR:O | 1:B:676:GLN:N | 2.33 | 0.45 |
| 1:C:228:ARG:HA | 1:C:231:ASP:CB | 2.46 | 0.45 |
| 1:C:235:PRO:HG2 | 1:C:238:LEU:HD12 | 1.98 | 0.45 |
| 1:C:590:VAL:O | 1:C:593:ALA:HB3 | 2.16 | 0.45 |
| 1:D:12:LEU:C | 1:D:16:THR:H | 2.25 | 0.45 |
| 1:D:170:TYR:O | 1:D:246:LEU:HD13 | 2.16 | 0.45 |
| 1:D:197:ILE:O | 1:D:200:LEU:HB2 | 2.16 | 0.45 |
| 1:D:283:ILE:HB | 1:D:313:ILE:O | 2.16 | 0.45 |
| 1:D:291:GLY:N | 1:D:294:LYS:HG2 | 2.31 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:369:ASP:HA | 1:D:372:LEU:CB | 2.45 | 0.45 |
| 1:D:377:GLN:HA | 1:D:380:LYS:HB3 | 1.98 | 0.45 |
| 1:D:549:THR:HG22 | 1:D:553:LEU:HD12 | 1.98 | 0.45 |
| 1:D:559:LYS:HG2 | 1:D:559:LYS:HZ2 | 1.47 | 0.45 |
| 1:D:585:ASP:HA | 1:D:588:LYS:HG3 | 1.98 | 0.45 |
| 1:D:599:SER:HG | 1:D:600:GLY:H | 1.62 | 0.45 |
| 1:D:611:LEU:O | 1:D:726:THR:HB | 2.16 | 0.45 |
| 1:D:684:LEU:HD12 | 1:D:724:ILE:O | 2.17 | 0.45 |
| 1:D:818:GLY:O | 1:D:819:TYR:C | 2.59 | 0.45 |
| 1:E:205:LYS:NZ | 1:E:334:ARG:C | 2.68 | 0.45 |
| 1:E:356:GLN:CD | 1:E:367:ILE:HD12 | 2.41 | 0.45 |
| 1:E:429:LYS:NZ | 1:E:432:GLU:CD | 2.71 | 0.45 |
| 1:E:469:GLU:O | 1:E:473:HIS:N | 2.38 | 0.45 |
| 1:E:833:GLN:O | 1:E:834:ASN:C | 2.60 | 0.45 |
| 1:F:176:GLU:CD | 1:F:177:GLN:H | 2.25 | 0.45 |
| 1:F:244:PHE:O | 1:F:281:LEU:HD13 | 2.16 | 0.45 |
| 1:F:389:PRO:C | 1:F:393:LEU:HG | 2.41 | 0.45 |
| 1:A:228:ARG:HA | 1:A:231:ASP:OD2 | 2.17 | 0.45 |
| 1:A:283:ILE:HD12 | 1:A:288:MET:CB | 2.47 | 0.45 |
| 1:A:331:PHE:HZ | 1:A:335:PHE:CE2 | 2.34 | 0.45 |
| 1:A:549:THR:CA | 1:A:552:ARG:HH12 | 2.29 | 0.45 |
| 1:A:560:LYS:N | 1:A:562:SER:OG | 2.49 | 0.45 |
| 1:A:606:GLN:HE21 | 1:A:608:ALA:HA | 1.82 | 0.45 |
| 1:A:733:PHE:HE2 | 1:A:750:VAL:HA | 1.82 | 0.45 |
| 1:B:228:ARG:HH22 | 1:B:233:ASP:CB | 2.28 | 0.45 |
| 1:B:646:LEU:HG | 1:B:690:LYS:HB2 | 1.99 | 0.45 |
| 1:B:673:ASN:HA | 1:B:676:GLN:OE1 | 2.17 | 0.45 |
| 1:B:704:ASP:CB | 1:B:707:ARG:NH1 | 2.78 | 0.45 |
| 1:B:790:GLU:CD | 1:B:791:ILE:HG13 | 2.41 | 0.45 |
| 1:C:221:ILE:C | 1:C:223:GLU:N | 2.73 | 0.45 |
| 1:C:352:LEU:HG | 1:C:352:LEU:H | 1.52 | 0.45 |
| 1:C:375:ALA:HA | 1:C:378:LEU:HB2 | 1.98 | 0.45 |
| 1:C:659:THR:HG23 | 1:C:712:GLN:HA | 1.99 | 0.45 |
| 1:C:752:GLY:O | 1:C:755:ARG:N | 2.49 | 0.45 |
| 1:C:773:ASN:C | 1:C:773:ASN:OD1 | 2.59 | 0.45 |
| 1:C:784:VAL:O | 1:C:787:ARG:HB2 | 2.16 | 0.45 |
| 1:D:380:LYS:HZ2 | 1:D:381:ARG:HB3 | 1.82 | 0.45 |
| 1:D:409:SER:O | 1:D:410:LYS:HB2 | 2.16 | 0.45 |
| 1:D:462:LEU:CD2 | 1:D:465:ARG:HH11 | 2.30 | 0.45 |
| 1:D:785:ASP:C | 1:D:788:LEU:H | 2.23 | 0.45 |
| 1:E:198:ARG:HD3 | 1:F:401:ALA:CB | 2.39 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:214:PRO:O | 1:E:218:LYS:NZ | 2.43 | 0.45 |
| 1:E:248:LEU:O | 1:E:251:LEU:N | 2.50 | 0.45 |
| 1:E:284:ASP:HA | 1:E:314:GLY:HA2 | 1.99 | 0.45 |
| 1:E:330:ALA:O | 1:E:334:ARG:HG3 | 2.16 | 0.45 |
| 1:E:375:ALA:O | 1:E:376:ALA:C | 2.58 | 0.45 |
| 1:E:761:GLU:HG2 | 1:E:762:PHE:N | 2.31 | 0.45 |
| 1:E:802:TYR:HB3 | 1:E:852:LYS:C | 2.41 | 0.45 |
| 1:E:820:SER:HB3 | 1:E:823:MET:C | 2.41 | 0.45 |
| 1:F:166:TYR:HD2 | 1:F:264:ARG:O | 2.00 | 0.45 |
| 1:F:199:VAL:HA | 1:F:202:ARG:CB | 2.47 | 0.45 |
| 1:F:205:LYS:HG3 | 1:F:334:ARG:C | 2.41 | 0.45 |
| 1:F:285:GLU:HB2 | 1:F:288:MET:HG2 | 1.99 | 0.45 |
| 1:F:609:SER:O | 1:F:724:ILE:HG22 | 2.16 | 0.45 |
| 1:F:789:LYS:O | 1:F:792:GLU:OE2 | 2.34 | 0.45 |
| 1:A:262:GLU:HB3 | 1:A:266:LYS:HB2 | 1.99 | 0.45 |
| 1:A:306:SER:HA | 1:A:310:LEU:HB3 | 1.98 | 0.45 |
| 1:A:767:SER:OG | 1:A:768:SER:N | 2.50 | 0.45 |
| 1:A:830:ARG:O | 1:A:833:GLN:HB3 | 2.16 | 0.45 |
| 1:B:225:VAL:HG12 | 1:B:229:ILE:HD11 | 1.99 | 0.45 |
| 1:B:349:VAL:HG12 | 1:B:353:ARG:HG2 | 1.99 | 0.45 |
| 1:C:189:ARG:NH2 | 1:C:341:ALA:C | 2.75 | 0.45 |
| 1:C:201:ALA:HB2 | 1:C:238:LEU:HD21 | 1.99 | 0.45 |
| 1:C:218:LYS:HE2 | 1:C:218:LYS:HB2 | 1.70 | 0.45 |
| 1:C:573:GLU:HA | 1:C:576:LEU:HG | 1.99 | 0.45 |
| 1:C:671:LEU:HB2 | 1:C:675:LEU:HD11 | 1.98 | 0.45 |
| 1:C:697:THR:O | 1:C:698:VAL:C | 2.59 | 0.45 |
| 1:C:841:ALA:O | 1:C:844:ILE:N | 2.50 | 0.45 |
| 1:D:167:LEU:HG | 1:D:170:TYR:CD2 | 2.52 | 0.45 |
| 1:D:301:LEU:HD12 | 1:D:302:LYS:H | 1.81 | 0.45 |
| 1:D:330:ALA:O | 1:D:333:ARG:HB2 | 2.17 | 0.45 |
| 1:D:469:GLU:OE2 | 1:D:536:MET:HB2 | 2.17 | 0.45 |
| 1:D:654:LYS:CE | 1:D:656:LEU:HB2 | 2.45 | 0.45 |
| 1:D:694:ASP:O | 1:D:698:VAL:HG23 | 2.17 | 0.45 |
| 1:D:787:ARG:O | 1:D:791:ILE:HG12 | 2.16 | 0.45 |
| 1:D:840:LEU:CD1 | 1:D:844:ILE:HD12 | 2.47 | 0.45 |
| 1:E:243:LEU:HA | 1:E:280:VAL:N | 2.32 | 0.45 |
| 1:E:248:LEU:O | 1:E:252:THR:HG23 | 2.16 | 0.45 |
| 1:E:572:MET:H | 1:E:595:ARG:NH2 | 2.15 | 0.45 |
| 1:E:611:LEU:HD13 | 1:E:726:THR:HA | 1.98 | 0.45 |
| 1:E:790:GLU:HA | 1:E:793:GLU:OE1 | 2.17 | 0.45 |
| 1:F:363:HIS:CE1 | 1:F:397:ASP:CG | 2.76 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:584:MET:HE3 | 1:F:588:LYS:HZ1 | 1.82 | 0.45 |
| 1:F:669:GLY:HA2 | 1:F:672:THR:HG1 | 1.81 | 0.45 |
| 1:F:683:LEU:HD13 | 1:F:685:PHE:HZ | 1.82 | 0.45 |
| 1:F:744:GLU:HB2 | 1:F:747:LYS:HE2 | 1.98 | 0.45 |
| 1:F:748:ASN:O | 1:F:751:MET:HB3 | 2.17 | 0.45 |
| 1:F:848:GLU:O | 1:F:849:ILE:HB | 2.16 | 0.45 |
| 1:A:192:GLU:HA | 1:A:195:SER:HB2 | 1.97 | 0.45 |
| 1:A:262:GLU:OE2 | 1:A:296:ASP:OD2 | 2.35 | 0.45 |
| 1:A:286:ILE:HG22 | 1:A:314:GLY:HA3 | 1.99 | 0.45 |
| 1:A:579:GLU:CD | 1:A:580:VAL:HG23 | 2.42 | 0.45 |
| 1:A:586:ALA:O | 1:A:590:VAL:N | 2.37 | 0.45 |
| 1:A:590:VAL:O | 1:A:593:ALA:HB3 | 2.16 | 0.45 |
| 1:A:809:GLU:OE1 | 1:A:810:ALA:N | 2.50 | 0.45 |
| 1:A:809:GLU:OE2 | 1:A:857:VAL:HG12 | 2.16 | 0.45 |
| 1:A:816:LYS:HA | 1:A:819:TYR:HE2 | 1.81 | 0.45 |
| 1:B:190:GLU:O | 1:B:191:GLU:C | 2.60 | 0.45 |
| 1:B:191:GLU:N | 1:B:191:GLU:CD | 2.66 | 0.45 |
| 1:B:207:ASN:ND2 | 1:B:335:PHE:HA | 2.32 | 0.45 |
| 1:B:337:LYS:HA | 1:B:337:LYS:HD2 | 1.75 | 0.45 |
| 1:B:393:LEU:O | 1:B:397:ASP:N | 2.48 | 0.45 |
| 1:B:541:VAL:O | 1:B:542:ASP:OD1 | 2.34 | 0.45 |
| 1:B:547:SER:HA | 1:B:550:ALA:HB3 | 1.99 | 0.45 |
| 1:B:666:ASP:OD2 | 1:B:669:GLY:O | 2.34 | 0.45 |
| 1:C:328:ASP:CG | 1:C:329:GLY:H | 2.25 | 0.45 |
| 1:C:378:LEU:O | 1:C:382:TYR:CD2 | 2.69 | 0.45 |
| 1:C:698:VAL:HA | 1:C:701:GLN:HB3 | 1.99 | 0.45 |
| 1:C:759:ARG:HG3 | 1:C:761:GLU:H | 1.82 | 0.45 |
| 1:C:805:ASN:O | 1:C:856:ASN:HA | 2.17 | 0.45 |
| 1:C:807:THR:OG1 | 1:C:856:ASN:OD1 | 2.35 | 0.45 |
| 1:D:468:GLU:C | 1:D:471:HIS:HB3 | 2.42 | 0.45 |
| 1:D:542:ASP:HB2 | 1:D:546:ILE:HD11 | 1.98 | 0.45 |
| 1:D:543:SER:O | 1:D:547:SER:OG | 2.25 | 0.45 |
| 1:D:603:ASN:ND2 | 1:D:606:GLN:HB2 | 2.32 | 0.45 |
| 1:E:172:ILE:C | 1:E:245:SER:H | 2.25 | 0.45 |
| 1:E:256:LYS:HZ1 | 1:E:264:ARG:HG2 | 1.82 | 0.45 |
| 1:E:270:LYS:HZ2 | 1:E:274:GLU:CB | 2.30 | 0.45 |
| 1:E:303:PRO:O | 1:E:307:ARG:HG3 | 2.17 | 0.45 |
| 1:E:349:VAL:HG12 | 1:E:353:ARG:CG | 2.43 | 0.45 |
| 1:E:386:ARG:HA | 1:E:386:ARG:HD3 | 1.77 | 0.45 |
| 1:E:486:LEU:HD23 | 1:E:489:LYS:HZ1 | 1.82 | 0.45 |
| 1:E:712:GLN:OE1 | 1:E:714:LYS:NZ | 2.48 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:800:LYS:HE3 | 1:E:802:TYR:HH | 1.82 | 0.45 |
| 1:F:216:ILE:HG22 | 1:F:388:LEU:HD11 | 1.97 | 0.45 |
| 1:F:349:VAL:O | 1:F:353:ARG:HG2 | 2.17 | 0.45 |
| 1:F:615:LEU:HB2 | 1:F:772:PHE:CD1 | 2.51 | 0.45 |
| 1:F:778:LYS:HB2 | 1:F:781:HIS:CD2 | 2.51 | 0.45 |
| 1:F:819:TYR:HE1 | 1:F:827:PRO:HD2 | 1.82 | 0.45 |
| 1:A:174:MET:C | 1:A:243:LEU:HD11 | 2.42 | 0.45 |
| 1:A:285:GLU:O | 1:A:288:MET:HB2 | 2.17 | 0.45 |
| 1:A:287:HIS:NE2 | 1:A:290:MET:HB2 | 2.31 | 0.45 |
| 1:A:628:ALA:C | 1:A:630:PHE:N | 2.74 | 0.45 |
| 1:A:642:ASP:HB3 | 1:A:645:GLU:CD | 2.42 | 0.45 |
| 1:A:822:ASP:CB | 1:F:333:ARG:NH1 | 2.77 | 0.45 |
| 1:A:835:GLU:HA | 1:A:838:ASN:ND2 | 2.30 | 0.45 |
| 1:A:854:THR:O | 1:A:880:LEU:HD22 | 2.17 | 0.45 |
| 1:B:180:GLN:HG2 | 1:B:182:LYS:NZ | 2.30 | 0.45 |
| 1:B:198:ARG:HB3 | 1:C:405:VAL:HG23 | 1.99 | 0.45 |
| 1:B:246:LEU:C | 1:B:283:ILE:HG12 | 2.42 | 0.45 |
| 1:B:607:PRO:HG2 | 1:B:703:LEU:HA | 1.97 | 0.45 |
| 1:B:770:VAL:O | 1:B:771:ILE:HG13 | 2.17 | 0.45 |
| 1:B:784:VAL:HG12 | 1:B:788:LEU:HD21 | 1.99 | 0.45 |
| 1:C:262:GLU:HG2 | 1:C:263:GLU:OE2 | 2.17 | 0.45 |
| 1:C:281:LEU:HG | 1:C:311:LYS:C | 2.42 | 0.45 |
| 1:C:377:GLN:O | 1:C:380:LYS:N | 2.50 | 0.45 |
| 1:C:560:LYS:C | 1:C:562:SER:N | 2.71 | 0.45 |
| 1:C:630:PHE:CD1 | 1:C:631:LEU:HA | 2.52 | 0.45 |
| 1:C:659:THR:HA | 1:C:712:GLN:CD | 2.42 | 0.45 |
| 1:C:786:ILE:CD1 | 1:C:789:LYS:HZ3 | 2.29 | 0.45 |
| 1:C:791:ILE:O | 1:C:795:PHE:HB2 | 2.16 | 0.45 |
| 1:D:33:ILE:H | 1:D:71:ARG:C | 2.25 | 0.45 |
| 1:D:270:LYS:O | 1:D:273:GLU:HG2 | 2.16 | 0.45 |
| 1:D:393:LEU:O | 1:D:396:VAL:N | 2.50 | 0.45 |
| 1:D:618:SER:OG | 1:D:772:PHE:HE2 | 2.00 | 0.45 |
| 1:D:631:LEU:HB3 | 1:D:632:PHE:CE2 | 2.52 | 0.45 |
| 1:D:779:ALA:C | 1:D:782:LYS:HZ1 | 2.08 | 0.45 |
| 1:D:794:ARG:NH1 | 1:D:794:ARG:HG2 | 2.31 | 0.45 |
| 1:D:810:ALA:O | 1:D:813:PHE:HB3 | 2.17 | 0.45 |
| 1:D:830:ARG:O | 1:D:833:GLN:HG2 | 2.16 | 0.45 |
| 1:E:166:TYR:CE2 | 1:E:167:LEU:HG | 2.52 | 0.45 |
| 1:E:211:ILE:O | 1:E:339:GLU:HG3 | 2.17 | 0.45 |
| 1:E:256:LYS:HE2 | 1:E:260:ASP:CG | 2.41 | 0.45 |
| 1:E:262:GLU:HG3 | 1:E:265:PHE:HD2 | 1.82 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:288:MET:HG2 | 1:E:290:MET:HB3 | 1.99 | 0.45 |
| 1:E:390:ASP:O | 1:E:394:ASP:N | 2.42 | 0.45 |
| 1:E:467:ASN:O | 1:E:470:LYS:HB3 | 2.17 | 0.45 |
| 1:E:473:HIS:HA | 1:E:521:GLU:HG2 | 1.99 | 0.45 |
| 1:E:476:LEU:HD11 | 1:E:517:ILE:HA | 1.99 | 0.45 |
| 1:E:679:PRO:O | 1:E:720:ASN:HB2 | 2.16 | 0.45 |
| 1:E:786:ILE:HA | 1:E:789:LYS:CE | 2.47 | 0.45 |
| 1:E:802:TYR:HB2 | 1:E:804:LEU:HD11 | 1.99 | 0.45 |
| 1:F:221:ILE:O | 1:F:225:VAL:HG23 | 2.17 | 0.45 |
| 1:F:307:ARG:HH12 | 1:F:333:ARG:HH12 | 1.56 | 0.45 |
| 1:F:609:SER:C | 1:F:724:ILE:HG22 | 2.42 | 0.45 |
| 1:A:215:GLY:HA3 | 1:A:218:LYS:HE3 | 1.99 | 0.45 |
| 1:A:248:LEU:HB3 | 1:A:288:MET:HE1 | 1.98 | 0.45 |
| 1:A:270:LYS:CA | 1:A:273:GLU:HB2 | 2.47 | 0.45 |
| 1:A:285:GLU:CD | 1:A:287:HIS:H | 2.23 | 0.45 |
| 1:A:612:PHE:H | 1:A:770:VAL:H | 1.65 | 0.45 |
| 1:A:622:GLU:O | 1:A:625:LYS:N | 2.50 | 0.45 |
| 1:A:689:GLU:HA | 1:A:757:HIS:ND1 | 2.31 | 0.45 |
| 1:A:777:ARG:HH22 | 1:A:816:LYS:H | 1.63 | 0.45 |
| 1:A:802:TYR:HA | 1:A:852:LYS:HA | 1.99 | 0.45 |
| 1:A:802:TYR:CD2 | 1:A:804:LEU:HB2 | 2.52 | 0.45 |
| 1:A:814:LEU:HD11 | 1:A:835:GLU:CD | 2.42 | 0.45 |
| 1:B:262:GLU:C | 1:B:265:PHE:H | 2.24 | 0.45 |
| 1:B:378:LEU:O | 1:B:381:ARG:HG2 | 2.17 | 0.45 |
| 1:B:384:PRO:HD2 | 1:B:386:ARG:CG | 2.46 | 0.45 |
| 1:B:543:SER:CA | 1:B:546:ILE:HB | 2.46 | 0.45 |
| 1:B:764:ASN:C | 1:B:765:ARG:NH1 | 2.74 | 0.45 |
| 1:B:765:ARG:HD3 | 1:B:765:ARG:HA | 1.41 | 0.45 |
| 1:B:795:PHE:HB3 | 1:B:798:ASN:OD1 | 2.17 | 0.45 |
| 1:C:198:ARG:CD | 1:D:405:VAL:HG22 | 2.47 | 0.45 |
| 1:C:268:VAL:HA | 1:C:271:GLU:HG3 | 1.97 | 0.45 |
| 1:C:281:LEU:HD12 | 1:C:312:VAL:CB | 2.40 | 0.45 |
| 1:C:296:ASP:OD1 | 1:C:299:ASN:N | 2.50 | 0.45 |
| 1:C:396:VAL:O | 1:C:400:CYS:N | 2.33 | 0.45 |
| 1:C:468:GLU:O | 1:C:472:GLY:N | 2.45 | 0.45 |
| 1:C:763:LEU:O | 1:C:766:ILE:N | 2.41 | 0.45 |
| 1:C:839:LYS:HZ2 | 1:C:881:PRO:CD | 2.29 | 0.45 |
| 1:D:166:TYR:O | 1:D:170:TYR:CD1 | 2.70 | 0.45 |
| 1:D:176:GLU:O | 1:D:179:ARG:HB2 | 2.17 | 0.45 |
| 1:D:248:LEU:CD1 | 1:D:251:LEU:HD12 | 2.44 | 0.45 |
| 1:D:328:ASP:HB3 | 1:D:331:PHE:CB | 2.45 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:580:VAL:HA | 1:D:626:LYS:HE2 | 1.98 | 0.45 |
| 1:D:585:ASP:HA | 1:D:588:LYS:HZ3 | 1.81 | 0.45 |
| 1:D:781:HIS:CE1 | 1:D:808:GLN:HE22 | 2.35 | 0.45 |
| 1:D:808:GLN:CA | 1:D:811:LYS:HD3 | 2.47 | 0.45 |
| 1:D:859:LEU:O | 1:D:877:LEU:N | 2.50 | 0.45 |
| 1:E:205:LYS:HD2 | 1:E:334:ARG:O | 2.17 | 0.45 |
| 1:E:216:ILE:CD1 | 1:E:389:PRO:HD2 | 2.47 | 0.45 |
| 1:E:260:ASP:O | 1:E:261:PHE:C | 2.60 | 0.45 |
| 1:E:301:LEU:O | 1:E:304:ALA:N | 2.50 | 0.45 |
| 1:E:322:ARG:CG | 1:E:323:SER:H | 2.30 | 0.45 |
| 1:E:361:ILE:O | 1:E:362:HIS:C | 2.59 | 0.45 |
| 1:E:386:ARG:HB2 | 1:E:391:SER:HB2 | 1.98 | 0.45 |
| 1:E:570:ILE:HG13 | 1:E:571:HIS:N | 2.33 | 0.45 |
| 1:E:591:SER:O | 1:E:595:ARG:HG3 | 2.17 | 0.45 |
| 1:E:745:SER:O | 1:E:748:ASN:N | 2.50 | 0.45 |
| 1:F:175:THR:HG22 | 1:F:243:LEU:HD12 | 1.99 | 0.45 |
| 1:F:320:GLU:HB3 | 1:F:321:TYR:H | 1.48 | 0.45 |
| 1:F:689:GLU:OE2 | 1:F:758:PHE:CG | 2.70 | 0.45 |
| 1:F:836:ILE:HG22 | 1:F:840:LEU:CD1 | 2.47 | 0.45 |
| 1:A:213:GLU:CB | 1:A:387:ARG:HH21 | 2.29 | 0.44 |
| 1:A:236:THR:O | 1:A:238:LEU:N | 2.50 | 0.44 |
| 1:A:596:LEU:CD2 | 1:B:838:ASN:HA | 2.46 | 0.44 |
| 1:A:683:LEU:O | 1:A:723:VAL:HB | 2.17 | 0.44 |
| 1:B:281:LEU:HD12 | 1:B:282:PHE:CD1 | 2.52 | 0.44 |
| 1:B:302:LYS:HZ3 | 1:B:306:SER:N | 2.12 | 0.44 |
| 1:B:369:ASP:O | 1:B:372:LEU:N | 2.50 | 0.44 |
| 1:B:718:CYS:HG | 1:B:720:ASN:HB3 | 1.81 | 0.44 |
| 1:B:739:GLY:HA2 | 1:B:774:LYS:HD2 | 1.99 | 0.44 |
| 1:B:798:ASN:HB3 | 1:B:802:TYR:HE1 | 1.82 | 0.44 |
| 1:C:174:MET:HE2 | 1:C:244:PHE:CA | 2.36 | 0.44 |
| 1:C:281:LEU:H | 1:C:311:LYS:HG3 | 1.82 | 0.44 |
| 1:C:310:LEU:HA | 1:C:310:LEU:HD23 | 1.81 | 0.44 |
| 1:C:536:MET:C | 1:C:538:GLN:H | 2.25 | 0.44 |
| 1:C:620:LYS:HB3 | 1:C:772:PHE:CE1 | 2.52 | 0.44 |
| 1:C:838:ASN:O | 1:C:842:LEU:HB2 | 2.17 | 0.44 |
| 1:D:172:ILE:C | 1:D:244:PHE:HA | 2.42 | 0.44 |
| 1:D:189:ARG:HH12 | 1:D:341:ALA:CB | 2.14 | 0.44 |
| 1:D:190:GLU:N | 1:D:192:GLU:OE2 | 2.50 | 0.44 |
| 1:D:200:LEU:HD23 | 1:D:200:LEU:HA | 1.75 | 0.44 |
| 1:D:299:ASN:C | 1:D:301:LEU:HG | 2.42 | 0.44 |
| 1:D:343:PRO:HB2 | 1:D:347:GLN:HB3 | 1.98 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:557:PRO:CB | 1:D:558:VAL:HG23 | 2.47 | 0.44 |
| 1:D:559:LYS:HE2 | 1:D:560:LYS:HZ2 | 1.82 | 0.44 |
| 1:D:592:ASN:HB3 | 1:E:838:ASN:HD21 | 1.82 | 0.44 |
| 1:D:630:PHE:CD2 | 1:D:631:LEU:N | 2.86 | 0.44 |
| 1:D:684:LEU:CG | 1:D:726:THR:H | 2.30 | 0.44 |
| 1:D:702:MET:SD | 1:D:706:GLY:HA2 | 2.57 | 0.44 |
| 1:D:874:GLU:CB | 1:D:876:CYS:HB2 | 2.47 | 0.44 |
| 1:E:213:GLU:O | 1:E:218:LYS:HE3 | 2.16 | 0.44 |
| 1:E:216:ILE:HG12 | 1:E:217:GLY:H | 1.81 | 0.44 |
| 1:E:234:VAL:CG2 | 1:E:238:LEU:HB2 | 2.47 | 0.44 |
| 1:E:368:LEU:H | 1:E:540:VAL:CB | 2.26 | 0.44 |
| 1:E:473:HIS:O | 1:E:477:THR:N | 2.28 | 0.44 |
| 1:E:659:THR:OG1 | 1:E:667:GLU:OE1 | 2.34 | 0.44 |
| 1:E:809:GLU:O | 1:E:810:ALA:C | 2.60 | 0.44 |
| 1:F:266:LYS:HA | 1:F:269:LEU:HD12 | 1.99 | 0.44 |
| 1:F:287:HIS:NE2 | 1:F:322:ARG:CB | 2.80 | 0.44 |
| 1:F:351:ILE:HG22 | 1:F:355:LEU:HD22 | 1.99 | 0.44 |
| 1:F:616:SER:OG | 2:F:1002:AGS:O3B | 2.34 | 0.44 |
| 1:F:796:GLU:OE1 | 1:F:798:ASN:HB3 | 2.17 | 0.44 |
| 1:A:629:GLY:HA3 | 1:A:635:GLU:CG | 2.48 | 0.44 |
| 1:A:781:HIS:NE2 | 1:A:782:LYS:HG3 | 2.32 | 0.44 |
| 1:B:193:ILE:O | 1:B:197:ILE:HG13 | 2.17 | 0.44 |
| 1:B:198:ARG:C | 1:B:200:LEU:H | 2.23 | 0.44 |
| 1:B:202:ARG:NH1 | 1:B:204:ILE:O | 2.49 | 0.44 |
| 1:B:284:ASP:OD2 | 1:B:285:GLU:HA | 2.17 | 0.44 |
| 1:B:374:THR:O | 1:B:375:ALA:C | 2.60 | 0.44 |
| 1:B:549:THR:O | 1:B:550:ALA:C | 2.60 | 0.44 |
| 1:B:629:GLY:HA2 | 1:B:634:ASP:CA | 2.43 | 0.44 |
| 1:B:739:GLY:CA | 1:B:774:LYS:HD2 | 2.47 | 0.44 |
| 1:B:853:GLU:OE2 | 1:B:855:VAL:HG23 | 2.17 | 0.44 |
| 1:C:222:ILE:H | 1:C:222:ILE:HG13 | 1.56 | 0.44 |
| 1:C:579:GLU:HB2 | 1:C:626:LYS:CE | 2.46 | 0.44 |
| 1:C:583:GLN:CD | 1:C:583:GLN:N | 2.74 | 0.44 |
| 1:C:584:MET:HG3 | 1:C:585:ASP:OD1 | 2.17 | 0.44 |
| 1:C:598:ARG:HA | 1:C:598:ARG:HD3 | 1.35 | 0.44 |
| 1:C:638:MET:HE3 | 1:C:640:ARG:CD | 2.48 | 0.44 |
| 1:C:783:ILE:O | 1:C:786:ILE:HB | 2.17 | 0.44 |
| 1:C:785:ASP:CG | 1:C:786:ILE:HD12 | 2.42 | 0.44 |
| 1:C:825:ALA:N | 1:C:827:PRO:HG2 | 2.29 | 0.44 |
| 1:D:190:GLU:N | 1:D:192:GLU:OE1 | 2.50 | 0.44 |
| 1:D:224:GLY:O | 1:D:228:ARG:HG2 | 2.17 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:348:THR:O | 1:D:349:VAL:C | 2.57 | 0.44 |
| 1:D:378:LEU:O | 1:D:379:ALA:C | 2.59 | 0.44 |
| 1:D:425:GLN:O | 1:D:428:ILE:HB | 2.16 | 0.44 |
| 1:D:525:ALA:C | 1:D:534:ASN:HD21 | 2.25 | 0.44 |
| 1:D:591:SER:O | 1:D:594:VAL:HB | 2.17 | 0.44 |
| 1:D:641:VAL:HG12 | 1:D:642:ASP:H | 1.83 | 0.44 |
| 1:E:296:ASP:O | 1:E:296:ASP:CG | 2.60 | 0.44 |
| 1:E:400:CYS:O | 1:E:403:VAL:HB | 2.15 | 0.44 |
| 1:E:556:ILE:HB | 1:E:560:LYS:CD | 2.43 | 0.44 |
| 1:E:622:GLU:O | 1:E:623:LEU:C | 2.59 | 0.44 |
| 1:E:684:LEU:N | 1:E:723:VAL:HG23 | 2.32 | 0.44 |
| 1:E:689:GLU:HA | 1:E:758:PHE:HZ | 1.83 | 0.44 |
| 1:E:701:GLN:CG | 1:E:707:ARG:HB2 | 2.42 | 0.44 |
| 1:E:770:VAL:HA | 1:E:771:ILE:HD12 | 1.99 | 0.44 |
| 1:E:777:ARG:CA | 1:E:780:ILE:HG22 | 2.45 | 0.44 |
| 1:E:808:GLN:CD | 1:E:809:GLU:N | 2.75 | 0.44 |
| 1:E:839:LYS:O | 1:E:843:ARG:HG2 | 2.16 | 0.44 |
| 1:F:310:LEU:HG | 1:F:311:LYS:H | 1.82 | 0.44 |
| 1:F:823:MET:C | 1:F:825:ALA:N | 2.73 | 0.44 |
| 1:A:278:LEU:C | 1:A:279:ILE:HG13 | 2.42 | 0.44 |
| 1:A:674:GLN:NE2 | 1:A:677:TYR:HE2 | 2.14 | 0.44 |
| 1:B:211:ILE:N | 1:B:339:GLU:CD | 2.75 | 0.44 |
| 1:B:302:LYS:HD2 | 1:B:302:LYS:HA | 1.76 | 0.44 |
| 1:B:390:ASP:C | 1:B:392:ALA:N | 2.73 | 0.44 |
| 1:B:646:LEU:CB | 1:B:690:LYS:H | 2.27 | 0.44 |
| 1:C:129:ILE:O | 1:C:131:LYS:N | 2.50 | 0.44 |
| 1:C:335:PHE:N | 1:C:335:PHE:CD1 | 2.86 | 0.44 |
| 1:C:345:VAL:HG21 | 1:C:380:LYS:HD3 | 1.98 | 0.44 |
| 1:C:366:ARG:O | 1:C:539:ASN:HA | 2.17 | 0.44 |
| 1:C:396:VAL:O | 1:C:399:SER:HB2 | 2.17 | 0.44 |
| 1:C:558:VAL:HG13 | 1:C:561:LEU:CD1 | 2.47 | 0.44 |
| 1:C:563:GLU:OE2 | 1:C:564:SER:O | 2.34 | 0.44 |
| 1:C:573:GLU:HA | 1:C:576:LEU:CD1 | 2.46 | 0.44 |
| 1:C:616:SER:C | 1:C:823:MET:HE1 | 2.43 | 0.44 |
| 1:C:799:ASP:O | 1:C:801:HIS:CE1 | 2.71 | 0.44 |
| 1:C:833:GLN:NE2 | 1:C:834:ASN:HD21 | 2.15 | 0.44 |
| 1:D:171:ALA:HB1 | 1:D:244:PHE:C | 2.43 | 0.44 |
| 1:D:299:ASN:CG | 1:D:300:ILE:N | 2.72 | 0.44 |
| 1:D:376:ALA:O | 1:D:377:GLN:C | 2.61 | 0.44 |
| 1:D:381:ARG:HG3 | 1:D:382:TYR:CD1 | 2.52 | 0.44 |
| 1:D:556:ILE:HG21 | 1:D:633:ASN:ND2 | 2.32 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:566:ASN:C | 1:D:570:ILE:HG13 | 2.43 | 0.44 |
| 1:D:605:ARG:HG3 | 1:D:704:ASP:HA | 1.98 | 0.44 |
| 1:D:857:VAL:HG12 | 1:D:859:LEU:N | 2.06 | 0.44 |
| 1:E:242:LYS:O | 1:E:280:VAL:N | 2.47 | 0.44 |
| 1:E:301:LEU:O | 1:E:305:LEU:HG | 2.18 | 0.44 |
| 1:E:363:HIS:CD2 | 1:E:400:CYS:HB3 | 2.53 | 0.44 |
| 1:E:363:HIS:HD2 | 1:E:400:CYS:SG | 2.40 | 0.44 |
| 1:E:392:ALA:O | 1:E:396:VAL:HG23 | 2.17 | 0.44 |
| 1:E:596:LEU:HB3 | 1:F:837:LEU:HD21 | 2.00 | 0.44 |
| 1:E:619:GLY:O | 1:E:623:LEU:N | 2.24 | 0.44 |
| 1:E:723:VAL:HG22 | 1:E:724:ILE:C | 2.42 | 0.44 |
| 1:F:219:THR:HA | 1:F:222:ILE:CG1 | 2.44 | 0.44 |
| 1:F:549:THR:O | 1:F:552:ARG:HB3 | 2.17 | 0.44 |
| 1:F:563:GLU:HA | 1:F:568:LYS:HD3 | 1.99 | 0.44 |
| 1:F:721:CYS:O | 1:F:722:ILE:HD13 | 2.17 | 0.44 |
| 1:F:808:GLN:N | 1:F:811:LYS:HZ1 | 2.14 | 0.44 |
| 1:A:235:PRO:HD2 | 1:A:238:LEU:HD11 | 1.99 | 0.44 |
| 1:A:317:THR:O | 1:A:322:ARG:HB2 | 2.18 | 0.44 |
| 1:A:387:ARG:O | 1:A:390:ASP:HB3 | 2.17 | 0.44 |
| 1:A:643:CYS:CB | 1:A:685:PHE:HB3 | 2.47 | 0.44 |
| 1:A:843:ARG:NH2 | 1:A:880:LEU:O | 2.51 | 0.44 |
| 1:B:226:ALA:O | 1:B:229:ILE:HB | 2.18 | 0.44 |
| 1:B:286:ILE:HG12 | 1:B:316:THR:CB | 2.48 | 0.44 |
| 1:B:539:ASN:CG | 1:B:540:VAL:N | 2.75 | 0.44 |
| 1:B:569:LEU:O | 1:B:570:ILE:C | 2.60 | 0.44 |
| 1:B:782:LYS:HA | 1:B:785:ASP:CG | 2.43 | 0.44 |
| 1:C:170:TYR:HH | 1:C:250:ALA:N | 1.80 | 0.44 |
| 1:C:215:GLY:O | 2:C:1001:AGS:O2B | 2.36 | 0.44 |
| 1:C:282:PHE:CZ | 1:C:284:ASP:HA | 2.52 | 0.44 |
| 1:C:319:ASN:ND2 | 1:C:713:GLY:O | 2.51 | 0.44 |
| 1:C:374:THR:O | 1:C:378:LEU:HG | 2.16 | 0.44 |
| 1:C:394:ASP:O | 1:C:395:LEU:C | 2.58 | 0.44 |
| 1:C:557:PRO:CB | 1:C:560:LYS:HB2 | 2.48 | 0.44 |
| 1:C:618:SER:C | 1:C:826:ARG:CZ | 2.90 | 0.44 |
| 1:C:622:GLU:O | 1:C:623:LEU:C | 2.60 | 0.44 |
| 1:C:699:MET:O | 1:C:703:LEU:HD13 | 2.16 | 0.44 |
| 1:C:746:THR:C | 1:C:748:ASN:N | 2.73 | 0.44 |
| 1:C:798:ASN:HA | 1:C:801:HIS:HE2 | 1.83 | 0.44 |
| 1:C:814:LEU:O | 1:C:818:GLY:CA | 2.66 | 0.44 |
| 1:D:198:ARG:CG | 1:E:404:ALA:HB3 | 2.43 | 0.44 |
| 1:D:344:SER:CB | 1:D:345:VAL:HG23 | 2.48 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:369:ASP:O | 1:D:373:VAL:N | 2.37 | 0.44 |
| 1:D:381:ARG:NH1 | 1:D:382:TYR:CE1 | 2.75 | 0.44 |
| 1:D:610:PHE:O | 1:D:724:ILE:HG23 | 2.17 | 0.44 |
| 1:D:785:ASP:HA | 1:D:788:LEU:HB2 | 1.98 | 0.44 |
| 1:E:360:GLU:OE2 | 1:E:365:VAL:HG22 | 2.17 | 0.44 |
| 1:E:573:GLU:HA | 1:E:576:LEU:HB2 | 2.00 | 0.44 |
| 1:E:843:ARG:CZ | 1:E:882:ASN:HD22 | 2.30 | 0.44 |
| 1:F:194:ARG:N | 1:F:228:ARG:NH1 | 2.49 | 0.44 |
| 1:F:331:PHE:CD1 | 1:F:334:ARG:O | 2.57 | 0.44 |
| 1:F:389:PRO:O | 1:F:392:ALA:N | 2.51 | 0.44 |
| 1:F:707:ARG:CB | 1:F:715:THR:HG21 | 2.47 | 0.44 |
| 1:A:203:ARG:O | 1:A:204:ILE:HG12 | 2.17 | 0.44 |
| 1:A:205:LYS:HZ3 | 1:B:397:ASP:CB | 2.16 | 0.44 |
| 1:A:235:PRO:O | 1:A:238:LEU:HG | 2.18 | 0.44 |
| 1:A:346:ARG:NH1 | 1:A:349:VAL:CG1 | 2.81 | 0.44 |
| 1:A:565:GLU:HA | 1:A:568:LYS:CD | 2.48 | 0.44 |
| 1:A:595:ARG:NH1 | 1:B:842:LEU:HD12 | 2.32 | 0.44 |
| 1:A:643:CYS:HG | 1:A:725:MET:HB3 | 1.82 | 0.44 |
| 1:A:813:PHE:CZ | 1:A:857:VAL:HG21 | 2.51 | 0.44 |
| 1:A:839:LYS:HD2 | 1:A:842:LEU:HD12 | 2.00 | 0.44 |
| 1:A:841:ALA:HA | 1:A:844:ILE:HG22 | 1.99 | 0.44 |
| 1:B:65:PHE:N | 1:B:70:ASN:H | 2.15 | 0.44 |
| 1:B:205:LYS:HB3 | 1:B:336:GLN:CB | 2.47 | 0.44 |
| 1:B:210:LEU:HD12 | 1:B:210:LEU:N | 2.32 | 0.44 |
| 1:B:328:ASP:OD1 | 1:B:328:ASP:O | 2.35 | 0.44 |
| 1:B:391:SER:HA | 1:B:394:ASP:OD2 | 2.18 | 0.44 |
| 1:B:759:ARG:HD3 | 1:B:760:PRO:CD | 2.48 | 0.44 |
| 1:B:808:GLN:O | 1:B:809:GLU:C | 2.61 | 0.44 |
| 1:C:337:LYS:O | 1:C:337:LYS:HG3 | 2.18 | 0.44 |
| 1:C:595:ARG:HD3 | 1:D:841:ALA:HB1 | 2.00 | 0.44 |
| 1:C:622:GLU:HG2 | 1:C:826:ARG:HH22 | 1.83 | 0.44 |
| 1:C:641:VAL:HG12 | 1:C:642:ASP:N | 2.32 | 0.44 |
| 1:C:743:GLN:HB3 | 1:C:745:SER:HB2 | 1.98 | 0.44 |
| 1:C:834:ASN:HA | 1:C:837:LEU:CG | 2.47 | 0.44 |
| 1:D:263:GLU:O | 1:D:264:ARG:C | 2.61 | 0.44 |
| 1:D:564:SER:O | 1:D:568:LYS:N | 2.43 | 0.44 |
| 1:D:839:LYS:HZ2 | 1:D:879:VAL:C | 2.13 | 0.44 |
| 1:E:270:LYS:O | 1:E:271:GLU:C | 2.60 | 0.44 |
| 1:E:303:PRO:CA | 1:E:334:ARG:HH12 | 2.31 | 0.44 |
| 1:E:529:ARG:CZ | 1:E:535:SER:HB3 | 2.47 | 0.44 |
| 1:E:543:SER:C | 1:E:547:SER:H | 2.26 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:583:GLN:HE22 | 1:E:772:PHE:HA | 1.82 | 0.44 |
| 1:E:632:PHE:HB2 | 1:E:634:ASP:HB2 | 1.99 | 0.44 |
| 1:E:688:VAL:CG1 | 1:E:690:LYS:H | 2.22 | 0.44 |
| 1:E:709:THR:C | 1:E:716:ILE:H | 2.24 | 0.44 |
| 1:E:747:LYS:O | 1:E:750:VAL:HB | 2.18 | 0.44 |
| 1:E:789:LYS:O | 1:E:790:GLU:C | 2.60 | 0.44 |
| 1:F:197:ILE:CG1 | 1:F:228:ARG:NH1 | 2.75 | 0.44 |
| 1:F:322:ARG:NH1 | 1:F:326:GLU:HA | 2.32 | 0.44 |
| 1:F:344:SER:C | 1:F:347:GLN:HE22 | 2.19 | 0.44 |
| 1:F:651:ALA:O | 1:F:654:LYS:HG3 | 2.17 | 0.44 |
| 1:F:700:LEU:HB3 | 1:F:761:GLU:CD | 2.43 | 0.44 |
| 1:F:826:ARG:N | 1:F:827:PRO:HD3 | 2.32 | 0.44 |
| 1:A:176:GLU:OE1 | 1:A:176:GLU:N | 2.50 | 0.44 |
| 1:A:610:PHE:HA | 1:A:768:SER:O | 2.18 | 0.44 |
| 1:A:736:SER:HB2 | 1:A:738:GLN:HE21 | 1.83 | 0.44 |
| 1:B:550:ALA:CA | 1:B:552:ARG:NH1 | 2.80 | 0.44 |
| 1:B:693:PRO:HD2 | 1:B:694:ASP:N | 2.22 | 0.44 |
| 1:B:778:LYS:C | 1:B:781:HIS:HB3 | 2.43 | 0.44 |
| 1:B:843:ARG:HH11 | 1:B:848:GLU:CG | 2.30 | 0.44 |
| 1:C:230:ILE:C | 1:C:232:ASP:N | 2.74 | 0.44 |
| 1:C:328:ASP:OD1 | 1:C:329:GLY:N | 2.50 | 0.44 |
| 1:C:393:LEU:HA | 1:C:396:VAL:HB | 1.99 | 0.44 |
| 1:C:403:VAL:O | 1:C:404:ALA:C | 2.60 | 0.44 |
| 1:C:570:ILE:O | 1:C:573:GLU:OE1 | 2.36 | 0.44 |
| 1:D:243:LEU:HD23 | 1:D:244:PHE:N | 2.32 | 0.44 |
| 1:D:262:GLU:O | 1:D:265:PHE:HB3 | 2.18 | 0.44 |
| 1:D:353:ARG:O | 1:D:354:GLY:C | 2.59 | 0.44 |
| 1:D:763:LEU:CA | 1:D:766:ILE:HG12 | 2.48 | 0.44 |
| 1:D:835:GLU:OE2 | 1:D:878:GLU:CB | 2.65 | 0.44 |
| 1:D:855:VAL:CG2 | 1:D:880:LEU:HD22 | 2.46 | 0.44 |
| 1:E:181:GLY:C | 1:E:488:ASN:HD21 | 2.24 | 0.44 |
| 1:E:219:THR:O | 1:E:222:ILE:HB | 2.18 | 0.44 |
| 1:E:245:SER:HA | 1:E:281:LEU:HG | 1.99 | 0.44 |
| 1:E:270:LYS:CD | 1:E:273:GLU:HB2 | 2.47 | 0.44 |
| 1:E:307:ARG:O | 1:E:309:GLN:HG3 | 2.17 | 0.44 |
| 1:E:454:SER:O | 1:E:457:GLU:N | 2.41 | 0.44 |
| 1:E:510:ILE:H | 1:E:513:ILE:HG12 | 1.82 | 0.44 |
| 1:E:613:LEU:HG | 1:E:728:ALA:CB | 2.48 | 0.44 |
| 1:E:614:GLY:H | 1:E:728:ALA:CB | 2.30 | 0.44 |
| 1:E:637:MET:HG3 | 1:E:682:VAL:CG1 | 2.48 | 0.44 |
| 1:E:639:ILE:CB | 1:E:683:LEU:HA | 2.45 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:654:LYS:HZ2 | 1:E:698:VAL:CG1 | 2.29 | 0.44 |
| 1:E:834:ASN:HA | 1:E:837:LEU:HD12 | 1.99 | 0.44 |
| 1:F:383:LEU:HD23 | 1:F:383:LEU:HA | 1.67 | 0.44 |
| 1:F:390:ASP:HA | 1:F:393:LEU:HB2 | 2.00 | 0.44 |
| 1:F:616:SER:HA | 1:F:620:LYS:HB2 | 2.00 | 0.44 |
| 1:F:625:LYS:NZ | 1:F:636:ASP:O | 2.44 | 0.44 |
| 1:F:733:PHE:HB3 | 1:F:746:THR:CG2 | 2.47 | 0.44 |
| 1:A:206:SER:N | 1:A:334:ARG:HB3 | 2.18 | 0.44 |
| 1:A:218:LYS:O | 1:A:221:ILE:HB | 2.18 | 0.44 |
| 1:A:285:GLU:HG3 | 1:A:287:HIS:N | 2.32 | 0.44 |
| 1:A:374:THR:O | 1:A:377:GLN:N | 2.51 | 0.44 |
| 1:B:223:GLU:N | 1:B:223:GLU:CD | 2.67 | 0.44 |
| 1:B:384:PRO:HG2 | 1:B:385:TYR:H | 1.82 | 0.44 |
| 1:B:683:LEU:HD22 | 1:B:723:VAL:O | 2.18 | 0.44 |
| 1:B:710:SER:OG | 1:B:712:GLN:HB3 | 2.18 | 0.44 |
| 1:B:777:ARG:HA | 1:B:780:ILE:HG12 | 2.00 | 0.44 |
| 1:B:839:LYS:O | 1:B:842:LEU:HD22 | 2.18 | 0.44 |
| 1:C:186:VAL:CG1 | 1:C:187:ILE:N | 2.81 | 0.44 |
| 1:C:286:ILE:O | 1:C:287:HIS:C | 2.61 | 0.44 |
| 1:C:288:MET:HG3 | 1:C:320:GLU:OE2 | 2.17 | 0.44 |
| 1:C:577:SER:HA | 1:C:581:VAL:N | 2.19 | 0.44 |
| 1:C:637:MET:HG3 | 1:C:678:LYS:HE3 | 1.99 | 0.44 |
| 1:C:769:ILE:O | 1:C:770:VAL:HB | 2.18 | 0.44 |
| 1:C:845:LEU:HG | 1:C:845:LEU:H | 1.59 | 0.44 |
| 1:D:283:ILE:HG22 | 1:D:284:ASP:C | 2.43 | 0.44 |
| 1:D:404:ALA:CA | 1:D:407:ARG:HE | 2.30 | 0.44 |
| 1:D:446:LYS:HG3 | 1:D:447:LEU:HD12 | 2.00 | 0.44 |
| 1:D:474:GLU:O | 1:D:478:GLN:HG3 | 2.17 | 0.44 |
| 1:D:485:GLU:O | 1:D:489:LYS:HG3 | 2.17 | 0.44 |
| 1:D:616:SER:C | 1:D:823:MET:HE2 | 2.42 | 0.44 |
| 1:D:639:ILE:HG21 | 1:D:639:ILE:HD13 | 1.60 | 0.44 |
| 1:D:696:LEU:HB3 | 1:D:699:MET:HE2 | 1.99 | 0.44 |
| 1:D:775:LEU:CB | 1:D:780:ILE:HD11 | 2.47 | 0.44 |
| 1:E:203:ARG:CD | 1:F:359:TYR:CE1 | 2.90 | 0.44 |
| 1:E:349:VAL:HA | 1:E:352:LEU:CD1 | 2.46 | 0.44 |
| 1:E:366:ARG:HH12 | 1:E:368:LEU:CA | 2.30 | 0.44 |
| 1:E:383:LEU:HD23 | 1:E:385:TYR:N | 2.32 | 0.44 |
| 1:E:387:ARG:O | 1:E:388:LEU:C | 2.59 | 0.44 |
| 1:E:410:LYS:O | 1:E:411:PRO:C | 2.61 | 0.44 |
| 1:E:512:ASP:O | 1:E:513:ILE:C | 2.61 | 0.44 |
| 1:E:553:LEU:HA | 1:E:553:LEU:HD23 | 1.63 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:612:PHE:CA | 1:E:771:ILE:HG13 | 2.48 | 0.44 |
| 1:E:626:LYS:HD3 | 1:E:626:LYS:HA | 1.69 | 0.44 |
| 1:F:243:LEU:C | 1:F:281:LEU:HB2 | 2.42 | 0.44 |
| 1:F:243:LEU:HA | 1:F:281:LEU:HA | 2.00 | 0.44 |
| 1:F:394:ASP:O | 1:F:395:LEU:C | 2.61 | 0.44 |
| 1:F:683:LEU:HD22 | 1:F:685:PHE:CE1 | 2.53 | 0.44 |
| 1:F:701:GLN:C | 1:F:703:LEU:HD12 | 2.43 | 0.44 |
| 1:F:755:ARG:NH1 | 1:F:763:LEU:O | 2.49 | 0.44 |
| 1:F:796:GLU:CD | 1:F:798:ASN:HB3 | 2.42 | 0.44 |
| 1:F:843:ARG:HH21 | 1:F:849:ILE:HD13 | 1.82 | 0.44 |
| 1:A:352:LEU:O | 1:A:355:LEU:HD13 | 2.18 | 0.44 |
| 1:A:583:GLN:NE2 | 1:A:773:ASN:N | 2.66 | 0.44 |
| 1:B:173:ASP:O | 1:B:174:MET:C | 2.60 | 0.44 |
| 1:B:213:GLU:HG2 | 1:B:387:ARG:HD2 | 2.00 | 0.44 |
| 1:B:228:ARG:NH1 | 1:B:231:ASP:CG | 2.76 | 0.44 |
| 1:B:235:PRO:HB3 | 1:C:408:ASP:C | 2.42 | 0.44 |
| 1:B:315:ALA:C | 1:B:316:THR:HG1 | 2.22 | 0.44 |
| 1:B:359:TYR:CA | 1:B:362:HIS:HB3 | 2.43 | 0.44 |
| 1:B:605:ARG:HG3 | 1:B:606:GLN:HG2 | 2.00 | 0.44 |
| 1:B:632:PHE:CE2 | 1:B:680:TYR:HB3 | 2.53 | 0.44 |
| 1:B:655:LEU:HA | 1:B:671:LEU:HD21 | 2.00 | 0.44 |
| 1:C:174:MET:HB2 | 1:C:242:LYS:HD2 | 2.00 | 0.44 |
| 1:C:261:PHE:C | 1:C:263:GLU:N | 2.72 | 0.44 |
| 1:C:313:ILE:O | 1:C:313:ILE:HG22 | 2.17 | 0.44 |
| 1:C:385:TYR:CD2 | 1:C:386:ARG:N | 2.86 | 0.44 |
| 1:C:394:ASP:C | 1:C:398:ILE:HD12 | 2.42 | 0.44 |
| 1:C:549:THR:HG22 | 1:C:553:LEU:HD11 | 1.99 | 0.44 |
| 1:C:675:LEU:C | 1:C:678:LYS:H | 2.26 | 0.44 |
| 1:C:731:ALA:O | 1:C:732:GLU:C | 2.60 | 0.44 |
| 1:C:742:ILE:HG22 | 1:C:743:GLN:N | 2.32 | 0.44 |
| 1:D:192:GLU:O | 1:D:196:THR:OG1 | 2.18 | 0.44 |
| 1:D:193:ILE:HG22 | 1:D:197:ILE:HD11 | 1.99 | 0.44 |
| 1:D:195:SER:O | 1:D:198:ARG:N | 2.51 | 0.44 |
| 1:D:218:LYS:HG2 | 2:D:1001:AGS:PB | 2.58 | 0.44 |
| 1:D:245:SER:HA | 1:D:282:PHE:CD2 | 2.52 | 0.44 |
| 1:D:286:ILE:C | 1:D:289:LEU:H | 2.26 | 0.44 |
| 1:D:296:ASP:O | 1:D:299:ASN:N | 2.45 | 0.44 |
| 1:D:340:VAL:HG12 | 1:D:341:ALA:N | 2.33 | 0.44 |
| 1:D:462:LEU:HG | 1:D:465:ARG:CZ | 2.48 | 0.44 |
| 1:D:470:LYS:HE3 | 1:D:470:LYS:HB3 | 1.68 | 0.44 |
| 1:D:731:ALA:O | 1:D:732:GLU:C | 2.61 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:D:805:ASN:OD1 | 1:D:855:VAL:O | 2.36 | 0.44 |
| 1:E:205:LYS:HE3 | 1:E:336:GLN:NE2 | 2.33 | 0.44 |
| 1:E:216:ILE:O | 2:E:1001:AGS:PA | 2.75 | 0.44 |
| 1:E:227:GLN:O | 1:E:231:ASP:N | 2.42 | 0.44 |
| 1:E:307:ARG:NH2 | 1:F:248:LEU:HD11 | 2.33 | 0.44 |
| 1:E:364:GLY:O | 1:E:407:ARG:CZ | 2.65 | 0.44 |
| 1:E:408:ASP:OD2 | 1:E:414:LEU:HD12 | 2.18 | 0.44 |
| 1:E:429:LYS:HE3 | 1:E:429:LYS:HB3 | 1.84 | 0.44 |
| 1:E:657:GLY:HA3 | 1:E:667:GLU:CA | 2.46 | 0.44 |
| 1:E:703:LEU:O | 1:E:704:ASP:C | 2.59 | 0.44 |
| 1:E:780:ILE:HA | 1:E:783:ILE:HB | 2.00 | 0.44 |
| 1:E:841:ALA:O | 1:E:844:ILE:HB | 2.17 | 0.44 |
| 1:F:210:LEU:CD1 | 1:F:339:GLU:HA | 2.43 | 0.44 |
| 1:F:226:ALA:C | 1:F:229:ILE:H | 2.25 | 0.44 |
| 1:F:242:LYS:O | 1:F:281:LEU:HB3 | 2.17 | 0.44 |
| 1:F:347:GLN:HG2 | 1:F:351:ILE:CD1 | 2.48 | 0.44 |
| 1:F:593:ALA:HB3 | 1:F:608:ALA:O | 2.17 | 0.44 |
| 1:F:792:GLU:HG2 | 1:F:793:GLU:N | 2.32 | 0.44 |
| 1:F:837:LEU:HA | 1:F:840:LEU:HD13 | 1.98 | 0.44 |
| 1:A:378:LEU:HA | 1:A:381:ARG:HD2 | 1.99 | 0.44 |
| 1:A:557:PRO:O | 1:A:561:LEU:HB2 | 2.17 | 0.44 |
| 1:A:571:HIS:CD2 | 1:A:574:ARG:CZ | 3.00 | 0.44 |
| 1:A:753:ALA:O | 1:A:756:GLN:HG2 | 2.18 | 0.44 |
| 1:B:210:LEU:HB3 | 1:B:339:GLU:HB3 | 2.00 | 0.44 |
| 1:B:234:VAL:CG1 | 1:B:238:LEU:HG | 2.48 | 0.44 |
| 1:B:347:GLN:O | 1:B:350:ALA:HB3 | 2.17 | 0.44 |
| 1:B:357:PRO:O | 1:B:358:LYS:C | 2.61 | 0.44 |
| 1:B:552:ARG:HG3 | 1:B:553:LEU:N | 2.33 | 0.44 |
| 1:B:672:THR:HA | 1:B:675:LEU:HD12 | 1.99 | 0.44 |
| 1:B:685:PHE:HB2 | 1:B:725:MET:HG2 | 1.99 | 0.44 |
| 1:B:685:PHE:HE2 | 1:B:687:GLU:OE2 | 2.01 | 0.44 |
| 1:B:709:THR:C | 1:B:715:THR:HG22 | 2.43 | 0.44 |
| 1:B:736:SER:HG | 1:B:774:LYS:NZ | 2.14 | 0.44 |
| 1:B:761:GLU:CA | 1:B:764:ASN:HB3 | 2.42 | 0.44 |
| 1:C:228:ARG:NH1 | 1:D:409:SER:OG | 2.44 | 0.44 |
| 1:C:266:LYS:O | 1:C:270:LYS:HG2 | 2.18 | 0.44 |
| 1:C:270:LYS:HA | 1:C:270:LYS:HD3 | 1.67 | 0.44 |
| 1:C:526:GLU:H | 1:C:533:ALA:HB2 | 1.81 | 0.44 |
| 1:C:546:ILE:O | 1:C:549:THR:N | 2.51 | 0.44 |
| 1:C:710:SER:C | 1:C:713:GLY:H | 2.26 | 0.44 |
| 1:C:798:ASN:HA | 1:C:801:HIS:NE2 | 2.32 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:836:ILE:O | 1:C:839:LYS:N | 2.50 | 0.44 |
| 1:D:174:MET:C | 1:D:176:GLU:N | 2.71 | 0.44 |
| 1:D:227:GLN:CD | 1:D:230:ILE:HB | 2.43 | 0.44 |
| 1:D:331:PHE:CE2 | 1:D:335:PHE:HZ | 2.36 | 0.44 |
| 1:D:348:THR:O | 1:D:351:ILE:HB | 2.17 | 0.44 |
| 1:D:658:THR:OG1 | 1:D:662:TYR:HB2 | 2.18 | 0.44 |
| 1:D:696:LEU:HA | 1:D:699:MET:CB | 2.42 | 0.44 |
| 1:D:733:PHE:CE2 | 1:D:746:THR:O | 2.71 | 0.44 |
| 1:D:835:GLU:HA | 1:D:838:ASN:ND2 | 2.33 | 0.44 |
| 1:E:268:VAL:O | 1:E:269:LEU:C | 2.60 | 0.44 |
| 1:E:310:LEU:HG | 1:E:311:LYS:O | 2.18 | 0.44 |
| 1:E:338:ILE:HG22 | 1:E:339:GLU:N | 2.27 | 0.44 |
| 1:E:457:GLU:C | 1:E:460:GLU:H | 2.24 | 0.44 |
| 1:E:462:LEU:HG | 1:E:466:TYR:HE2 | 1.83 | 0.44 |
| 1:E:510:ILE:HA | 1:E:513:ILE:HG12 | 2.00 | 0.44 |
| 1:E:625:LYS:HE2 | 1:E:626:LYS:NZ | 2.33 | 0.44 |
| 1:E:650:TYR:HD1 | 1:E:656:LEU:HG | 1.83 | 0.44 |
| 1:E:742:ILE:HD11 | 1:E:773:ASN:HA | 2.00 | 0.44 |
| 1:E:748:ASN:HA | 1:E:751:MET:CG | 2.24 | 0.44 |
| 1:E:806:LEU:HD11 | 1:E:856:ASN:HA | 2.00 | 0.44 |
| 1:E:807:THR:C | 1:E:811:LYS:HG3 | 2.43 | 0.44 |
| 1:F:193:ILE:C | 1:F:228:ARG:NH1 | 2.76 | 0.44 |
| 1:F:592:ASN:HB2 | 1:F:610:PHE:HE1 | 1.82 | 0.44 |
| 1:F:593:ALA:HB1 | 1:F:596:LEU:HB2 | 1.98 | 0.44 |
| 1:F:778:LYS:O | 1:F:780:ILE:N | 2.51 | 0.44 |
| 1:F:820:SER:HB3 | 1:F:824:GLY:N | 2.33 | 0.44 |
| 1:A:235:PRO:HA | 1:B:408:ASP:OD1 | 2.18 | 0.43 |
| 1:A:387:ARG:HB2 | 1:A:390:ASP:HB3 | 2.00 | 0.43 |
| 1:A:564:SER:HB2 | 1:A:567:GLU:OE2 | 2.18 | 0.43 |
| 1:A:606:GLN:NE2 | 1:A:608:ALA:HA | 2.33 | 0.43 |
| 1:A:623:LEU:HA | 1:A:626:LYS:HB2 | 2.00 | 0.43 |
| 1:A:689:GLU:HG3 | 1:A:757:HIS:CD2 | 2.52 | 0.43 |
| 1:A:762:PHE:CD2 | 1:A:766:ILE:HD11 | 2.53 | 0.43 |
| 1:A:813:PHE:CG | 1:A:857:VAL:HG11 | 2.52 | 0.43 |
| 1:B:88:PRO:N | 1:B:93:GLY:HA3 | 2.33 | 0.43 |
| 1:B:159:ASP:C | 1:B:161:ASN:H | 2.26 | 0.43 |
| 1:B:551:ALA:O | 1:B:554:THR:N | 2.50 | 0.43 |
| 1:B:619:GLY:O | 1:B:620:LYS:C | 2.60 | 0.43 |
| 1:B:637:MET:HE2 | 1:B:680:TYR:C | 2.42 | 0.43 |
| 1:B:641:VAL:N | 1:B:684:LEU:HD22 | 2.32 | 0.43 |
| 1:B:778:LYS:O | 1:B:782:LYS:N | 2.45 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:189:ARG:HA | 1:C:192:GLU:OE2 | 2.18 | 0.43 |
| 1:C:221:ILE:HG22 | 1:C:225:VAL:HG23 | 1.99 | 0.43 |
| 1:C:243:LEU:CD1 | 1:C:280:VAL:HB | 2.48 | 0.43 |
| 1:C:245:SER:HA | 1:C:283:ILE:HA | 1.99 | 0.43 |
| 1:C:282:PHE:HA | 1:C:312:VAL:CG2 | 2.30 | 0.43 |
| 1:C:291:GLY:O | 1:C:294:LYS:HG3 | 2.18 | 0.43 |
| 1:C:776:SER:O | 1:C:779:ALA:HB3 | 2.17 | 0.43 |
| 1:D:175:THR:HA | 1:D:178:ALA:CB | 2.45 | 0.43 |
| 1:D:344:SER:O | 1:D:345:VAL:C | 2.60 | 0.43 |
| 1:D:375:ALA:O | 1:D:376:ALA:C | 2.61 | 0.43 |
| 1:D:462:LEU:HG | 1:D:465:ARG:NH1 | 2.32 | 0.43 |
| 1:D:552:ARG:HD3 | 1:D:552:ARG:HA | 1.63 | 0.43 |
| 1:D:655:LEU:HA | 1:D:668:GLY:HA3 | 2.00 | 0.43 |
| 1:D:655:LEU:HG | 1:D:671:LEU:HD11 | 2.00 | 0.43 |
| 1:D:710:SER:O | 1:D:713:GLY:N | 2.48 | 0.43 |
| 1:D:733:PHE:CE2 | 1:D:750:VAL:N | 2.86 | 0.43 |
| 1:D:769:ILE:HG23 | 1:D:769:ILE:O | 2.17 | 0.43 |
| 1:D:792:GLU:OE2 | 1:D:801:HIS:HA | 2.18 | 0.43 |
| 1:E:200:LEU:HD23 | 1:E:206:SER:O | 2.18 | 0.43 |
| 1:E:230:ILE:C | 1:E:232:ASP:H | 2.26 | 0.43 |
| 1:E:251:LEU:HD23 | 1:E:254:GLY:C | 2.43 | 0.43 |
| 1:E:255:ALA:C | 1:E:256:LYS:HG3 | 2.43 | 0.43 |
| 1:E:407:ARG:HA | 1:E:536:MET:CE | 2.48 | 0.43 |
| 1:E:483:LEU:HD12 | 1:E:513:ILE:CG2 | 2.48 | 0.43 |
| 1:E:546:ILE:O | 1:E:547:SER:C | 2.59 | 0.43 |
| 1:E:676:GLN:CD | 1:E:677:TYR:H | 2.26 | 0.43 |
| 1:E:758:PHE:O | 1:E:761:GLU:OE2 | 2.36 | 0.43 |
| 1:E:826:ARG:HB2 | 1:E:827:PRO:HD3 | 2.00 | 0.43 |
| 1:F:269:LEU:HA | 1:F:269:LEU:HD23 | 1.81 | 0.43 |
| 1:F:269:LEU:CA | 1:F:272:ILE:HG12 | 2.47 | 0.43 |
| 1:F:280:VAL:N | 1:F:310:LEU:HD11 | 2.33 | 0.43 |
| 1:F:553:LEU:HD23 | 1:F:553:LEU:HA | 1.76 | 0.43 |
| 1:F:748:ASN:HB2 | 1:F:749:LEU:HG | 1.99 | 0.43 |
| 1:F:769:ILE:HG22 | 1:F:770:VAL:N | 2.33 | 0.43 |
| 1:F:789:LYS:CA | 1:F:792:GLU:OE2 | 2.65 | 0.43 |
| 1:F:812:ASP:CB | 1:F:816:LYS:HZ2 | 2.31 | 0.43 |
| 1:F:820:SER:OG | 1:F:822:ASP:N | 2.50 | 0.43 |
| 2:F:1001:AGS:O2G | 2:F:1001:AGS:O1B | 2.35 | 0.43 |
| 1:A:168:SER:C | 1:A:171:ALA:H | 2.25 | 0.43 |
| 1:A:176:GLU:HA | 1:A:179:ARG:CB | 2.34 | 0.43 |
| 1:A:204:ILE:HD12 | 1:A:334:ARG:NH2 | 2.33 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:287:HIS:HA | 1:A:290:MET:HG3 | 1.99 | 0.43 |
| 1:A:289:LEU:O | 1:A:290:MET:HG3 | 2.18 | 0.43 |
| 1:A:594:VAL:O | 1:A:597:SER:OG | 2.13 | 0.43 |
| 1:A:605:ARG:HA | 1:A:705:ASP:HA | 2.01 | 0.43 |
| 1:A:656:LEU:O | 1:A:669:GLY:N | 2.51 | 0.43 |
| 1:A:804:LEU:HD12 | 1:A:855:VAL:CG2 | 2.48 | 0.43 |
| 1:A:828:LEU:O | 1:A:831:LEU:HB3 | 2.18 | 0.43 |
| 1:B:169:LYS:HG3 | 1:B:170:TYR:N | 2.33 | 0.43 |
| 1:B:208:PRO:HA | 1:B:337:LYS:CB | 2.48 | 0.43 |
| 1:B:210:LEU:CA | 1:B:339:GLU:HB3 | 2.47 | 0.43 |
| 1:B:234:VAL:HG12 | 1:B:239:GLN:HG3 | 1.99 | 0.43 |
| 1:B:247:ASP:C | 1:B:249:ALA:N | 2.74 | 0.43 |
| 1:B:252:THR:C | 1:B:254:GLY:H | 2.26 | 0.43 |
| 1:B:296:ASP:CB | 1:B:300:ILE:HB | 2.48 | 0.43 |
| 1:B:304:ALA:O | 1:B:307:ARG:HB2 | 2.17 | 0.43 |
| 1:B:623:LEU:HG | 1:B:624:ALA:N | 2.32 | 0.43 |
| 1:B:630:PHE:CZ | 1:B:631:LEU:HD23 | 2.53 | 0.43 |
| 1:B:634:ASP:HB2 | 1:B:635:GLU:OE1 | 2.18 | 0.43 |
| 1:B:751:MET:C | 1:B:755:ARG:HH12 | 2.25 | 0.43 |
| 1:C:48:VAL:C | 1:C:54:LEU:H | 2.26 | 0.43 |
| 1:C:189:ARG:C | 1:C:192:GLU:CD | 2.86 | 0.43 |
| 1:C:194:ARG:O | 1:C:195:SER:C | 2.60 | 0.43 |
| 1:C:336:GLN:OE1 | 1:C:336:GLN:N | 2.51 | 0.43 |
| 1:C:356:GLN:N | 1:C:357:PRO:HD2 | 2.33 | 0.43 |
| 1:C:391:SER:O | 1:C:392:ALA:C | 2.61 | 0.43 |
| 1:C:543:SER:OG | 1:C:544:ASP:N | 2.39 | 0.43 |
| 1:C:640:ARG:NE | 1:C:684:LEU:HD13 | 2.33 | 0.43 |
| 1:C:655:LEU:HB2 | 1:C:671:LEU:HD11 | 2.00 | 0.43 |
| 1:C:785:ASP:CG | 1:C:811:LYS:HZ2 | 2.26 | 0.43 |
| 1:C:804:LEU:C | 1:C:854:THR:HG23 | 2.43 | 0.43 |
| 1:D:180:GLN:HB3 | 1:D:182:LYS:CG | 2.42 | 0.43 |
| 1:D:281:LEU:CD1 | 1:D:312:VAL:HG12 | 2.42 | 0.43 |
| 1:D:418:GLU:O | 1:D:423:LEU:HG | 2.18 | 0.43 |
| 1:D:543:SER:O | 1:D:546:ILE:HB | 2.18 | 0.43 |
| 1:D:559:LYS:HA | 1:D:562:SER:OG | 2.18 | 0.43 |
| 1:D:585:ASP:N | 1:D:588:LYS:NZ | 2.65 | 0.43 |
| 1:D:752:GLY:HA2 | 1:D:755:ARG:CZ | 2.48 | 0.43 |
| 1:D:779:ALA:O | 1:D:780:ILE:C | 2.61 | 0.43 |
| 1:D:792:GLU:HA | 1:D:795:PHE:CZ | 2.52 | 0.43 |
| 1:D:802:TYR:CG | 1:D:853:GLU:OE2 | 2.71 | 0.43 |
| 1:E:216:ILE:C | 2:E:1001:AGS:H4' | 2.42 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:245:SER:O | 1:E:246:LEU:HB2 | 2.18 | 0.43 |
| 1:E:283:ILE:HG22 | 1:E:284:ASP:N | 2.34 | 0.43 |
| 1:E:409:SER:HB2 | 1:E:470:LYS:NZ | 2.33 | 0.43 |
| 1:E:523:GLN:HA | 1:E:526:GLU:HB2 | 1.99 | 0.43 |
| 1:E:549:THR:HG22 | 1:E:553:LEU:CD1 | 2.48 | 0.43 |
| 1:E:621:THR:OG1 | 2:E:1002:AGS:PA | 2.76 | 0.43 |
| 1:E:650:TYR:CE1 | 1:E:694:ASP:OD2 | 2.70 | 0.43 |
| 1:E:807:THR:CA | 1:E:811:LYS:NZ | 2.81 | 0.43 |
| 1:F:179:ARG:HA | 1:F:179:ARG:HD2 | 1.74 | 0.43 |
| 1:F:323:SER:HA | 1:F:326:GLU:HB3 | 1.99 | 0.43 |
| 1:F:542:ASP:O | 1:F:543:SER:HB3 | 2.18 | 0.43 |
| 1:F:811:LYS:HA | 1:F:814:LEU:HB2 | 2.00 | 0.43 |
| 1:F:853:GLU:OE2 | 1:F:854:THR:O | 2.37 | 0.43 |
| 1:A:209:CYS:HA | 1:A:315:ALA:HA | 2.00 | 0.43 |
| 1:A:306:SER:C | 1:A:307:ARG:HG3 | 2.43 | 0.43 |
| 1:A:325:VAL:HA | 1:A:328:ASP:HB2 | 2.00 | 0.43 |
| 1:A:579:GLU:OE1 | 1:A:580:VAL:N | 2.52 | 0.43 |
| 1:A:591:SER:O | 1:A:594:VAL:N | 2.51 | 0.43 |
| 1:A:642:ASP:HA | 1:A:686:ASP:HB2 | 1.99 | 0.43 |
| 1:A:777:ARG:O | 1:A:778:LYS:C | 2.61 | 0.43 |
| 1:A:823:MET:HE2 | 1:F:307:ARG:HB2 | 2.00 | 0.43 |
| 1:B:237:ILE:HG13 | 1:B:238:LEU:N | 2.34 | 0.43 |
| 1:B:286:ILE:HG13 | 1:B:320:GLU:OE2 | 2.19 | 0.43 |
| 1:B:303:PRO:O | 1:B:306:SER:OG | 2.11 | 0.43 |
| 1:B:375:ALA:HA | 1:B:378:LEU:HB2 | 2.01 | 0.43 |
| 1:B:551:ALA:HA | 1:B:554:THR:CG2 | 2.45 | 0.43 |
| 1:B:566:ASN:O | 1:B:567:GLU:C | 2.62 | 0.43 |
| 1:B:581:VAL:HG12 | 1:B:582:GLY:N | 2.33 | 0.43 |
| 1:B:583:GLN:HE21 | 1:B:773:ASN:CB | 2.31 | 0.43 |
| 1:C:212:GLY:O | 1:C:213:GLU:HB2 | 2.17 | 0.43 |
| 1:C:225:VAL:C | 1:C:227:GLN:N | 2.71 | 0.43 |
| 1:C:287:HIS:CG | 1:C:288:MET:N | 2.87 | 0.43 |
| 1:C:380:LYS:CG | 1:C:381:ARG:N | 2.81 | 0.43 |
| 1:C:502:ALA:O | 1:C:506:ARG:HD3 | 2.17 | 0.43 |
| 1:C:585:ASP:O | 1:C:586:ALA:C | 2.60 | 0.43 |
| 1:C:785:ASP:HB2 | 1:C:789:LYS:HZ2 | 1.83 | 0.43 |
| 1:D:266:LYS:HA | 1:D:269:LEU:CD1 | 2.47 | 0.43 |
| 1:D:346:ARG:O | 1:D:347:GLN:C | 2.61 | 0.43 |
| 1:D:349:VAL:O | 1:D:352:LEU:N | 2.51 | 0.43 |
| 1:D:378:LEU:C | 1:D:382:TYR:CD2 | 2.97 | 0.43 |
| 1:D:414:LEU:HD13 | 1:D:459:LEU:HD21 | 2.00 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:425:GLN:NE2 | 1:D:456:GLN:HE22 | 2.17 | 0.43 |
| 1:D:458:GLU:O | 1:D:461:PRO:HD2 | 2.18 | 0.43 |
| 1:D:462:LEU:HD21 | 1:D:465:ARG:HH11 | 1.83 | 0.43 |
| 1:D:558:VAL:CA | 1:D:561:LEU:HD13 | 2.48 | 0.43 |
| 1:D:575:ASP:C | 1:D:577:SER:N | 2.75 | 0.43 |
| 1:D:674:GLN:O | 1:D:675:LEU:C | 2.61 | 0.43 |
| 1:D:689:GLU:HB2 | 1:D:729:LEU:HD12 | 2.00 | 0.43 |
| 1:D:699:MET:O | 1:D:702:MET:N | 2.51 | 0.43 |
| 1:D:747:LYS:O | 1:D:751:MET:HB3 | 2.18 | 0.43 |
| 1:D:791:ILE:C | 1:D:793:GLU:N | 2.75 | 0.43 |
| 1:E:324:ILE:HA | 1:E:327:LYS:NZ | 2.33 | 0.43 |
| 1:E:352:LEU:HA | 1:E:355:LEU:HG | 2.00 | 0.43 |
| 1:E:366:ARG:NH1 | 1:E:539:ASN:CG | 2.64 | 0.43 |
| 1:E:428:ILE:HG12 | 1:E:449:ARG:HD3 | 2.00 | 0.43 |
| 1:E:544:ASP:HB2 | 1:E:545:THR:H | 1.42 | 0.43 |
| 1:E:580:VAL:HG23 | 1:E:581:VAL:H | 1.83 | 0.43 |
| 1:E:587:ILE:O | 1:E:591:SER:OG | 2.31 | 0.43 |
| 1:E:651:ALA:HA | 1:E:656:LEU:HD12 | 2.00 | 0.43 |
| 1:E:759:ARG:HB3 | 1:E:761:GLU:CD | 2.43 | 0.43 |
| 1:E:803:LYS:HZ1 | 1:E:854:THR:CG2 | 2.31 | 0.43 |
| 1:E:805:ASN:HB2 | 1:E:807:THR:HG22 | 2.00 | 0.43 |
| 1:E:821:ASP:O | 1:E:822:ASP:C | 2.60 | 0.43 |
| 1:F:170:TYR:CG | 1:F:250:ALA:HB2 | 2.53 | 0.43 |
| 1:F:220:ALA:O | 1:F:223:GLU:HB2 | 2.18 | 0.43 |
| 1:F:378:LEU:O | 1:F:383:LEU:HD12 | 2.19 | 0.43 |
| 1:F:389:PRO:HB2 | 1:F:393:LEU:HG | 2.00 | 0.43 |
| 1:F:787:ARG:HA | 1:F:787:ARG:HD3 | 1.73 | 0.43 |
| 1:F:792:GLU:N | 1:F:792:GLU:CD | 2.76 | 0.43 |
| 1:A:193:ILE:O | 1:A:194:ARG:C | 2.61 | 0.43 |
| 1:A:216:ILE:HD13 | 1:A:216:ILE:HA | 1.89 | 0.43 |
| 1:A:230:ILE:HG21 | 1:A:243:LEU:HD23 | 2.00 | 0.43 |
| 1:A:836:ILE:O | 1:A:840:LEU:HG | 2.18 | 0.43 |
| 1:B:229:ILE:HA | 1:B:238:LEU:HD22 | 2.00 | 0.43 |
| 1:B:361:ILE:O | 1:B:362:HIS:C | 2.60 | 0.43 |
| 1:B:362:HIS:CD2 | 1:B:363:HIS:CE1 | 3.06 | 0.43 |
| 1:B:396:VAL:O | 1:B:399:SER:HB2 | 2.18 | 0.43 |
| 1:B:617:GLY:CA | 1:B:826:ARG:HH11 | 2.30 | 0.43 |
| 1:B:681:SER:OG | 1:B:683:LEU:HB2 | 2.18 | 0.43 |
| 1:B:699:MET:O | 1:B:703:LEU:HG | 2.19 | 0.43 |
| 1:B:798:ASN:C | 1:B:800:LYS:H | 2.26 | 0.43 |
| 1:C:259:GLY:O | 1:C:260:ASP:C | 2.61 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:284:ASP:O | 1:C:287:HIS:CD2 | 2.71 | 0.43 |
| 1:C:333:ARG:NH1 | 1:C:334:ARG:HG3 | 2.33 | 0.43 |
| 1:C:343:PRO:HB2 | 1:C:347:GLN:HB2 | 2.01 | 0.43 |
| 1:C:433:ARG:HD3 | 1:C:434:ASP:H | 1.82 | 0.43 |
| 1:C:541:VAL:O | 1:C:545:THR:OG1 | 2.34 | 0.43 |
| 1:C:571:HIS:O | 1:C:572:MET:C | 2.58 | 0.43 |
| 1:C:638:MET:HG3 | 1:C:682:VAL:HG13 | 1.98 | 0.43 |
| 1:C:754:VAL:O | 1:C:758:PHE:CE2 | 2.71 | 0.43 |
| 1:C:789:LYS:HB3 | 1:C:793:GLU:CD | 2.42 | 0.43 |
| 1:D:208:PRO:N | 1:D:336:GLN:HB3 | 2.33 | 0.43 |
| 1:D:211:ILE:HD13 | 1:D:340:VAL:HG21 | 1.99 | 0.43 |
| 1:D:278:LEU:HA | 1:D:278:LEU:HD23 | 1.81 | 0.43 |
| 1:D:377:GLN:C | 1:D:380:LYS:HB3 | 2.43 | 0.43 |
| 1:D:462:LEU:HD21 | 1:D:465:ARG:NH1 | 2.33 | 0.43 |
| 1:D:575:ASP:O | 1:D:577:SER:N | 2.51 | 0.43 |
| 1:D:637:MET:CA | 1:D:678:LYS:NZ | 2.81 | 0.43 |
| 1:D:670:PHE:CG | 1:D:671:LEU:N | 2.84 | 0.43 |
| 1:D:800:LYS:HG2 | 1:D:800:LYS:H | 1.53 | 0.43 |
| 1:E:186:VAL:HA | 2:E:1001:AGS:N6 | 2.31 | 0.43 |
| 1:E:358:LYS:NZ | 1:E:362:HIS:HE1 | 2.03 | 0.43 |
| 1:E:462:LEU:HG | 1:E:466:TYR:CE2 | 2.53 | 0.43 |
| 1:E:566:ASN:O | 1:E:570:ILE:N | 2.49 | 0.43 |
| 1:E:596:LEU:HB3 | 1:F:837:LEU:CD2 | 2.49 | 0.43 |
| 1:E:786:ILE:O | 1:E:787:ARG:C | 2.60 | 0.43 |
| 1:F:226:ALA:HA | 1:F:229:ILE:HB | 2.01 | 0.43 |
| 1:F:290:MET:CG | 1:F:293:GLY:HA2 | 2.45 | 0.43 |
| 1:F:331:PHE:CG | 1:F:331:PHE:O | 2.70 | 0.43 |
| 1:F:583:GLN:HE22 | 1:F:741:LYS:NZ | 2.16 | 0.43 |
| 1:F:605:ARG:NH1 | 1:F:605:ARG:HG2 | 2.34 | 0.43 |
| 1:F:610:PHE:CA | 1:F:768:SER:HB3 | 2.32 | 0.43 |
| 1:F:639:ILE:O | 1:F:684:LEU:HD23 | 2.19 | 0.43 |
| 1:F:698:VAL:HG12 | 1:F:699:MET:HE2 | 2.00 | 0.43 |
| 1:F:780:ILE:O | 1:F:781:HIS:C | 2.61 | 0.43 |
| 1:F:785:ASP:C | 1:F:789:LYS:NZ | 2.77 | 0.43 |
| 1:A:295:ASP:C | 1:A:297:ALA:H | 2.27 | 0.43 |
| 1:A:301:LEU:C | 1:A:303:PRO:HD2 | 2.44 | 0.43 |
| 1:A:642:ASP:OD1 | 1:A:644:SER:OG | 2.34 | 0.43 |
| 1:A:747:LYS:HG3 | 1:A:748:ASN:N | 2.33 | 0.43 |
| 1:B:383:LEU:HB2 | 1:B:386:ARG:CG | 2.48 | 0.43 |
| 1:B:666:ASP:OD2 | 1:B:669:GLY:C | 2.62 | 0.43 |
| 1:B:669:GLY:C | 1:B:671:LEU:N | 2.77 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:759:ARG:HA | 1:B:760:PRO:HD3 | 1.91 | 0.43 |
| 1:C:200:LEU:HD23 | 1:C:200:LEU:HA | 1.50 | 0.43 |
| 1:C:274:GLU:H | 1:C:276:LYS:NZ | 2.15 | 0.43 |
| 1:C:360:GLU:HB2 | 1:C:367:ILE:HD11 | 2.00 | 0.43 |
| 1:C:371:ALA:HA | 1:C:374:THR:HG23 | 2.00 | 0.43 |
| 1:C:544:ASP:O | 1:C:545:THR:C | 2.61 | 0.43 |
| 1:C:628:ALA:C | 1:C:631:LEU:H | 2.26 | 0.43 |
| 1:C:682:VAL:HG23 | 1:C:723:VAL:HG13 | 2.00 | 0.43 |
| 1:C:799:ASP:O | 1:C:801:HIS:ND1 | 2.51 | 0.43 |
| 1:C:801:HIS:O | 1:C:853:GLU:HG3 | 2.19 | 0.43 |
| 1:C:808:GLN:HG3 | 1:C:812:ASP:CG | 2.44 | 0.43 |
| 1:C:809:GLU:N | 1:C:809:GLU:CD | 2.76 | 0.43 |
| 1:D:186:VAL:HG23 | 1:D:186:VAL:O | 2.18 | 0.43 |
| 1:D:193:ILE:HG22 | 1:D:197:ILE:CD1 | 2.49 | 0.43 |
| 1:D:368:LEU:O | 1:D:369:ASP:HB3 | 2.18 | 0.43 |
| 1:D:380:LYS:O | 1:D:381:ARG:C | 2.61 | 0.43 |
| 1:D:460:GLU:O | 1:D:463:ARG:HB3 | 2.18 | 0.43 |
| 1:D:473:HIS:CE1 | 1:D:536:MET:HE1 | 2.53 | 0.43 |
| 1:D:536:MET:N | 1:D:538:GLN:H | 2.16 | 0.43 |
| 1:D:618:SER:OG | 1:D:772:PHE:CE2 | 2.71 | 0.43 |
| 1:D:699:MET:HB3 | 1:D:699:MET:HE2 | 1.92 | 0.43 |
| 1:D:748:ASN:O | 1:D:749:LEU:C | 2.61 | 0.43 |
| 1:D:831:LEU:H | 1:D:831:LEU:HG | 1.38 | 0.43 |
| 1:E:191:GLU:CG | 1:E:192:GLU:N | 2.82 | 0.43 |
| 1:E:266:LYS:HA | 1:E:269:LEU:CD1 | 2.49 | 0.43 |
| 1:E:687:GLU:CA | 1:E:727:SER:HA | 2.48 | 0.43 |
| 1:E:699:MET:O | 1:E:703:LEU:N | 2.36 | 0.43 |
| 1:E:734:ILE:O | 1:E:737:GLN:N | 2.50 | 0.43 |
| 1:E:760:PRO:HA | 1:E:763:LEU:CB | 2.37 | 0.43 |
| 1:E:791:ILE:O | 1:E:794:ARG:N | 2.52 | 0.43 |
| 1:E:814:LEU:HA | 1:E:814:LEU:HD23 | 1.61 | 0.43 |
| 1:E:850:LYS:HE2 | 1:E:850:LYS:HB2 | 1.65 | 0.43 |
| 1:F:167:LEU:N | 1:F:169:LYS:NZ | 2.46 | 0.43 |
| 1:F:299:ASN:O | 1:F:300:ILE:C | 2.62 | 0.43 |
| 1:F:783:ILE:HD11 | 1:F:787:ARG:CZ | 2.49 | 0.43 |
| 1:F:785:ASP:O | 1:F:788:LEU:HB3 | 2.18 | 0.43 |
| 1:A:198:ARG:O | 1:A:199:VAL:C | 2.62 | 0.43 |
| 1:A:213:GLU:HB3 | 1:A:214:PRO:CD | 2.48 | 0.43 |
| 1:A:218:LYS:HZ2 | 1:A:387:ARG:HG3 | 1.83 | 0.43 |
| 1:A:564:SER:CB | 1:A:567:GLU:OE2 | 2.66 | 0.43 |
| 1:A:607:PRO:HD3 | 1:A:706:GLY:CA | 2.49 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:784:VAL:O | 1:A:785:ASP:C | 2.60 | 0.43 |
| 1:A:848:GLU:H | 1:A:849:ILE:HG22 | 1.83 | 0.43 |
| 1:B:174:MET:SD | 1:B:243:LEU:O | 2.76 | 0.43 |
| 1:B:213:GLU:HG3 | 1:B:341:ALA:O | 2.18 | 0.43 |
| 1:B:244:PHE:CD1 | 1:B:279:ILE:HG22 | 2.46 | 0.43 |
| 1:B:383:LEU:HD12 | 1:B:383:LEU:O | 2.18 | 0.43 |
| 1:C:117:LEU:C | 1:C:141:LYS:H | 2.26 | 0.43 |
| 1:C:210:LEU:C | 1:C:338:ILE:HG13 | 2.43 | 0.43 |
| 1:C:212:GLY:H | 1:C:340:VAL:HG13 | 1.83 | 0.43 |
| 1:C:563:GLU:HG2 | 1:C:565:GLU:OE1 | 2.19 | 0.43 |
| 1:C:654:LYS:HB2 | 1:C:671:LEU:HD23 | 1.99 | 0.43 |
| 1:C:718:CYS:C | 1:C:719:SER:HG | 2.27 | 0.43 |
| 1:C:801:HIS:CE1 | 1:C:851:ASP:OD2 | 2.71 | 0.43 |
| 1:C:841:ALA:O | 1:C:844:ILE:HB | 2.18 | 0.43 |
| 1:D:211:ILE:HG22 | 1:D:212:GLY:O | 2.18 | 0.43 |
| 1:D:362:HIS:CD2 | 1:D:363:HIS:CD2 | 2.94 | 0.43 |
| 1:D:399:SER:O | 1:D:403:VAL:HG23 | 2.18 | 0.43 |
| 1:D:404:ALA:N | 1:D:407:ARG:HE | 2.16 | 0.43 |
| 1:D:630:PHE:CD2 | 1:D:631:LEU:HA | 2.54 | 0.43 |
| 1:D:654:LYS:HE2 | 1:D:656:LEU:N | 2.33 | 0.43 |
| 1:D:684:LEU:CG | 1:D:725:MET:HA | 2.38 | 0.43 |
| 1:D:692:HIS:CE1 | 1:D:694:ASP:HB2 | 2.53 | 0.43 |
| 1:D:748:ASN:N | 1:D:748:ASN:ND2 | 2.65 | 0.43 |
| 1:D:765:ARG:NH2 | 1:E:640:ARG:NH1 | 2.61 | 0.43 |
| 1:D:805:ASN:O | 1:D:856:ASN:HB3 | 2.19 | 0.43 |
| 1:E:173:ASP:OD2 | 1:E:176:GLU:OE1 | 2.36 | 0.43 |
| 1:E:193:ILE:HG22 | 1:E:197:ILE:CD1 | 2.48 | 0.43 |
| 1:E:200:LEU:C | 1:E:206:SER:HB3 | 2.44 | 0.43 |
| 1:E:211:ILE:HB | 1:E:318:ASN:N | 2.33 | 0.43 |
| 1:E:224:GLY:O | 1:E:227:GLN:HB3 | 2.18 | 0.43 |
| 1:E:585:ASP:OD1 | 1:E:586:ALA:N | 2.50 | 0.43 |
| 1:E:773:ASN:HB2 | 1:E:775:LEU:HG | 1.99 | 0.43 |
| 1:F:207:ASN:HB2 | 1:F:335:PHE:CE1 | 2.53 | 0.43 |
| 1:F:607:PRO:CD | 1:F:705:ASP:C | 2.91 | 0.43 |
| 1:F:612:PHE:CD1 | 1:F:770:VAL:HG21 | 2.54 | 0.43 |
| 1:F:614:GLY:HA3 | 1:F:727:SER:C | 2.44 | 0.43 |
| 1:F:617:GLY:C | 1:F:620:LYS:HE2 | 2.43 | 0.43 |
| 1:F:689:GLU:OE2 | 1:F:758:PHE:CD1 | 2.71 | 0.43 |
| 1:F:723:VAL:HG12 | 1:F:724:ILE:N | 2.32 | 0.43 |
| 1:A:297:ALA:HA | 1:A:301:LEU:HD22 | 2.01 | 0.43 |
| 1:A:332:GLU:OE2 | 1:A:334:ARG:CZ | 2.61 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:625:LYS:NZ | 1:A:635:GLU:C | 2.77 | 0.43 |
| 1:B:261:PHE:HB2 | 1:B:265:PHE:CE2 | 2.54 | 0.43 |
| 1:B:261:PHE:CD2 | 1:B:262:GLU:N | 2.81 | 0.43 |
| 1:B:324:ILE:HG22 | 1:B:332:GLU:OE2 | 2.19 | 0.43 |
| 1:C:198:ARG:CZ | 1:D:405:VAL:HG22 | 2.49 | 0.43 |
| 1:C:286:ILE:CG1 | 1:C:289:LEU:HB2 | 2.47 | 0.43 |
| 1:C:333:ARG:HH12 | 1:C:334:ARG:NE | 2.15 | 0.43 |
| 1:C:349:VAL:HA | 1:C:352:LEU:CG | 2.48 | 0.43 |
| 1:C:376:ALA:O | 1:C:379:ALA:HB3 | 2.19 | 0.43 |
| 1:C:504:ASP:O | 1:C:507:TYR:HB3 | 2.19 | 0.43 |
| 1:C:610:PHE:CA | 1:C:768:SER:HB3 | 2.48 | 0.43 |
| 1:C:628:ALA:HA | 1:C:631:LEU:H | 1.84 | 0.43 |
| 1:C:646:LEU:O | 1:C:692:HIS:HB2 | 2.18 | 0.43 |
| 1:C:762:PHE:CE1 | 1:C:766:ILE:HD11 | 2.53 | 0.43 |
| 1:C:782:LYS:C | 1:C:784:VAL:N | 2.76 | 0.43 |
| 1:C:803:LYS:HZ2 | 1:C:853:GLU:C | 2.27 | 0.43 |
| 1:D:246:LEU:N | 1:D:282:PHE:HD2 | 2.16 | 0.43 |
| 1:D:414:LEU:HD22 | 1:D:459:LEU:HD22 | 2.01 | 0.43 |
| 1:D:542:ASP:O | 1:D:544:ASP:N | 2.51 | 0.43 |
| 1:D:680:TYR:HA | 1:D:720:ASN:O | 2.19 | 0.43 |
| 1:D:751:MET:O | 1:D:752:GLY:C | 2.61 | 0.43 |
| 1:D:759:ARG:HA | 1:D:760:PRO:HD3 | 1.76 | 0.43 |
| 1:D:833:GLN:HA | 1:D:836:ILE:HG12 | 2.00 | 0.43 |
| 1:E:354:GLY:C | 1:E:357:PRO:HD2 | 2.43 | 0.43 |
| 1:E:577:SER:HG | 1:E:578:SER:H | 1.66 | 0.43 |
| 1:E:627:VAL:HG12 | 1:E:631:LEU:HD11 | 2.00 | 0.43 |
| 1:E:713:GLY:O | 1:E:715:THR:HG23 | 2.19 | 0.43 |
| 1:E:760:PRO:O | 1:E:761:GLU:C | 2.61 | 0.43 |
| 1:F:298:ALA:O | 1:F:299:ASN:C | 2.62 | 0.43 |
| 1:F:392:ALA:O | 1:F:395:LEU:N | 2.52 | 0.43 |
| 1:F:751:MET:C | 1:F:755:ARG:HG2 | 2.42 | 0.43 |
| 1:F:800:LYS:HA | 1:F:802:TYR:CD1 | 2.54 | 0.43 |
| 1:F:839:LYS:HD3 | 1:F:880:LEU:N | 2.34 | 0.43 |
| 1:A:169:LYS:HZ1 | 1:A:264:ARG:CZ | 2.28 | 0.43 |
| 1:A:196:THR:HA | 1:A:199:VAL:HG23 | 2.01 | 0.43 |
| 1:A:208:PRO:CB | 1:A:338:ILE:HD12 | 2.48 | 0.43 |
| 1:A:220:ALA:O | 1:A:224:GLY:N | 2.46 | 0.43 |
| 1:A:249:ALA:O | 1:A:264:ARG:NH2 | 2.52 | 0.43 |
| 1:A:289:LEU:HD23 | 1:A:289:LEU:HA | 1.74 | 0.43 |
| 1:A:617:GLY:HA2 | 1:A:620:LYS:CD | 2.39 | 0.43 |
| 1:A:646:LEU:HD12 | 1:A:647:SER:N | 2.34 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:748:ASN:O | 1:A:752:GLY:N | 2.51 | 0.43 |
| 1:A:806:LEU:CA | 1:A:810:ALA:HB3 | 2.48 | 0.43 |
| 1:A:814:LEU:HA | 1:A:817:TYR:HD2 | 1.83 | 0.43 |
| 1:B:234:VAL:HG12 | 1:B:238:LEU:HG | 2.00 | 0.43 |
| 1:B:271:GLU:C | 1:B:271:GLU:CD | 2.86 | 0.43 |
| 1:B:362:HIS:NE2 | 1:B:363:HIS:CE1 | 2.86 | 0.43 |
| 1:B:547:SER:C | 1:B:560:LYS:HZ2 | 2.25 | 0.43 |
| 1:B:551:ALA:C | 1:B:554:THR:H | 2.27 | 0.43 |
| 1:B:610:PHE:CB | 1:B:768:SER:HB3 | 2.48 | 0.43 |
| 1:B:627:VAL:O | 1:B:630:PHE:CE1 | 2.72 | 0.43 |
| 1:B:785:ASP:HA | 1:B:788:LEU:CD1 | 2.49 | 0.43 |
| 1:B:814:LEU:HD23 | 1:B:814:LEU:HA | 1.52 | 0.43 |
| 1:C:189:ARG:C | 1:C:193:ILE:HD12 | 2.44 | 0.43 |
| 1:C:203:ARG:NH1 | 1:D:362:HIS:HB3 | 2.33 | 0.43 |
| 1:C:225:VAL:O | 1:C:227:GLN:N | 2.51 | 0.43 |
| 1:C:270:LYS:O | 1:C:271:GLU:C | 2.58 | 0.43 |
| 1:C:306:SER:O | 1:C:307:ARG:C | 2.61 | 0.43 |
| 1:C:333:ARG:O | 1:C:335:PHE:CD1 | 2.72 | 0.43 |
| 1:C:704:ASP:CG | 1:C:705:ASP:N | 2.77 | 0.43 |
| 1:D:249:ALA:C | 1:D:251:LEU:H | 2.27 | 0.43 |
| 1:D:375:ALA:O | 1:D:378:LEU:HB2 | 2.19 | 0.43 |
| 1:D:393:LEU:O | 1:D:396:VAL:HB | 2.19 | 0.43 |
| 1:D:589:ALA:O | 1:D:590:VAL:C | 2.59 | 0.43 |
| 1:D:613:LEU:HG | 1:D:614:GLY:N | 2.29 | 0.43 |
| 1:D:714:LYS:HG3 | 1:D:715:THR:N | 2.34 | 0.43 |
| 1:D:721:CYS:SG | 1:D:722:ILE:O | 2.77 | 0.43 |
| 1:D:759:ARG:NE | 1:D:763:LEU:HD21 | 2.32 | 0.43 |
| 1:D:857:VAL:HG13 | 1:D:879:VAL:O | 2.19 | 0.43 |
| 1:E:174:MET:HE3 | 1:E:177:GLN:HB3 | 2.00 | 0.43 |
| 1:E:187:ILE:HB | 1:E:351:ILE:HD11 | 2.01 | 0.43 |
| 1:E:200:LEU:CB | 1:E:311:LYS:HE3 | 2.48 | 0.43 |
| 1:E:318:ASN:O | 1:E:321:TYR:CE2 | 2.72 | 0.43 |
| 1:E:650:TYR:O | 1:E:654:LYS:HG2 | 2.18 | 0.43 |
| 1:F:200:LEU:HB3 | 1:F:238:LEU:HG | 2.00 | 0.43 |
| 1:F:283:ILE:HB | 1:F:289:LEU:CD2 | 2.48 | 0.43 |
| 1:F:378:LEU:HA | 1:F:381:ARG:CB | 2.44 | 0.43 |
| 1:F:806:LEU:O | 1:F:807:THR:C | 2.62 | 0.43 |
| 1:F:815:ALA:O | 1:F:816:LYS:C | 2.62 | 0.43 |
| 1:F:829:ASN:C | 1:F:831:LEU:N | 2.76 | 0.43 |
| 1:A:219:THR:O | 1:A:223:GLU:HG2 | 2.18 | 0.43 |
| 1:A:299:ASN:OD1 | 1:A:299:ASN:N | 2.52 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:571:HIS:CD2 | 1:A:574:ARG:HD2 | 2.51 | 0.43 |
| 1:A:592:ASN:O | 1:A:595:ARG:HB3 | 2.18 | 0.43 |
| 1:A:858:VAL:HB | 1:A:877:LEU:HD13 | 1.99 | 0.43 |
| 1:A:858:VAL:HG23 | 1:A:877:LEU:HD22 | 2.00 | 0.43 |
| 1:B:310:LEU:HA | 1:B:310:LEU:HD23 | 1.71 | 0.43 |
| 1:B:393:LEU:HD21 | 1:B:397:ASP:HB2 | 2.00 | 0.43 |
| 1:B:541:VAL:HB | 1:B:543:SER:O | 2.19 | 0.43 |
| 1:B:571:HIS:O | 1:B:574:ARG:N | 2.51 | 0.43 |
| 1:B:612:PHE:HB2 | 1:B:770:VAL:HB | 2.01 | 0.43 |
| 1:B:637:MET:C | 1:B:682:VAL:HB | 2.44 | 0.43 |
| 1:B:671:LEU:HD12 | 1:B:672:THR:N | 2.33 | 0.43 |
| 1:B:740:SER:C | 1:B:742:ILE:HD12 | 2.44 | 0.43 |
| 1:B:843:ARG:CZ | 1:B:846:LYS:HE2 | 2.49 | 0.43 |
| 1:C:208:PRO:HD2 | 1:C:313:ILE:HA | 2.00 | 0.43 |
| 1:C:213:GLU:O | 1:C:218:LYS:HE3 | 2.19 | 0.43 |
| 1:C:297:ALA:O | 1:C:301:LEU:HD21 | 2.19 | 0.43 |
| 1:C:302:LYS:O | 1:C:303:PRO:C | 2.61 | 0.43 |
| 1:C:330:ALA:C | 1:C:332:GLU:N | 2.75 | 0.43 |
| 1:C:371:ALA:HA | 1:C:374:THR:CG2 | 2.47 | 0.43 |
| 1:C:490:ALA:HB2 | 1:C:505:LEU:HD23 | 2.00 | 0.43 |
| 1:C:595:ARG:HG3 | 1:C:595:ARG:H | 1.55 | 0.43 |
| 1:C:639:ILE:C | 1:C:683:LEU:HD12 | 2.44 | 0.43 |
| 1:C:780:ILE:C | 1:C:782:LYS:N | 2.77 | 0.43 |
| 1:C:789:LYS:O | 1:C:790:GLU:C | 2.61 | 0.43 |
| 1:D:211:ILE:HB | 1:D:321:TYR:CE2 | 2.54 | 0.43 |
| 1:D:217:GLY:C | 1:D:219:THR:N | 2.75 | 0.43 |
| 1:D:231:ASP:OD1 | 1:D:231:ASP:N | 2.49 | 0.43 |
| 1:D:245:SER:HA | 1:D:282:PHE:CB | 2.49 | 0.43 |
| 1:D:246:LEU:HD23 | 1:D:247:ASP:C | 2.44 | 0.43 |
| 1:D:352:LEU:HG | 1:D:352:LEU:H | 1.60 | 0.43 |
| 1:D:473:HIS:HA | 1:D:476:LEU:CD1 | 2.49 | 0.43 |
| 1:D:560:LYS:O | 1:D:563:GLU:OE2 | 2.37 | 0.43 |
| 1:D:696:LEU:CA | 1:D:699:MET:HB3 | 2.41 | 0.43 |
| 1:D:704:ASP:O | 1:D:705:ASP:HB3 | 2.18 | 0.43 |
| 1:D:705:ASP:C | 1:D:707:ARG:H | 2.26 | 0.43 |
| 1:D:731:ALA:HA | 1:D:734:ILE:HB | 2.00 | 0.43 |
| 1:D:810:ALA:C | 1:D:812:ASP:N | 2.73 | 0.43 |
| 1:D:827:PRO:O | 1:D:829:ASN:N | 2.52 | 0.43 |
| 1:E:248:LEU:O | 1:E:249:ALA:C | 2.60 | 0.43 |
| 1:E:262:GLU:HA | 1:E:265:PHE:CE2 | 2.54 | 0.43 |
| 1:E:265:PHE:CE2 | 1:E:298:ALA:HB2 | 2.54 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:268:VAL:O | 1:E:272:ILE:HG12 | 2.19 | 0.43 |
| 1:E:610:PHE:O | 1:E:725:MET:HE3 | 2.18 | 0.43 |
| 1:E:620:LYS:HG2 | 2:E:1002:AGS:PA | 2.59 | 0.43 |
| 1:E:675:LEU:N | 1:E:676:GLN:OE1 | 2.52 | 0.43 |
| 1:E:683:LEU:HB3 | 1:E:723:VAL:CB | 2.49 | 0.43 |
| 1:E:840:LEU:O | 1:E:844:ILE:HG13 | 2.19 | 0.43 |
| 1:E:842:LEU:HA | 1:E:845:LEU:CD2 | 2.49 | 0.43 |
| 1:F:375:ALA:C | 1:F:378:LEU:H | 2.25 | 0.43 |
| 1:F:673:ASN:HA | 1:F:676:GLN:OE1 | 2.19 | 0.43 |
| 1:F:685:PHE:HB2 | 1:F:726:THR:H | 1.82 | 0.43 |
| 1:A:172:ILE:HD12 | 1:A:247:ASP:H | 1.83 | 0.43 |
| 1:A:183:LEU:HD23 | 1:A:185:PRO:HD3 | 2.01 | 0.43 |
| 1:A:211:ILE:N | 1:A:316:THR:N | 2.66 | 0.43 |
| 1:A:225:VAL:O | 1:A:227:GLN:N | 2.52 | 0.43 |
| 1:A:599:SER:HB2 | 1:A:601:LEU:CG | 2.49 | 0.43 |
| 1:A:623:LEU:O | 1:A:626:LYS:HB2 | 2.19 | 0.43 |
| 1:B:173:ASP:OD1 | 1:B:177:GLN:N | 2.51 | 0.43 |
| 1:B:211:ILE:HG12 | 1:B:318:ASN:CA | 2.47 | 0.43 |
| 1:B:248:LEU:C | 1:B:264:ARG:NH2 | 2.77 | 0.43 |
| 1:B:366:ARG:CG | 1:B:407:ARG:HH22 | 2.32 | 0.43 |
| 1:B:544:ASP:CA | 1:B:560:LYS:NZ | 2.82 | 0.43 |
| 1:B:552:ARG:CG | 1:B:553:LEU:N | 2.81 | 0.43 |
| 1:B:591:SER:O | 1:B:595:ARG:HG3 | 2.18 | 0.43 |
| 1:C:194:ARG:CA | 1:C:197:ILE:HG12 | 2.49 | 0.43 |
| 1:C:246:LEU:O | 1:C:283:ILE:HG22 | 2.19 | 0.43 |
| 1:C:359:TYR:CZ | 1:C:397:ASP:OD2 | 2.72 | 0.43 |
| 1:C:368:LEU:HB3 | 1:C:372:LEU:HD21 | 2.00 | 0.43 |
| 1:C:416:SER:O | 1:C:419:ARG:N | 2.52 | 0.43 |
| 1:C:503:ALA:HB1 | 1:D:433:ARG:HG3 | 2.01 | 0.43 |
| 1:C:530:ARG:HH21 | 1:C:535:SER:C | 2.26 | 0.43 |
| 1:C:591:SER:CB | 1:C:595:ARG:NH1 | 2.82 | 0.43 |
| 1:C:688:VAL:HB | 1:C:725:MET:CB | 2.45 | 0.43 |
| 1:C:803:LYS:HD2 | 1:C:853:GLU:HG2 | 2.01 | 0.43 |
| 1:D:215:GLY:N | 2:D:1001:AGS:O2G | 2.52 | 0.43 |
| 1:D:272:ILE:CA | 1:D:276:LYS:HZ2 | 2.32 | 0.43 |
| 1:D:421:LEU:HD23 | 1:D:452:GLU:OE2 | 2.19 | 0.43 |
| 1:D:576:LEU:CD1 | 1:D:630:PHE:HB2 | 2.49 | 0.43 |
| 1:D:610:PHE:H | 1:D:724:ILE:CG2 | 2.29 | 0.43 |
| 1:D:627:VAL:O | 1:D:630:PHE:HB3 | 2.19 | 0.43 |
| 1:D:644:SER:HA | 1:D:692:HIS:H | 1.84 | 0.43 |
| 1:D:797:GLN:NE2 | 1:D:800:LYS:NZ | 2.59 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:166:TYR:HB2 | 1:E:271:GLU:CD | 2.44 | 0.43 |
| 1:E:167:LEU:HD12 | 1:E:168:SER:N | 2.33 | 0.43 |
| 1:E:172:ILE:HB | 1:E:245:SER:C | 2.44 | 0.43 |
| 1:E:173:ASP:O | 1:E:175:THR:OG1 | 2.34 | 0.43 |
| 1:E:173:ASP:OD2 | 1:E:175:THR:OG1 | 2.37 | 0.43 |
| 1:E:186:VAL:HA | 2:E:1001:AGS:C5 | 2.47 | 0.43 |
| 1:E:221:ILE:O | 1:E:224:GLY:N | 2.52 | 0.43 |
| 1:E:228:ARG:HH22 | 1:E:232:ASP:C | 2.26 | 0.43 |
| 1:E:247:ASP:CB | 1:E:249:ALA:HB3 | 2.49 | 0.43 |
| 1:E:356:GLN:O | 1:E:357:PRO:C | 2.62 | 0.43 |
| 1:E:359:TYR:CD1 | 1:E:362:HIS:CE1 | 3.07 | 0.43 |
| 1:E:424:ILE:O | 1:E:428:ILE:HG13 | 2.18 | 0.43 |
| 1:E:429:LYS:HG2 | 1:E:432:GLU:OE1 | 2.18 | 0.43 |
| 1:E:611:LEU:HB3 | 1:E:769:ILE:CG1 | 2.48 | 0.43 |
| 1:E:672:THR:O | 1:E:676:GLN:OE1 | 2.37 | 0.43 |
| 1:E:687:GLU:C | 1:E:727:SER:HB2 | 2.44 | 0.43 |
| 1:E:853:GLU:OE1 | 1:E:881:PRO:HB2 | 2.19 | 0.43 |
| 1:F:375:ALA:O | 1:F:376:ALA:C | 2.61 | 0.43 |
| 1:F:569:LEU:O | 1:F:573:GLU:N | 2.48 | 0.43 |
| 1:F:671:LEU:HD23 | 1:F:671:LEU:HA | 1.53 | 0.43 |
| 1:F:796:GLU:HG3 | 1:F:799:ASP:N | 2.20 | 0.43 |
| 1:F:798:ASN:O | 1:F:801:HIS:CE1 | 2.72 | 0.43 |
| 1:A:297:ALA:HA | 1:A:301:LEU:HB2 | 2.01 | 0.42 |
| 1:A:299:ASN:O | 1:A:303:PRO:HG3 | 2.19 | 0.42 |
| 1:A:652:VAL:HG13 | 1:A:658:THR:HG21 | 2.01 | 0.42 |
| 1:A:781:HIS:CE1 | 1:A:782:LYS:HG3 | 2.54 | 0.42 |
| 1:B:210:LEU:HD23 | 1:B:339:GLU:HA | 2.00 | 0.42 |
| 1:B:252:THR:HG21 | 1:B:256:LYS:HZ3 | 1.83 | 0.42 |
| 1:B:252:THR:OG1 | 1:B:260:ASP:OD1 | 2.36 | 0.42 |
| 1:B:273:GLU:C | 1:B:275:SER:N | 2.77 | 0.42 |
| 1:B:286:ILE:HG21 | 1:B:320:GLU:CG | 2.49 | 0.42 |
| 1:B:344:SER:N | 1:B:347:GLN:NE2 | 2.66 | 0.42 |
| 1:B:386:ARG:HA | 1:B:386:ARG:HD3 | 1.75 | 0.42 |
| 1:B:585:ASP:CA | 1:B:588:LYS:HD3 | 2.41 | 0.42 |
| 1:B:634:ASP:CG | 1:B:635:GLU:N | 2.72 | 0.42 |
| 1:B:754:VAL:O | 1:B:758:PHE:CD2 | 2.72 | 0.42 |
| 1:C:282:PHE:CE1 | 1:C:283:ILE:O | 2.72 | 0.42 |
| 1:C:289:LEU:O | 1:C:290:MET:HB2 | 2.18 | 0.42 |
| 1:C:397:ASP:N | 1:C:397:ASP:OD1 | 2.51 | 0.42 |
| 1:C:465:ARG:HH12 | 1:C:529:ARG:CZ | 2.29 | 0.42 |
| 1:C:573:GLU:C | 1:C:575:ASP:N | 2.75 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:605:ARG:HE | 1:C:606:GLN:HB2 | 1.83 | 0.42 |
| 1:C:625:LYS:O | 1:C:635:GLU:CD | 2.62 | 0.42 |
| 1:C:716:ILE:HG22 | 1:C:717:ASP:OD1 | 2.19 | 0.42 |
| 1:C:754:VAL:O | 1:C:755:ARG:C | 2.62 | 0.42 |
| 1:C:797:GLN:CD | 1:C:797:GLN:N | 2.77 | 0.42 |
| 1:D:177:GLN:O | 1:D:180:GLN:HB2 | 2.19 | 0.42 |
| 1:D:320:GLU:HG3 | 1:D:712:GLN:NE2 | 2.33 | 0.42 |
| 1:D:414:LEU:O | 1:D:415:ASP:C | 2.59 | 0.42 |
| 1:D:503:ALA:O | 1:D:507:TYR:CG | 2.72 | 0.42 |
| 1:D:555:GLY:O | 1:D:560:LYS:HE3 | 2.18 | 0.42 |
| 1:D:612:PHE:N | 1:D:770:VAL:O | 2.52 | 0.42 |
| 1:D:618:SER:CA | 1:D:826:ARG:HH11 | 2.31 | 0.42 |
| 1:D:804:LEU:CA | 1:D:854:THR:HA | 2.45 | 0.42 |
| 1:D:808:GLN:O | 1:D:809:GLU:C | 2.62 | 0.42 |
| 1:E:202:ARG:CG | 1:E:204:ILE:H | 2.30 | 0.42 |
| 1:E:290:MET:H | 1:E:295:ASP:CG | 2.27 | 0.42 |
| 1:E:541:VAL:HB | 1:E:545:THR:OG1 | 2.18 | 0.42 |
| 1:E:581:VAL:HG12 | 1:E:582:GLY:H | 1.83 | 0.42 |
| 1:E:641:VAL:HB | 1:E:684:LEU:CD2 | 2.49 | 0.42 |
| 1:E:643:CYS:C | 1:E:649:LYS:NZ | 2.77 | 0.42 |
| 1:E:733:PHE:HA | 1:E:736:SER:HB2 | 2.00 | 0.42 |
| 1:E:761:GLU:CG | 1:E:762:PHE:N | 2.82 | 0.42 |
| 1:F:265:PHE:CZ | 1:F:269:LEU:HD21 | 2.53 | 0.42 |
| 1:F:395:LEU:HA | 1:F:395:LEU:HD23 | 1.80 | 0.42 |
| 1:F:781:HIS:O | 1:F:784:VAL:HG13 | 2.19 | 0.42 |
| 1:F:781:HIS:CD2 | 1:F:782:LYS:HZ2 | 2.32 | 0.42 |
| 1:F:819:TYR:CE2 | 1:F:828:LEU:HD12 | 2.54 | 0.42 |
| 1:F:838:ASN:O | 1:F:839:LYS:C | 2.62 | 0.42 |
| 1:F:877:LEU:HD23 | 1:F:877:LEU:HA | 1.83 | 0.42 |
| 1:A:219:THR:HA | 1:A:222:ILE:HG12 | 2.00 | 0.42 |
| 1:A:355:LEU:O | 1:A:357:PRO:HD3 | 2.18 | 0.42 |
| 1:A:543:SER:CA | 1:A:547:SER:HB3 | 2.38 | 0.42 |
| 1:A:625:LYS:HA | 1:A:628:ALA:CB | 2.46 | 0.42 |
| 1:A:806:LEU:HA | 1:A:810:ALA:HB3 | 1.99 | 0.42 |
| 1:B:166:TYR:CB | 1:B:169:LYS:NZ | 2.82 | 0.42 |
| 1:B:186:VAL:HG22 | 1:B:355:LEU:HD11 | 2.01 | 0.42 |
| 1:B:268:VAL:CA | 1:B:271:GLU:HB2 | 2.45 | 0.42 |
| 1:B:603:ASN:HB3 | 1:B:605:ARG:NE | 2.34 | 0.42 |
| 1:B:615:LEU:HD23 | 1:B:615:LEU:HA | 1.81 | 0.42 |
| 1:B:820:SER:N | 1:B:828:LEU:HD11 | 2.34 | 0.42 |
| 1:B:839:LYS:HB3 | 1:B:878:GLU:CD | 2.43 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:C:195:SER:O | 1:C:196:THR:C | 2.62 | 0.42 |
| 1:C:223:GLU:HA | 1:C:226:ALA:HB3 | 2.01 | 0.42 |
| 1:C:356:GLN:HG3 | 1:C:367:ILE:CD1 | 2.42 | 0.42 |
| 1:C:359:TYR:O | 1:C:360:GLU:C | 2.61 | 0.42 |
| 1:C:407:ARG:NH1 | 1:C:539:ASN:H | 2.16 | 0.42 |
| 1:C:524:VAL:HG13 | 1:C:533:ALA:HB3 | 2.00 | 0.42 |
| 1:C:585:ASP:HB3 | 1:C:588:LYS:HE2 | 2.01 | 0.42 |
| 1:C:596:LEU:HA | 1:C:596:LEU:HD23 | 1.61 | 0.42 |
| 1:C:607:PRO:HB2 | 1:C:722:ILE:HA | 2.01 | 0.42 |
| 1:C:689:GLU:OE2 | 1:C:729:LEU:HD13 | 2.19 | 0.42 |
| 1:C:713:GLY:C | 1:C:714:LYS:NZ | 2.74 | 0.42 |
| 1:C:722:ILE:HG13 | 1:C:723:VAL:N | 2.34 | 0.42 |
| 1:C:843:ARG:NH1 | 1:C:848:GLU:CB | 2.71 | 0.42 |
| 1:D:227:GLN:O | 1:D:230:ILE:HB | 2.18 | 0.42 |
| 1:D:299:ASN:N | 1:D:301:LEU:HD21 | 2.34 | 0.42 |
| 1:D:351:ILE:HG23 | 2:D:1001:AGS:C2 | 2.49 | 0.42 |
| 1:D:390:ASP:O | 1:D:394:ASP:N | 2.49 | 0.42 |
| 1:D:507:TYR:CD2 | 1:E:429:LYS:HD3 | 2.54 | 0.42 |
| 1:D:684:LEU:C | 1:D:725:MET:HG2 | 2.44 | 0.42 |
| 1:D:708:ILE:HB | 1:D:715:THR:C | 2.43 | 0.42 |
| 1:E:173:ASP:HB3 | 1:E:176:GLU:OE2 | 2.20 | 0.42 |
| 1:E:200:LEU:HG | 1:E:200:LEU:H | 1.66 | 0.42 |
| 1:E:211:ILE:HB | 1:E:317:THR:C | 2.44 | 0.42 |
| 1:E:276:LYS:HG2 | 1:E:277:THR:O | 2.18 | 0.42 |
| 1:E:298:ALA:CA | 1:E:301:LEU:HB3 | 2.49 | 0.42 |
| 1:E:454:SER:HA | 1:E:457:GLU:CD | 2.45 | 0.42 |
| 1:E:473:HIS:O | 1:E:521:GLU:OE2 | 2.37 | 0.42 |
| 1:E:619:GLY:CA | 2:E:1002:AGS:H5'2 | 2.48 | 0.42 |
| 1:E:632:PHE:C | 1:E:634:ASP:N | 2.77 | 0.42 |
| 1:E:649:LYS:O | 1:E:651:ALA:N | 2.50 | 0.42 |
| 1:F:205:LYS:NZ | 1:F:334:ARG:C | 2.73 | 0.42 |
| 1:F:205:LYS:HB2 | 1:F:205:LYS:HE2 | 1.71 | 0.42 |
| 1:F:239:GLN:N | 1:F:278:LEU:HD12 | 2.27 | 0.42 |
| 1:F:349:VAL:O | 1:F:350:ALA:C | 2.62 | 0.42 |
| 1:F:556:ILE:HG12 | 1:F:559:LYS:HZ2 | 1.78 | 0.42 |
| 1:F:575:ASP:O | 1:F:579:GLU:N | 2.51 | 0.42 |
| 1:F:606:GLN:O | 1:F:606:GLN:HG3 | 2.20 | 0.42 |
| 1:F:613:LEU:O | 1:F:772:PHE:CE1 | 2.72 | 0.42 |
| 1:F:731:ALA:CA | 1:F:734:ILE:HB | 2.42 | 0.42 |
| 1:F:749:LEU:HD23 | 1:F:749:LEU:HA | 1.80 | 0.42 |
| 1:F:790:GLU:C | 1:F:793:GLU:OE2 | 2.62 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:260:ASP:O | 1:A:263:GLU:HB2 | 2.19 | 0.42 |
| 1:A:287:HIS:CD2 | 1:A:321:TYR:OH | 2.72 | 0.42 |
| 1:A:758:PHE:CG | 1:A:759:ARG:N | 2.86 | 0.42 |
| 1:B:196:THR:O | 1:B:197:ILE:C | 2.62 | 0.42 |
| 1:B:196:THR:HA | 1:B:199:VAL:CG2 | 2.49 | 0.42 |
| 1:B:282:PHE:HD2 | 1:B:283:ILE:C | 2.27 | 0.42 |
| 1:B:290:MET:HE2 | 1:B:293:GLY:O | 2.20 | 0.42 |
| 1:B:357:PRO:O | 1:B:360:GLU:HB3 | 2.19 | 0.42 |
| 1:B:360:GLU:HG3 | 1:B:367:ILE:HD12 | 2.01 | 0.42 |
| 1:B:376:ALA:O | 1:B:377:GLN:C | 2.62 | 0.42 |
| 1:B:545:THR:O | 1:B:546:ILE:C | 2.62 | 0.42 |
| 1:B:630:PHE:CD2 | 1:B:631:LEU:N | 2.88 | 0.42 |
| 1:B:750:VAL:O | 1:B:754:VAL:HG23 | 2.19 | 0.42 |
| 1:B:762:PHE:HA | 1:B:765:ARG:HG2 | 2.00 | 0.42 |
| 1:C:193:ILE:O | 1:C:196:THR:HB | 2.20 | 0.42 |
| 1:C:299:ASN:OD1 | 1:C:300:ILE:HG13 | 2.19 | 0.42 |
| 1:C:648:GLU:N | 1:C:648:GLU:CD | 2.76 | 0.42 |
| 1:C:709:THR:HA | 1:C:716:ILE:H | 1.84 | 0.42 |
| 1:C:835:GLU:O | 1:C:838:ASN:OD1 | 2.38 | 0.42 |
| 1:D:191:GLU:O | 1:D:192:GLU:C | 2.61 | 0.42 |
| 1:D:234:VAL:O | 1:D:239:GLN:HB2 | 2.18 | 0.42 |
| 1:D:276:LYS:HE2 | 1:D:279:ILE:CD1 | 2.50 | 0.42 |
| 1:D:360:GLU:OE2 | 1:D:366:ARG:HA | 2.19 | 0.42 |
| 1:D:362:HIS:CD2 | 1:D:363:HIS:N | 2.88 | 0.42 |
| 1:D:386:ARG:HG2 | 1:D:391:SER:HB3 | 2.00 | 0.42 |
| 1:D:405:VAL:O | 1:D:406:ALA:C | 2.61 | 0.42 |
| 1:D:515:LYS:HA | 1:D:518:GLU:HB3 | 2.00 | 0.42 |
| 1:D:548:GLU:O | 1:D:552:ARG:HG2 | 2.20 | 0.42 |
| 1:D:714:LYS:CG | 1:D:715:THR:N | 2.83 | 0.42 |
| 1:D:808:GLN:HB3 | 1:D:812:ASP:OD2 | 2.19 | 0.42 |
| 1:D:842:LEU:CD2 | 1:D:843:ARG:HE | 2.33 | 0.42 |
| 1:E:300:ILE:CD1 | 1:F:249:ALA:HB3 | 2.49 | 0.42 |
| 1:E:401:ALA:O | 1:E:402:GLY:C | 2.62 | 0.42 |
| 1:E:534:ASN:HD21 | 1:E:538:GLN:N | 2.04 | 0.42 |
| 1:E:541:VAL:O | 1:E:542:ASP:C | 2.62 | 0.42 |
| 1:E:548:GLU:O | 1:E:551:ALA:HB3 | 2.19 | 0.42 |
| 1:E:562:SER:N | 1:E:563:GLU:OE1 | 2.52 | 0.42 |
| 1:E:612:PHE:HA | 1:E:770:VAL:O | 2.19 | 0.42 |
| 1:E:743:GLN:C | 1:E:746:THR:HG1 | 2.27 | 0.42 |
| 1:E:786:ILE:HA | 1:E:789:LYS:HZ3 | 1.82 | 0.42 |
| 1:E:811:LYS:O | 1:E:812:ASP:C | 2.61 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:819:TYR:CZ | 1:E:821:ASP:HA | 2.53 | 0.42 |
| 1:F:352:LEU:O | 1:F:355:LEU:HB2 | 2.19 | 0.42 |
| 1:F:356:GLN:HE22 | 1:F:372:LEU:HD11 | 1.83 | 0.42 |
| 1:F:388:LEU:HB3 | 1:F:389:PRO:HD2 | 2.01 | 0.42 |
| 1:F:638:MET:HB3 | 1:F:682:VAL:C | 2.44 | 0.42 |
| 1:F:715:THR:O | 1:F:715:THR:HG22 | 2.18 | 0.42 |
| 1:F:853:GLU:CD | 1:F:854:THR:N | 2.77 | 0.42 |
| 1:A:177:GLN:C | 1:A:182:LYS:HZ3 | 2.26 | 0.42 |
| 1:A:597:SER:HA | 1:A:602:ALA:HB2 | 2.00 | 0.42 |
| 1:A:687:GLU:HA | 1:A:726:THR:O | 2.19 | 0.42 |
| 1:A:748:ASN:HA | 1:A:751:MET:HB3 | 2.01 | 0.42 |
| 1:A:790:GLU:HG2 | 1:A:791:ILE:HG13 | 2.02 | 0.42 |
| 1:A:804:LEU:HD12 | 1:A:855:VAL:HG21 | 2.00 | 0.42 |
| 1:A:820:SER:HG | 1:A:822:ASP:H | 1.66 | 0.42 |
| 1:A:826:ARG:HH22 | 1:F:304:ALA:HB1 | 1.84 | 0.42 |
| 1:B:174:MET:HB2 | 1:B:175:THR:H | 1.53 | 0.42 |
| 1:B:211:ILE:O | 1:B:317:THR:HA | 2.20 | 0.42 |
| 1:B:245:SER:HB2 | 1:B:283:ILE:HA | 2.02 | 0.42 |
| 1:B:246:LEU:O | 1:B:283:ILE:HG21 | 2.19 | 0.42 |
| 1:B:321:TYR:HD2 | 1:B:322:ARG:HG3 | 1.84 | 0.42 |
| 1:B:352:LEU:HG | 1:B:352:LEU:H | 1.60 | 0.42 |
| 1:B:359:TYR:C | 1:B:362:HIS:HB3 | 2.44 | 0.42 |
| 1:B:560:LYS:O | 1:B:561:LEU:C | 2.63 | 0.42 |
| 1:B:625:LYS:O | 1:B:627:VAL:N | 2.53 | 0.42 |
| 1:C:266:LYS:HA | 1:C:269:LEU:CG | 2.49 | 0.42 |
| 1:C:374:THR:HG23 | 1:C:374:THR:H | 1.58 | 0.42 |
| 1:C:472:GLY:HA2 | 1:C:475:GLU:CD | 2.44 | 0.42 |
| 1:C:577:SER:O | 1:C:578:SER:C | 2.63 | 0.42 |
| 1:C:803:LYS:HA | 1:C:803:LYS:HD2 | 1.86 | 0.42 |
| 1:C:809:GLU:O | 1:C:813:PHE:N | 2.38 | 0.42 |
| 1:D:191:GLU:CD | 1:D:194:ARG:HD2 | 2.44 | 0.42 |
| 1:D:507:TYR:CD1 | 1:E:426:VAL:HA | 2.55 | 0.42 |
| 1:D:542:ASP:C | 1:D:545:THR:HG1 | 2.21 | 0.42 |
| 1:D:587:ILE:C | 1:D:591:SER:HG | 2.27 | 0.42 |
| 1:D:594:VAL:O | 1:D:597:SER:HB2 | 2.19 | 0.42 |
| 1:D:610:PHE:H | 1:D:724:ILE:CG1 | 2.32 | 0.42 |
| 1:D:640:ARG:HA | 1:D:683:LEU:HD11 | 2.00 | 0.42 |
| 1:D:751:MET:CG | 1:D:769:ILE:HD11 | 2.49 | 0.42 |
| 1:D:794:ARG:HH11 | 1:D:794:ARG:HG2 | 1.83 | 0.42 |
| 1:D:813:PHE:HE2 | 1:D:874:GLU:OE1 | 2.02 | 0.42 |
| 1:E:304:ALA:HA | 1:E:307:ARG:CD | 2.49 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:E:443:ASP:O | 1:E:447:LEU:N | 2.34 | 0.42 |
| 1:E:510:ILE:HA | 1:E:513:ILE:H | 1.84 | 0.42 |
| 1:E:529:ARG:NH2 | 1:E:535:SER:HB3 | 2.33 | 0.42 |
| 1:E:595:ARG:O | 1:E:598:ARG:N | 2.52 | 0.42 |
| 1:E:605:ARG:HA | 1:E:706:GLY:HA2 | 2.01 | 0.42 |
| 1:E:613:LEU:O | 1:E:771:ILE:HG23 | 2.19 | 0.42 |
| 1:E:680:TYR:HA | 1:E:720:ASN:CG | 2.44 | 0.42 |
| 1:E:699:MET:HE2 | 1:E:762:PHE:CE1 | 2.53 | 0.42 |
| 1:E:855:VAL:HA | 1:E:880:LEU:CD2 | 2.48 | 0.42 |
| 1:F:369:ASP:OD1 | 1:F:369:ASP:N | 2.51 | 0.42 |
| 1:F:743:GLN:C | 1:F:747:LYS:HZ3 | 2.26 | 0.42 |
| 1:F:787:ARG:HA | 1:F:790:GLU:OE1 | 2.18 | 0.42 |
| 1:F:831:LEU:O | 1:F:832:ILE:C | 2.61 | 0.42 |
| 1:A:168:SER:HA | 1:A:171:ALA:HB3 | 2.01 | 0.42 |
| 1:A:194:ARG:C | 1:A:198:ARG:NH1 | 2.77 | 0.42 |
| 1:A:264:ARG:O | 1:A:268:VAL:HG13 | 2.20 | 0.42 |
| 1:A:268:VAL:CA | 1:A:271:GLU:HB3 | 2.49 | 0.42 |
| 1:A:387:ARG:HA | 1:A:387:ARG:HD3 | 1.81 | 0.42 |
| 1:A:873:ALA:HB2 | 1:F:202:ARG:HA | 2.00 | 0.42 |
| 1:B:173:ASP:CG | 1:B:177:GLN:N | 2.78 | 0.42 |
| 1:B:187:ILE:CG1 | 1:B:351:ILE:HD13 | 2.49 | 0.42 |
| 1:B:238:LEU:C | 1:B:241:ALA:H | 2.28 | 0.42 |
| 1:B:251:LEU:H | 1:B:264:ARG:CZ | 2.29 | 0.42 |
| 1:B:585:ASP:OD1 | 1:B:585:ASP:N | 2.52 | 0.42 |
| 1:B:595:ARG:O | 1:B:599:SER:N | 2.51 | 0.42 |
| 1:B:673:ASN:O | 1:B:676:GLN:HB3 | 2.20 | 0.42 |
| 1:B:747:LYS:C | 1:B:751:MET:HE3 | 2.45 | 0.42 |
| 1:B:787:ARG:C | 1:B:790:GLU:H | 2.27 | 0.42 |
| 1:C:291:GLY:HA2 | 1:C:327:LYS:HE2 | 2.01 | 0.42 |
| 1:C:331:PHE:HD1 | 1:C:335:PHE:HE2 | 1.68 | 0.42 |
| 1:C:342:GLU:OE2 | 1:C:388:LEU:HB3 | 2.19 | 0.42 |
| 1:C:359:TYR:CD2 | 1:C:359:TYR:C | 2.97 | 0.42 |
| 1:C:399:SER:O | 1:C:400:CYS:C | 2.63 | 0.42 |
| 1:C:420:GLN:NE2 | 1:C:455:LEU:O | 2.52 | 0.42 |
| 1:C:629:GLY:N | 1:C:635:GLU:OE2 | 2.32 | 0.42 |
| 1:C:682:VAL:HA | 1:C:723:VAL:HG22 | 2.01 | 0.42 |
| 1:C:716:ILE:CG2 | 1:C:717:ASP:N | 2.83 | 0.42 |
| 1:C:792:GLU:O | 1:C:793:GLU:C | 2.63 | 0.42 |
| 1:D:219:THR:O | 1:D:220:ALA:C | 2.62 | 0.42 |
| 1:D:387:ARG:O | 1:D:388:LEU:C | 2.63 | 0.42 |
| 1:D:434:ASP:O | 1:D:435:GLU:C | 2.62 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:458:GLU:C | 1:D:461:PRO:HD2 | 2.44 | 0.42 |
| 1:D:530:ARG:NH2 | 1:D:535:SER:HA | 2.35 | 0.42 |
| 1:D:554:THR:O | 1:D:556:ILE:HG13 | 2.19 | 0.42 |
| 1:D:585:ASP:N | 1:D:588:LYS:HZ3 | 2.18 | 0.42 |
| 1:D:799:ASP:CG | 1:D:800:LYS:H | 2.26 | 0.42 |
| 1:D:813:PHE:HD1 | 1:D:814:LEU:HD23 | 1.84 | 0.42 |
| 1:E:186:VAL:HG22 | 2:E:1001:AGS:C4 | 2.50 | 0.42 |
| 1:E:358:LYS:HZ2 | 1:E:362:HIS:CE1 | 2.34 | 0.42 |
| 1:E:502:ALA:HB3 | 1:E:506:ARG:NH1 | 2.35 | 0.42 |
| 1:E:585:ASP:HA | 1:E:588:LYS:HB3 | 2.00 | 0.42 |
| 1:E:610:PHE:O | 1:E:725:MET:HG2 | 2.19 | 0.42 |
| 1:E:802:TYR:HB3 | 1:E:804:LEU:HG | 2.02 | 0.42 |
| 1:E:856:ASN:ND2 | 1:E:880:LEU:C | 2.78 | 0.42 |
| 1:F:192:GLU:O | 1:F:196:THR:OG1 | 2.25 | 0.42 |
| 1:F:557:PRO:C | 1:F:559:LYS:N | 2.77 | 0.42 |
| 1:F:594:VAL:H | 1:F:610:PHE:HZ | 1.67 | 0.42 |
| 1:F:656:LEU:HD13 | 1:F:711:GLY:HA2 | 1.93 | 0.42 |
| 1:F:804:LEU:HB3 | 1:F:855:VAL:CG2 | 2.41 | 0.42 |
| 1:A:238:LEU:HA | 1:A:278:LEU:HD23 | 2.02 | 0.42 |
| 1:A:262:GLU:HA | 1:A:266:LYS:H | 1.84 | 0.42 |
| 1:A:373:VAL:O | 1:A:374:THR:C | 2.63 | 0.42 |
| 1:A:378:LEU:HA | 1:A:378:LEU:HD23 | 1.80 | 0.42 |
| 1:A:848:GLU:O | 1:A:849:ILE:C | 2.61 | 0.42 |
| 1:B:173:ASP:HB3 | 1:B:177:GLN:HG3 | 2.01 | 0.42 |
| 1:B:194:ARG:O | 1:B:197:ILE:HB | 2.20 | 0.42 |
| 1:B:209:CYS:N | 1:B:337:LYS:HB3 | 2.34 | 0.42 |
| 1:B:265:PHE:O | 1:B:266:LYS:C | 2.60 | 0.42 |
| 1:B:272:ILE:O | 1:B:274:GLU:N | 2.53 | 0.42 |
| 1:B:277:THR:O | 1:B:278:LEU:HD12 | 2.19 | 0.42 |
| 1:B:285:GLU:OE2 | 1:B:287:HIS:N | 2.49 | 0.42 |
| 1:B:358:LYS:HG3 | 1:B:359:TYR:N | 2.29 | 0.42 |
| 1:B:611:LEU:O | 1:B:770:VAL:N | 2.52 | 0.42 |
| 1:C:180:GLN:HG2 | 1:C:182:LYS:HE3 | 2.01 | 0.42 |
| 1:C:217:GLY:O | 1:C:221:ILE:HG13 | 2.20 | 0.42 |
| 1:C:345:VAL:HG21 | 1:C:377:GLN:HB2 | 2.01 | 0.42 |
| 1:C:620:LYS:C | 1:C:623:LEU:HB3 | 2.45 | 0.42 |
| 1:C:620:LYS:N | 1:C:772:PHE:HE1 | 2.18 | 0.42 |
| 1:C:646:LEU:HD23 | 1:C:646:LEU:HA | 1.67 | 0.42 |
| 1:C:709:THR:OG1 | 1:C:715:THR:HA | 2.20 | 0.42 |
| 1:C:777:ARG:HA | 1:C:780:ILE:HG12 | 2.02 | 0.42 |
| 1:C:777:ARG:CA | 1:C:780:ILE:HG12 | 2.49 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:786:ILE:CD1 | 1:C:789:LYS:NZ | 2.83 | 0.42 |
| 1:D:404:ALA:O | 1:D:408:ASP:N | 2.39 | 0.42 |
| 1:D:465:ARG:O | 1:D:534:ASN:HB2 | 2.19 | 0.42 |
| 1:D:524:VAL:HG22 | 1:D:532:GLY:C | 2.45 | 0.42 |
| 1:D:616:SER:HA | 1:D:620:LYS:CE | 2.50 | 0.42 |
| 1:D:692:HIS:HB3 | 1:D:695:VAL:CG2 | 2.50 | 0.42 |
| 1:D:715:THR:HG22 | 1:D:716:ILE:O | 2.20 | 0.42 |
| 1:D:836:ILE:O | 1:D:837:LEU:C | 2.63 | 0.42 |
| 1:D:837:LEU:O | 1:D:838:ASN:C | 2.63 | 0.42 |
| 1:E:187:ILE:HD12 | 2:E:1001:AGS:N6 | 2.28 | 0.42 |
| 1:E:194:ARG:O | 1:E:197:ILE:HB | 2.18 | 0.42 |
| 1:E:262:GLU:OE2 | 1:E:297:ALA:O | 2.38 | 0.42 |
| 1:E:544:ASP:O | 1:E:548:GLU:HG2 | 2.19 | 0.42 |
| 1:E:570:ILE:HG13 | 1:E:571:HIS:ND1 | 2.35 | 0.42 |
| 1:E:680:TYR:N | 1:E:680:TYR:CD1 | 2.88 | 0.42 |
| 1:E:770:VAL:CA | 1:E:771:ILE:HD12 | 2.50 | 0.42 |
| 1:E:837:LEU:HA | 1:E:840:LEU:HD22 | 2.00 | 0.42 |
| 1:F:275:SER:OG | 1:F:310:LEU:HB2 | 2.19 | 0.42 |
| 1:F:286:ILE:O | 1:F:289:LEU:HB2 | 2.19 | 0.42 |
| 1:F:707:ARG:CZ | 1:F:707:ARG:HB2 | 2.48 | 0.42 |
| 1:F:730:GLY:HA3 | 1:F:750:VAL:HG11 | 2.00 | 0.42 |
| 1:F:775:LEU:HD12 | 1:F:776:SER:O | 2.19 | 0.42 |
| 1:A:243:LEU:HD12 | 1:A:244:PHE:O | 2.20 | 0.42 |
| 1:A:283:ILE:HD13 | 1:A:283:ILE:HA | 1.74 | 0.42 |
| 1:A:385:TYR:CE2 | 1:A:386:ARG:HG3 | 2.54 | 0.42 |
| 1:A:541:VAL:HB | 1:A:545:THR:H | 1.84 | 0.42 |
| 1:A:556:ILE:HG22 | 1:A:559:LYS:O | 2.19 | 0.42 |
| 1:A:823:MET:CE | 1:F:303:PRO:HB2 | 2.50 | 0.42 |
| 1:B:236:THR:O | 1:B:239:GLN:HB2 | 2.20 | 0.42 |
| 1:B:322:ARG:O | 1:B:326:GLU:HG2 | 2.20 | 0.42 |
| 1:B:379:ALA:O | 1:B:380:LYS:C | 2.60 | 0.42 |
| 1:B:404:ALA:O | 1:B:405:VAL:C | 2.60 | 0.42 |
| 1:B:542:ASP:O | 1:B:543:SER:OG | 2.31 | 0.42 |
| 1:B:591:SER:HB3 | 1:B:595:ARG:HH12 | 1.85 | 0.42 |
| 1:B:632:PHE:O | 1:B:633:ASN:C | 2.63 | 0.42 |
| 1:B:645:GLU:OE1 | 1:B:691:ALA:HB1 | 2.20 | 0.42 |
| 1:B:735:ASN:OD1 | 1:B:774:LYS:HE3 | 2.20 | 0.42 |
| 1:B:839:LYS:O | 1:B:842:LEU:HB2 | 2.20 | 0.42 |
| 1:B:854:THR:HG22 | 1:B:855:VAL:O | 2.20 | 0.42 |
| 1:C:189:ARG:HH12 | 1:C:341:ALA:H | 1.62 | 0.42 |
| 1:C:195:SER:HB3 | 1:C:198:ARG:HH21 | 1.84 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:224:GLY:HA2 | 1:C:227:GLN:HB2 | 2.02 | 0.42 |
| 1:C:227:GLN:O | 1:C:230:ILE:N | 2.52 | 0.42 |
| 1:C:301:LEU:O | 1:C:302:LYS:C | 2.59 | 0.42 |
| 1:C:343:PRO:HG2 | 1:C:388:LEU:HD23 | 2.02 | 0.42 |
| 1:C:344:SER:O | 1:C:347:GLN:HB2 | 2.19 | 0.42 |
| 1:C:354:GLY:O | 1:C:357:PRO:HD2 | 2.20 | 0.42 |
| 1:C:355:LEU:HD13 | 1:C:358:LYS:CE | 2.49 | 0.42 |
| 1:C:498:ASP:HB3 | 1:C:501:THR:H | 1.85 | 0.42 |
| 1:C:685:PHE:CB | 1:C:688:VAL:HA | 2.49 | 0.42 |
| 1:C:693:PRO:O | 1:C:697:THR:HG23 | 2.19 | 0.42 |
| 1:D:186:VAL:HG21 | 2:D:1001:AGS:H2' | 2.01 | 0.42 |
| 1:D:190:GLU:O | 1:D:194:ARG:HG3 | 2.18 | 0.42 |
| 1:D:193:ILE:O | 1:D:196:THR:N | 2.52 | 0.42 |
| 1:D:248:LEU:C | 1:D:251:LEU:HG | 2.44 | 0.42 |
| 1:D:281:LEU:HB2 | 1:D:312:VAL:CB | 2.50 | 0.42 |
| 1:D:351:ILE:O | 1:D:352:LEU:C | 2.60 | 0.42 |
| 1:D:383:LEU:HB3 | 1:D:385:TYR:CZ | 2.54 | 0.42 |
| 1:D:417:LYS:O | 1:D:421:LEU:N | 2.52 | 0.42 |
| 1:D:507:TYR:HB3 | 1:E:429:LYS:HB2 | 2.01 | 0.42 |
| 1:D:585:ASP:HA | 1:D:588:LYS:CG | 2.50 | 0.42 |
| 1:D:618:SER:HA | 1:D:826:ARG:HG3 | 2.01 | 0.42 |
| 1:D:635:GLU:O | 1:D:638:MET:HG3 | 2.20 | 0.42 |
| 1:D:684:LEU:HD23 | 1:D:685:PHE:C | 2.45 | 0.42 |
| 1:D:689:GLU:CD | 1:D:727:SER:HB2 | 2.44 | 0.42 |
| 1:D:744:GLU:O | 1:D:747:LYS:HG3 | 2.19 | 0.42 |
| 1:E:369:ASP:O | 1:E:370:SER:C | 2.62 | 0.42 |
| 1:E:379:ALA:HB2 | 1:E:395:LEU:HD21 | 2.02 | 0.42 |
| 1:E:389:PRO:O | 1:E:390:ASP:C | 2.62 | 0.42 |
| 1:E:617:GLY:CA | 2:E:1002:AGS:O1B | 2.65 | 0.42 |
| 1:E:674:GLN:OE1 | 1:E:678:LYS:N | 2.53 | 0.42 |
| 1:E:764:ASN:O | 1:E:765:ARG:C | 2.62 | 0.42 |
| 1:E:855:VAL:HG12 | 1:E:856:ASN:N | 2.34 | 0.42 |
| 1:F:174:MET:O | 1:F:175:THR:C | 2.63 | 0.42 |
| 1:F:191:GLU:O | 1:F:194:ARG:N | 2.52 | 0.42 |
| 1:F:234:VAL:HB | 1:F:235:PRO:HD2 | 2.02 | 0.42 |
| 1:F:270:LYS:O | 1:F:273:GLU:HB2 | 2.20 | 0.42 |
| 1:F:320:GLU:O | 1:F:324:ILE:HG12 | 2.19 | 0.42 |
| 1:F:570:ILE:O | 1:F:573:GLU:HB2 | 2.19 | 0.42 |
| 1:F:657:GLY:CA | 1:F:667:GLU:HB2 | 2.38 | 0.42 |
| 1:F:708:ILE:N | 1:F:715:THR:CG2 | 2.82 | 0.42 |
| 1:F:835:GLU:O | 1:F:838:ASN:HB2 | 2.19 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:210:LEU:HD13 | 1:A:339:GLU:CD | 2.45 | 0.42 |
| 1:A:226:ALA:HB1 | 1:A:230:ILE:HG12 | 2.01 | 0.42 |
| 1:A:246:LEU:HB3 | 1:A:282:PHE:C | 2.45 | 0.42 |
| 1:A:368:LEU:HD21 | 1:A:539:ASN:HB2 | 2.02 | 0.42 |
| 1:A:612:PHE:N | 1:A:770:VAL:N | 2.68 | 0.42 |
| 1:A:612:PHE:C | 1:A:613:LEU:HD12 | 2.44 | 0.42 |
| 1:B:166:TYR:HA | 1:B:169:LYS:HZ2 | 1.85 | 0.42 |
| 1:B:281:LEU:O | 1:B:312:VAL:HG12 | 2.19 | 0.42 |
| 1:B:649:LYS:HB3 | 1:B:692:HIS:HE1 | 1.78 | 0.42 |
| 1:B:698:VAL:HA | 1:B:701:GLN:CB | 2.26 | 0.42 |
| 1:C:203:ARG:NE | 1:D:362:HIS:CG | 2.87 | 0.42 |
| 1:C:280:VAL:HA | 1:C:311:LYS:CG | 2.49 | 0.42 |
| 1:C:287:HIS:CG | 1:C:288:MET:H | 2.37 | 0.42 |
| 1:C:299:ASN:O | 1:C:303:PRO:HG2 | 2.20 | 0.42 |
| 1:C:401:ALA:O | 1:C:402:GLY:C | 2.59 | 0.42 |
| 1:C:475:GLU:OE2 | 1:C:523:GLN:HB3 | 2.20 | 0.42 |
| 1:C:475:GLU:C | 1:C:520:LEU:HD22 | 2.45 | 0.42 |
| 1:C:596:LEU:HA | 1:C:599:SER:CB | 2.50 | 0.42 |
| 1:C:674:GLN:O | 1:C:675:LEU:C | 2.63 | 0.42 |
| 1:C:675:LEU:O | 1:C:676:GLN:C | 2.63 | 0.42 |
| 1:C:722:ILE:HD12 | 1:C:722:ILE:HA | 1.88 | 0.42 |
| 1:C:801:HIS:ND1 | 1:C:851:ASP:OD2 | 2.52 | 0.42 |
| 1:C:857:VAL:HA | 1:C:880:LEU:CB | 2.37 | 0.42 |
| 1:D:166:TYR:HB2 | 1:D:264:ARG:CZ | 2.49 | 0.42 |
| 1:D:193:ILE:O | 1:D:194:ARG:C | 2.60 | 0.42 |
| 1:D:221:ILE:HD11 | 2:D:1001:AGS:C8 | 2.50 | 0.42 |
| 1:D:413:GLU:OE1 | 1:D:462:LEU:HD22 | 2.19 | 0.42 |
| 1:D:544:ASP:O | 1:D:548:GLU:HG2 | 2.20 | 0.42 |
| 1:D:558:VAL:N | 1:D:561:LEU:HD13 | 2.34 | 0.42 |
| 1:D:593:ALA:O | 1:D:594:VAL:C | 2.63 | 0.42 |
| 1:D:622:GLU:HG3 | 1:D:826:ARG:NH2 | 2.35 | 0.42 |
| 1:D:680:TYR:HD1 | 1:D:720:ASN:O | 2.03 | 0.42 |
| 1:D:691:ALA:HB1 | 1:D:696:LEU:HD21 | 2.01 | 0.42 |
| 1:D:829:ASN:O | 1:D:833:GLN:N | 2.24 | 0.42 |
| 1:E:205:LYS:HB2 | 1:E:205:LYS:HE3 | 1.61 | 0.42 |
| 1:E:270:LYS:HA | 1:E:273:GLU:HB2 | 2.00 | 0.42 |
| 1:E:289:LEU:O | 1:E:290:MET:C | 2.63 | 0.42 |
| 1:E:330:ALA:O | 1:E:331:PHE:C | 2.63 | 0.42 |
| 1:E:342:GLU:OE2 | 1:E:388:LEU:HD22 | 2.20 | 0.42 |
| 1:E:613:LEU:CD1 | 1:E:728:ALA:HA | 2.50 | 0.42 |
| 1:E:807:THR:O | 1:E:811:LYS:HG3 | 2.19 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:205:LYS:HD3 | 1:F:336:GLN:N | 2.34 | 0.42 |
| 1:F:547:SER:OG | 1:F:548:GLU:N | 2.53 | 0.42 |
| 1:F:585:ASP:O | 1:F:586:ALA:C | 2.62 | 0.42 |
| 1:F:646:LEU:HB2 | 1:F:691:ALA:HA | 2.01 | 0.42 |
| 1:F:646:LEU:HA | 1:F:692:HIS:NE2 | 2.34 | 0.42 |
| 1:F:744:GLU:OE2 | 1:F:747:LYS:C | 2.63 | 0.42 |
| 1:A:211:ILE:H | 1:A:316:THR:CG2 | 2.32 | 0.42 |
| 1:A:228:ARG:HA | 1:A:231:ASP:CB | 2.50 | 0.42 |
| 1:A:261:PHE:CD2 | 1:A:262:GLU:N | 2.88 | 0.42 |
| 1:A:586:ALA:O | 1:A:590:VAL:HG23 | 2.20 | 0.42 |
| 1:A:742:ILE:HD12 | 1:A:746:THR:HG21 | 2.01 | 0.42 |
| 1:A:786:ILE:HA | 1:A:789:LYS:CE | 2.50 | 0.42 |
| 1:A:792:GLU:HB3 | 1:A:793:GLU:OE1 | 2.19 | 0.42 |
| 1:A:879:VAL:HG12 | 1:A:880:LEU:H | 1.85 | 0.42 |
| 1:B:213:GLU:OE2 | 1:B:342:GLU:HG3 | 2.20 | 0.42 |
| 1:B:313:ILE:HG22 | 1:B:314:GLY:N | 2.33 | 0.42 |
| 1:B:594:VAL:HG22 | 1:B:610:PHE:HE2 | 1.85 | 0.42 |
| 1:B:646:LEU:HD12 | 1:B:690:LYS:N | 2.25 | 0.42 |
| 1:B:669:GLY:O | 1:B:670:PHE:C | 2.62 | 0.42 |
| 1:B:732:GLU:O | 1:B:735:ASN:N | 2.52 | 0.42 |
| 1:C:186:VAL:HA | 2:C:1001:AGS:N1 | 2.34 | 0.42 |
| 1:C:214:PRO:CA | 1:C:218:LYS:HE3 | 2.49 | 0.42 |
| 1:C:216:ILE:O | 2:C:1001:AGS:H1' | 2.20 | 0.42 |
| 1:C:225:VAL:HG12 | 1:C:229:ILE:CD1 | 2.49 | 0.42 |
| 1:C:247:ASP:C | 1:C:248:LEU:HD12 | 2.44 | 0.42 |
| 1:C:261:PHE:O | 1:C:265:PHE:HB3 | 2.18 | 0.42 |
| 1:C:467:ASN:HA | 1:C:470:LYS:HB3 | 2.01 | 0.42 |
| 1:C:571:HIS:C | 1:C:574:ARG:HG2 | 2.44 | 0.42 |
| 1:C:587:ILE:C | 1:C:590:VAL:HB | 2.45 | 0.42 |
| 1:C:696:LEU:HA | 1:C:699:MET:CG | 2.48 | 0.42 |
| 1:D:190:GLU:HG2 | 1:D:191:GLU:N | 2.35 | 0.42 |
| 1:D:369:ASP:HA | 1:D:372:LEU:CD1 | 2.38 | 0.42 |
| 1:D:514:LYS:O | 1:D:517:ILE:HB | 2.19 | 0.42 |
| 1:D:620:LYS:O | 1:D:623:LEU:HB2 | 2.20 | 0.42 |
| 1:D:779:ALA:C | 1:D:782:LYS:HZ2 | 2.28 | 0.42 |
| 1:E:174:MET:CG | 1:E:177:GLN:HB2 | 2.29 | 0.42 |
| 1:E:225:VAL:O | 1:E:226:ALA:C | 2.63 | 0.42 |
| 1:E:303:PRO:N | 1:E:334:ARG:HH12 | 2.17 | 0.42 |
| 1:E:356:GLN:N | 1:E:357:PRO:HD2 | 2.35 | 0.42 |
| 1:E:701:GLN:HE22 | 1:E:708:ILE:C | 2.27 | 0.42 |
| 1:E:707:ARG:NH2 | 1:E:718:CYS:SG | 2.93 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:772:PHE:CG | 1:E:773:ASN:N | 2.87 | 0.42 |
| 1:E:782:LYS:N | 1:E:782:LYS:HD2 | 2.35 | 0.42 |
| 1:F:356:GLN:C | 1:F:360:GLU:HB3 | 2.44 | 0.42 |
| 1:F:675:LEU:HA | 1:F:678:LYS:O | 2.20 | 0.42 |
| 1:F:698:VAL:C | 1:F:699:MET:HE2 | 2.45 | 0.42 |
| 1:F:702:MET:CB | 1:F:708:ILE:CB | 2.97 | 0.42 |
| 1:F:774:LYS:HG2 | 1:F:775:LEU:HG | 2.02 | 0.42 |
| 1:F:778:LYS:O | 1:F:779:ALA:C | 2.61 | 0.42 |
| 1:F:829:ASN:OD1 | 1:F:830:ARG:HG2 | 2.19 | 0.42 |
| 1:F:829:ASN:C | 1:F:831:LEU:H | 2.28 | 0.42 |
| 1:A:166:TYR:O | 1:A:170:TYR:CD2 | 2.73 | 0.42 |
| 1:A:335:PHE:CD1 | 1:A:335:PHE:N | 2.83 | 0.42 |
| 1:A:638:MET:HE1 | 1:A:684:LEU:HB3 | 2.01 | 0.42 |
| 1:A:791:ILE:O | 1:A:792:GLU:C | 2.62 | 0.42 |
| 1:A:803:LYS:CB | 1:A:852:LYS:HE3 | 2.49 | 0.42 |
| 1:B:225:VAL:HG12 | 1:B:229:ILE:CD1 | 2.49 | 0.42 |
| 1:B:339:GLU:N | 1:B:339:GLU:OE1 | 2.52 | 0.42 |
| 1:B:399:SER:O | 1:B:403:VAL:HG23 | 2.19 | 0.42 |
| 1:B:619:GLY:CA | 1:B:622:GLU:HB3 | 2.45 | 0.42 |
| 1:B:736:SER:OG | 1:B:738:GLN:N | 2.44 | 0.42 |
| 1:B:780:ILE:HA | 1:B:783:ILE:HB | 2.00 | 0.42 |
| 1:C:196:THR:HB | 1:C:197:ILE:HD13 | 2.02 | 0.42 |
| 1:C:325:VAL:O | 1:C:328:ASP:HB2 | 2.19 | 0.42 |
| 1:C:370:SER:O | 1:C:371:ALA:C | 2.62 | 0.42 |
| 1:C:573:GLU:O | 1:C:576:LEU:N | 2.40 | 0.42 |
| 1:C:630:PHE:C | 1:C:630:PHE:CD1 | 2.98 | 0.42 |
| 1:C:644:SER:OG | 1:C:645:GLU:OE2 | 2.30 | 0.42 |
| 1:C:695:VAL:O | 1:C:696:LEU:C | 2.63 | 0.42 |
| 1:C:786:ILE:N | 1:C:789:LYS:HZ3 | 2.17 | 0.42 |
| 1:D:175:THR:CG2 | 1:D:230:ILE:HG13 | 2.50 | 0.42 |
| 1:D:265:PHE:O | 1:D:266:LYS:C | 2.63 | 0.42 |
| 1:D:352:LEU:HD23 | 1:D:352:LEU:HA | 1.80 | 0.42 |
| 1:D:375:ALA:HB2 | 1:D:546:ILE:CD1 | 2.50 | 0.42 |
| 1:D:383:LEU:HD22 | 1:D:385:TYR:HE2 | 1.84 | 0.42 |
| 1:D:388:LEU:HB2 | 1:D:389:PRO:HD3 | 2.02 | 0.42 |
| 1:D:530:ARG:NH1 | 1:D:538:GLN:N | 2.68 | 0.42 |
| 1:D:587:ILE:O | 1:D:588:LYS:C | 2.61 | 0.42 |
| 1:D:785:ASP:OD1 | 1:D:788:LEU:C | 2.57 | 0.42 |
| 1:E:349:VAL:HA | 1:E:352:LEU:CG | 2.50 | 0.42 |
| 1:E:456:GLN:HG3 | 1:E:460:GLU:HB2 | 2.01 | 0.42 |
| 1:E:541:VAL:HG12 | 1:E:544:ASP:HB2 | 2.00 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:639:ILE:HD12 | 1:E:682:VAL:HG13 | 2.02 | 0.42 |
| 1:E:641:VAL:HG12 | 1:E:643:CYS:SG | 2.60 | 0.42 |
| 1:E:674:GLN:OE1 | 1:E:677:TYR:C | 2.63 | 0.42 |
| 1:E:698:VAL:HG23 | 1:E:699:MET:N | 2.34 | 0.42 |
| 1:E:753:ALA:O | 1:E:756:GLN:NE2 | 2.53 | 0.42 |
| 1:E:759:ARG:CZ | 1:E:759:ARG:HB2 | 2.48 | 0.42 |
| 1:F:166:TYR:OH | 1:F:263:GLU:OE2 | 2.34 | 0.42 |
| 1:F:217:GLY:H | 2:F:1001:AGS:PG | 2.42 | 0.42 |
| 1:F:318:ASN:CG | 1:F:337:LYS:NZ | 2.78 | 0.42 |
| 1:F:394:ASP:O | 1:F:397:ASP:N | 2.53 | 0.42 |
| 1:F:732:GLU:HA | 1:F:735:ASN:HB2 | 2.02 | 0.42 |
| 1:F:778:LYS:C | 1:F:781:HIS:CD2 | 2.93 | 0.42 |
| 1:F:793:GLU:HA | 1:F:797:GLN:CG | 2.50 | 0.42 |
| 1:A:218:LYS:NZ | 1:A:387:ARG:HG3 | 2.35 | 0.41 |
| 1:A:240:GLY:O | 1:A:241:ALA:C | 2.63 | 0.41 |
| 1:A:358:LYS:NZ | 1:A:400:CYS:HB3 | 2.34 | 0.41 |
| 1:B:12:LEU:C | 1:B:15:LEU:H | 2.27 | 0.41 |
| 1:B:198:ARG:CG | 1:B:199:VAL:N | 2.82 | 0.41 |
| 1:B:221:ILE:H | 1:B:221:ILE:HG13 | 1.41 | 0.41 |
| 1:B:271:GLU:O | 1:B:274:GLU:OE1 | 2.38 | 0.41 |
| 1:B:541:VAL:HG12 | 1:B:544:ASP:CG | 2.45 | 0.41 |
| 1:B:543:SER:C | 1:B:546:ILE:HB | 2.45 | 0.41 |
| 1:B:637:MET:HB3 | 1:B:682:VAL:CG2 | 2.50 | 0.41 |
| 1:B:638:MET:C | 1:B:674:GLN:HE22 | 2.28 | 0.41 |
| 1:B:773:ASN:N | 1:B:773:ASN:OD1 | 2.47 | 0.41 |
| 1:B:791:ILE:HD13 | 1:B:833:GLN:HG3 | 2.01 | 0.41 |
| 1:C:210:LEU:CD1 | 1:C:337:LYS:HA | 2.47 | 0.41 |
| 1:C:214:PRO:HA | 1:C:218:LYS:CE | 2.48 | 0.41 |
| 1:C:274:GLU:H | 1:C:276:LYS:HZ1 | 1.66 | 0.41 |
| 1:C:285:GLU:OE1 | 1:C:287:HIS:NE2 | 2.52 | 0.41 |
| 1:C:290:MET:HG2 | 1:C:299:ASN:HD22 | 1.85 | 0.41 |
| 1:C:427:GLU:HB3 | 1:C:452:GLU:CD | 2.43 | 0.41 |
| 1:C:474:GLU:HG3 | 1:C:478:GLN:CD | 2.44 | 0.41 |
| 1:C:606:GLN:OE1 | 1:C:705:ASP:N | 2.53 | 0.41 |
| 1:C:650:TYR:CD2 | 1:C:650:TYR:C | 2.98 | 0.41 |
| 1:C:782:LYS:C | 1:C:784:VAL:H | 2.24 | 0.41 |
| 1:C:798:ASN:OD1 | 1:C:801:HIS:CE1 | 2.73 | 0.41 |
| 1:D:258:LYS:HZ2 | 1:D:262:GLU:CD | 2.28 | 0.41 |
| 1:D:299:ASN:O | 1:D:300:ILE:C | 2.63 | 0.41 |
| 1:D:302:LYS:O | 1:D:303:PRO:C | 2.62 | 0.41 |
| 1:D:311:LYS:HE2 | 1:D:311:LYS:HB2 | 1.72 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:411:PRO:HB2 | 1:D:538:GLN:HB3 | 2.02 | 0.41 |
| 1:D:467:ASN:HA | 1:D:470:LYS:HE3 | 2.01 | 0.41 |
| 1:D:570:ILE:HA | 1:D:595:ARG:CZ | 2.47 | 0.41 |
| 1:D:642:ASP:OD2 | 1:D:645:GLU:OE1 | 2.38 | 0.41 |
| 1:D:693:PRO:HA | 1:D:696:LEU:HD12 | 2.02 | 0.41 |
| 1:D:794:ARG:HG2 | 1:D:795:PHE:HD1 | 1.85 | 0.41 |
| 1:D:802:TYR:CD2 | 1:D:802:TYR:C | 2.95 | 0.41 |
| 1:E:231:ASP:HA | 1:E:495:ARG:NH2 | 2.35 | 0.41 |
| 1:E:342:GLU:HG3 | 1:E:343:PRO:HD2 | 2.02 | 0.41 |
| 1:E:370:SER:O | 1:E:371:ALA:C | 2.62 | 0.41 |
| 1:E:373:VAL:O | 1:E:376:ALA:N | 2.53 | 0.41 |
| 1:E:472:GLY:HA2 | 1:E:475:GLU:CD | 2.45 | 0.41 |
| 1:E:607:PRO:HG3 | 1:E:707:ARG:CZ | 2.50 | 0.41 |
| 1:E:659:THR:HA | 1:E:667:GLU:OE1 | 2.20 | 0.41 |
| 1:E:771:ILE:HG22 | 1:E:772:PHE:N | 2.33 | 0.41 |
| 1:E:777:ARG:O | 1:E:780:ILE:HG22 | 2.19 | 0.41 |
| 1:E:779:ALA:O | 1:E:783:ILE:HG13 | 2.20 | 0.41 |
| 1:E:836:ILE:O | 1:E:840:LEU:HD13 | 2.20 | 0.41 |
| 1:F:290:MET:HG2 | 1:F:293:GLY:CA | 2.42 | 0.41 |
| 1:F:317:THR:HG22 | 1:F:318:ASN:N | 2.33 | 0.41 |
| 1:F:369:ASP:O | 1:F:372:LEU:HB2 | 2.19 | 0.41 |
| 1:F:580:VAL:CG2 | 1:F:623:LEU:HD22 | 2.50 | 0.41 |
| 1:F:744:GLU:OE2 | 1:F:748:ASN:OD1 | 2.37 | 0.41 |
| 1:F:880:LEU:HG | 1:F:881:PRO:N | 2.32 | 0.41 |
| 1:A:302:LYS:HE2 | 1:A:305:LEU:O | 2.20 | 0.41 |
| 1:A:378:LEU:HG | 1:A:378:LEU:H | 1.64 | 0.41 |
| 1:A:389:PRO:O | 1:A:392:ALA:HB3 | 2.21 | 0.41 |
| 1:A:576:LEU:HD21 | 1:A:630:PHE:CD1 | 2.55 | 0.41 |
| 1:A:589:ALA:O | 1:A:592:ASN:N | 2.52 | 0.41 |
| 1:A:759:ARG:HA | 1:A:760:PRO:HD3 | 1.87 | 0.41 |
| 1:A:830:ARG:NH2 | 1:F:275:SER:HB2 | 2.35 | 0.41 |
| 1:B:280:VAL:CG1 | 1:B:310:LEU:HA | 2.44 | 0.41 |
| 1:B:596:LEU:H | 1:B:596:LEU:HG | 1.69 | 0.41 |
| 1:B:617:GLY:HA2 | 1:B:620:LYS:HZ2 | 1.72 | 0.41 |
| 1:B:620:LYS:O | 1:B:623:LEU:HB3 | 2.19 | 0.41 |
| 1:B:641:VAL:H | 1:B:684:LEU:HD22 | 1.85 | 0.41 |
| 1:B:777:ARG:O | 1:B:780:ILE:HG12 | 2.20 | 0.41 |
| 1:C:237:ILE:HD13 | 1:D:362:HIS:CE1 | 2.55 | 0.41 |
| 1:C:262:GLU:CA | 1:C:265:PHE:HB3 | 2.49 | 0.41 |
| 1:C:355:LEU:O | 1:C:356:GLN:C | 2.62 | 0.41 |
| 1:C:412:GLU:CB | 1:C:536:MET:HE1 | 2.50 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:461:PRO:O | 1:C:464:GLN:HB2 | 2.21 | 0.41 |
| 1:C:603:ASN:OD1 | 1:C:603:ASN:C | 2.62 | 0.41 |
| 1:C:672:THR:H | 1:C:672:THR:HG23 | 1.59 | 0.41 |
| 1:C:723:VAL:HG11 | 1:C:725:MET:HE2 | 2.01 | 0.41 |
| 1:C:828:LEU:HB3 | 1:C:832:ILE:HD11 | 2.02 | 0.41 |
| 1:C:837:LEU:O | 1:C:838:ASN:C | 2.62 | 0.41 |
| 1:D:211:ILE:N | 1:D:316:THR:O | 2.53 | 0.41 |
| 1:D:508:PHE:CZ | 1:D:512:ASP:HB3 | 2.54 | 0.41 |
| 1:D:587:ILE:HG22 | 1:D:591:SER:OG | 2.20 | 0.41 |
| 1:D:605:ARG:NH1 | 1:D:707:ARG:HB3 | 2.35 | 0.41 |
| 1:D:722:ILE:CG2 | 1:D:723:VAL:H | 2.19 | 0.41 |
| 1:D:802:TYR:CE2 | 1:D:853:GLU:HG3 | 2.54 | 0.41 |
| 1:D:826:ARG:N | 1:D:827:PRO:CD | 2.83 | 0.41 |
| 1:E:219:THR:O | 1:E:223:GLU:N | 2.40 | 0.41 |
| 1:E:356:GLN:HG3 | 1:E:367:ILE:HD12 | 2.02 | 0.41 |
| 1:E:428:ILE:HG12 | 1:E:449:ARG:CG | 2.49 | 0.41 |
| 1:E:536:MET:CG | 1:E:538:GLN:HB3 | 2.45 | 0.41 |
| 1:E:622:GLU:N | 1:E:625:LYS:HD3 | 2.35 | 0.41 |
| 1:E:697:THR:O | 1:E:700:LEU:HB3 | 2.21 | 0.41 |
| 1:E:723:VAL:HG13 | 1:E:724:ILE:N | 2.34 | 0.41 |
| 1:E:794:ARG:NH2 | 1:E:797:GLN:NE2 | 2.68 | 0.41 |
| 1:E:813:PHE:HD2 | 1:E:857:VAL:HG11 | 1.84 | 0.41 |
| 1:E:825:ALA:CB | 1:E:828:LEU:HB3 | 2.41 | 0.41 |
| 1:F:166:TYR:CZ | 1:F:264:ARG:NH1 | 2.88 | 0.41 |
| 1:F:699:MET:O | 1:F:702:MET:HG2 | 2.20 | 0.41 |
| 1:F:763:LEU:HA | 1:F:763:LEU:HD23 | 1.79 | 0.41 |
| 1:F:808:GLN:CA | 1:F:811:LYS:NZ | 2.83 | 0.41 |
| 1:A:235:PRO:HD2 | 1:A:238:LEU:CD1 | 2.50 | 0.41 |
| 1:A:378:LEU:CD2 | 1:A:381:ARG:HD2 | 2.50 | 0.41 |
| 1:A:576:LEU:O | 1:A:579:GLU:HB3 | 2.20 | 0.41 |
| 1:A:612:PHE:HD2 | 1:A:770:VAL:CA | 2.33 | 0.41 |
| 1:B:166:TYR:HA | 1:B:169:LYS:CG | 2.44 | 0.41 |
| 1:B:193:ILE:HB | 1:B:225:VAL:HG22 | 2.02 | 0.41 |
| 1:B:195:SER:O | 1:B:197:ILE:N | 2.52 | 0.41 |
| 1:B:566:ASN:OD1 | 1:B:570:ILE:HG13 | 2.21 | 0.41 |
| 1:B:592:ASN:O | 1:B:596:LEU:HG | 2.20 | 0.41 |
| 1:B:599:SER:O | 1:B:602:ALA:HB3 | 2.20 | 0.41 |
| 1:B:607:PRO:HD3 | 1:B:705:ASP:O | 2.19 | 0.41 |
| 1:B:637:MET:O | 1:B:638:MET:C | 2.64 | 0.41 |
| 1:B:762:PHE:C | 1:B:765:ARG:H | 2.28 | 0.41 |
| 1:C:189:ARG:O | 1:C:190:GLU:C | 2.64 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:318:ASN:O | 1:C:321:TYR:HB3 | 2.20 | 0.41 |
| 1:C:333:ARG:HH11 | 1:C:334:ARG:NE | 2.18 | 0.41 |
| 1:C:392:ALA:HA | 1:C:395:LEU:HG | 2.02 | 0.41 |
| 1:C:417:LYS:CG | 1:C:456:GLN:HE22 | 2.30 | 0.41 |
| 1:C:472:GLY:C | 1:C:475:GLU:HG2 | 2.46 | 0.41 |
| 1:C:492:ASP:O | 1:C:495:ARG:HB2 | 2.19 | 0.41 |
| 1:C:514:LYS:O | 1:C:517:ILE:HB | 2.20 | 0.41 |
| 1:C:534:ASN:OD1 | 1:C:538:GLN:HB2 | 2.20 | 0.41 |
| 1:C:546:ILE:O | 1:C:549:THR:HB | 2.21 | 0.41 |
| 1:C:816:LYS:NZ | 1:C:817:TYR:CE1 | 2.88 | 0.41 |
| 1:D:178:ALA:O | 1:D:181:GLY:N | 2.53 | 0.41 |
| 1:D:237:ILE:O | 1:D:240:GLY:N | 2.54 | 0.41 |
| 1:D:270:LYS:O | 1:D:274:GLU:CD | 2.63 | 0.41 |
| 1:D:323:SER:O | 1:D:326:GLU:OE2 | 2.38 | 0.41 |
| 1:D:356:GLN:HE21 | 1:D:366:ARG:HA | 1.86 | 0.41 |
| 1:D:462:LEU:HA | 1:D:465:ARG:CD | 2.50 | 0.41 |
| 1:D:569:LEU:O | 1:D:573:GLU:CD | 2.63 | 0.41 |
| 1:D:618:SER:O | 1:D:622:GLU:CD | 2.63 | 0.41 |
| 1:D:683:LEU:O | 1:D:723:VAL:HG13 | 2.20 | 0.41 |
| 1:D:846:LYS:HE2 | 1:D:846:LYS:HB2 | 1.73 | 0.41 |
| 1:E:194:ARG:C | 1:E:198:ARG:HH11 | 2.29 | 0.41 |
| 1:E:194:ARG:C | 1:E:198:ARG:NH1 | 2.79 | 0.41 |
| 1:E:205:LYS:NZ | 1:E:334:ARG:CA | 2.83 | 0.41 |
| 1:E:244:PHE:CB | 1:E:281:LEU:HD12 | 2.50 | 0.41 |
| 1:E:262:GLU:CB | 1:E:297:ALA:HB1 | 2.45 | 0.41 |
| 1:E:344:SER:O | 1:E:345:VAL:C | 2.63 | 0.41 |
| 1:E:366:ARG:HD3 | 1:E:539:ASN:CG | 2.45 | 0.41 |
| 1:E:400:CYS:C | 1:E:403:VAL:HB | 2.45 | 0.41 |
| 1:E:453:ALA:O | 1:E:457:GLU:HG3 | 2.20 | 0.41 |
| 1:E:502:ALA:O | 1:E:506:ARG:HG3 | 2.19 | 0.41 |
| 1:E:610:PHE:C | 1:E:725:MET:HE3 | 2.44 | 0.41 |
| 1:E:701:GLN:O | 1:E:702:MET:C | 2.63 | 0.41 |
| 1:E:745:SER:H | 1:E:747:LYS:CE | 2.34 | 0.41 |
| 1:E:747:LYS:HB2 | 1:E:747:LYS:HE2 | 1.60 | 0.41 |
| 1:E:802:TYR:HH | 1:E:850:LYS:C | 2.15 | 0.41 |
| 1:E:807:THR:HA | 1:E:811:LYS:CD | 2.50 | 0.41 |
| 1:E:807:THR:HA | 1:E:811:LYS:HG3 | 2.03 | 0.41 |
| 1:E:814:LEU:HB3 | 1:E:828:LEU:HD21 | 2.02 | 0.41 |
| 1:F:203:ARG:O | 1:F:204:ILE:C | 2.63 | 0.41 |
| 1:F:249:ALA:C | 1:F:251:LEU:N | 2.78 | 0.41 |
| 1:F:363:HIS:CD2 | 1:F:400:CYS:HG | 2.27 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:F:402:GLY:O | 1:F:405:VAL:HB | 2.20 | 0.41 |
| 1:F:616:SER:HB3 | 2:F:1002:AGS:O2A | 2.20 | 0.41 |
| 1:F:745:SER:O | 1:F:749:LEU:HG | 2.20 | 0.41 |
| 1:F:790:GLU:O | 1:F:793:GLU:OE2 | 2.38 | 0.41 |
| 1:F:833:GLN:HG3 | 1:F:834:ASN:N | 2.35 | 0.41 |
| 1:A:266:LYS:O | 1:A:269:LEU:HB3 | 2.20 | 0.41 |
| 1:A:279:ILE:H | 1:A:309:GLN:CG | 2.33 | 0.41 |
| 1:A:355:LEU:N | 1:A:360:GLU:OE1 | 2.53 | 0.41 |
| 1:A:374:THR:O | 1:A:375:ALA:C | 2.64 | 0.41 |
| 1:A:625:LYS:O | 1:A:628:ALA:N | 2.53 | 0.41 |
| 1:A:689:GLU:CD | 1:A:727:SER:HB2 | 2.46 | 0.41 |
| 1:A:739:GLY:O | 1:A:742:ILE:HG12 | 2.21 | 0.41 |
| 1:A:763:LEU:HA | 1:A:766:ILE:HD12 | 2.01 | 0.41 |
| 1:B:176:GLU:O | 1:B:177:GLN:C | 2.62 | 0.41 |
| 1:B:207:ASN:O | 1:B:335:PHE:CZ | 2.73 | 0.41 |
| 1:B:265:PHE:HA | 1:B:268:VAL:CG2 | 2.50 | 0.41 |
| 1:B:287:HIS:HA | 1:B:290:MET:CB | 2.46 | 0.41 |
| 1:B:372:LEU:H | 1:B:372:LEU:HG | 1.31 | 0.41 |
| 1:B:542:ASP:OD1 | 1:B:544:ASP:HB2 | 2.20 | 0.41 |
| 1:B:599:SER:C | 1:B:602:ALA:H | 2.28 | 0.41 |
| 1:B:611:LEU:O | 1:B:770:VAL:HB | 2.20 | 0.41 |
| 1:B:642:ASP:O | 1:B:643:CYS:C | 2.63 | 0.41 |
| 1:C:203:ARG:CG | 1:C:204:ILE:N | 2.83 | 0.41 |
| 1:C:208:PRO:HD3 | 1:C:313:ILE:CG2 | 2.48 | 0.41 |
| 1:C:652:VAL:HB | 1:C:654:LYS:NZ | 2.36 | 0.41 |
| 1:C:683:LEU:H | 1:C:723:VAL:HG13 | 1.85 | 0.41 |
| 1:C:800:LYS:HA | 1:C:851:ASP:OD1 | 2.20 | 0.41 |
| 1:D:249:ALA:C | 1:D:251:LEU:N | 2.78 | 0.41 |
| 1:D:260:ASP:OD1 | 1:D:264:ARG:HB2 | 2.21 | 0.41 |
| 1:D:356:GLN:O | 1:D:357:PRO:C | 2.63 | 0.41 |
| 1:D:380:LYS:NZ | 1:D:381:ARG:HB3 | 2.35 | 0.41 |
| 1:D:411:PRO:CB | 1:D:538:GLN:HB3 | 2.50 | 0.41 |
| 1:D:565:GLU:CG | 1:D:566:ASN:H | 2.29 | 0.41 |
| 1:D:584:MET:O | 1:D:587:ILE:HB | 2.20 | 0.41 |
| 1:D:620:LYS:HZ1 | 1:D:621:THR:HG23 | 1.85 | 0.41 |
| 1:D:642:ASP:HA | 1:D:685:PHE:CE2 | 2.56 | 0.41 |
| 1:D:671:LEU:C | 1:D:675:LEU:HG | 2.45 | 0.41 |
| 1:D:704:ASP:OD1 | 1:D:704:ASP:C | 2.60 | 0.41 |
| 1:D:779:ALA:HA | 1:D:782:LYS:NZ | 2.36 | 0.41 |
| 1:D:805:ASN:CA | 1:D:856:ASN:HB3 | 2.50 | 0.41 |
| 1:D:831:LEU:HA | 1:D:834:ASN:ND2 | 2.34 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:186:VAL:HA | 2:E:1001:AGS:N1 | 2.31 | 0.41 |
| 1:E:189:ARG:HB3 | 1:E:192:GLU:CD | 2.45 | 0.41 |
| 1:E:206:SER:O | 1:E:208:PRO:HD2 | 2.20 | 0.41 |
| 1:E:219:THR:O | 1:E:222:ILE:N | 2.53 | 0.41 |
| 1:E:228:ARG:HH12 | 1:E:232:ASP:N | 2.18 | 0.41 |
| 1:E:372:LEU:H | 1:E:372:LEU:HG | 1.26 | 0.41 |
| 1:E:424:ILE:HB | 1:E:452:GLU:CD | 2.45 | 0.41 |
| 1:E:598:ARG:HD3 | 1:E:598:ARG:HA | 1.27 | 0.41 |
| 1:E:626:LYS:O | 1:E:630:PHE:N | 2.40 | 0.41 |
| 1:E:730:GLY:O | 1:E:731:ALA:C | 2.63 | 0.41 |
| 1:E:754:VAL:O | 1:E:756:GLN:N | 2.53 | 0.41 |
| 1:E:828:LEU:HG | 1:E:832:ILE:CG1 | 2.48 | 0.41 |
| 1:E:831:LEU:C | 1:E:834:ASN:OD1 | 2.63 | 0.41 |
| 1:F:242:LYS:HD3 | 1:F:242:LYS:HA | 1.62 | 0.41 |
| 1:F:321:TYR:CD1 | 1:F:321:TYR:N | 2.88 | 0.41 |
| 1:F:321:TYR:CD2 | 1:F:322:ARG:N | 2.89 | 0.41 |
| 1:F:382:TYR:CE2 | 1:F:383:LEU:HD21 | 2.55 | 0.41 |
| 1:F:678:LYS:HG2 | 1:F:678:LYS:HZ2 | 1.65 | 0.41 |
| 1:F:704:ASP:H | 1:F:765:ARG:NH1 | 2.18 | 0.41 |
| 1:F:806:LEU:O | 1:F:811:LYS:HG3 | 2.20 | 0.41 |
| 1:A:174:MET:O | 1:A:175:THR:C | 2.64 | 0.41 |
| 1:A:283:ILE:O | 1:A:313:ILE:O | 2.39 | 0.41 |
| 1:A:358:LYS:HZ1 | 1:A:400:CYS:HB3 | 1.85 | 0.41 |
| 1:A:552:ARG:HB3 | 1:A:552:ARG:CZ | 2.50 | 0.41 |
| 1:A:607:PRO:HB3 | 1:A:719:SER:O | 2.20 | 0.41 |
| 1:A:613:LEU:CD1 | 1:A:727:SER:H | 2.32 | 0.41 |
| 1:A:639:ILE:HG22 | 1:A:640:ARG:N | 2.36 | 0.41 |
| 1:A:742:ILE:HD13 | 1:A:742:ILE:HA | 1.89 | 0.41 |
| 1:A:785:ASP:OD1 | 1:A:789:LYS:NZ | 2.53 | 0.41 |
| 1:A:813:PHE:CD2 | 1:A:814:LEU:N | 2.89 | 0.41 |
| 1:B:165:GLU:O | 1:B:169:LYS:HD3 | 2.21 | 0.41 |
| 1:B:282:PHE:CE2 | 1:B:284:ASP:HA | 2.56 | 0.41 |
| 1:B:287:HIS:CD2 | 1:B:288:MET:N | 2.89 | 0.41 |
| 1:B:299:ASN:C | 1:B:299:ASN:OD1 | 2.63 | 0.41 |
| 1:B:300:ILE:CG2 | 1:C:248:LEU:HD23 | 2.50 | 0.41 |
| 1:B:583:GLN:HG3 | 1:B:772:PHE:HA | 2.01 | 0.41 |
| 1:B:587:ILE:O | 1:B:590:VAL:HB | 2.20 | 0.41 |
| 1:B:615:LEU:HD12 | 1:B:772:PHE:HE2 | 1.85 | 0.41 |
| 1:B:700:LEU:HA | 1:B:703:LEU:HD12 | 2.03 | 0.41 |
| 1:B:730:GLY:C | 1:B:732:GLU:N | 2.78 | 0.41 |
| 1:B:748:ASN:O | 1:B:749:LEU:C | 2.63 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:784:VAL:O | 1:B:788:LEU:HG | 2.20 | 0.41 |
| 1:C:203:ARG:HE | 1:D:363:HIS:CD2 | 2.39 | 0.41 |
| 1:C:360:GLU:OE2 | 1:C:364:GLY:C | 2.58 | 0.41 |
| 1:C:465:ARG:NH2 | 1:C:466:TYR:CZ | 2.89 | 0.41 |
| 1:C:611:LEU:HB3 | 1:C:769:ILE:CA | 2.50 | 0.41 |
| 1:C:642:ASP:HA | 1:C:686:ASP:CG | 2.46 | 0.41 |
| 1:C:644:SER:C | 1:C:646:LEU:H | 2.29 | 0.41 |
| 1:C:658:THR:HG22 | 1:C:665:TYR:CE1 | 2.54 | 0.41 |
| 1:C:687:GLU:C | 1:C:689:GLU:H | 2.27 | 0.41 |
| 1:C:710:SER:HG | 1:C:712:GLN:C | 2.27 | 0.41 |
| 1:C:831:LEU:O | 1:C:833:GLN:N | 2.54 | 0.41 |
| 1:D:207:ASN:CG | 1:D:312:VAL:HG22 | 2.45 | 0.41 |
| 1:D:317:THR:HG1 | 1:D:321:TYR:N | 2.18 | 0.41 |
| 1:D:331:PHE:O | 1:D:332:GLU:C | 2.61 | 0.41 |
| 1:D:373:VAL:O | 1:D:376:ALA:N | 2.44 | 0.41 |
| 1:D:570:ILE:HG23 | 1:D:595:ARG:HH12 | 1.85 | 0.41 |
| 1:D:583:GLN:HE22 | 1:D:772:PHE:C | 2.28 | 0.41 |
| 1:D:613:LEU:HD11 | 1:D:728:ALA:HA | 2.03 | 0.41 |
| 1:D:656:LEU:O | 1:D:667:GLU:HB3 | 2.21 | 0.41 |
| 1:D:777:ARG:HG3 | 1:D:778:LYS:N | 2.36 | 0.41 |
| 1:D:791:ILE:CG2 | 1:D:795:PHE:HZ | 2.27 | 0.41 |
| 1:E:191:GLU:HG2 | 1:E:192:GLU:H | 1.85 | 0.41 |
| 1:E:221:ILE:C | 1:E:225:VAL:HG23 | 2.45 | 0.41 |
| 1:E:322:ARG:O | 1:E:323:SER:C | 2.64 | 0.41 |
| 1:E:344:SER:OG | 1:E:344:SER:O | 2.38 | 0.41 |
| 1:E:352:LEU:HD23 | 1:E:355:LEU:HD12 | 2.01 | 0.41 |
| 1:E:378:LEU:HG | 1:E:381:ARG:HB3 | 2.03 | 0.41 |
| 1:E:583:GLN:O | 1:E:586:ALA:N | 2.53 | 0.41 |
| 1:E:603:ASN:HD21 | 1:F:794:ARG:CZ | 2.34 | 0.41 |
| 1:E:632:PHE:HE1 | 1:E:680:TYR:HD2 | 1.68 | 0.41 |
| 1:E:782:LYS:O | 1:E:785:ASP:CG | 2.64 | 0.41 |
| 1:E:858:VAL:HB | 1:E:877:LEU:CD1 | 2.48 | 0.41 |
| 1:F:189:ARG:HH11 | 1:F:340:VAL:HB | 1.84 | 0.41 |
| 1:F:319:ASN:CA | 1:F:323:SER:OG | 2.53 | 0.41 |
| 1:F:638:MET:HG3 | 1:F:674:GLN:HE22 | 1.85 | 0.41 |
| 1:F:674:GLN:O | 1:F:677:TYR:HB2 | 2.20 | 0.41 |
| 1:F:702:MET:HE3 | 1:F:708:ILE:CG1 | 2.50 | 0.41 |
| 1:F:858:VAL:CA | 1:F:878:GLU:HA | 2.42 | 0.41 |
| 1:A:218:LYS:CG | 1:A:219:THR:H | 2.20 | 0.41 |
| 1:A:246:LEU:HD22 | 1:A:281:LEU:HB3 | 2.01 | 0.41 |
| 1:A:270:LYS:C | 1:A:272:ILE:N | 2.77 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:542:ASP:OD1 | 1:A:542:ASP:N | 2.51 | 0.41 |
| 1:A:607:PRO:HD2 | 1:A:703:LEU:O | 2.21 | 0.41 |
| 1:A:698:VAL:O | 1:A:702:MET:HG2 | 2.20 | 0.41 |
| 1:A:781:HIS:CD2 | 1:A:782:LYS:HG3 | 2.55 | 0.41 |
| 1:A:788:LEU:HD13 | 1:A:802:TYR:OH | 2.21 | 0.41 |
| 1:B:170:TYR:CE1 | 1:B:251:LEU:HD23 | 2.55 | 0.41 |
| 1:B:273:GLU:C | 1:B:273:GLU:CD | 2.89 | 0.41 |
| 1:B:322:ARG:O | 1:B:323:SER:C | 2.62 | 0.41 |
| 1:B:362:HIS:CD2 | 1:B:363:HIS:CD2 | 3.05 | 0.41 |
| 1:B:372:LEU:O | 1:B:373:VAL:C | 2.63 | 0.41 |
| 1:B:393:LEU:CD2 | 1:B:397:ASP:HB2 | 2.51 | 0.41 |
| 1:B:544:ASP:N | 1:B:560:LYS:HZ1 | 2.17 | 0.41 |
| 1:B:553:LEU:HD12 | 1:B:553:LEU:HA | 1.85 | 0.41 |
| 1:B:573:GLU:C | 1:B:575:ASP:N | 2.76 | 0.41 |
| 1:B:619:GLY:HA2 | 1:B:622:GLU:OE1 | 2.20 | 0.41 |
| 1:B:656:LEU:HB2 | 1:B:667:GLU:HB2 | 2.02 | 0.41 |
| 1:B:657:GLY:H | 1:B:668:GLY:HA3 | 1.86 | 0.41 |
| 1:B:672:THR:O | 1:B:673:ASN:C | 2.64 | 0.41 |
| 1:B:799:ASP:O | 1:B:801:HIS:CE1 | 2.72 | 0.41 |
| 1:B:804:LEU:O | 1:B:855:VAL:N | 2.48 | 0.41 |
| 1:C:290:MET:HB3 | 1:C:294:LYS:HZ2 | 1.85 | 0.41 |
| 1:C:291:GLY:CA | 1:C:294:LYS:HZ3 | 2.33 | 0.41 |
| 1:C:568:LYS:NZ | 1:C:630:PHE:HA | 2.34 | 0.41 |
| 1:C:709:THR:C | 1:C:716:ILE:HG13 | 2.45 | 0.41 |
| 1:C:761:GLU:O | 1:C:762:PHE:C | 2.62 | 0.41 |
| 1:C:803:LYS:NZ | 1:C:855:VAL:HG13 | 2.35 | 0.41 |
| 1:C:814:LEU:HA | 1:C:814:LEU:HD23 | 1.76 | 0.41 |
| 1:D:324:ILE:O | 1:D:325:VAL:C | 2.63 | 0.41 |
| 1:D:352:LEU:HA | 1:D:355:LEU:CD2 | 2.49 | 0.41 |
| 1:D:380:LYS:C | 1:D:382:TYR:N | 2.72 | 0.41 |
| 1:D:460:GLU:O | 1:D:464:GLN:HG3 | 2.21 | 0.41 |
| 1:D:785:ASP:HA | 1:D:788:LEU:CD1 | 2.50 | 0.41 |
| 1:D:800:LYS:N | 1:D:801:HIS:HD2 | 2.19 | 0.41 |
| 1:E:483:LEU:CD1 | 1:E:514:LYS:HG3 | 2.51 | 0.41 |
| 1:E:585:ASP:O | 1:E:586:ALA:C | 2.63 | 0.41 |
| 1:E:644:SER:CB | 1:E:690:LYS:HE3 | 2.51 | 0.41 |
| 1:E:841:ALA:C | 1:E:844:ILE:H | 2.29 | 0.41 |
| 1:F:556:ILE:H | 1:F:559:LYS:NZ | 2.19 | 0.41 |
| 1:F:786:ILE:O | 1:F:787:ARG:C | 2.63 | 0.41 |
| 1:A:221:ILE:C | 1:A:225:VAL:HG23 | 2.46 | 0.41 |
| 1:A:334:ARG:HD3 | 1:A:334:ARG:HA | 1.51 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:374:THR:O | 1:A:377:GLN:HB2 | 2.21 | 0.41 |
| 1:A:403:VAL:HG11 | 1:A:407:ARG:HH12 | 1.84 | 0.41 |
| 1:A:613:LEU:HB3 | 1:A:728:ALA:HA | 2.03 | 0.41 |
| 1:A:655:LEU:HD12 | 1:A:671:LEU:HB3 | 2.03 | 0.41 |
| 1:A:708:ILE:H | 1:A:717:ASP:HA | 1.86 | 0.41 |
| 1:A:780:ILE:O | 1:A:781:HIS:C | 2.63 | 0.41 |
| 1:A:782:LYS:NZ | 1:A:782:LYS:HB2 | 2.34 | 0.41 |
| 1:A:783:ILE:O | 1:A:784:VAL:C | 2.63 | 0.41 |
| 1:B:345:VAL:O | 1:B:349:VAL:HG23 | 2.21 | 0.41 |
| 1:B:543:SER:O | 1:B:544:ASP:C | 2.63 | 0.41 |
| 1:B:719:SER:C | 1:B:721:CYS:N | 2.75 | 0.41 |
| 1:B:759:ARG:HD3 | 1:B:759:ARG:HA | 1.83 | 0.41 |
| 1:B:798:ASN:HB3 | 1:B:802:TYR:CE1 | 2.55 | 0.41 |
| 1:C:197:ILE:N | 1:C:197:ILE:HD13 | 2.35 | 0.41 |
| 1:C:211:ILE:HD13 | 1:C:315:ALA:HA | 2.03 | 0.41 |
| 1:C:235:PRO:HB2 | 1:C:238:LEU:HB2 | 2.03 | 0.41 |
| 1:C:259:GLY:HA3 | 1:C:262:GLU:OE1 | 2.20 | 0.41 |
| 1:C:619:GLY:O | 1:C:620:LYS:C | 2.63 | 0.41 |
| 1:D:165:GLU:CD | 1:D:170:TYR:OH | 2.64 | 0.41 |
| 1:D:259:GLY:O | 1:D:263:GLU:HG3 | 2.20 | 0.41 |
| 1:D:365:VAL:HG11 | 1:D:540:VAL:HG11 | 2.01 | 0.41 |
| 1:D:371:ALA:O | 1:D:374:THR:N | 2.54 | 0.41 |
| 1:D:487:GLU:O | 1:D:491:LEU:N | 2.34 | 0.41 |
| 1:D:595:ARG:O | 1:D:596:LEU:C | 2.64 | 0.41 |
| 1:D:619:GLY:O | 1:D:623:LEU:N | 2.33 | 0.41 |
| 1:D:650:TYR:CD2 | 1:D:650:TYR:O | 2.73 | 0.41 |
| 1:D:729:LEU:HD22 | 1:D:754:VAL:CG2 | 2.51 | 0.41 |
| 1:D:735:ASN:O | 1:D:736:SER:C | 2.64 | 0.41 |
| 1:D:777:ARG:N | 1:D:780:ILE:HD12 | 2.35 | 0.41 |
| 1:D:792:GLU:HG2 | 1:D:801:HIS:HA | 2.03 | 0.41 |
| 1:D:814:LEU:O | 1:D:817:TYR:C | 2.63 | 0.41 |
| 1:D:849:ILE:HG21 | 1:D:852:LYS:HG2 | 2.02 | 0.41 |
| 1:E:459:LEU:HG | 1:E:463:ARG:NE | 2.36 | 0.41 |
| 1:E:613:LEU:N | 1:E:771:ILE:HG23 | 2.36 | 0.41 |
| 1:F:286:ILE:CD1 | 1:F:322:ARG:HG3 | 2.24 | 0.41 |
| 1:F:335:PHE:N | 1:F:335:PHE:CD1 | 2.85 | 0.41 |
| 1:F:556:ILE:CG1 | 1:F:559:LYS:HG3 | 2.50 | 0.41 |
| 1:F:687:GLU:CG | 1:F:728:ALA:H | 2.32 | 0.41 |
| 1:F:808:GLN:HA | 1:F:811:LYS:HB2 | 2.02 | 0.41 |
| 1:F:832:ILE:O | 1:F:833:GLN:C | 2.60 | 0.41 |
| 1:A:263:GLU:O | 1:A:267:GLY:HA3 | 2.20 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:546:ILE:O | 1:A:547:SER:C | 2.63 | 0.41 |
| 1:A:563:GLU:C | 1:A:568:LYS:HB3 | 2.46 | 0.41 |
| 1:A:625:LYS:NZ | 1:A:638:MET:CG | 2.84 | 0.41 |
| 1:A:843:ARG:C | 1:A:846:LYS:H | 2.29 | 0.41 |
| 1:B:198:ARG:O | 1:B:199:VAL:C | 2.62 | 0.41 |
| 1:B:252:THR:C | 1:B:264:ARG:NH2 | 2.78 | 0.41 |
| 1:B:349:VAL:HA | 1:B:352:LEU:HD12 | 2.02 | 0.41 |
| 1:B:387:ARG:HD3 | 1:B:387:ARG:HA | 1.76 | 0.41 |
| 1:B:403:VAL:HA | 1:B:406:ALA:HB3 | 2.03 | 0.41 |
| 1:B:583:GLN:H | 1:B:773:ASN:CG | 2.28 | 0.41 |
| 1:B:617:GLY:C | 1:B:826:ARG:HH11 | 2.28 | 0.41 |
| 1:B:744:GLU:HG3 | 1:B:748:ASN:HD21 | 1.86 | 0.41 |
| 1:C:240:GLY:H | 1:C:278:LEU:HD12 | 1.86 | 0.41 |
| 1:C:535:SER:C | 1:C:537:ILE:N | 2.77 | 0.41 |
| 1:C:618:SER:OG | 1:C:772:PHE:CZ | 2.74 | 0.41 |
| 1:C:659:THR:CG2 | 1:C:712:GLN:HA | 2.51 | 0.41 |
| 1:C:692:HIS:HB3 | 1:C:695:VAL:CG2 | 2.51 | 0.41 |
| 1:C:699:MET:O | 1:C:700:LEU:C | 2.62 | 0.41 |
| 1:C:718:CYS:C | 1:C:720:ASN:N | 2.76 | 0.41 |
| 1:C:839:LYS:HZ2 | 1:C:881:PRO:HD3 | 1.85 | 0.41 |
| 1:C:859:LEU:HG | 1:C:876:CYS:SG | 2.61 | 0.41 |
| 1:D:191:GLU:HA | 1:D:194:ARG:HB2 | 2.01 | 0.41 |
| 1:D:207:ASN:CG | 1:D:312:VAL:H | 2.28 | 0.41 |
| 1:D:355:LEU:HD12 | 1:D:356:GLN:HA | 2.01 | 0.41 |
| 1:D:356:GLN:HE22 | 1:D:367:ILE:H | 1.68 | 0.41 |
| 1:D:374:THR:C | 1:D:377:GLN:OE1 | 2.64 | 0.41 |
| 1:D:378:LEU:HA | 1:D:378:LEU:HD23 | 1.88 | 0.41 |
| 1:D:571:HIS:O | 1:D:574:ARG:N | 2.54 | 0.41 |
| 1:D:596:LEU:HG | 1:E:838:ASN:OD1 | 2.21 | 0.41 |
| 1:D:619:GLY:O | 1:D:620:LYS:C | 2.63 | 0.41 |
| 1:D:655:LEU:HD23 | 1:D:656:LEU:HA | 2.02 | 0.41 |
| 1:D:655:LEU:HD23 | 1:D:667:GLU:O | 2.21 | 0.41 |
| 1:D:656:LEU:HG | 1:D:710:SER:CA | 2.51 | 0.41 |
| 1:D:824:GLY:C | 1:D:828:LEU:HD21 | 2.45 | 0.41 |
| 1:E:216:ILE:HG21 | 1:E:387:ARG:CZ | 2.50 | 0.41 |
| 1:E:241:ALA:CA | 1:E:278:LEU:HB3 | 2.50 | 0.41 |
| 1:E:480:LYS:NZ | 1:E:521:GLU:CD | 2.71 | 0.41 |
| 1:E:621:THR:O | 1:E:622:GLU:C | 2.62 | 0.41 |
| 1:E:643:CYS:N | 1:E:649:LYS:NZ | 2.66 | 0.41 |
| 1:E:687:GLU:OE2 | 1:E:728:ALA:O | 2.39 | 0.41 |
| 1:E:696:LEU:HA | 1:E:699:MET:CG | 2.46 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:750:VAL:O | 1:E:751:MET:C | 2.62 | 0.41 |
| 1:E:752:GLY:HA2 | 1:E:755:ARG:CG | 2.50 | 0.41 |
| 1:E:796:GLU:HB3 | 1:E:797:GLN:H | 1.73 | 0.41 |
| 1:E:803:LYS:NZ | 1:E:854:THR:CG2 | 2.84 | 0.41 |
| 1:F:192:GLU:CG | 1:F:338:ILE:HG22 | 2.51 | 0.41 |
| 1:F:583:GLN:HB2 | 1:F:586:ALA:HB2 | 2.03 | 0.41 |
| 1:F:627:VAL:O | 1:F:631:LEU:HG | 2.21 | 0.41 |
| 1:F:687:GLU:HB3 | 1:F:728:ALA:O | 2.19 | 0.41 |
| 1:F:833:GLN:CG | 1:F:834:ASN:N | 2.83 | 0.41 |
| 1:A:190:GLU:C | 1:A:190:GLU:CD | 2.89 | 0.41 |
| 1:A:216:ILE:O | 1:A:219:THR:N | 2.53 | 0.41 |
| 1:A:228:ARG:NH1 | 1:A:233:ASP:CG | 2.79 | 0.41 |
| 1:A:243:LEU:HD12 | 1:A:244:PHE:N | 2.36 | 0.41 |
| 1:A:316:THR:HG23 | 1:A:317:THR:O | 2.21 | 0.41 |
| 1:A:332:GLU:CD | 1:A:334:ARG:NH1 | 2.70 | 0.41 |
| 1:A:351:ILE:HD13 | 1:A:389:PRO:HA | 2.03 | 0.41 |
| 1:A:355:LEU:N | 1:A:360:GLU:OE2 | 2.54 | 0.41 |
| 1:A:366:ARG:C | 1:A:368:LEU:H | 2.28 | 0.41 |
| 1:A:368:LEU:HD23 | 1:A:539:ASN:ND2 | 2.36 | 0.41 |
| 1:A:571:HIS:HD2 | 1:A:574:ARG:CD | 2.32 | 0.41 |
| 1:A:583:GLN:NE2 | 1:A:771:ILE:C | 2.76 | 0.41 |
| 1:A:621:THR:HB | 1:A:684:LEU:HD22 | 2.03 | 0.41 |
| 1:A:675:LEU:CD1 | 1:A:716:ILE:HG13 | 2.51 | 0.41 |
| 1:A:682:VAL:CG1 | 1:A:683:LEU:N | 2.84 | 0.41 |
| 1:A:780:ILE:CA | 1:A:783:ILE:HB | 2.40 | 0.41 |
| 1:B:175:THR:H | 1:B:175:THR:HG23 | 1.53 | 0.41 |
| 1:B:227:GLN:C | 1:B:229:ILE:N | 2.79 | 0.41 |
| 1:B:286:ILE:O | 1:B:287:HIS:C | 2.63 | 0.41 |
| 1:B:312:VAL:C | 1:B:313:ILE:HG13 | 2.46 | 0.41 |
| 1:B:333:ARG:NH1 | 1:B:334:ARG:HG3 | 2.36 | 0.41 |
| 1:B:382:TYR:O | 1:B:383:LEU:C | 2.63 | 0.41 |
| 1:B:393:LEU:HG | 1:B:397:ASP:HB2 | 2.03 | 0.41 |
| 1:B:583:GLN:CG | 1:B:772:PHE:HA | 2.51 | 0.41 |
| 1:B:612:PHE:HD1 | 1:B:770:VAL:HG12 | 1.86 | 0.41 |
| 1:B:637:MET:O | 1:B:639:ILE:HG13 | 2.21 | 0.41 |
| 1:B:654:LYS:HZ1 | 1:B:694:ASP:H | 1.69 | 0.41 |
| 1:B:683:LEU:H | 1:B:723:VAL:CG1 | 2.33 | 0.41 |
| 1:B:685:PHE:CE2 | 1:B:687:GLU:OE2 | 2.73 | 0.41 |
| 1:B:697:THR:O | 1:B:701:GLN:HG3 | 2.21 | 0.41 |
| 1:B:705:ASP:O | 1:B:719:SER:HB3 | 2.21 | 0.41 |
| 1:B:740:SER:OG | 1:B:773:ASN:HB2 | 2.21 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:B:746:THR:HA | 1:B:749:LEU:HB2 | 2.03 | 0.41 |
| 1:B:762:PHE:O | 1:B:765:ARG:N | 2.54 | 0.41 |
| 1:B:786:ILE:O | 1:B:787:ARG:C | 2.64 | 0.41 |
| 1:B:808:GLN:NE2 | 1:B:808:GLN:O | 2.54 | 0.41 |
| 1:C:169:LYS:NZ | 1:C:264:ARG:CD | 2.69 | 0.41 |
| 1:C:170:TYR:HE2 | 1:C:250:ALA:N | 2.05 | 0.41 |
| 1:C:175:THR:HA | 1:C:230:ILE:CD1 | 2.51 | 0.41 |
| 1:C:175:THR:O | 1:C:179:ARG:HB2 | 2.20 | 0.41 |
| 1:C:178:ALA:C | 1:C:181:GLY:H | 2.23 | 0.41 |
| 1:C:189:ARG:NH1 | 1:C:341:ALA:C | 2.79 | 0.41 |
| 1:C:191:GLU:OE2 | 1:C:194:ARG:HB2 | 2.21 | 0.41 |
| 1:C:210:LEU:HB3 | 1:C:338:ILE:H | 1.78 | 0.41 |
| 1:C:228:ARG:NH1 | 1:C:233:ASP:C | 2.79 | 0.41 |
| 1:C:241:ALA:CB | 1:C:280:VAL:HG23 | 2.51 | 0.41 |
| 1:C:262:GLU:HA | 1:C:265:PHE:HB3 | 2.03 | 0.41 |
| 1:C:276:LYS:CB | 1:C:279:ILE:HD12 | 2.48 | 0.41 |
| 1:C:342:GLU:CD | 1:C:388:LEU:HB3 | 2.46 | 0.41 |
| 1:C:368:LEU:HD13 | 1:C:540:VAL:C | 2.46 | 0.41 |
| 1:C:385:TYR:CG | 1:C:386:ARG:N | 2.89 | 0.41 |
| 1:C:402:GLY:O | 1:C:405:VAL:HB | 2.21 | 0.41 |
| 1:C:599:SER:CB | 1:C:602:ALA:H | 2.33 | 0.41 |
| 1:C:634:ASP:HB2 | 1:C:636:ASP:OD1 | 2.20 | 0.41 |
| 1:C:643:CYS:HG | 1:C:686:ASP:HB2 | 1.86 | 0.41 |
| 1:C:685:PHE:O | 1:C:688:VAL:N | 2.45 | 0.41 |
| 1:C:826:ARG:N | 1:C:827:PRO:CD | 2.84 | 0.41 |
| 1:C:839:LYS:NZ | 1:C:881:PRO:CD | 2.84 | 0.41 |
| 1:C:874:GLU:HB3 | 1:C:877:LEU:HD21 | 2.03 | 0.41 |
| 1:D:166:TYR:CE2 | 1:D:169:LYS:O | 2.74 | 0.41 |
| 1:D:166:TYR:CZ | 1:D:169:LYS:HB3 | 2.55 | 0.41 |
| 1:D:172:ILE:H | 1:D:245:SER:C | 2.28 | 0.41 |
| 1:D:213:GLU:OE1 | 1:D:389:PRO:HD2 | 2.21 | 0.41 |
| 1:D:221:ILE:HD11 | 2:D:1001:AGS:H5'2 | 2.03 | 0.41 |
| 1:D:231:ASP:CB | 1:D:495:ARG:HG3 | 2.47 | 0.41 |
| 1:D:337:LYS:HE3 | 1:D:339:GLU:OE2 | 2.20 | 0.41 |
| 1:D:417:LYS:O | 1:D:420:GLN:N | 2.53 | 0.41 |
| 1:D:643:CYS:SG | 1:D:649:LYS:HD3 | 2.61 | 0.41 |
| 1:D:644:SER:CB | 1:D:691:ALA:HA | 2.41 | 0.41 |
| 1:D:654:LYS:HG3 | 1:D:655:LEU:C | 2.46 | 0.41 |
| 1:D:797:GLN:HG3 | 1:D:801:HIS:NE2 | 2.36 | 0.41 |
| 1:D:799:ASP:N | 1:D:799:ASP:OD1 | 2.53 | 0.41 |
| 1:D:808:GLN:HA | 1:D:811:LYS:HD3 | 2.01 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:829:ASN:O | 1:D:830:ARG:C | 2.61 | 0.41 |
| 1:E:174:MET:HG2 | 1:E:178:ALA:HB2 | 2.03 | 0.41 |
| 1:E:184:ASP:OD2 | 1:E:358:LYS:HD3 | 2.20 | 0.41 |
| 1:E:195:SER:O | 1:E:199:VAL:N | 2.38 | 0.41 |
| 1:E:207:ASN:ND2 | 1:E:312:VAL:O | 2.53 | 0.41 |
| 1:E:216:ILE:HD11 | 1:E:389:PRO:CD | 2.51 | 0.41 |
| 1:E:217:GLY:O | 1:E:221:ILE:HG13 | 2.21 | 0.41 |
| 1:E:218:LYS:HA | 1:E:221:ILE:HD12 | 2.03 | 0.41 |
| 1:E:346:ARG:HD2 | 1:E:347:GLN:NE2 | 2.36 | 0.41 |
| 1:E:360:GLU:O | 1:E:362:HIS:N | 2.54 | 0.41 |
| 1:E:418:GLU:CD | 1:E:421:LEU:HD12 | 2.45 | 0.41 |
| 1:E:460:GLU:O | 1:E:464:GLN:NE2 | 2.53 | 0.41 |
| 1:E:462:LEU:CD1 | 1:E:465:ARG:NH1 | 2.82 | 0.41 |
| 1:E:467:ASN:OD1 | 1:E:471:HIS:NE2 | 2.54 | 0.41 |
| 1:E:494:GLU:HA | 1:E:501:THR:HG22 | 2.03 | 0.41 |
| 1:E:496:ARG:O | 1:E:496:ARG:HG3 | 2.21 | 0.41 |
| 1:E:545:THR:O | 1:E:548:GLU:HB2 | 2.21 | 0.41 |
| 1:E:573:GLU:O | 1:E:574:ARG:C | 2.63 | 0.41 |
| 1:E:580:VAL:HG23 | 1:E:581:VAL:N | 2.36 | 0.41 |
| 1:E:607:PRO:CG | 1:E:707:ARG:HH12 | 2.34 | 0.41 |
| 1:E:622:GLU:CA | 1:E:625:LYS:HB2 | 2.49 | 0.41 |
| 1:E:623:LEU:O | 1:E:624:ALA:C | 2.64 | 0.41 |
| 1:E:709:THR:H | 1:E:716:ILE:N | 1.98 | 0.41 |
| 1:E:744:GLU:C | 1:E:747:LYS:NZ | 2.79 | 0.41 |
| 1:E:777:ARG:O | 1:E:778:LYS:C | 2.63 | 0.41 |
| 1:E:777:ARG:HA | 1:E:780:ILE:CG2 | 2.46 | 0.41 |
| 1:E:787:ARG:HE | 1:E:832:ILE:CD1 | 2.34 | 0.41 |
| 1:E:833:GLN:HA | 1:E:836:ILE:CG2 | 2.48 | 0.41 |
| 1:E:839:LYS:HZ2 | 1:E:879:VAL:CA | 2.28 | 0.41 |
| 1:E:876:CYS:SG | 1:E:878:GLU:OE2 | 2.74 | 0.41 |
| 1:F:195:SER:O | 1:F:198:ARG:HB2 | 2.20 | 0.41 |
| 1:F:262:GLU:OE2 | 1:F:299:ASN:HA | 2.20 | 0.41 |
| 1:F:265:PHE:HE2 | 1:F:299:ASN:HD22 | 1.68 | 0.41 |
| 1:F:301:LEU:HG | 1:F:303:PRO:CD | 2.48 | 0.41 |
| 1:F:381:ARG:CZ | 1:F:565:GLU:OE2 | 2.67 | 0.41 |
| 1:F:395:LEU:HD22 | 1:F:545:THR:HG22 | 2.02 | 0.41 |
| 1:F:552:ARG:HG2 | 1:F:553:LEU:CD2 | 2.51 | 0.41 |
| 1:F:591:SER:O | 1:F:595:ARG:CZ | 2.65 | 0.41 |
| 1:F:618:SER:HB2 | 2:F:1002:AGS:C6 | 2.50 | 0.41 |
| 1:F:655:LEU:CA | 1:F:668:GLY:HA3 | 2.46 | 0.41 |
| 1:F:787:ARG:O | 1:F:790:GLU:HB2 | 2.21 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:793:GLU:O | 1:F:794:ARG:C | 2.63 | 0.41 |
| 1:A:344:SER:HB3 | 1:A:347:GLN:NE2 | 2.36 | 0.41 |
| 1:A:609:SER:CB | 1:A:724:ILE:HG13 | 2.43 | 0.41 |
| 1:A:727:SER:C | 1:A:729:LEU:N | 2.79 | 0.41 |
| 1:B:218:LYS:HZ2 | 1:B:218:LYS:HG3 | 1.61 | 0.41 |
| 1:B:221:ILE:C | 1:B:223:GLU:OE1 | 2.64 | 0.41 |
| 1:B:226:ALA:O | 1:B:230:ILE:HG23 | 2.21 | 0.41 |
| 1:B:286:ILE:O | 1:B:289:LEU:N | 2.53 | 0.41 |
| 1:B:342:GLU:CD | 1:B:388:LEU:H | 2.29 | 0.41 |
| 1:B:372:LEU:HA | 1:B:372:LEU:HD23 | 1.82 | 0.41 |
| 1:B:583:GLN:NE2 | 1:B:771:ILE:HG22 | 2.35 | 0.41 |
| 1:B:641:VAL:N | 1:B:684:LEU:HB3 | 2.29 | 0.41 |
| 1:B:645:GLU:HB3 | 1:B:692:HIS:CG | 2.55 | 0.41 |
| 1:B:809:GLU:O | 1:B:810:ALA:C | 2.64 | 0.41 |
| 1:C:170:TYR:OH | 1:C:249:ALA:CA | 2.53 | 0.41 |
| 1:C:351:ILE:O | 1:C:352:LEU:C | 2.62 | 0.41 |
| 1:C:365:VAL:CG1 | 1:C:366:ARG:N | 2.84 | 0.41 |
| 1:C:370:SER:N | 1:C:372:LEU:HG | 2.36 | 0.41 |
| 1:C:394:ASP:O | 1:C:398:ILE:HB | 2.20 | 0.41 |
| 1:C:407:ARG:CZ | 1:C:539:ASN:O | 2.68 | 0.41 |
| 1:C:420:GLN:HE21 | 1:C:455:LEU:CA | 2.34 | 0.41 |
| 1:C:490:ALA:O | 1:C:494:GLU:HG3 | 2.21 | 0.41 |
| 1:C:548:GLU:O | 1:C:549:THR:C | 2.63 | 0.41 |
| 1:C:572:MET:HB3 | 1:C:630:PHE:CD2 | 2.56 | 0.41 |
| 1:C:607:PRO:HB2 | 1:C:722:ILE:CD1 | 2.48 | 0.41 |
| 1:C:675:LEU:HA | 1:C:678:LYS:HB3 | 2.03 | 0.41 |
| 1:C:758:PHE:HB3 | 1:C:762:PHE:HD2 | 1.86 | 0.41 |
| 1:D:166:TYR:CB | 1:D:264:ARG:HE | 2.34 | 0.41 |
| 1:D:179:ARG:HD3 | 1:D:179:ARG:HA | 1.85 | 0.41 |
| 1:D:244:PHE:O | 1:D:282:PHE:HB3 | 2.21 | 0.41 |
| 1:D:317:THR:HG1 | 1:D:321:TYR:H | 1.69 | 0.41 |
| 1:D:349:VAL:O | 1:D:350:ALA:C | 2.62 | 0.41 |
| 1:D:352:LEU:O | 1:D:355:LEU:HG | 2.21 | 0.41 |
| 1:D:473:HIS:HA | 1:D:476:LEU:HB2 | 2.02 | 0.41 |
| 1:D:585:ASP:CA | 1:D:588:LYS:HZ3 | 2.34 | 0.41 |
| 1:D:643:CYS:HA | 1:D:645:GLU:OE1 | 2.21 | 0.41 |
| 1:D:698:VAL:O | 1:D:701:GLN:OE1 | 2.38 | 0.41 |
| 1:D:777:ARG:C | 1:D:780:ILE:HB | 2.45 | 0.41 |
| 1:D:791:ILE:C | 1:D:793:GLU:H | 2.28 | 0.41 |
| 1:D:804:LEU:HD11 | 1:D:880:LEU:HD13 | 2.03 | 0.41 |
| 1:E:228:ARG:HD2 | 1:E:231:ASP:CB | 2.48 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:230:ILE:C | 1:E:232:ASP:N | 2.79 | 0.41 |
| 1:E:351:ILE:O | 1:E:352:LEU:C | 2.64 | 0.41 |
| 1:E:472:GLY:HA2 | 1:E:475:GLU:OE1 | 2.20 | 0.41 |
| 1:E:512:ASP:O | 1:E:512:ASP:OD1 | 2.38 | 0.41 |
| 1:E:542:ASP:OD1 | 1:E:544:ASP:OD2 | 2.38 | 0.41 |
| 1:E:605:ARG:O | 1:E:705:ASP:HA | 2.21 | 0.41 |
| 1:E:616:SER:HA | 2:E:1002:AGS:O1B | 2.20 | 0.41 |
| 1:E:625:LYS:HB3 | 1:E:635:GLU:CD | 2.43 | 0.41 |
| 1:E:692:HIS:CE1 | 1:E:694:ASP:HB2 | 2.55 | 0.41 |
| 1:E:777:ARG:HG3 | 1:E:777:ARG:NH1 | 2.36 | 0.41 |
| 1:F:175:THR:OG1 | 1:F:244:PHE:HZ | 2.03 | 0.41 |
| 1:F:215:GLY:C | 2:F:1001:AGS:O2B | 2.64 | 0.41 |
| 1:F:254:GLY:HA2 | 1:F:264:ARG:HD3 | 2.02 | 0.41 |
| 1:F:287:HIS:NE2 | 1:F:321:TYR:HD2 | 2.19 | 0.41 |
| 1:F:542:ASP:HB3 | 1:F:544:ASP:CG | 2.46 | 0.41 |
| 1:F:566:ASN:O | 1:F:570:ILE:HG12 | 2.21 | 0.41 |
| 1:F:786:ILE:HG22 | 1:F:790:GLU:OE2 | 2.21 | 0.41 |
| 1:F:807:THR:HB | 1:F:856:ASN:OD1 | 2.21 | 0.41 |
| 1:F:832:ILE:HG23 | 1:F:835:GLU:OE2 | 2.21 | 0.41 |
| 1:A:173:ASP:CG | 1:A:175:THR:H | 2.26 | 0.40 |
| 1:A:286:ILE:HD11 | 1:A:321:TYR:HD2 | 1.84 | 0.40 |
| 1:A:611:LEU:HB2 | 1:A:724:ILE:CG2 | 2.50 | 0.40 |
| 1:A:674:GLN:O | 1:A:677:TYR:HB2 | 2.21 | 0.40 |
| 1:A:822:ASP:CB | 1:F:333:ARG:HH11 | 2.34 | 0.40 |
| 1:B:218:LYS:HZ1 | 1:B:219:THR:CG2 | 2.34 | 0.40 |
| 1:B:321:TYR:O | 1:B:322:ARG:C | 2.64 | 0.40 |
| 1:B:607:PRO:HA | 1:B:722:ILE:CD1 | 2.51 | 0.40 |
| 1:B:625:LYS:O | 1:B:626:LYS:C | 2.64 | 0.40 |
| 1:B:738:GLN:N | 1:B:774:LYS:NZ | 2.69 | 0.40 |
| 1:B:762:PHE:O | 1:B:765:ARG:HB2 | 2.21 | 0.40 |
| 1:B:764:ASN:HD22 | 1:B:765:ARG:HH12 | 1.69 | 0.40 |
| 1:B:793:GLU:C | 1:B:798:ASN:HD21 | 2.28 | 0.40 |
| 1:B:799:ASP:OD1 | 1:B:799:ASP:N | 2.52 | 0.40 |
| 1:B:835:GLU:O | 1:B:838:ASN:HB2 | 2.21 | 0.40 |
| 1:C:14:ILE:N | 1:C:159:ASP:CA | 2.82 | 0.40 |
| 1:C:173:ASP:CG | 1:C:177:GLN:N | 2.77 | 0.40 |
| 1:C:208:PRO:CD | 1:C:313:ILE:HA | 2.50 | 0.40 |
| 1:C:226:ALA:O | 1:C:227:GLN:C | 2.63 | 0.40 |
| 1:C:355:LEU:C | 1:C:357:PRO:HD2 | 2.46 | 0.40 |
| 1:C:356:GLN:CG | 1:C:357:PRO:CD | 3.00 | 0.40 |
| 1:C:631:LEU:HD12 | 1:C:631:LEU:N | 2.36 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:658:THR:HB | 1:C:664:GLY:O | 2.21 | 0.40 |
| 1:C:699:MET:CG | 1:C:700:LEU:N | 2.84 | 0.40 |
| 1:C:731:ALA:HB1 | 1:C:734:ILE:HG22 | 2.03 | 0.40 |
| 1:C:780:ILE:HA | 1:C:784:VAL:HG13 | 2.02 | 0.40 |
| 1:C:790:GLU:CG | 1:C:794:ARG:HE | 2.34 | 0.40 |
| 1:C:796:GLU:CD | 1:C:797:GLN:N | 2.79 | 0.40 |
| 1:D:172:ILE:N | 1:D:245:SER:O | 2.54 | 0.40 |
| 1:D:203:ARG:CZ | 1:E:363:HIS:CE1 | 3.04 | 0.40 |
| 1:D:207:ASN:HD21 | 1:D:311:LYS:CA | 2.34 | 0.40 |
| 1:D:509:ALA:HA | 1:D:512:ASP:OD2 | 2.21 | 0.40 |
| 1:D:642:ASP:C | 1:D:644:SER:N | 2.79 | 0.40 |
| 1:D:744:GLU:N | 1:D:747:LYS:NZ | 2.68 | 0.40 |
| 1:D:789:LYS:O | 1:D:790:GLU:C | 2.65 | 0.40 |
| 1:E:277:THR:O | 1:E:279:ILE:N | 2.54 | 0.40 |
| 1:E:321:TYR:HA | 1:E:324:ILE:HB | 2.03 | 0.40 |
| 1:E:373:VAL:O | 1:E:374:THR:C | 2.65 | 0.40 |
| 1:E:378:LEU:O | 1:E:379:ALA:C | 2.60 | 0.40 |
| 1:E:384:PRO:HB3 | 1:E:680:TYR:HE1 | 1.87 | 0.40 |
| 1:E:644:SER:HB3 | 1:E:690:LYS:HE3 | 2.02 | 0.40 |
| 1:E:787:ARG:CZ | 1:E:829:ASN:HB3 | 2.50 | 0.40 |
| 1:E:788:LEU:O | 1:E:789:LYS:C | 2.64 | 0.40 |
| 1:E:807:THR:CA | 1:E:811:LYS:HZ3 | 2.28 | 0.40 |
| 1:F:248:LEU:HB3 | 1:F:249:ALA:H | 1.57 | 0.40 |
| 1:F:287:HIS:NE2 | 1:F:321:TYR:CD2 | 2.89 | 0.40 |
| 1:F:592:ASN:HA | 1:F:595:ARG:NH1 | 2.36 | 0.40 |
| 1:F:733:PHE:CG | 1:F:750:VAL:HG21 | 2.56 | 0.40 |
| 1:F:742:ILE:CG2 | 1:F:747:LYS:NZ | 2.73 | 0.40 |
| 1:A:348:THR:O | 1:A:351:ILE:N | 2.52 | 0.40 |
| 1:A:625:LYS:HB3 | 1:A:635:GLU:CD | 2.46 | 0.40 |
| 1:A:692:HIS:HB3 | 1:A:694:ASP:HB2 | 2.02 | 0.40 |
| 1:A:693:PRO:HA | 1:A:696:LEU:HD11 | 2.03 | 0.40 |
| 1:A:693:PRO:CA | 1:A:696:LEU:HD11 | 2.52 | 0.40 |
| 1:A:709:THR:HG22 | 1:A:713:GLY:HA2 | 2.02 | 0.40 |
| 1:A:784:VAL:HG13 | 1:A:785:ASP:N | 2.36 | 0.40 |
| 1:A:787:ARG:HE | 1:A:790:GLU:CD | 2.21 | 0.40 |
| 1:B:193:ILE:HG13 | 1:B:194:ARG:H | 1.87 | 0.40 |
| 1:B:193:ILE:HD12 | 1:B:197:ILE:HG13 | 2.03 | 0.40 |
| 1:B:204:ILE:O | 1:B:206:SER:N | 2.54 | 0.40 |
| 1:B:212:GLY:O | 1:B:317:THR:HA | 2.21 | 0.40 |
| 1:B:301:LEU:HD12 | 1:B:301:LEU:C | 2.46 | 0.40 |
| 1:B:391:SER:O | 1:B:394:ASP:N | 2.53 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:392:ALA:HA | 1:B:395:LEU:HD12 | 2.04 | 0.40 |
| 1:B:587:ILE:CA | 1:B:590:VAL:HB | 2.43 | 0.40 |
| 1:B:598:ARG:O | 1:B:599:SER:C | 2.64 | 0.40 |
| 1:B:609:SER:OG | 1:B:765:ARG:O | 2.28 | 0.40 |
| 1:B:675:LEU:CB | 1:B:717:ASP:OD2 | 2.68 | 0.40 |
| 1:B:736:SER:CB | 1:B:738:GLN:H | 2.33 | 0.40 |
| 1:B:740:SER:HB3 | 1:B:773:ASN:HB2 | 2.02 | 0.40 |
| 1:B:766:ILE:N | 1:C:830:ARG:HH22 | 2.18 | 0.40 |
| 1:B:858:VAL:HG12 | 1:B:859:LEU:O | 2.22 | 0.40 |
| 1:C:189:ARG:CB | 1:C:193:ILE:HG13 | 2.51 | 0.40 |
| 1:C:201:ALA:O | 1:C:206:SER:OG | 2.33 | 0.40 |
| 1:C:208:PRO:O | 1:C:210:LEU:N | 2.55 | 0.40 |
| 1:C:210:LEU:HD22 | 1:C:338:ILE:N | 2.36 | 0.40 |
| 1:C:241:ALA:HA | 1:C:279:ILE:HA | 2.04 | 0.40 |
| 1:C:243:LEU:HD23 | 1:C:282:PHE:O | 2.21 | 0.40 |
| 1:C:302:LYS:HZ2 | 1:C:306:SER:CA | 2.26 | 0.40 |
| 1:C:355:LEU:HB3 | 1:C:358:LYS:HE3 | 2.03 | 0.40 |
| 1:C:383:LEU:HD23 | 1:C:383:LEU:HA | 1.62 | 0.40 |
| 1:C:405:VAL:O | 1:C:406:ALA:C | 2.64 | 0.40 |
| 1:C:458:GLU:CA | 1:C:461:PRO:HD2 | 2.50 | 0.40 |
| 1:C:557:PRO:HA | 1:C:560:LYS:HB2 | 2.02 | 0.40 |
| 1:C:567:GLU:O | 1:C:570:ILE:HB | 2.21 | 0.40 |
| 1:C:610:PHE:CB | 1:C:768:SER:HB3 | 2.51 | 0.40 |
| 1:C:679:PRO:O | 1:C:721:CYS:HB2 | 2.20 | 0.40 |
| 1:C:747:LYS:C | 1:C:750:VAL:HB | 2.47 | 0.40 |
| 1:C:747:LYS:HA | 1:C:750:VAL:HG21 | 2.03 | 0.40 |
| 1:C:786:ILE:HA | 1:C:789:LYS:HD2 | 2.02 | 0.40 |
| 1:D:164:LEU:C | 1:D:165:GLU:HG2 | 2.46 | 0.40 |
| 1:D:177:GLN:CA | 1:D:180:GLN:HB2 | 2.48 | 0.40 |
| 1:D:218:LYS:HD3 | 1:D:221:ILE:HD13 | 2.02 | 0.40 |
| 1:D:243:LEU:HD11 | 1:D:313:ILE:HG12 | 2.01 | 0.40 |
| 1:D:317:THR:OG1 | 1:D:321:TYR:N | 2.54 | 0.40 |
| 1:D:395:LEU:O | 1:D:396:VAL:C | 2.64 | 0.40 |
| 1:D:464:GLN:HB3 | 1:D:468:GLU:HB3 | 2.03 | 0.40 |
| 1:D:490:ALA:C | 1:D:492:ASP:H | 2.29 | 0.40 |
| 1:D:543:SER:C | 1:D:546:ILE:HB | 2.46 | 0.40 |
| 1:D:564:SER:O | 1:D:565:GLU:C | 2.64 | 0.40 |
| 1:D:620:LYS:HG3 | 1:D:621:THR:HG23 | 2.03 | 0.40 |
| 1:D:633:ASN:O | 1:D:634:ASP:C | 2.65 | 0.40 |
| 1:D:639:ILE:N | 1:D:640:ARG:NH1 | 2.69 | 0.40 |
| 1:D:699:MET:HE3 | 1:D:762:PHE:CZ | 2.56 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:733:PHE:O | 1:D:736:SER:N | 2.32 | 0.40 |
| 1:D:830:ARG:HA | 1:D:833:GLN:CG | 2.49 | 0.40 |
| 1:E:173:ASP:C | 1:E:175:THR:N | 2.71 | 0.40 |
| 1:E:214:PRO:HD2 | 1:E:387:ARG:HD2 | 2.02 | 0.40 |
| 1:E:392:ALA:HA | 1:E:395:LEU:HD12 | 2.02 | 0.40 |
| 1:E:596:LEU:HD23 | 1:F:841:ALA:HB2 | 2.02 | 0.40 |
| 1:E:646:LEU:C | 1:E:649:LYS:HB2 | 2.46 | 0.40 |
| 1:E:730:GLY:HA3 | 1:E:734:ILE:HG12 | 2.03 | 0.40 |
| 1:E:785:ASP:O | 1:E:786:ILE:C | 2.65 | 0.40 |
| 1:F:238:LEU:HD22 | 1:F:278:LEU:HB3 | 2.02 | 0.40 |
| 1:F:564:SER:HB3 | 1:F:568:LYS:HD2 | 2.03 | 0.40 |
| 1:F:583:GLN:HB2 | 1:F:586:ALA:CB | 2.51 | 0.40 |
| 1:F:673:ASN:O | 1:F:676:GLN:N | 2.53 | 0.40 |
| 1:A:278:LEU:CD1 | 1:A:309:GLN:HA | 2.51 | 0.40 |
| 1:A:620:LYS:O | 1:A:621:THR:C | 2.64 | 0.40 |
| 1:A:625:LYS:HG2 | 1:A:638:MET:SD | 2.62 | 0.40 |
| 1:A:705:ASP:OD2 | 1:A:707:ARG:CZ | 2.66 | 0.40 |
| 1:B:247:ASP:N | 1:B:283:ILE:HG12 | 2.36 | 0.40 |
| 1:B:260:ASP:HA | 1:B:263:GLU:HB3 | 2.03 | 0.40 |
| 1:B:321:TYR:CD2 | 1:B:322:ARG:N | 2.90 | 0.40 |
| 1:B:565:GLU:O | 1:B:569:LEU:HG | 2.22 | 0.40 |
| 1:B:573:GLU:CD | 1:B:595:ARG:CZ | 2.95 | 0.40 |
| 1:B:583:GLN:HG2 | 1:B:773:ASN:OD1 | 2.21 | 0.40 |
| 1:B:608:ALA:HB1 | 1:B:610:PHE:CE1 | 2.56 | 0.40 |
| 1:B:611:LEU:HD12 | 1:B:611:LEU:C | 2.47 | 0.40 |
| 1:B:630:PHE:CD1 | 1:B:630:PHE:N | 2.89 | 0.40 |
| 1:B:685:PHE:HE2 | 1:B:687:GLU:CD | 2.29 | 0.40 |
| 1:B:813:PHE:O | 1:B:816:LYS:HB2 | 2.22 | 0.40 |
| 1:B:839:LYS:NZ | 1:B:877:LEU:CD2 | 2.82 | 0.40 |
| 1:B:842:LEU:C | 1:B:846:LYS:HG3 | 2.46 | 0.40 |
| 1:C:251:LEU:HD12 | 1:C:252:THR:N | 2.31 | 0.40 |
| 1:C:407:ARG:HH11 | 1:C:539:ASN:C | 2.21 | 0.40 |
| 1:C:490:ALA:O | 1:C:493:ALA:N | 2.54 | 0.40 |
| 1:C:599:SER:O | 1:C:601:LEU:N | 2.50 | 0.40 |
| 1:C:731:ALA:CA | 1:C:734:ILE:HG22 | 2.51 | 0.40 |
| 1:C:809:GLU:O | 1:C:812:ASP:HB2 | 2.21 | 0.40 |
| 1:C:813:PHE:HZ | 1:C:877:LEU:HD23 | 1.86 | 0.40 |
| 1:D:241:ALA:HA | 1:D:278:LEU:HA | 2.03 | 0.40 |
| 1:D:351:ILE:HG12 | 2:D:1001:AGS:N1 | 2.37 | 0.40 |
| 1:D:355:LEU:HD12 | 1:D:356:GLN:CA | 2.51 | 0.40 |
| 1:D:475:GLU:O | 1:D:476:LEU:C | 2.63 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:536:MET:H | 1:D:538:GLN:H | 1.69 | 0.40 |
| 1:D:634:ASP:HB3 | 1:D:637:MET:HE2 | 2.04 | 0.40 |
| 1:D:672:THR:O | 1:D:676:GLN:HG3 | 2.22 | 0.40 |
| 1:D:683:LEU:N | 1:D:722:ILE:O | 2.54 | 0.40 |
| 1:E:173:ASP:C | 1:E:176:GLU:OE2 | 2.64 | 0.40 |
| 1:E:202:ARG:HH11 | 1:E:336:GLN:NE2 | 2.17 | 0.40 |
| 1:E:204:ILE:HG22 | 1:E:205:LYS:HG3 | 2.03 | 0.40 |
| 1:E:277:THR:HG1 | 1:E:278:LEU:H | 1.69 | 0.40 |
| 1:E:282:PHE:CD2 | 1:E:282:PHE:C | 2.95 | 0.40 |
| 1:E:676:GLN:NE2 | 1:E:677:TYR:HB2 | 2.36 | 0.40 |
| 1:E:784:VAL:O | 1:E:785:ASP:C | 2.65 | 0.40 |
| 1:F:215:GLY:CA | 2:F:1001:AGS:O1B | 2.66 | 0.40 |
| 1:F:273:GLU:HG3 | 1:F:274:GLU:N | 2.27 | 0.40 |
| 1:F:287:HIS:CE1 | 1:F:322:ARG:HD2 | 2.56 | 0.40 |
| 1:F:306:SER:HA | 1:F:310:LEU:O | 2.21 | 0.40 |
| 1:F:552:ARG:HH11 | 1:F:552:ARG:CB | 2.34 | 0.40 |
| 1:F:584:MET:O | 1:F:587:ILE:HB | 2.21 | 0.40 |
| 1:F:819:TYR:OH | 1:F:828:LEU:HB2 | 2.22 | 0.40 |
| 1:F:827:PRO:C | 1:F:831:LEU:HG | 2.46 | 0.40 |
| 1:F:841:ALA:C | 1:F:845:LEU:HG | 2.46 | 0.40 |
| 1:A:175:THR:OG1 | 1:A:243:LEU:HG | 2.21 | 0.40 |
| 1:A:547:SER:O | 1:A:550:ALA:HB3 | 2.21 | 0.40 |
| 1:A:563:GLU:CD | 1:A:568:LYS:HB2 | 2.45 | 0.40 |
| 1:A:629:GLY:H | 1:A:635:GLU:HG2 | 1.87 | 0.40 |
| 1:A:678:LYS:O | 1:A:681:SER:OG | 2.25 | 0.40 |
| 1:A:814:LEU:O | 1:A:817:TYR:HB2 | 2.21 | 0.40 |
| 1:B:166:TYR:HA | 1:B:169:LYS:HZ3 | 1.86 | 0.40 |
| 1:B:166:TYR:C | 1:B:169:LYS:H | 2.29 | 0.40 |
| 1:B:195:SER:O | 1:B:198:ARG:N | 2.50 | 0.40 |
| 1:B:247:ASP:CG | 1:B:288:MET:HG2 | 2.47 | 0.40 |
| 1:B:281:LEU:HA | 1:B:313:ILE:HD12 | 2.04 | 0.40 |
| 1:B:285:GLU:O | 1:B:288:MET:HB3 | 2.21 | 0.40 |
| 1:B:285:GLU:CD | 1:B:287:HIS:N | 2.80 | 0.40 |
| 1:B:353:ARG:NH1 | 1:B:369:ASP:O | 2.55 | 0.40 |
| 1:B:388:LEU:HB3 | 1:B:389:PRO:HD3 | 2.03 | 0.40 |
| 1:B:758:PHE:CB | 1:B:763:LEU:HD21 | 2.49 | 0.40 |
| 1:B:759:ARG:C | 1:B:763:LEU:HG | 2.46 | 0.40 |
| 1:B:790:GLU:C | 1:B:793:GLU:HG2 | 2.47 | 0.40 |
| 1:B:842:LEU:O | 1:B:846:LYS:HG3 | 2.21 | 0.40 |
| 1:C:302:LYS:N | 1:C:303:PRO:HD2 | 2.37 | 0.40 |
| 1:C:363:HIS:CG | 1:C:400:CYS:HB3 | 2.56 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:419:ARG:HG3 | 1:C:423:LEU:CD1 | 2.52 | 0.40 |
| 1:C:476:LEU:O | 1:C:480:LYS:HG3 | 2.21 | 0.40 |
| 1:C:611:LEU:HB2 | 1:C:612:PHE:O | 2.22 | 0.40 |
| 1:C:619:GLY:CA | 1:C:622:GLU:HG2 | 2.50 | 0.40 |
| 1:C:652:VAL:O | 1:C:655:LEU:O | 2.40 | 0.40 |
| 1:C:659:THR:HG23 | 1:C:712:GLN:OE1 | 2.22 | 0.40 |
| 1:C:792:GLU:O | 1:C:802:TYR:CE1 | 2.75 | 0.40 |
| 1:D:229:ILE:O | 1:D:232:ASP:HA | 2.21 | 0.40 |
| 1:D:252:THR:HA | 1:D:261:PHE:CE1 | 2.56 | 0.40 |
| 1:D:276:LYS:HB3 | 1:D:279:ILE:HD12 | 2.03 | 0.40 |
| 1:D:457:GLU:O | 1:D:460:GLU:N | 2.46 | 0.40 |
| 1:D:473:HIS:O | 1:D:476:LEU:HB2 | 2.22 | 0.40 |
| 1:D:524:VAL:HG13 | 1:D:532:GLY:C | 2.47 | 0.40 |
| 1:D:686:ASP:CG | 1:D:687:GLU:N | 2.79 | 0.40 |
| 1:D:692:HIS:HA | 1:D:693:PRO:HD3 | 1.96 | 0.40 |
| 1:D:696:LEU:HA | 1:D:696:LEU:HD23 | 1.75 | 0.40 |
| 1:D:751:MET:HG3 | 1:D:769:ILE:HD11 | 2.04 | 0.40 |
| 1:D:759:ARG:HE | 1:D:763:LEU:HD11 | 1.86 | 0.40 |
| 1:D:779:ALA:CA | 1:D:782:LYS:NZ | 2.83 | 0.40 |
| 1:E:383:LEU:HD22 | 1:E:386:ARG:CG | 2.52 | 0.40 |
| 1:E:471:HIS:O | 1:E:474:GLU:N | 2.53 | 0.40 |
| 1:E:492:ASP:O | 1:E:495:ARG:N | 2.53 | 0.40 |
| 1:E:597:SER:C | 1:E:599:SER:N | 2.80 | 0.40 |
| 1:E:611:LEU:HD13 | 1:E:725:MET:HG3 | 2.03 | 0.40 |
| 1:E:649:LYS:HG2 | 1:E:650:TYR:H | 1.86 | 0.40 |
| 1:E:700:LEU:O | 1:E:701:GLN:C | 2.64 | 0.40 |
| 1:E:723:VAL:HG22 | 1:E:724:ILE:O | 2.20 | 0.40 |
| 1:E:783:ILE:O | 1:E:786:ILE:HD12 | 2.22 | 0.40 |
| 1:E:856:ASN:O | 1:E:878:GLU:C | 2.65 | 0.40 |
| 1:F:166:TYR:CG | 1:F:264:ARG:NH1 | 2.89 | 0.40 |
| 1:F:654:LYS:HG2 | 1:F:692:HIS:CD2 | 2.57 | 0.40 |
| 1:F:818:GLY:HA3 | 1:F:828:LEU:CG | 2.51 | 0.40 |
| 1:A:177:GLN:C | 1:A:182:LYS:NZ | 2.79 | 0.40 |
| 1:A:357:PRO:CA | 1:A:360:GLU:HB3 | 2.46 | 0.40 |
| 1:A:564:SER:HB2 | 1:A:567:GLU:CD | 2.46 | 0.40 |
| 1:A:580:VAL:CG1 | 1:A:581:VAL:N | 2.84 | 0.40 |
| 1:A:657:GLY:HA3 | 1:A:668:GLY:CA | 2.52 | 0.40 |
| 1:A:822:ASP:CG | 1:F:333:ARG:HH11 | 2.26 | 0.40 |
| 1:B:169:LYS:NZ | 1:B:170:TYR:HE2 | 2.20 | 0.40 |
| 1:B:207:ASN:O | 1:B:336:GLN:O | 2.39 | 0.40 |
| 1:B:305:LEU:H | 1:B:305:LEU:HG | 1.66 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:320:GLU:O | 1:B:323:SER:HB2 | 2.22 | 0.40 |
| 1:B:346:ARG:N | 1:B:347:GLN:OE1 | 2.55 | 0.40 |
| 1:B:393:LEU:O | 1:B:394:ASP:C | 2.63 | 0.40 |
| 1:B:615:LEU:HB2 | 1:B:772:PHE:CE2 | 2.57 | 0.40 |
| 1:B:634:ASP:CG | 1:B:635:GLU:H | 2.28 | 0.40 |
| 1:B:654:LYS:NZ | 1:B:694:ASP:CB | 2.81 | 0.40 |
| 1:B:673:ASN:CA | 1:B:676:GLN:HB3 | 2.51 | 0.40 |
| 1:B:695:VAL:O | 1:B:696:LEU:C | 2.63 | 0.40 |
| 1:B:786:ILE:O | 1:B:788:LEU:N | 2.55 | 0.40 |
| 1:B:788:LEU:HB2 | 1:B:789:LYS:H | 1.72 | 0.40 |
| 1:B:789:LYS:CG | 1:B:790:GLU:N | 2.84 | 0.40 |
| 1:B:801:HIS:ND1 | 1:B:851:ASP:CG | 2.77 | 0.40 |
| 1:C:211:ILE:HG21 | 1:C:315:ALA:CA | 2.44 | 0.40 |
| 1:C:286:ILE:HA | 1:C:289:LEU:CG | 2.51 | 0.40 |
| 1:C:373:VAL:HA | 1:C:376:ALA:HB3 | 2.02 | 0.40 |
| 1:C:421:LEU:HD13 | 1:C:456:GLN:HG2 | 2.03 | 0.40 |
| 1:C:466:TYR:HE1 | 1:C:530:ARG:NH2 | 2.19 | 0.40 |
| 1:C:467:ASN:O | 1:C:471:HIS:CD2 | 2.75 | 0.40 |
| 1:C:496:ARG:O | 1:C:497:TYR:HB3 | 2.22 | 0.40 |
| 1:C:573:GLU:HA | 1:C:576:LEU:HD12 | 2.03 | 0.40 |
| 1:C:573:GLU:O | 1:C:574:ARG:C | 2.64 | 0.40 |
| 1:C:618:SER:C | 1:C:620:LYS:N | 2.79 | 0.40 |
| 1:C:628:ALA:C | 1:C:631:LEU:N | 2.79 | 0.40 |
| 1:C:707:ARG:C | 1:C:708:ILE:HG13 | 2.46 | 0.40 |
| 1:C:765:ARG:HA | 1:C:765:ARG:HD3 | 1.81 | 0.40 |
| 1:C:793:GLU:O | 1:C:802:TYR:CE2 | 2.74 | 0.40 |
| 1:C:853:GLU:OE1 | 1:C:853:GLU:N | 2.55 | 0.40 |
| 1:D:197:ILE:O | 1:D:198:ARG:C | 2.63 | 0.40 |
| 1:D:202:ARG:CZ | 1:D:205:LYS:O | 2.70 | 0.40 |
| 1:D:276:LYS:CB | 1:D:279:ILE:HD12 | 2.51 | 0.40 |
| 1:D:330:ALA:HA | 1:D:333:ARG:CD | 2.51 | 0.40 |
| 1:D:338:ILE:CG2 | 1:D:339:GLU:N | 2.83 | 0.40 |
| 1:D:559:LYS:O | 1:D:562:SER:HB2 | 2.21 | 0.40 |
| 1:D:575:ASP:O | 1:D:578:SER:OG | 2.29 | 0.40 |
| 1:D:587:ILE:O | 1:D:590:VAL:N | 2.55 | 0.40 |
| 1:D:651:ALA:HA | 1:D:654:LYS:HG2 | 2.04 | 0.40 |
| 1:D:682:VAL:HG22 | 1:D:722:ILE:CB | 2.35 | 0.40 |
| 1:D:693:PRO:O | 1:D:696:LEU:N | 2.55 | 0.40 |
| 1:D:793:GLU:C | 1:D:795:PHE:H | 2.30 | 0.40 |
| 1:D:802:TYR:HE2 | 1:D:804:LEU:CB | 2.24 | 0.40 |
| 1:D:805:ASN:HA | 1:D:856:ASN:CB | 2.51 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:805:ASN:HD21 | 1:D:880:LEU:HD11 | 1.87 | 0.40 |
| 1:E:174:MET:HG2 | 1:E:178:ALA:N | 2.37 | 0.40 |
| 1:E:218:LYS:HB2 | 2:E:1001:AGS:O3B | 2.21 | 0.40 |
| 1:E:405:VAL:C | 1:E:408:ASP:H | 2.29 | 0.40 |
| 1:E:471:HIS:HA | 1:E:474:GLU:OE1 | 2.22 | 0.40 |
| 1:E:522:ASP:OD1 | 1:E:526:GLU:OE2 | 2.39 | 0.40 |
| 1:E:570:ILE:HG22 | 1:F:845:LEU:HD22 | 2.02 | 0.40 |
| 1:E:571:HIS:HD2 | 1:E:574:ARG:CD | 2.33 | 0.40 |
| 1:E:582:GLY:O | 1:E:583:GLN:C | 2.64 | 0.40 |
| 1:E:591:SER:O | 1:E:592:ASN:C | 2.63 | 0.40 |
| 1:E:609:SER:HA | 1:E:724:ILE:HA | 2.03 | 0.40 |
| 1:E:624:ALA:O | 1:E:628:ALA:N | 2.41 | 0.40 |
| 1:E:784:VAL:HG11 | 1:E:815:ALA:CB | 2.49 | 0.40 |
| 1:E:845:LEU:HD12 | 1:E:846:LYS:HB3 | 2.04 | 0.40 |
| 1:F:189:ARG:HH22 | 1:F:343:PRO:HA | 1.86 | 0.40 |
| 1:F:199:VAL:HG11 | 1:F:207:ASN:OD1 | 2.20 | 0.40 |
| 1:F:356:GLN:O | 1:F:360:GLU:HB3 | 2.21 | 0.40 |
| 1:F:392:ALA:HA | 1:F:395:LEU:HD12 | 2.03 | 0.40 |
| 1:F:812:ASP:C | 1:F:816:LYS:HG3 | 2.47 | 0.40 |

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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 | 571/908 (63%) | 408 (72%) | 141 (25%) | 22 (4%) | 2 | 19 |
| 1 | B | 731/908 (80%) | 492 (67%) | 204 (28%) | 35 (5%) | 2 | 16 |
| 1 | C | 861/908 (95%) | 591 (69%) | 220 (26%) | 50 (6%) | 1 | 14 |
| 1 | D | 861/908 (95%) | 584 (68%) | 246 (29%) | 31 (4%) | 3 | 20 |
| 1 | E | 701/908 (77%) | 496 (71%) | 170 (24%) | 35 (5%) | 1 | 16 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-----------------|------------|------------|----------|-------------|----|
| 1 | F | 568/908 (63%) | 426 (75%) | 112 (20%) | 30 (5%) | 1 | 15 |
| All | All | 4293/5448 (79%) | 2997 (70%) | 1093 (26%) | 203 (5%) | 3 | 17 |

All (203) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 367 | ILE |
| 1 | B | 137 | ILE |
| 1 | C | 159 | ASP |
| 1 | C | 161 | ASN |
| 1 | C | 163 | PRO |
| 1 | C | 169 | LYS |
| 1 | C | 209 | CYS |
| 1 | C | 537 | ILE |
| 1 | C | 688 | VAL |
| 1 | D | 317 | THR |
| 1 | D | 643 | CYS |
| 1 | E | 174 | MET |
| 1 | F | 319 | ASN |
| 1 | F | 356 | GLN |
| 1 | F | 703 | LEU |
| 1 | F | 714 | LYS |
| 1 | F | 716 | ILE |
| 1 | F | 849 | ILE |
| 1 | A | 201 | ALA |
| 1 | B | 47 | SER |
| 1 | C | 211 | ILE |
| 1 | C | 627 | VAL |
| 1 | C | 754 | VAL |
| 1 | D | 111 | ILE |
| 1 | D | 126 | ILE |
| 1 | D | 135 | VAL |
| 1 | D | 211 | ILE |
| 1 | D | 558 | VAL |
| 1 | D | 703 | LEU |
| 1 | D | 742 | ILE |
| 1 | D | 784 | VAL |
| 1 | D | 879 | VAL |
| 1 | E | 175 | THR |
| 1 | E | 216 | ILE |
| 1 | E | 688 | VAL |
| 1 | E | 879 | VAL |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | F | 357 | PRO |
| 1 | F | 879 | VAL |
| 1 | A | 204 | ILE |
| 1 | A | 227 | GLN |
| 1 | A | 357 | PRO |
| 1 | A | 697 | THR |
| 1 | A | 794 | ARG |
| 1 | B | 208 | PRO |
| 1 | B | 292 | ASN |
| 1 | B | 667 | GLU |
| 1 | B | 676 | GLN |
| 1 | B | 754 | VAL |
| 1 | B | 788 | LEU |
| 1 | B | 799 | ASP |
| 1 | C | 40 | ILE |
| 1 | C | 140 | ILE |
| 1 | C | 792 | GLU |
| 1 | D | 77 | PRO |
| 1 | D | 86 | ILE |
| 1 | D | 170 | TYR |
| 1 | D | 797 | GLN |
| 1 | E | 583 | GLN |
| 1 | E | 649 | LYS |
| 1 | E | 725 | MET |
| 1 | E | 809 | GLU |
| 1 | F | 365 | VAL |
| 1 | F | 564 | SER |
| 1 | F | 670 | PHE |
| 1 | F | 715 | THR |
| 1 | A | 352 | LEU |
| 1 | A | 355 | LEU |
| 1 | A | 647 | SER |
| 1 | A | 675 | LEU |
| 1 | A | 790 | GLU |
| 1 | B | 40 | ILE |
| 1 | B | 220 | ALA |
| 1 | B | 286 | ILE |
| 1 | B | 316 | THR |
| 1 | B | 318 | ASN |
| 1 | B | 345 | VAL |
| 1 | B | 632 | PHE |
| 1 | B | 742 | ILE |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | B | 876 | CYS |
| 1 | C | 52 | GLN |
| 1 | C | 204 | ILE |
| 1 | C | 394 | ASP |
| 1 | C | 777 | ARG |
| 1 | C | 814 | LEU |
| 1 | C | 875 | GLU |
| 1 | D | 204 | ILE |
| 1 | D | 345 | VAL |
| 1 | D | 527 | GLU |
| 1 | D | 566 | ASN |
| 1 | D | 597 | SER |
| 1 | D | 755 | ARG |
| 1 | D | 781 | HIS |
| 1 | E | 252 | THR |
| 1 | E | 331 | PHE |
| 1 | E | 362 | HIS |
| 1 | E | 501 | THR |
| 1 | E | 656 | LEU |
| 1 | E | 700 | LEU |
| 1 | E | 724 | ILE |
| 1 | F | 701 | GLN |
| 1 | A | 231 | ASP |
| 1 | A | 265 | PHE |
| 1 | A | 799 | ASP |
| 1 | A | 849 | ILE |
| 1 | B | 86 | ILE |
| 1 | B | 221 | ILE |
| 1 | B | 321 | TYR |
| 1 | B | 756 | GLN |
| 1 | B | 784 | VAL |
| 1 | B | 786 | ILE |
| 1 | C | 135 | VAL |
| 1 | C | 153 | ILE |
| 1 | C | 154 | ASP |
| 1 | C | 175 | THR |
| 1 | C | 219 | THR |
| 1 | C | 227 | GLN |
| 1 | C | 261 | PHE |
| 1 | C | 756 | GLN |
| 1 | C | 797 | GLN |
| 1 | C | 810 | ALA |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | C | 812 | ASP |
| 1 | C | 816 | LYS |
| 1 | D | 399 | SER |
| 1 | D | 749 | LEU |
| 1 | E | 297 | ALA |
| 1 | E | 330 | ALA |
| 1 | E | 346 | ARG |
| 1 | E | 397 | ASP |
| 1 | E | 404 | ALA |
| 1 | E | 697 | THR |
| 1 | E | 779 | ALA |
| 1 | E | 853 | GLU |
| 1 | F | 822 | ASP |
| 1 | F | 878 | GLU |
| 1 | B | 84 | ALA |
| 1 | B | 175 | THR |
| 1 | B | 269 | LEU |
| 1 | B | 395 | LEU |
| 1 | B | 546 | ILE |
| 1 | B | 745 | SER |
| 1 | C | 13 | THR |
| 1 | C | 42 | THR |
| 1 | C | 125 | SER |
| 1 | C | 190 | GLU |
| 1 | C | 283 | ILE |
| 1 | C | 405 | VAL |
| 1 | C | 674 | GLN |
| 1 | C | 687 | GLU |
| 1 | D | 261 | PHE |
| 1 | D | 845 | LEU |
| 1 | E | 275 | SER |
| 1 | E | 517 | ILE |
| 1 | E | 695 | VAL |
| 1 | E | 734 | ILE |
| 1 | E | 837 | LEU |
| 1 | F | 303 | PRO |
| 1 | F | 351 | ILE |
| 1 | F | 631 | LEU |
| 1 | F | 807 | THR |
| 1 | F | 880 | LEU |
| 1 | A | 207 | ASN |
| 1 | B | 556 | ILE |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | C | 31 | GLN |
| 1 | D | 48 | VAL |
| 1 | D | 405 | VAL |
| 1 | E | 373 | VAL |
| 1 | E | 587 | ILE |
| 1 | F | 682 | VAL |
| 1 | A | 225 | VAL |
| 1 | A | 345 | VAL |
| 1 | A | 836 | ILE |
| 1 | B | 87 | THR |
| 1 | C | 213 | GLU |
| 1 | C | 396 | VAL |
| 1 | C | 428 | ILE |
| 1 | C | 581 | VAL |
| 1 | C | 770 | VAL |
| 1 | E | 229 | ILE |
| 1 | F | 345 | VAL |
| 1 | F | 396 | VAL |
| 1 | F | 759 | ARG |
| 1 | F | 766 | ILE |
| 1 | B | 384 | PRO |
| 1 | C | 27 | HIS |
| 1 | C | 35 | ILE |
| 1 | C | 590 | VAL |
| 1 | C | 879 | VAL |
| 1 | D | 237 | ILE |
| 1 | D | 410 | LYS |
| 1 | E | 537 | ILE |
| 1 | E | 652 | VAL |
| 1 | F | 581 | VAL |
| 1 | A | 693 | PRO |
| 1 | B | 879 | VAL |
| 1 | D | 49 | PRO |
| 1 | E | 556 | ILE |
| 1 | F | 221 | ILE |
| 1 | F | 367 | ILE |
| 1 | F | 713 | GLY |
| 1 | A | 759 | ARG |
| 1 | B | 48 | VAL |
| 1 | C | 55 | ILE |
| 1 | F | 594 | VAL |

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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 | 484/782 (62%) | 480 (99%) | 4 (1%) | 79 | 85 |
| 1 | B | 493/782 (63%) | 485 (98%) | 8 (2%) | 58 | 74 |
| 1 | C | 599/782 (77%) | 583 (97%) | 16 (3%) | 40 | 58 |
| 1 | D | 599/782 (77%) | 595 (99%) | 4 (1%) | 81 | 87 |
| 1 | E | 595/782 (76%) | 589 (99%) | 6 (1%) | 73 | 82 |
| 1 | F | 490/782 (63%) | 472 (96%) | 18 (4%) | 29 | 49 |
| All | All | 3260/4692 (70%) | 3204 (98%) | 56 (2%) | 56 | 72 |

All (56) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 221 | ILE |
| 1 | A | 248 | LEU |
| 1 | A | 566 | ASN |
| 1 | A | 655 | LEU |
| 1 | B | 172 | ILE |
| 1 | B | 173 | ASP |
| 1 | B | 187 | ILE |
| 1 | B | 193 | ILE |
| 1 | B | 238 | LEU |
| 1 | B | 243 | LEU |
| 1 | B | 671 | LEU |
| 1 | B | 790 | GLU |
| 1 | C | 169 | LYS |
| 1 | C | 170 | TYR |
| 1 | C | 172 | ILE |
| 1 | C | 192 | GLU |
| 1 | C | 210 | LEU |
| 1 | C | 263 | GLU |
| 1 | C | 281 | LEU |
| 1 | C | 372 | LEU |
| 1 | C | 513 | ILE |
| 1 | C | 544 | ASP |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | C | 611 | LEU |
| 1 | C | 764 | ASN |
| 1 | C | 788 | LEU |
| 1 | C | 837 | LEU |
| 1 | C | 844 | ILE |
| 1 | C | 857 | VAL |
| 1 | D | 301 | LEU |
| 1 | D | 585 | ASP |
| 1 | D | 748 | ASN |
| 1 | D | 812 | ASP |
| 1 | E | 544 | ASP |
| 1 | E | 575 | ASP |
| 1 | E | 623 | LEU |
| 1 | E | 636 | ASP |
| 1 | E | 723 | VAL |
| 1 | E | 805 | ASN |
| 1 | F | 319 | ASN |
| 1 | F | 320 | GLU |
| 1 | F | 322 | ARG |
| 1 | F | 356 | GLN |
| 1 | F | 357 | PRO |
| 1 | F | 358 | LYS |
| 1 | F | 360 | GLU |
| 1 | F | 361 | ILE |
| 1 | F | 365 | VAL |
| 1 | F | 407 | ARG |
| 1 | F | 683 | LEU |
| 1 | F | 703 | LEU |
| 1 | F | 705 | ASP |
| 1 | F | 707 | ARG |
| 1 | F | 708 | ILE |
| 1 | F | 709 | THR |
| 1 | F | 712 | GLN |
| 1 | F | 812 | ASP |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (69) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 177 | GLN |
| 1 | A | 571 | HIS |
| 1 | A | 583 | GLN |
| 1 | A | 633 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 738 | GLN |
| 1 | A | 808 | GLN |
| 1 | A | 829 | ASN |
| 1 | B | 177 | GLN |
| 1 | B | 336 | GLN |
| 1 | B | 347 | GLN |
| 1 | B | 356 | GLN |
| 1 | B | 362 | HIS |
| 1 | B | 583 | GLN |
| 1 | B | 712 | GLN |
| 1 | B | 743 | GLN |
| 1 | B | 808 | GLN |
| 1 | B | 856 | ASN |
| 1 | C | 319 | ASN |
| 1 | C | 362 | HIS |
| 1 | C | 363 | HIS |
| 1 | C | 456 | GLN |
| 1 | C | 488 | ASN |
| 1 | C | 583 | GLN |
| 1 | C | 633 | ASN |
| 1 | C | 673 | ASN |
| 1 | C | 674 | GLN |
| 1 | C | 781 | HIS |
| 1 | C | 833 | GLN |
| 1 | C | 856 | ASN |
| 1 | C | 882 | ASN |
| 1 | D | 177 | GLN |
| 1 | D | 319 | ASN |
| 1 | D | 336 | GLN |
| 1 | D | 356 | GLN |
| 1 | D | 362 | HIS |
| 1 | D | 363 | HIS |
| 1 | D | 471 | HIS |
| 1 | D | 534 | ASN |
| 1 | D | 712 | GLN |
| 1 | D | 720 | ASN |
| 1 | D | 748 | ASN |
| 1 | D | 797 | GLN |
| 1 | D | 801 | HIS |
| 1 | D | 838 | ASN |
| 1 | E | 292 | ASN |
| 1 | E | 319 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | E | 336 | GLN |
| 1 | E | 362 | HIS |
| 1 | E | 363 | HIS |
| 1 | E | 425 | GLN |
| 1 | E | 450 | GLN |
| 1 | E | 534 | ASN |
| 1 | E | 571 | HIS |
| 1 | E | 592 | ASN |
| 1 | E | 701 | GLN |
| 1 | E | 756 | GLN |
| 1 | E | 757 | HIS |
| 1 | E | 882 | ASN |
| 1 | F | 177 | GLN |
| 1 | F | 207 | ASN |
| 1 | F | 309 | GLN |
| 1 | F | 571 | HIS |
| 1 | F | 583 | GLN |
| 1 | F | 592 | ASN |
| 1 | F | 720 | ASN |
| 1 | F | 773 | ASN |
| 1 | F | 797 | GLN |
| 1 | F | 833 | GLN |
| 1 | F | 834 | ASN |

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

6 ligands 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 | $\# Z > 2$ |
| 2 | AGS | C | 1001 | - | 26,33,33 | 0.88 | 1 (3%) | 26,52,52 | 2.33 | 4 (15%) |
| 2 | AGS | F | 1002 | - | 26,33,33 | 0.87 | 2 (7%) | 26,52,52 | 1.25 | 2 (7%) |
| 2 | AGS | D | 1001 | - | 26,33,33 | 1.05 | 2 (7%) | 26,52,52 | 1.34 | 2 (7%) |
| 2 | AGS | E | 1002 | - | 26,33,33 | 0.90 | 1 (3%) | 26,52,52 | 1.53 | 2 (7%) |
| 2 | AGS | E | 1001 | - | 26,33,33 | 0.88 | 1 (3%) | 26,52,52 | 2.01 | 2 (7%) |
| 2 | AGS | F | 1001 | - | 26,33,33 | 0.78 | 0 | 26,52,52 | 1.29 | 1 (3%) |

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 |
|-----|------|-------|------|------|---------|------------|---------|
| 2 | AGS | C | 1001 | - | - | 4/17/38/38 | 0/3/3/3 |
| 2 | AGS | F | 1002 | - | - | 5/17/38/38 | 0/3/3/3 |
| 2 | AGS | D | 1001 | - | - | 8/17/38/38 | 0/3/3/3 |
| 2 | AGS | E | 1002 | - | - | 6/17/38/38 | 0/3/3/3 |
| 2 | AGS | E | 1001 | - | - | 4/17/38/38 | 0/3/3/3 |
| 2 | AGS | F | 1001 | - | - | 7/17/38/38 | 0/3/3/3 |

All (7) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 2 | D | 1001 | AGS | C4-N3 | -2.52 | 1.32 | 1.35 |
| 2 | F | 1002 | AGS | C8-N7 | -2.40 | 1.30 | 1.34 |
| 2 | E | 1002 | AGS | C8-N7 | -2.38 | 1.30 | 1.34 |
| 2 | C | 1001 | AGS | PB-O2B | -2.19 | 1.45 | 1.55 |
| 2 | D | 1001 | AGS | PA-O2A | -2.18 | 1.45 | 1.55 |
| 2 | F | 1002 | AGS | PG-S1G | 2.15 | 1.95 | 1.90 |
| 2 | E | 1001 | AGS | C8-N7 | -2.03 | 1.31 | 1.34 |

All (13) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|--------|-------------|----------|
| 2 | C | 1001 | AGS | PA-O3A-PB | -10.20 | 97.83 | 132.83 |
| 2 | E | 1001 | AGS | PA-O3A-PB | -9.19 | 101.31 | 132.83 |
| 2 | E | 1002 | AGS | PA-O3A-PB | -6.17 | 111.64 | 132.83 |
| 2 | D | 1001 | AGS | PA-O3A-PB | -5.11 | 115.31 | 132.83 |
| 2 | F | 1001 | AGS | PA-O3A-PB | -4.88 | 116.08 | 132.83 |
| 2 | F | 1002 | AGS | PA-O3A-PB | -4.37 | 117.84 | 132.83 |
| 2 | D | 1001 | AGS | C4-C5-N7 | 3.18 | 112.71 | 109.40 |
| 2 | C | 1001 | AGS | O2G-PG-O3B | 2.91 | 114.36 | 104.64 |
| 2 | E | 1002 | AGS | C5-C6-N6 | 2.73 | 124.50 | 120.35 |
| 2 | F | 1002 | AGS | C5-C6-N6 | 2.50 | 124.15 | 120.35 |
| 2 | C | 1001 | AGS | C4-C5-N7 | 2.41 | 111.91 | 109.40 |
| 2 | E | 1001 | AGS | C5-C6-N6 | 2.25 | 123.78 | 120.35 |
| 2 | C | 1001 | AGS | C5-C6-N6 | 2.21 | 123.70 | 120.35 |

There are no chirality outliers.

All (34) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 2 | C | 1001 | AGS | C4'-C5'-O5'-PA |
| 2 | D | 1001 | AGS | C5'-O5'-PA-O1A |
| 2 | D | 1001 | AGS | C5'-O5'-PA-O2A |
| 2 | D | 1001 | AGS | C3'-C4'-C5'-O5' |
| 2 | E | 1001 | AGS | C5'-O5'-PA-O1A |
| 2 | E | 1001 | AGS | C5'-O5'-PA-O2A |
| 2 | E | 1002 | AGS | O4'-C4'-C5'-O5' |
| 2 | E | 1002 | AGS | C3'-C4'-C5'-O5' |
| 2 | F | 1001 | AGS | C5'-O5'-PA-O1A |
| 2 | F | 1001 | AGS | C5'-O5'-PA-O2A |
| 2 | F | 1001 | AGS | C4'-C5'-O5'-PA |
| 2 | F | 1002 | AGS | PB-O3B-PG-O2G |
| 2 | F | 1002 | AGS | PB-O3B-PG-O3G |
| 2 | F | 1002 | AGS | C5'-O5'-PA-O1A |
| 2 | F | 1002 | AGS | C4'-C5'-O5'-PA |
| 2 | D | 1001 | AGS | O4'-C4'-C5'-O5' |
| 2 | E | 1002 | AGS | C4'-C5'-O5'-PA |
| 2 | F | 1001 | AGS | PA-O3A-PB-O1B |
| 2 | E | 1001 | AGS | C4'-C5'-O5'-PA |
| 2 | D | 1001 | AGS | C5'-O5'-PA-O3A |
| 2 | F | 1002 | AGS | C3'-C4'-C5'-O5' |
| 2 | D | 1001 | AGS | C4'-C5'-O5'-PA |
| 2 | F | 1001 | AGS | PB-O3A-PA-O2A |
| 2 | D | 1001 | AGS | PG-O3B-PB-O2B |
| 2 | E | 1002 | AGS | PB-O3B-PG-O2G |

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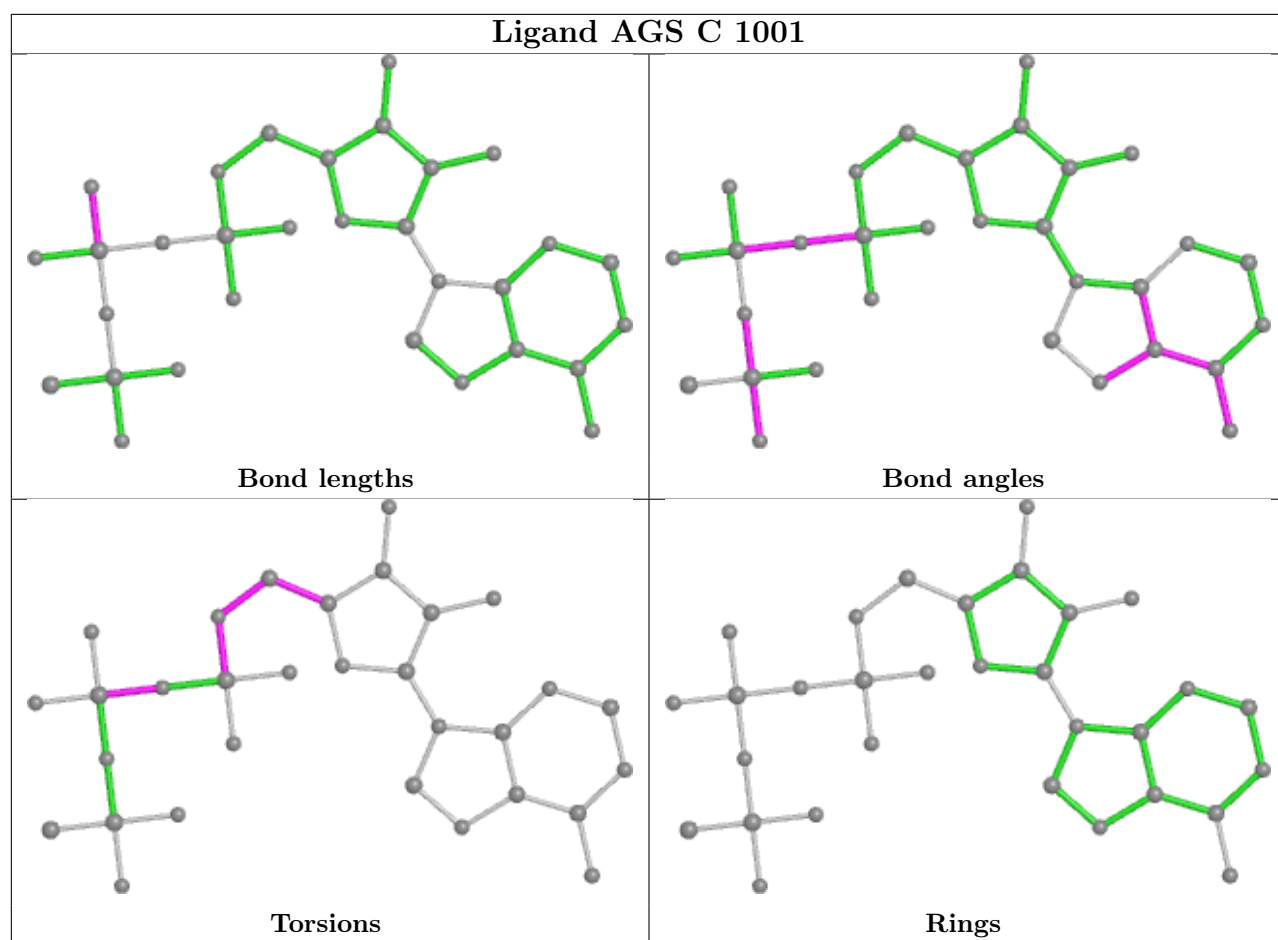
| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-----------------|
| 2 | C | 1001 | AGS | PA-O3A-PB-O1B |
| 2 | E | 1002 | AGS | PA-O3A-PB-O3B |
| 2 | D | 1001 | AGS | PG-O3B-PB-O1B |
| 2 | E | 1001 | AGS | C5'-O5'-PA-O3A |
| 2 | F | 1001 | AGS | C5'-O5'-PA-O3A |
| 2 | F | 1001 | AGS | O4'-C4'-C5'-O5' |
| 2 | E | 1002 | AGS | PA-O3A-PB-O1B |
| 2 | C | 1001 | AGS | C5'-O5'-PA-O1A |
| 2 | C | 1001 | AGS | O4'-C4'-C5'-O5' |

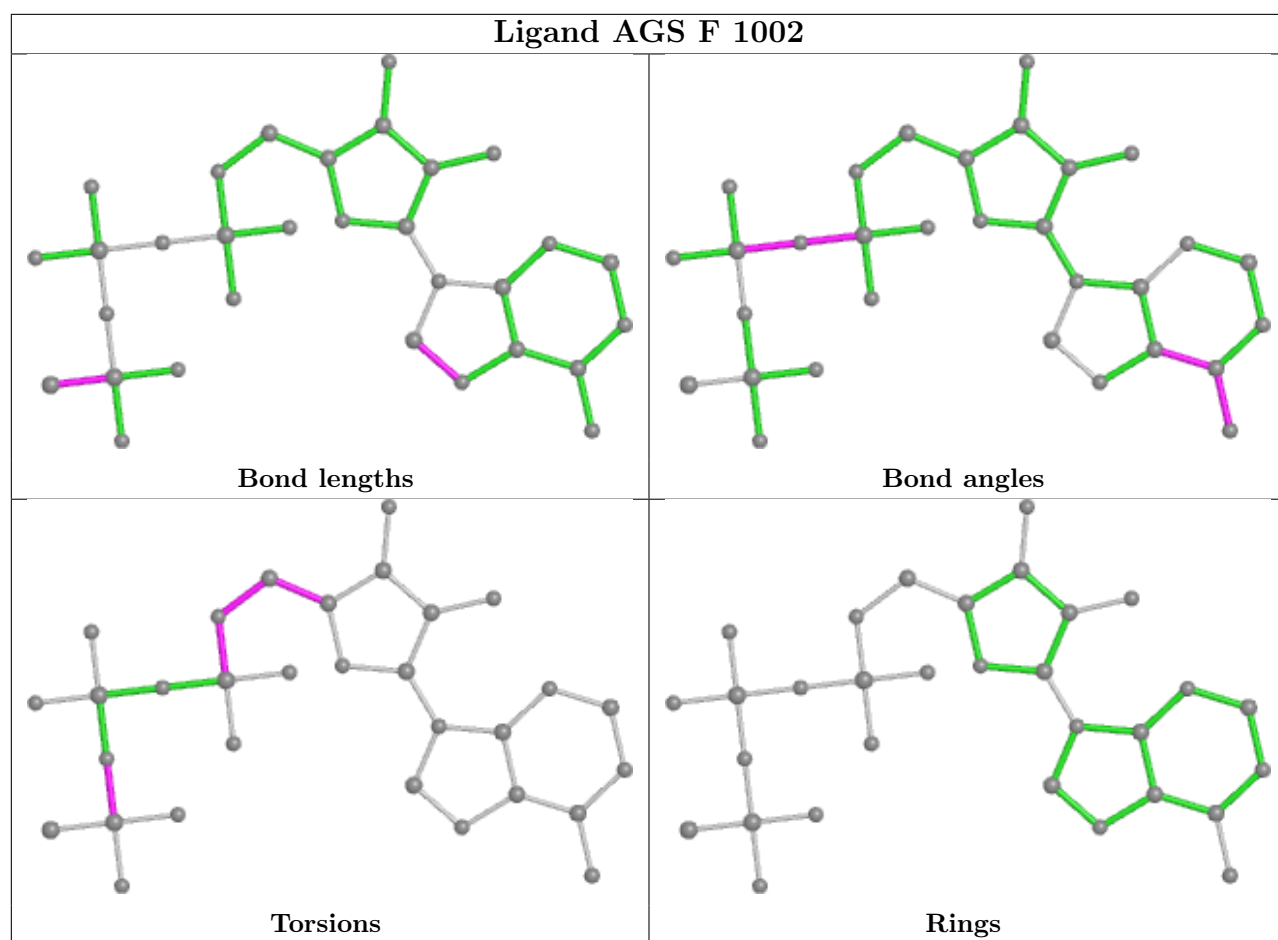
There are no ring outliers.

6 monomers are involved in 170 short contacts:

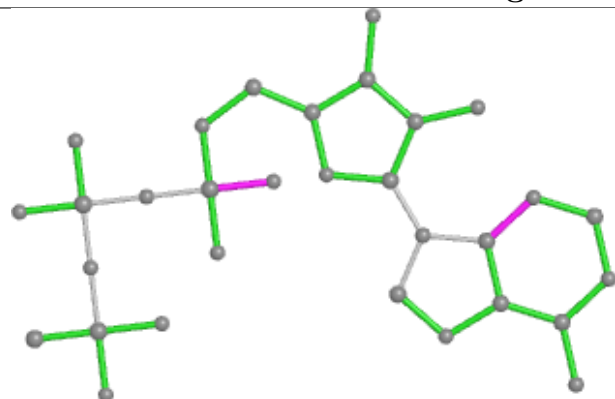
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 2 | C | 1001 | AGS | 29 | 0 |
| 2 | F | 1002 | AGS | 19 | 0 |
| 2 | D | 1001 | AGS | 38 | 0 |
| 2 | E | 1002 | AGS | 35 | 0 |
| 2 | E | 1001 | AGS | 30 | 0 |
| 2 | F | 1001 | AGS | 19 | 0 |

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

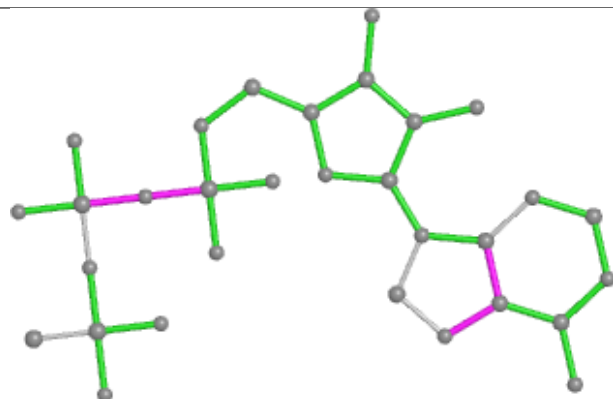




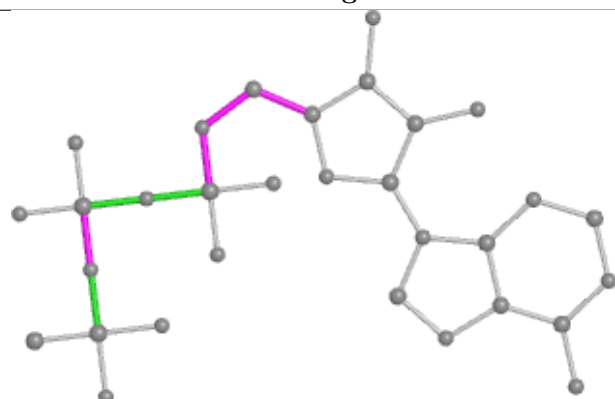
Ligand AGS D 1001



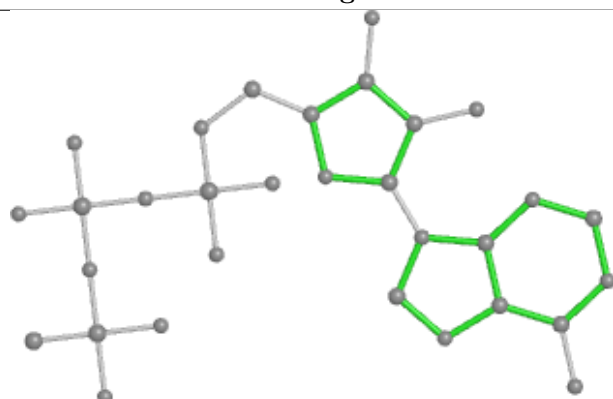
Bond lengths



Bond angles

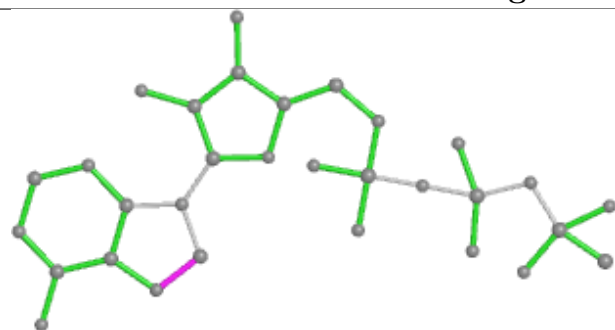


Torsions

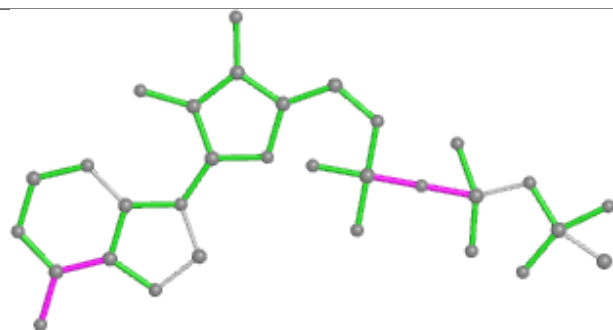


Rings

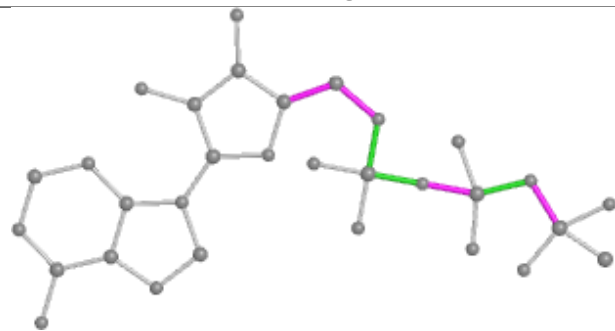
Ligand AGS E 1002



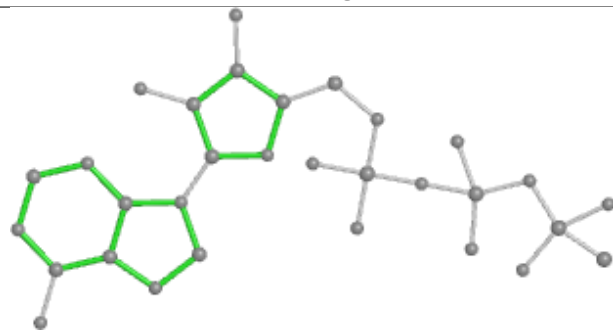
Bond lengths



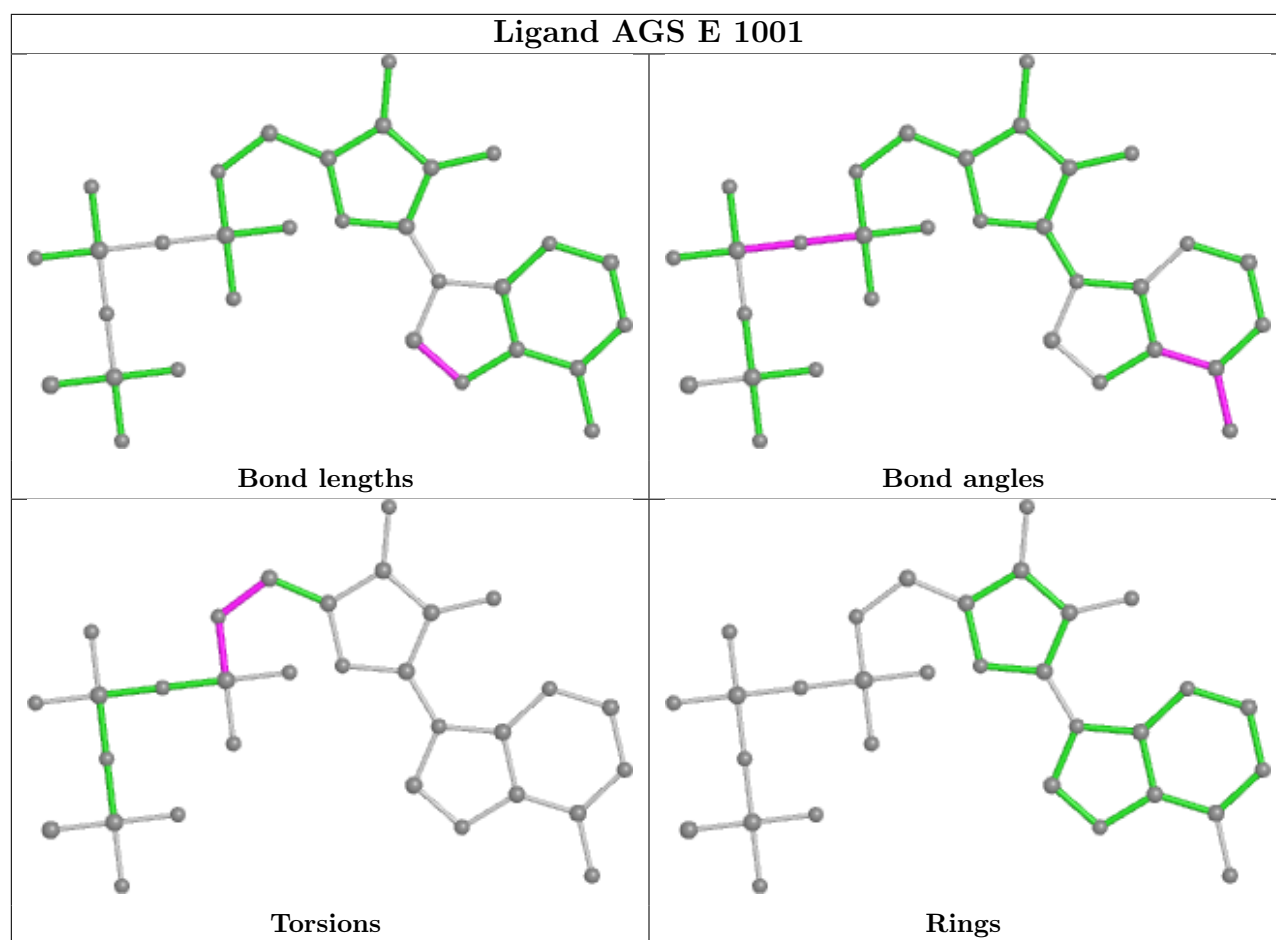
Bond angles

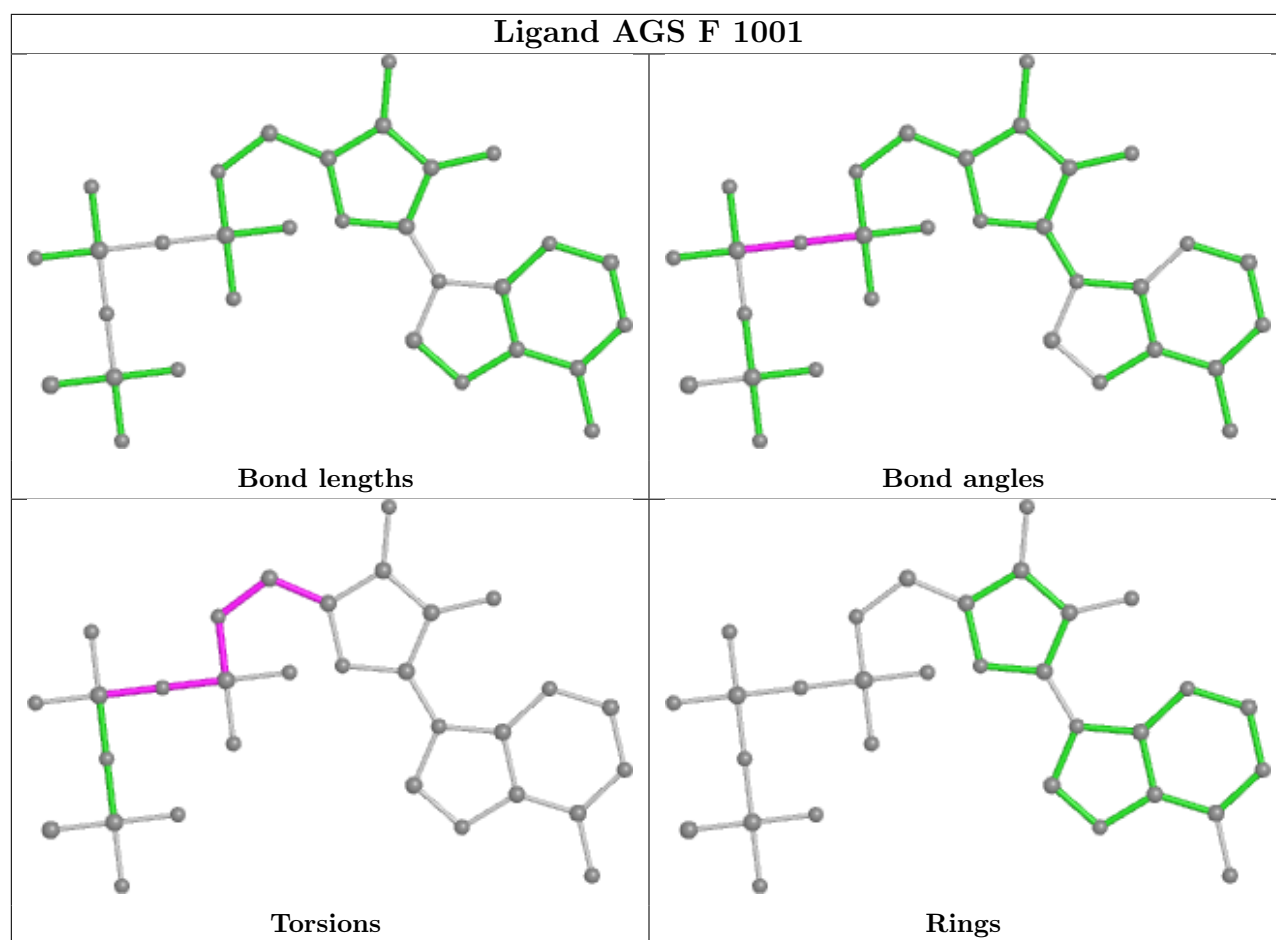


Torsions



Rings





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

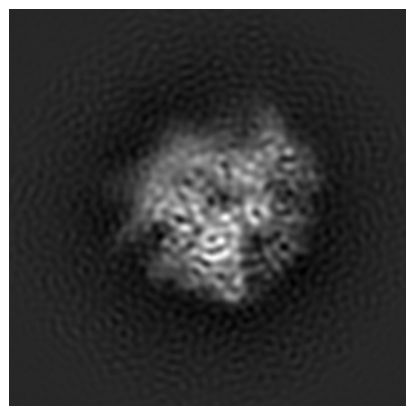
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-9625. These allow visual inspection of the internal detail of the map and identification of artifacts.

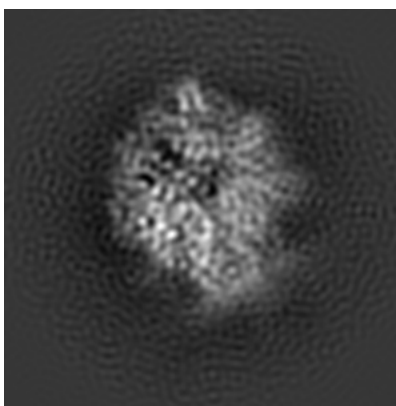
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

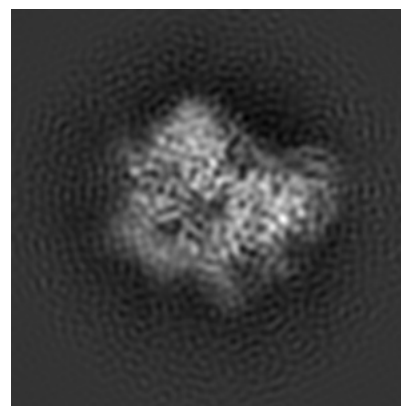
6.1.1 Primary map



X

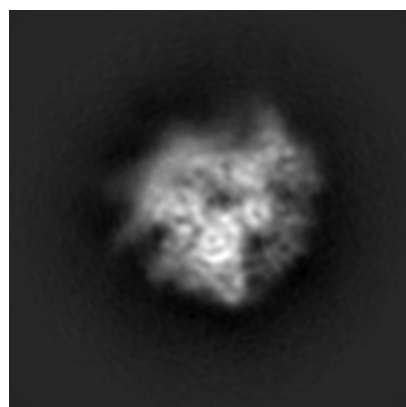


Y

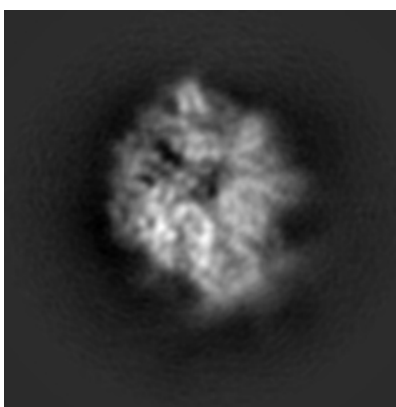


Z

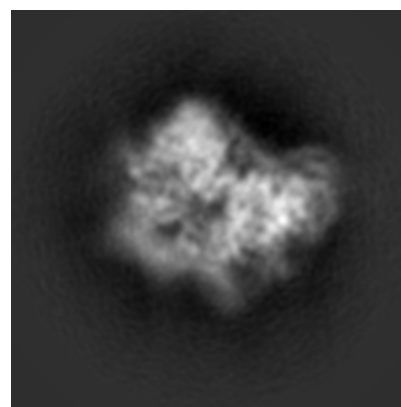
6.1.2 Raw map



X



Y

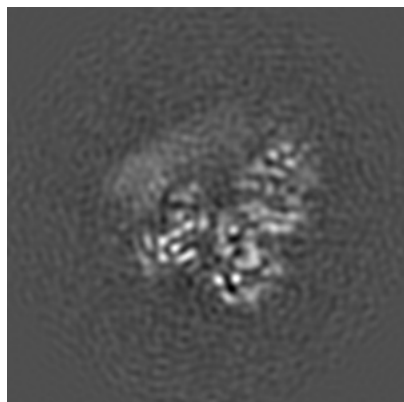


Z

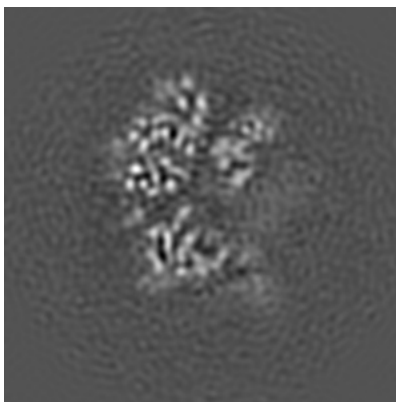
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

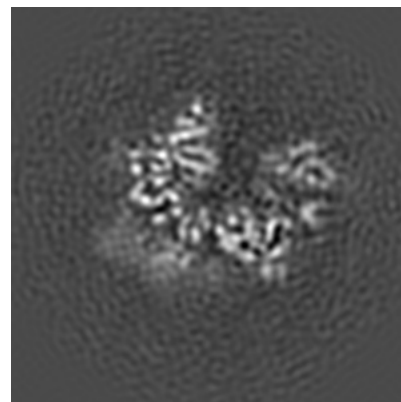
6.2.1 Primary map



X Index: 54

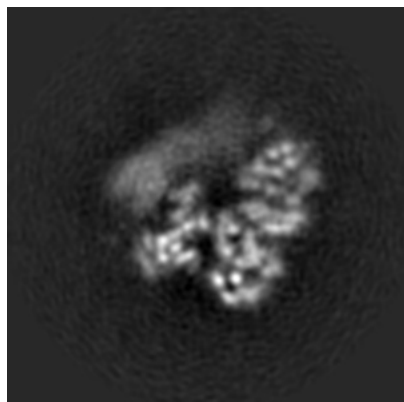


Y Index: 54

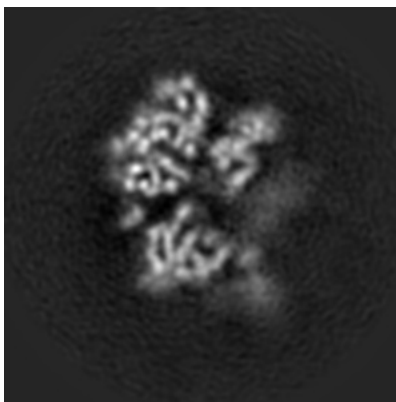


Z Index: 54

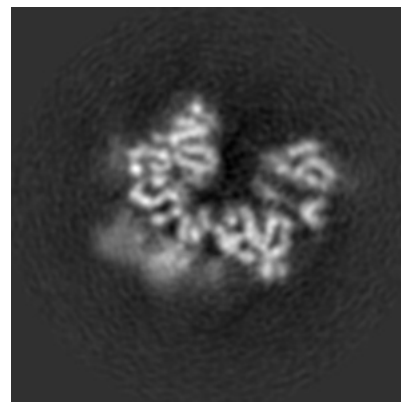
6.2.2 Raw map



X Index: 54



Y Index: 54

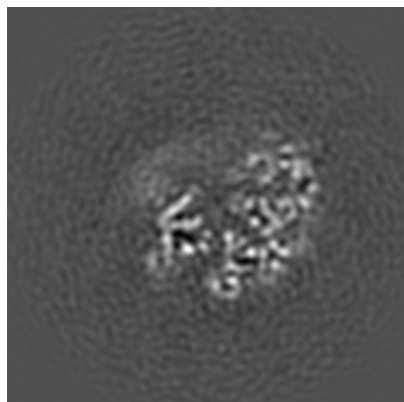


Z Index: 54

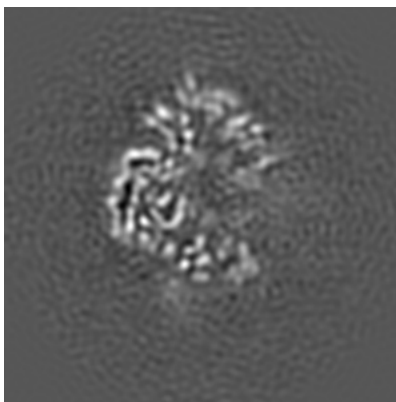
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

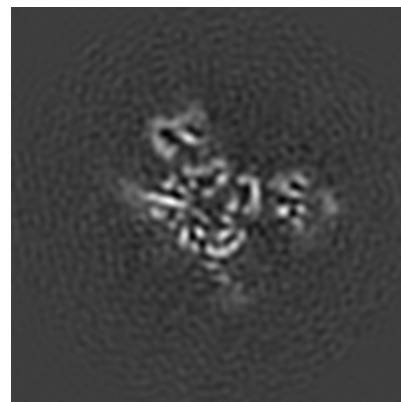
6.3.1 Primary map



X Index: 49

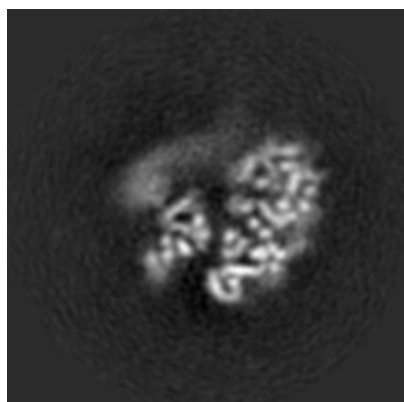


Y Index: 60

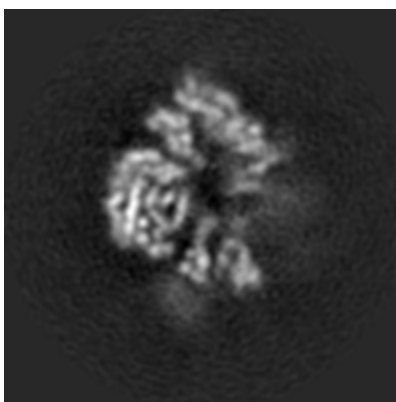


Z Index: 44

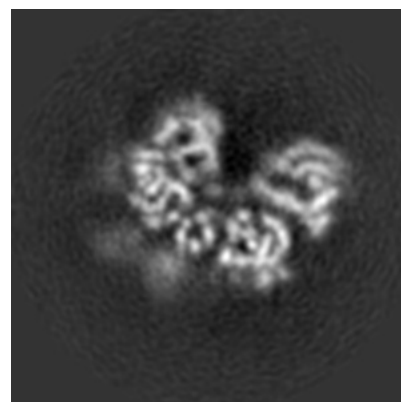
6.3.2 Raw map



X Index: 50



Y Index: 61

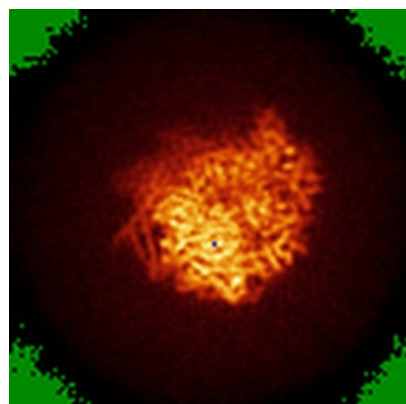


Z Index: 52

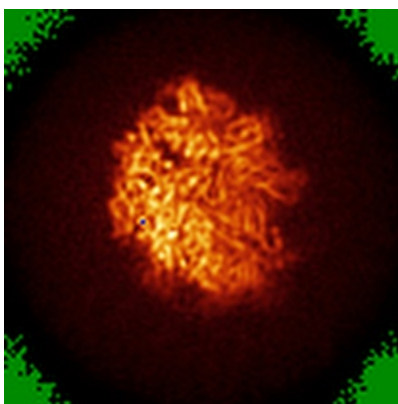
The images above show the largest variance slices of the map in three orthogonal directions.

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

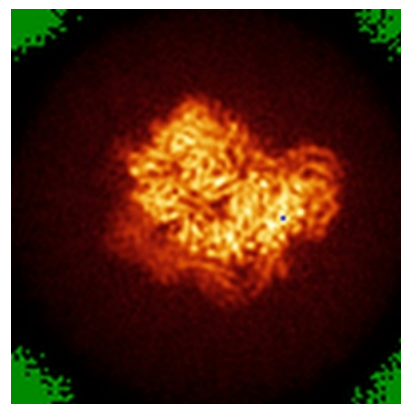
6.4.1 Primary map



X

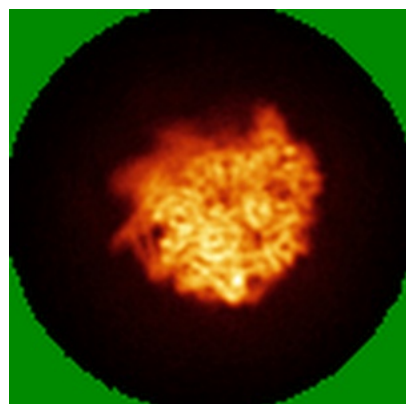


Y

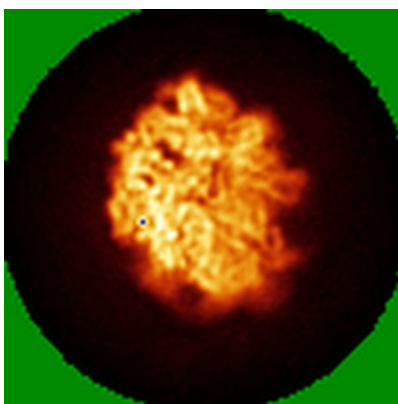


Z

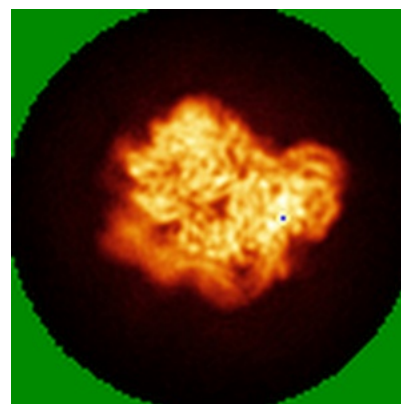
6.4.2 Raw map



X



Y

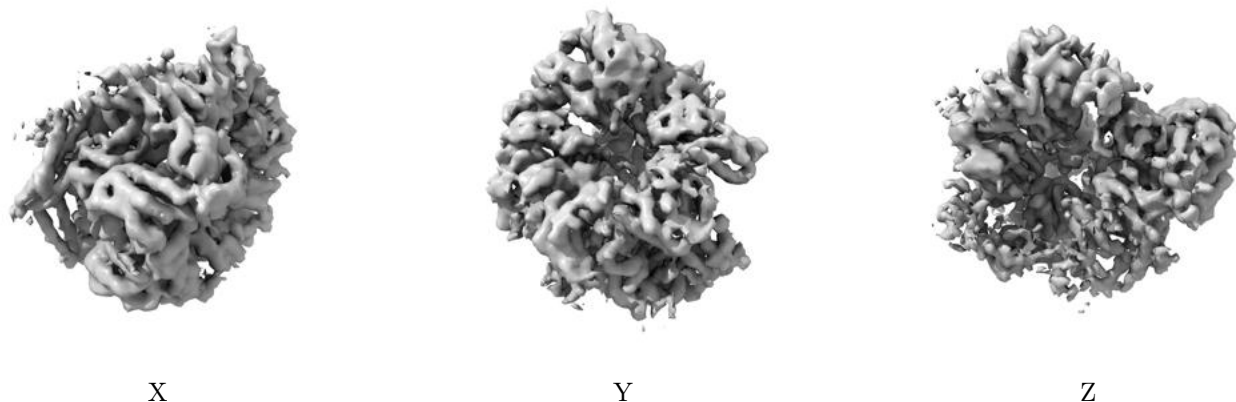


Z

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

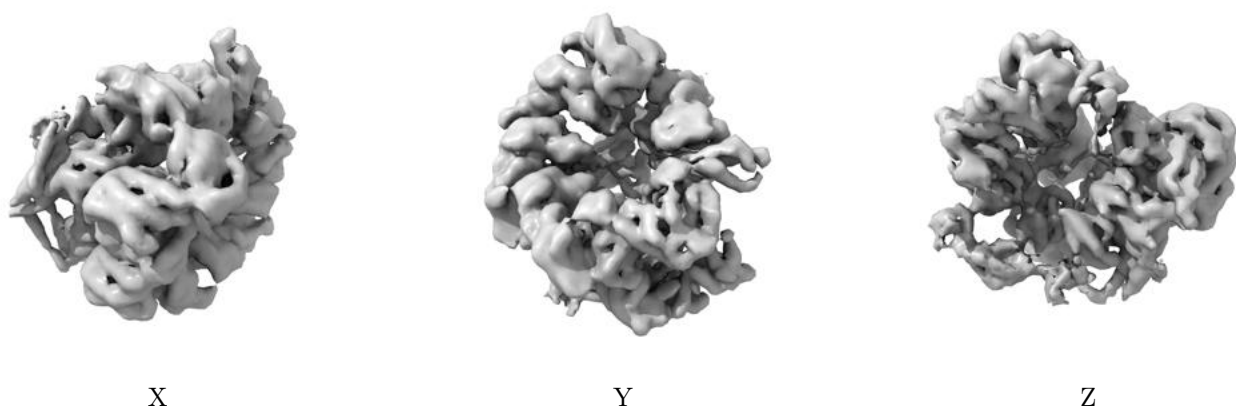
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.08. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

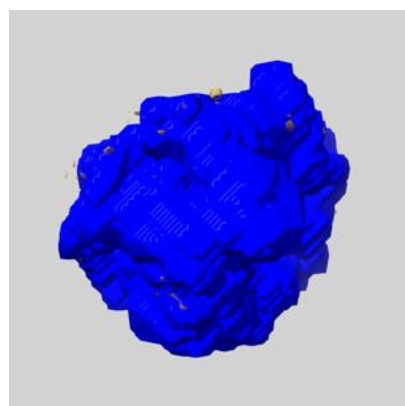
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

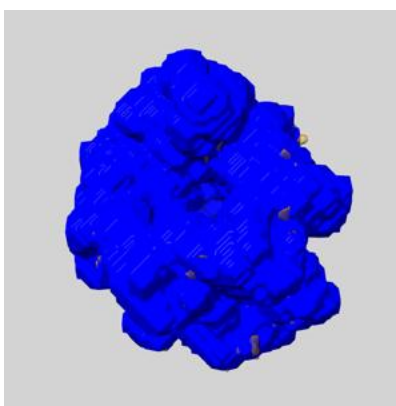
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

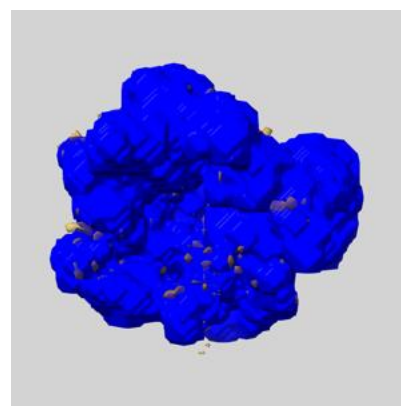
6.6.1 emd_9625_msk_1.map [i](#)



X



Y

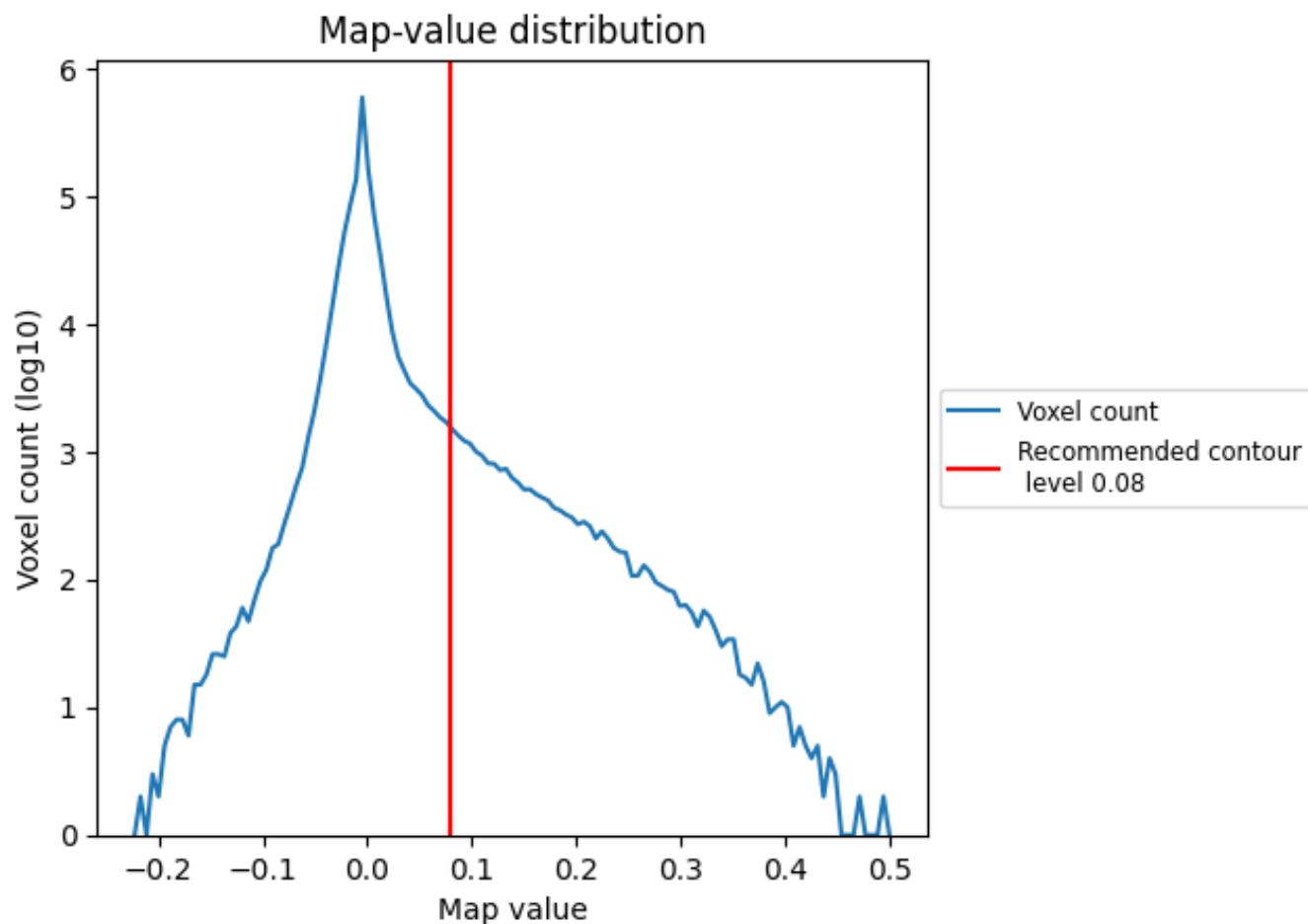


Z

7 Map analysis [i](#)

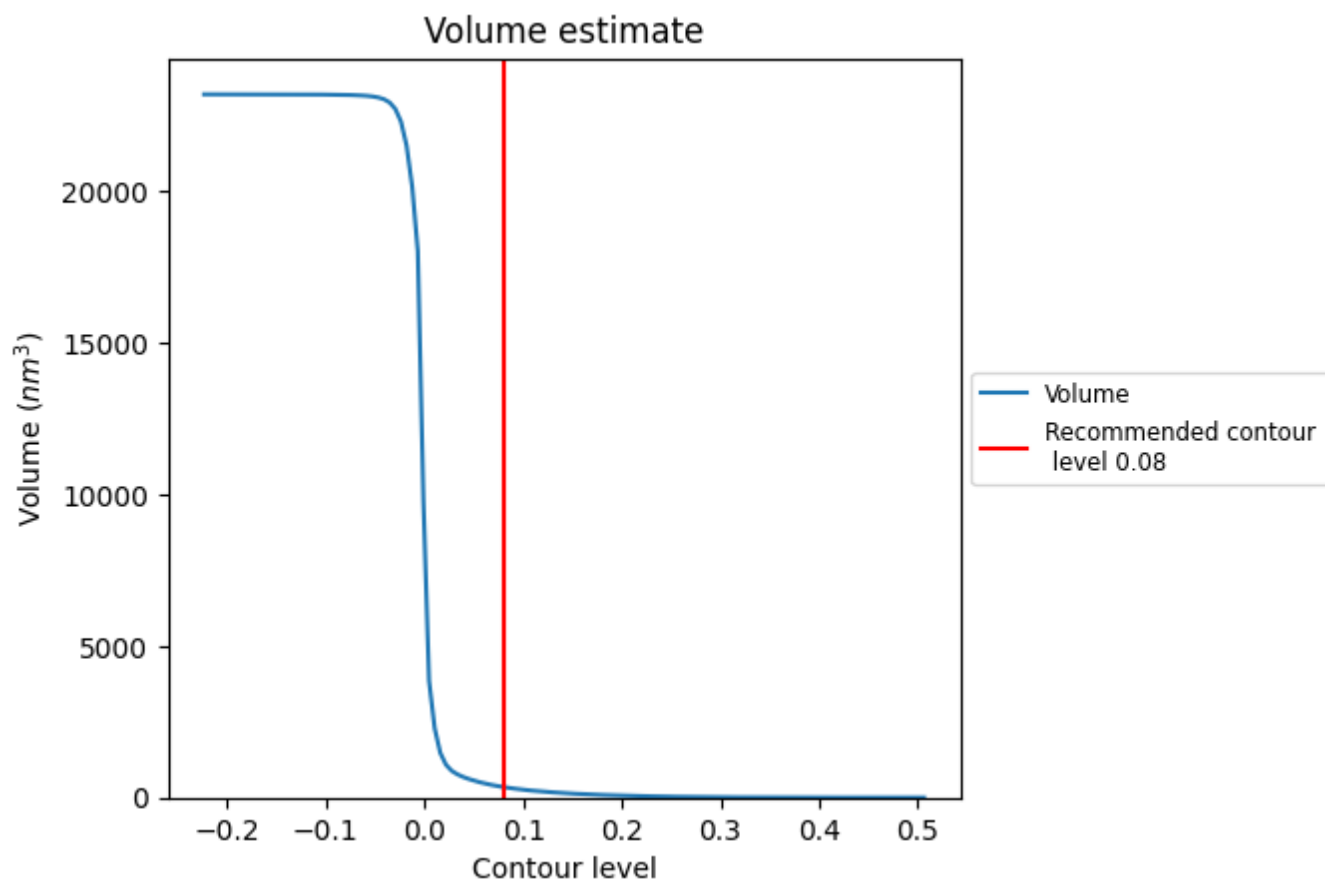
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

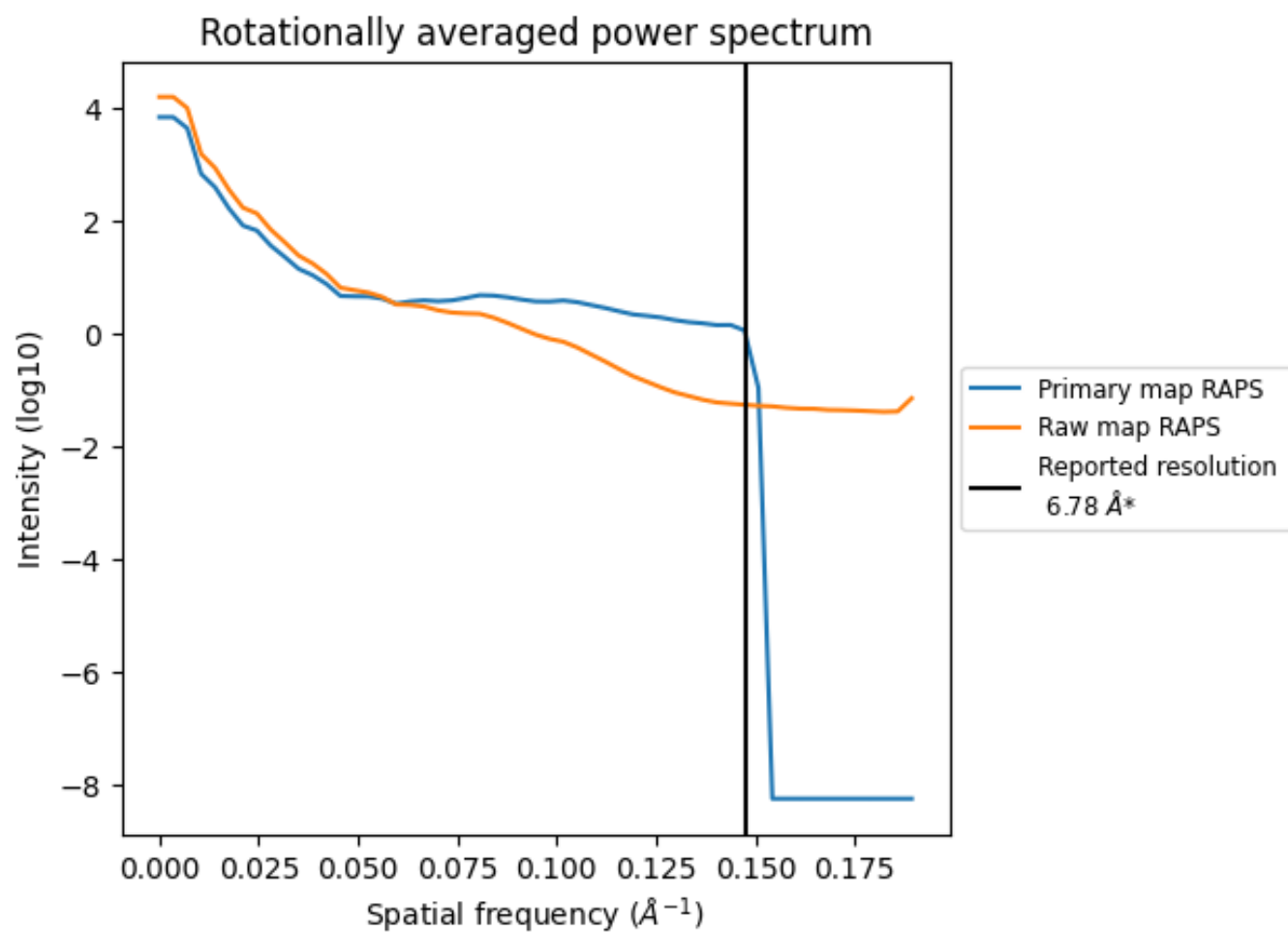
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 346 nm^3 ; this corresponds to an approximate mass of 313 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

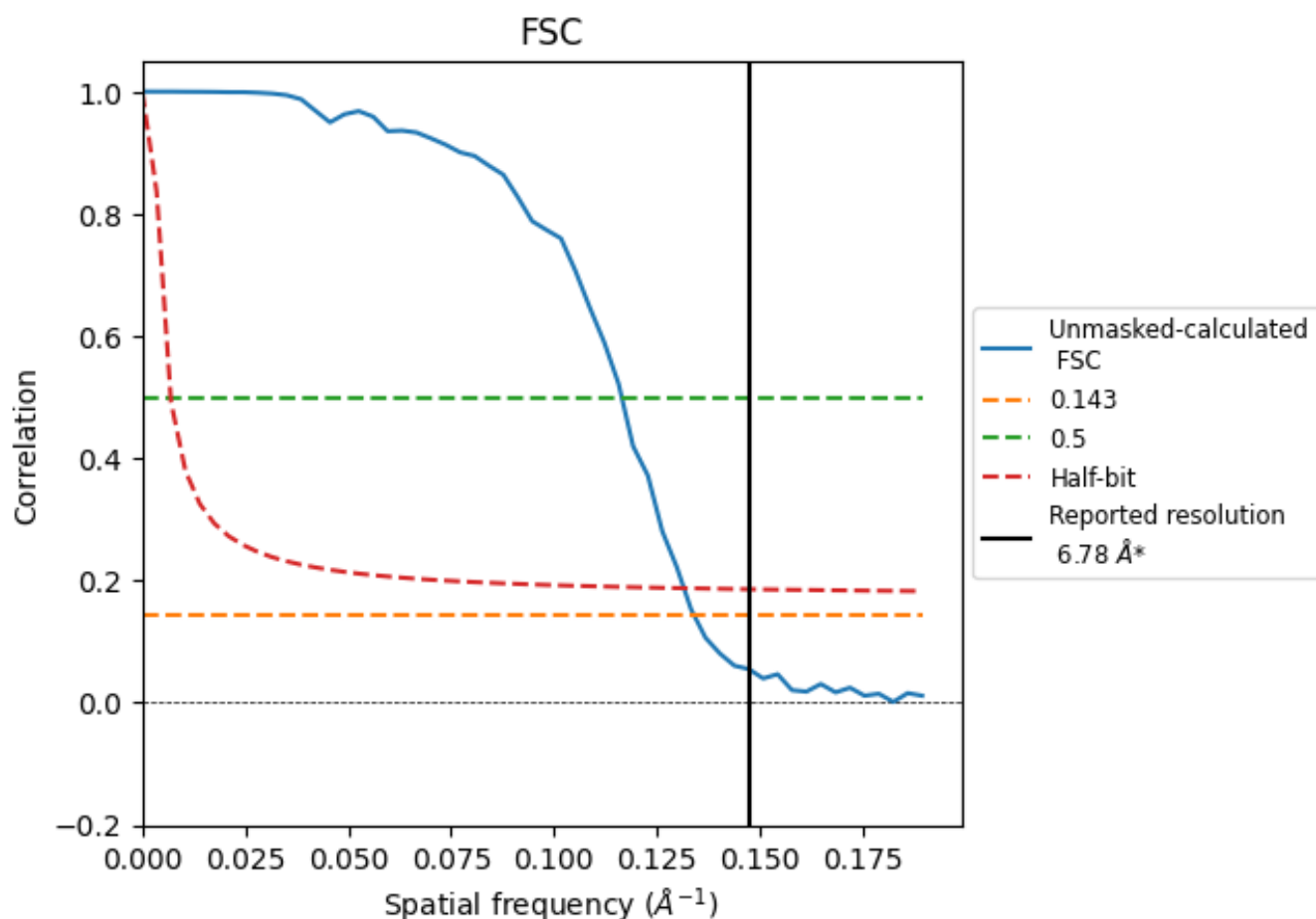


*Reported resolution corresponds to spatial frequency of 0.147 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.147 Å⁻¹

8.2 Resolution estimates [i](#)

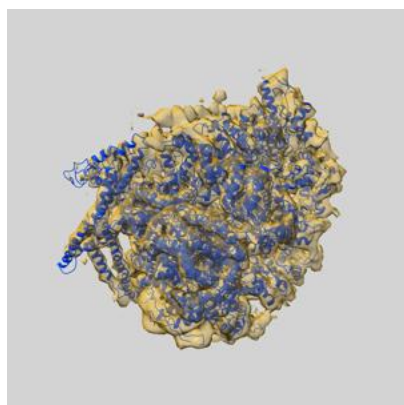
| Resolution estimate (Å) | Estimation criterion (FSC cut-off) | | |
|---------------------------|------------------------------------|------|----------|
| | 0.143 | 0.5 | Half-bit |
| Reported by author | 6.78 | - | - |
| Author-provided FSC curve | - | - | - |
| Unmasked-calculated* | 7.46 | 8.58 | 7.60 |

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 7.46 differs from the reported value 6.78 by more than 10 %

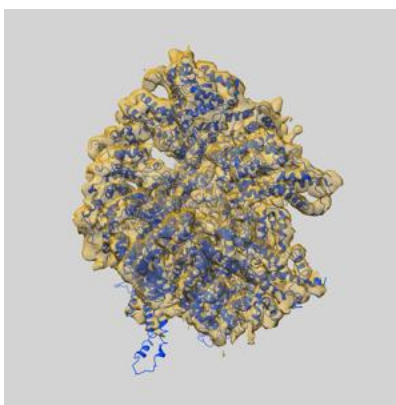
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-9625 and PDB model 6AHF. Per-residue inclusion information can be found in section [3](#) on page [6](#).

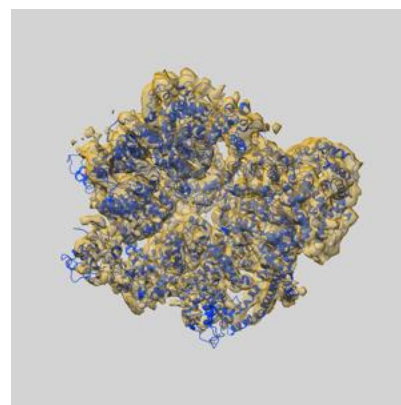
9.1 Map-model overlay [i](#)



X



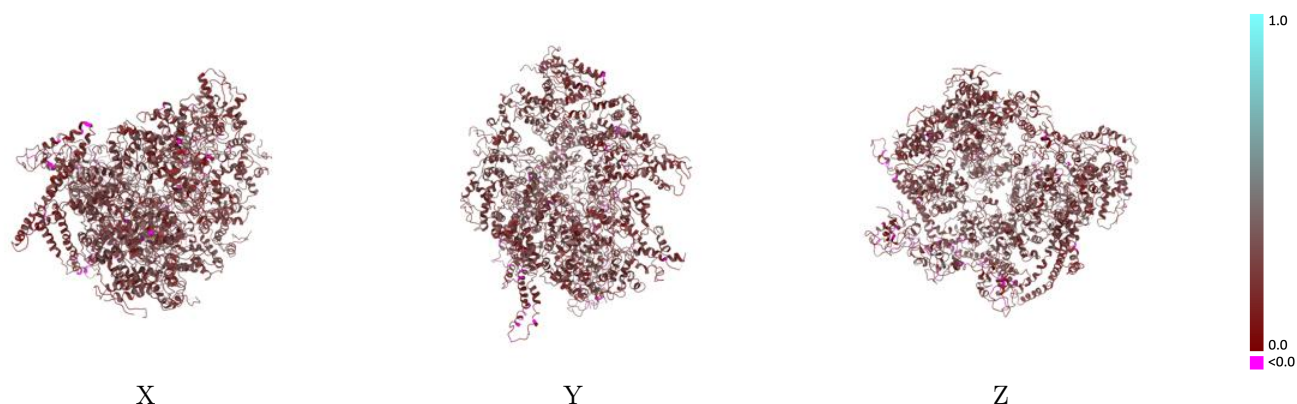
Y



Z

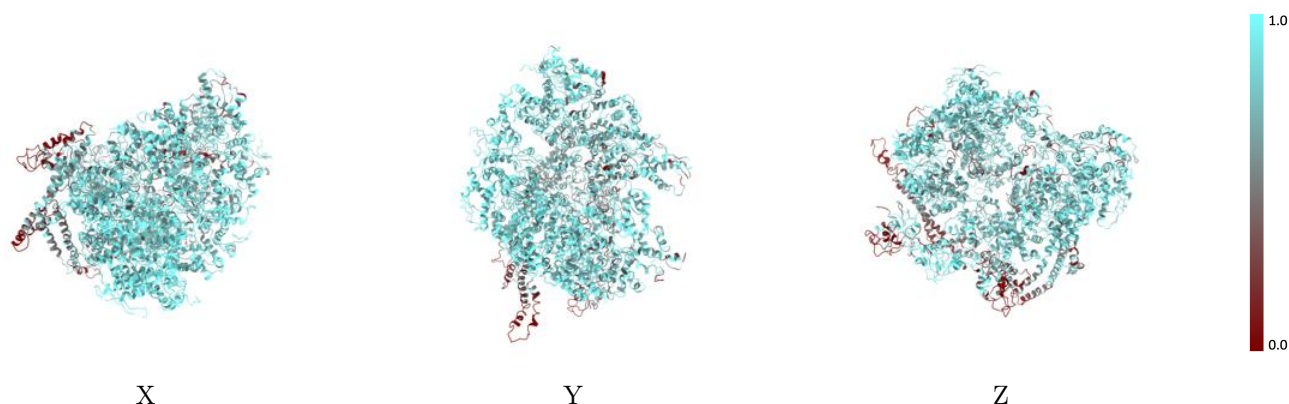
The images above show the 3D surface view of the map at the recommended contour level 0.08 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



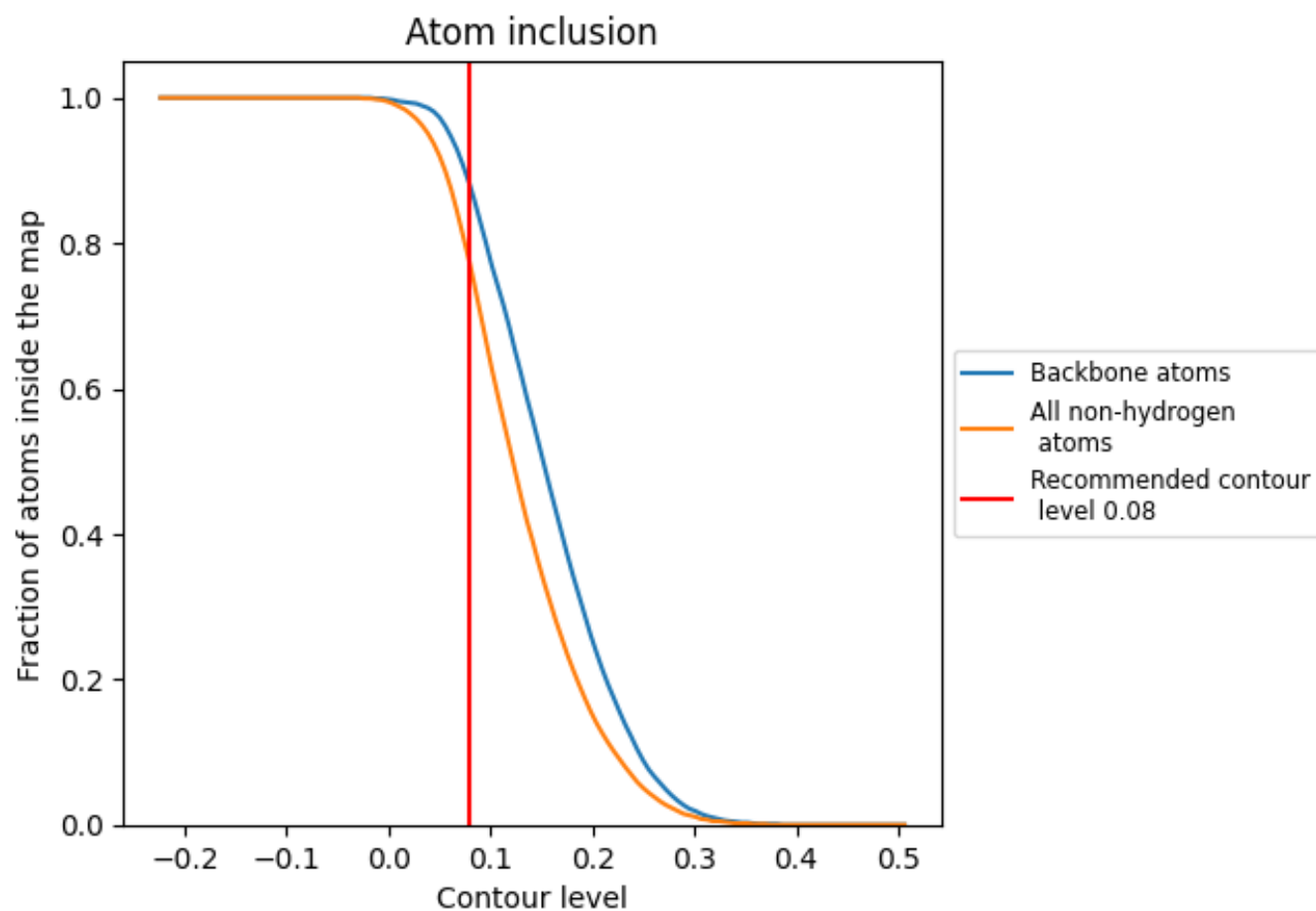
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.08).

9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 77% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.08) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion | Q-score |
|-------|------------------------------|------------------------------|
| All | <div><div></div>0.7720</div> | <div><div></div>0.2430</div> |
| A | <div><div></div>0.7290</div> | <div><div></div>0.2380</div> |
| B | <div><div></div>0.7940</div> | <div><div></div>0.2480</div> |
| C | <div><div></div>0.7520</div> | <div><div></div>0.2460</div> |
| D | <div><div></div>0.7680</div> | <div><div></div>0.2500</div> |
| E | <div><div></div>0.8060</div> | <div><div></div>0.2450</div> |
| F | <div><div></div>0.7800</div> | <div><div></div>0.2310</div> |

1.0

0.0

<0.0