# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 10, 2021 – 08:01 PM EDT

| | | |
|---|---|---|
| PDB ID | : | 3EXG |
| Title | : | Crystal structure of the pyruvate dehydrogenase (E1p) component of human pyruvate dehydrogenase complex |
| Authors | : | Kato, M.; Wynn, R.M.; Chuang, J.L.; Tso, S.-C.; Machius, M.; Li, J.; Chuang, D.T. |
| Deposited on | : | 2008-10-16 |
| Resolution | : | 3.01 Å(reported) |

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

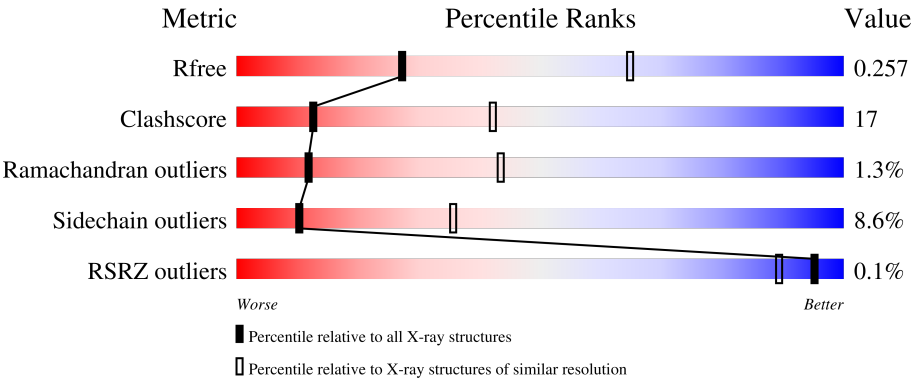
| | | |
|---|---|---|
| MolProbity | : | 4.02b-467 |
| Xtriage (Phenix) | : | 1.13 |
| EDS | : | 2.23.2 |
| Percentile statistics | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| Refmac | : | 5.8.0158 |
| CCP4 | : | 7.0.044 (Gargrove) |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | 2.23.2 |

# 1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.01 Å.

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




| Metric | Whole archive (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|---|---|---|
| $R_{free}$ | 130704 | 2399 (3.04-3.00) |
| Clashscore | 141614 | 2734 (3.04-3.00) |
| Ramachandran outliers | 138981 | 2640 (3.04-3.00) |
| Sidechain outliers | 138945 | 2643 (3.04-3.00) |
| RSRZ outliers | 127900 | 2287 (3.04-3.00) |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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 <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | 1 | 382 | 54% 29% • • 12% |
| 1 | 3 | 382 | 55% 28% 6% • 10% |
| 1 | 5 | 382 | 61% 22% 7% • 9% |
| 1 | A | 382 | 53% 31% 5% • 10% |
| 1 | C | 382 | 51% 34% • • 10% |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | E | 382 | 61% 25% 5% 9% |
| 1 | G | 382 | 60% 26% 9% |
| 1 | I | 382 | 58% 29% 10% |
| 1 | K | 382 | 62% 25% 9% |
| 1 | M | 382 | 61% 25% 5% 9% |
| 1 | O | 382 | 51% 31% 5% 13% |
| 1 | Q | 382 | 52% 32% 6% 10% |
| 1 | S | 382 | 57% 26% 5% 11% |
| 1 | U | 382 | 61% 25% 5% 9% |
| 1 | W | 382 | 59% 26% 10% |
| 1 | Y | 382 | 61% 26% 9% |
| 2 | 2 | 329 | 72% 25% |
| 2 | 4 | 329 | 70% 27% |
| 2 | 6 | 329 | 73% 22% 5% |
| 2 | B | 329 | 73% 25% |
| 2 | D | 329 | 70% 25% 5% |
| 2 | F | 329 | 69% 28% |
| 2 | H | 329 | 69% 27% |
| 2 | J | 329 | 65% 33% |
| 2 | L | 329 | 71% 25% |
| 2 | N | 329 | 67% 29% |
| 2 | P | 329 | 71% 25% |
| 2 | R | 329 | 68% 28% |
| 2 | T | 329 | 72% 23% 5% |
| 2 | V | 329 | 71% 26% |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 2 | X | 329 | |
| 2 | Z | 329 | |

## 2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 83339 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Pyruvate dehydrogenase E1 component subunit alpha, somatic form, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 1 | A | 342 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2677 | 1684 | 471 | 500 | 22 | | | |
| 1 | C | 342 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2677 | 1684 | 471 | 500 | 22 | | | |
| 1 | E | 349 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2728 | 1717 | 481 | 508 | 22 | | | |
| 1 | G | 346 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2712 | 1707 | 478 | 505 | 22 | | | |
| 1 | I | 344 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2693 | 1694 | 473 | 504 | 22 | | | |
| 1 | K | 347 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2712 | 1708 | 476 | 506 | 22 | | | |
| 1 | M | 349 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2728 | 1717 | 481 | 508 | 22 | | | |
| 1 | O | 332 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2580 | 1626 | 449 | 483 | 22 | | | |
| 1 | Q | 344 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2693 | 1694 | 473 | 504 | 22 | | | |
| 1 | S | 340 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2661 | 1675 | 466 | 498 | 22 | | | |
| 1 | U | 348 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2723 | 1714 | 480 | 507 | 22 | | | |
| 1 | W | 345 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2705 | 1702 | 477 | 504 | 22 | | | |
| 1 | Y | 349 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2728 | 1717 | 481 | 508 | 22 | | | |
| 1 | 1 | 335 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2614 | 1647 | 458 | 487 | 22 | | | |
| 1 | 3 | 342 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2676 | 1683 | 469 | 502 | 22 | | | |
| 1 | 5 | 347 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2712 | 1708 | 476 | 506 | 22 | | | |

There are 368 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| A | -20 | MET | - | expression tag | UNP P08559 |
| A | -19 | GLY | - | expression tag | UNP P08559 |
| A | -18 | SER | - | expression tag | UNP P08559 |
| A | -17 | SER | - | expression tag | UNP P08559 |
| A | -16 | HIS | - | expression tag | UNP P08559 |
| A | -15 | HIS | - | expression tag | UNP P08559 |
| A | -14 | HIS | - | expression tag | UNP P08559 |
| A | -13 | HIS | - | expression tag | UNP P08559 |
| A | -12 | HIS | - | expression tag | UNP P08559 |
| A | -11 | HIS | - | expression tag | UNP P08559 |
| A | -10 | SER | - | expression tag | UNP P08559 |
| A | -9 | SER | - | expression tag | UNP P08559 |
| A | -8 | GLY | - | expression tag | UNP P08559 |
| A | -7 | LEU | - | expression tag | UNP P08559 |
| A | -6 | VAL | - | expression tag | UNP P08559 |
| A | -5 | PRO | - | expression tag | UNP P08559 |
| A | -4 | ARG | - | expression tag | UNP P08559 |
| A | -3 | GLY | - | expression tag | UNP P08559 |
| A | -2 | SER | - | expression tag | UNP P08559 |
| A | -1 | HIS | - | expression tag | UNP P08559 |
| A | 0 | MET | - | expression tag | UNP P08559 |
| A | 203 | ALA | SER | engineered mutation | UNP P08559 |
| A | 271 | ALA | SER | engineered mutation | UNP P08559 |
| C | -20 | MET | - | expression tag | UNP P08559 |
| C | -19 | GLY | - | expression tag | UNP P08559 |
| C | -18 | SER | - | expression tag | UNP P08559 |
| C | -17 | SER | - | expression tag | UNP P08559 |
| C | -16 | HIS | - | expression tag | UNP P08559 |
| C | -15 | HIS | - | expression tag | UNP P08559 |
| C | -14 | HIS | - | expression tag | UNP P08559 |
| C | -13 | HIS | - | expression tag | UNP P08559 |
| C | -12 | HIS | - | expression tag | UNP P08559 |
| C | -11 | HIS | - | expression tag | UNP P08559 |
| C | -10 | SER | - | expression tag | UNP P08559 |
| C | -9 | SER | - | expression tag | UNP P08559 |
| C | -8 | GLY | - | expression tag | UNP P08559 |
| C | -7 | LEU | - | expression tag | UNP P08559 |
| C | -6 | VAL | - | expression tag | UNP P08559 |
| C | -5 | PRO | - | expression tag | UNP P08559 |
| C | -4 | ARG | - | expression tag | UNP P08559 |
| C | -3 | GLY | - | expression tag | UNP P08559 |
| C | -2 | SER | - | expression tag | UNP P08559 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| C | -1 | HIS | - | expression tag | UNP P08559 |
| C | 0 | MET | - | expression tag | UNP P08559 |
| C | 203 | ALA | SER | engineered mutation | UNP P08559 |
| C | 271 | ALA | SER | engineered mutation | UNP P08559 |
| E | -20 | MET | - | expression tag | UNP P08559 |
| E | -19 | GLY | - | expression tag | UNP P08559 |
| E | -18 | SER | - | expression tag | UNP P08559 |
| E | -17 | SER | - | expression tag | UNP P08559 |
| E | -16 | HIS | - | expression tag | UNP P08559 |
| E | -15 | HIS | - | expression tag | UNP P08559 |
| E | -14 | HIS | - | expression tag | UNP P08559 |
| E | -13 | HIS | - | expression tag | UNP P08559 |
| E | -12 | HIS | - | expression tag | UNP P08559 |
| E | -11 | HIS | - | expression tag | UNP P08559 |
| E | -10 | SER | - | expression tag | UNP P08559 |
| E | -9 | SER | - | expression tag | UNP P08559 |
| E | -8 | GLY | - | expression tag | UNP P08559 |
| E | -7 | LEU | - | expression tag | UNP P08559 |
| E | -6 | VAL | - | expression tag | UNP P08559 |
| E | -5 | PRO | - | expression tag | UNP P08559 |
| E | -4 | ARG | - | expression tag | UNP P08559 |
| E | -3 | GLY | - | expression tag | UNP P08559 |
| E | -2 | SER | - | expression tag | UNP P08559 |
| E | -1 | HIS | - | expression tag | UNP P08559 |
| E | 0 | MET | - | expression tag | UNP P08559 |
| E | 203 | ALA | SER | engineered mutation | UNP P08559 |
| E | 271 | ALA | SER | engineered mutation | UNP P08559 |
| G | -20 | MET | - | expression tag | UNP P08559 |
| G | -19 | GLY | - | expression tag | UNP P08559 |
| G | -18 | SER | - | expression tag | UNP P08559 |
| G | -17 | SER | - | expression tag | UNP P08559 |
| G | -16 | HIS | - | expression tag | UNP P08559 |
| G | -15 | HIS | - | expression tag | UNP P08559 |
| G | -14 | HIS | - | expression tag | UNP P08559 |
| G | -13 | HIS | - | expression tag | UNP P08559 |
| G | -12 | HIS | - | expression tag | UNP P08559 |
| G | -11 | HIS | - | expression tag | UNP P08559 |
| G | -10 | SER | - | expression tag | UNP P08559 |
| G | -9 | SER | - | expression tag | UNP P08559 |
| G | -8 | GLY | - | expression tag | UNP P08559 |
| G | -7 | LEU | - | expression tag | UNP P08559 |
| G | -6 | VAL | - | expression tag | UNP P08559 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| G | -5 | PRO | - | expression tag | UNP P08559 |
| G | -4 | ARG | - | expression tag | UNP P08559 |
| G | -3 | GLY | - | expression tag | UNP P08559 |
| G | -2 | SER | - | expression tag | UNP P08559 |
| G | -1 | HIS | - | expression tag | UNP P08559 |
| G | 0 | MET | - | expression tag | UNP P08559 |
| G | 203 | ALA | SER | engineered mutation | UNP P08559 |
| G | 271 | ALA | SER | engineered mutation | UNP P08559 |
| I | -20 | MET | - | expression tag | UNP P08559 |
| I | -19 | GLY | - | expression tag | UNP P08559 |
| I | -18 | SER | - | expression tag | UNP P08559 |
| I | -17 | SER | - | expression tag | UNP P08559 |
| I | -16 | HIS | - | expression tag | UNP P08559 |
| I | -15 | HIS | - | expression tag | UNP P08559 |
| I | -14 | HIS | - | expression tag | UNP P08559 |
| I | -13 | HIS | - | expression tag | UNP P08559 |
| I | -12 | HIS | - | expression tag | UNP P08559 |
| I | -11 | HIS | - | expression tag | UNP P08559 |
| I | -10 | SER | - | expression tag | UNP P08559 |
| I | -9 | SER | - | expression tag | UNP P08559 |
| I | -8 | GLY | - | expression tag | UNP P08559 |
| I | -7 | LEU | - | expression tag | UNP P08559 |
| I | -6 | VAL | - | expression tag | UNP P08559 |
| I | -5 | PRO | - | expression tag | UNP P08559 |
| I | -4 | ARG | - | expression tag | UNP P08559 |
| I | -3 | GLY | - | expression tag | UNP P08559 |
| I | -2 | SER | - | expression tag | UNP P08559 |
| I | -1 | HIS | - | expression tag | UNP P08559 |
| I | 0 | MET | - | expression tag | UNP P08559 |
| I | 203 | ALA | SER | engineered mutation | UNP P08559 |
| I | 271 | ALA | SER | engineered mutation | UNP P08559 |
| K | -20 | MET | - | expression tag | UNP P08559 |
| K | -19 | GLY | - | expression tag | UNP P08559 |
| K | -18 | SER | - | expression tag | UNP P08559 |
| K | -17 | SER | - | expression tag | UNP P08559 |
| K | -16 | HIS | - | expression tag | UNP P08559 |
| K | -15 | HIS | - | expression tag | UNP P08559 |
| K | -14 | HIS | - | expression tag | UNP P08559 |
| K | -13 | HIS | - | expression tag | UNP P08559 |
| K | -12 | HIS | - | expression tag | UNP P08559 |
| K | -11 | HIS | - | expression tag | UNP P08559 |
| K | -10 | SER | - | expression tag | UNP P08559 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| K | -9 | SER | - | expression tag | UNP P08559 |
| K | -8 | GLY | - | expression tag | UNP P08559 |
| K | -7 | LEU | - | expression tag | UNP P08559 |
| K | -6 | VAL | - | expression tag | UNP P08559 |
| K | -5 | PRO | - | expression tag | UNP P08559 |
| K | -4 | ARG | - | expression tag | UNP P08559 |
| K | -3 | GLY | - | expression tag | UNP P08559 |
| K | -2 | SER | - | expression tag | UNP P08559 |
| K | -1 | HIS | - | expression tag | UNP P08559 |
| K | 0 | MET | - | expression tag | UNP P08559 |
| K | 203 | ALA | SER | engineered mutation | UNP P08559 |
| K | 271 | ALA | SER | engineered mutation | UNP P08559 |
| M | -20 | MET | - | expression tag | UNP P08559 |
| M | -19 | GLY | - | expression tag | UNP P08559 |
| M | -18 | SER | - | expression tag | UNP P08559 |
| M | -17 | SER | - | expression tag | UNP P08559 |
| M | -16 | HIS | - | expression tag | UNP P08559 |
| M | -15 | HIS | - | expression tag | UNP P08559 |
| M | -14 | HIS | - | expression tag | UNP P08559 |
| M | -13 | HIS | - | expression tag | UNP P08559 |
| M | -12 | HIS | - | expression tag | UNP P08559 |
| M | -11 | HIS | - | expression tag | UNP P08559 |
| M | -10 | SER | - | expression tag | UNP P08559 |
| M | -9 | SER | - | expression tag | UNP P08559 |
| M | -8 | GLY | - | expression tag | UNP P08559 |
| M | -7 | LEU | - | expression tag | UNP P08559 |
| M | -6 | VAL | - | expression tag | UNP P08559 |
| M | -5 | PRO | - | expression tag | UNP P08559 |
| M | -4 | ARG | - | expression tag | UNP P08559 |
| M | -3 | GLY | - | expression tag | UNP P08559 |
| M | -2 | SER | - | expression tag | UNP P08559 |
| M | -1 | HIS | - | expression tag | UNP P08559 |
| M | 0 | MET | - | expression tag | UNP P08559 |
| M | 203 | ALA | SER | engineered mutation | UNP P08559 |
| M | 271 | ALA | SER | engineered mutation | UNP P08559 |
| O | -20 | MET | - | expression tag | UNP P08559 |
| O | -19 | GLY | - | expression tag | UNP P08559 |
| O | -18 | SER | - | expression tag | UNP P08559 |
| O | -17 | SER | - | expression tag | UNP P08559 |
| O | -16 | HIS | - | expression tag | UNP P08559 |
| O | -15 | HIS | - | expression tag | UNP P08559 |
| O | -14 | HIS | - | expression tag | UNP P08559 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| O | -13 | HIS | - | expression tag | UNP P08559 |
| O | -12 | HIS | - | expression tag | UNP P08559 |
| O | -11 | HIS | - | expression tag | UNP P08559 |
| O | -10 | SER | - | expression tag | UNP P08559 |
| O | -9 | SER | - | expression tag | UNP P08559 |
| O | -8 | GLY | - | expression tag | UNP P08559 |
| O | -7 | LEU | - | expression tag | UNP P08559 |
| O | -6 | VAL | - | expression tag | UNP P08559 |
| O | -5 | PRO | - | expression tag | UNP P08559 |
| O | -4 | ARG | - | expression tag | UNP P08559 |
| O | -3 | GLY | - | expression tag | UNP P08559 |
| O | -2 | SER | - | expression tag | UNP P08559 |
| O | -1 | HIS | - | expression tag | UNP P08559 |
| O | 0 | MET | - | expression tag | UNP P08559 |
| O | 203 | ALA | SER | engineered mutation | UNP P08559 |
| O | 271 | ALA | SER | engineered mutation | UNP P08559 |
| Q | -20 | MET | - | expression tag | UNP P08559 |
| Q | -19 | GLY | - | expression tag | UNP P08559 |
| Q | -18 | SER | - | expression tag | UNP P08559 |
| Q | -17 | SER | - | expression tag | UNP P08559 |
| Q | -16 | HIS | - | expression tag | UNP P08559 |
| Q | -15 | HIS | - | expression tag | UNP P08559 |
| Q | -14 | HIS | - | expression tag | UNP P08559 |
| Q | -13 | HIS | - | expression tag | UNP P08559 |
| Q | -12 | HIS | - | expression tag | UNP P08559 |
| Q | -11 | HIS | - | expression tag | UNP P08559 |
| Q | -10 | SER | - | expression tag | UNP P08559 |
| Q | -9 | SER | - | expression tag | UNP P08559 |
| Q | -8 | GLY | - | expression tag | UNP P08559 |
| Q | -7 | LEU | - | expression tag | UNP P08559 |
| Q | -6 | VAL | - | expression tag | UNP P08559 |
| Q | -5 | PRO | - | expression tag | UNP P08559 |
| Q | -4 | ARG | - | expression tag | UNP P08559 |
| Q | -3 | GLY | - | expression tag | UNP P08559 |
| Q | -2 | SER | - | expression tag | UNP P08559 |
| Q | -1 | HIS | - | expression tag | UNP P08559 |
| Q | 0 | MET | - | expression tag | UNP P08559 |
| Q | 203 | ALA | SER | engineered mutation | UNP P08559 |
| Q | 271 | ALA | SER | engineered mutation | UNP P08559 |
| S | -20 | MET | - | expression tag | UNP P08559 |
| S | -19 | GLY | - | expression tag | UNP P08559 |
| S | -18 | SER | - | expression tag | UNP P08559 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| S | -17 | SER | - | expression tag | UNP P08559 |
| S | -16 | HIS | - | expression tag | UNP P08559 |
| S | -15 | HIS | - | expression tag | UNP P08559 |
| S | -14 | HIS | - | expression tag | UNP P08559 |
| S | -13 | HIS | - | expression tag | UNP P08559 |
| S | -12 | HIS | - | expression tag | UNP P08559 |
| S | -11 | HIS | - | expression tag | UNP P08559 |
| S | -10 | SER | - | expression tag | UNP P08559 |
| S | -9 | SER | - | expression tag | UNP P08559 |
| S | -8 | GLY | - | expression tag | UNP P08559 |
| S | -7 | LEU | - | expression tag | UNP P08559 |
| S | -6 | VAL | - | expression tag | UNP P08559 |
| S | -5 | PRO | - | expression tag | UNP P08559 |
| S | -4 | ARG | - | expression tag | UNP P08559 |
| S | -3 | GLY | - | expression tag | UNP P08559 |
| S | -2 | SER | - | expression tag | UNP P08559 |
| S | -1 | HIS | - | expression tag | UNP P08559 |
| S | 0 | MET | - | expression tag | UNP P08559 |
| S | 203 | ALA | SER | engineered mutation | UNP P08559 |
| S | 271 | ALA | SER | engineered mutation | UNP P08559 |
| U | -20 | MET | - | expression tag | UNP P08559 |
| U | -19 | GLY | - | expression tag | UNP P08559 |
| U | -18 | SER | - | expression tag | UNP P08559 |
| U | -17 | SER | - | expression tag | UNP P08559 |
| U | -16 | HIS | - | expression tag | UNP P08559 |
| U | -15 | HIS | - | expression tag | UNP P08559 |
| U | -14 | HIS | - | expression tag | UNP P08559 |
| U | -13 | HIS | - | expression tag | UNP P08559 |
| U | -12 | HIS | - | expression tag | UNP P08559 |
| U | -11 | HIS | - | expression tag | UNP P08559 |
| U | -10 | SER | - | expression tag | UNP P08559 |
| U | -9 | SER | - | expression tag | UNP P08559 |
| U | -8 | GLY | - | expression tag | UNP P08559 |
| U | -7 | LEU | - | expression tag | UNP P08559 |
| U | -6 | VAL | - | expression tag | UNP P08559 |
| U | -5 | PRO | - | expression tag | UNP P08559 |
| U | -4 | ARG | - | expression tag | UNP P08559 |
| U | -3 | GLY | - | expression tag | UNP P08559 |
| U | -2 | SER | - | expression tag | UNP P08559 |
| U | -1 | HIS | - | expression tag | UNP P08559 |
| U | 0 | MET | - | expression tag | UNP P08559 |
| U | 203 | ALA | SER | engineered mutation | UNP P08559 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| U | 271 | ALA | SER | engineered mutation | UNP P08559 |
| W | -20 | MET | - | expression tag | UNP P08559 |
| W | -19 | GLY | - | expression tag | UNP P08559 |
| W | -18 | SER | - | expression tag | UNP P08559 |
| W | -17 | SER | - | expression tag | UNP P08559 |
| W | -16 | HIS | - | expression tag | UNP P08559 |
| W | -15 | HIS | - | expression tag | UNP P08559 |
| W | -14 | HIS | - | expression tag | UNP P08559 |
| W | -13 | HIS | - | expression tag | UNP P08559 |
| W | -12 | HIS | - | expression tag | UNP P08559 |
| W | -11 | HIS | - | expression tag | UNP P08559 |
| W | -10 | SER | - | expression tag | UNP P08559 |
| W | -9 | SER | - | expression tag | UNP P08559 |
| W | -8 | GLY | - | expression tag | UNP P08559 |
| W | -7 | LEU | - | expression tag | UNP P08559 |
| W | -6 | VAL | - | expression tag | UNP P08559 |
| W | -5 | PRO | - | expression tag | UNP P08559 |
| W | -4 | ARG | - | expression tag | UNP P08559 |
| W | -3 | GLY | - | expression tag | UNP P08559 |
| W | -2 | SER | - | expression tag | UNP P08559 |
| W | -1 | HIS | - | expression tag | UNP P08559 |
| W | 0 | MET | - | expression tag | UNP P08559 |
| W | 203 | ALA | SER | engineered mutation | UNP P08559 |
| W | 271 | ALA | SER | engineered mutation | UNP P08559 |
| Y | -20 | MET | - | expression tag | UNP P08559 |
| Y | -19 | GLY | - | expression tag | UNP P08559 |
| Y | -18 | SER | - | expression tag | UNP P08559 |
| Y | -17 | SER | - | expression tag | UNP P08559 |
| Y | -16 | HIS | - | expression tag | UNP P08559 |
| Y | -15 | HIS | - | expression tag | UNP P08559 |
| Y | -14 | HIS | - | expression tag | UNP P08559 |
| Y | -13 | HIS | - | expression tag | UNP P08559 |
| Y | -12 | HIS | - | expression tag | UNP P08559 |
| Y | -11 | HIS | - | expression tag | UNP P08559 |
| Y | -10 | SER | - | expression tag | UNP P08559 |
| Y | -9 | SER | - | expression tag | UNP P08559 |
| Y | -8 | GLY | - | expression tag | UNP P08559 |
| Y | -7 | LEU | - | expression tag | UNP P08559 |
| Y | -6 | VAL | - | expression tag | UNP P08559 |
| Y | -5 | PRO | - | expression tag | UNP P08559 |
| Y | -4 | ARG | - | expression tag | UNP P08559 |
| Y | -3 | GLY | - | expression tag | UNP P08559 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| Y | -2 | SER | - | expression tag | UNP P08559 |
| Y | -1 | HIS | - | expression tag | UNP P08559 |
| Y | 0 | MET | - | expression tag | UNP P08559 |
| Y | 203 | ALA | SER | engineered mutation | UNP P08559 |
| Y | 271 | ALA | SER | engineered mutation | UNP P08559 |
| 1 | -20 | MET | - | expression tag | UNP P08559 |
| 1 | -19 | GLY | - | expression tag | UNP P08559 |
| 1 | -18 | SER | - | expression tag | UNP P08559 |
| 1 | -17 | SER | - | expression tag | UNP P08559 |
| 1 | -16 | HIS | - | expression tag | UNP P08559 |
| 1 | -15 | HIS | - | expression tag | UNP P08559 |
| 1 | -14 | HIS | - | expression tag | UNP P08559 |
| 1 | -13 | HIS | - | expression tag | UNP P08559 |
| 1 | -12 | HIS | - | expression tag | UNP P08559 |
| 1 | -11 | HIS | - | expression tag | UNP P08559 |
| 1 | -10 | SER | - | expression tag | UNP P08559 |
| 1 | -9 | SER | - | expression tag | UNP P08559 |
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| 1 | -7 | LEU | - | expression tag | UNP P08559 |
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| 1 | -4 | ARG | - | expression tag | UNP P08559 |
| 1 | -3 | GLY | - | expression tag | UNP P08559 |
| 1 | -2 | SER | - | expression tag | UNP P08559 |
| 1 | -1 | HIS | - | expression tag | UNP P08559 |
| 1 | 0 | MET | - | expression tag | UNP P08559 |
| 1 | 203 | ALA | SER | engineered mutation | UNP P08559 |
| 1 | 271 | ALA | SER | engineered mutation | UNP P08559 |
| 3 | -20 | MET | - | expression tag | UNP P08559 |
| 3 | -19 | GLY | - | expression tag | UNP P08559 |
| 3 | -18 | SER | - | expression tag | UNP P08559 |
| 3 | -17 | SER | - | expression tag | UNP P08559 |
| 3 | -16 | HIS | - | expression tag | UNP P08559 |
| 3 | -15 | HIS | - | expression tag | UNP P08559 |
| 3 | -14 | HIS | - | expression tag | UNP P08559 |
| 3 | -13 | HIS | - | expression tag | UNP P08559 |
| 3 | -12 | HIS | - | expression tag | UNP P08559 |
| 3 | -11 | HIS | - | expression tag | UNP P08559 |
| 3 | -10 | SER | - | expression tag | UNP P08559 |
| 3 | -9 | SER | - | expression tag | UNP P08559 |
| 3 | -8 | GLY | - | expression tag | UNP P08559 |
| 3 | -7 | LEU | - | expression tag | UNP P08559 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| 3 | -6 | VAL | - | expression tag | UNP P08559 |
| 3 | -5 | PRO | - | expression tag | UNP P08559 |
| 3 | -4 | ARG | - | expression tag | UNP P08559 |
| 3 | -3 | GLY | - | expression tag | UNP P08559 |
| 3 | -2 | SER | - | expression tag | UNP P08559 |
| 3 | -1 | HIS | - | expression tag | UNP P08559 |
| 3 | 0 | MET | - | expression tag | UNP P08559 |
| 3 | 203 | ALA | SER | engineered mutation | UNP P08559 |
| 3 | 271 | ALA | SER | engineered mutation | UNP P08559 |
| 5 | -20 | MET | - | expression tag | UNP P08559 |
| 5 | -19 | GLY | - | expression tag | UNP P08559 |
| 5 | -18 | SER | - | expression tag | UNP P08559 |
| 5 | -17 | SER | - | expression tag | UNP P08559 |
| 5 | -16 | HIS | - | expression tag | UNP P08559 |
| 5 | -15 | HIS | - | expression tag | UNP P08559 |
| 5 | -14 | HIS | - | expression tag | UNP P08559 |
| 5 | -13 | HIS | - | expression tag | UNP P08559 |
| 5 | -12 | HIS | - | expression tag | UNP P08559 |
| 5 | -11 | HIS | - | expression tag | UNP P08559 |
| 5 | -10 | SER | - | expression tag | UNP P08559 |
| 5 | -9 | SER | - | expression tag | UNP P08559 |
| 5 | -8 | GLY | - | expression tag | UNP P08559 |
| 5 | -7 | LEU | - | expression tag | UNP P08559 |
| 5 | -6 | VAL | - | expression tag | UNP P08559 |
| 5 | -5 | PRO | - | expression tag | UNP P08559 |
| 5 | -4 | ARG | - | expression tag | UNP P08559 |
| 5 | -3 | GLY | - | expression tag | UNP P08559 |
| 5 | -2 | SER | - | expression tag | UNP P08559 |
| 5 | -1 | HIS | - | expression tag | UNP P08559 |
| 5 | 0 | MET | - | expression tag | UNP P08559 |
| 5 | 203 | ALA | SER | engineered mutation | UNP P08559 |
| 5 | 271 | ALA | SER | engineered mutation | UNP P08559 |

- Molecule 2 is a protein called Pyruvate dehydrogenase E1 component subunit beta, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 2 | B | 329 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2519 | 1604 | 427 | 469 | 19 | | | |
| 2 | D | 329 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2519 | 1604 | 427 | 469 | 19 | | | |
| 2 | F | 329 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2519 | 1604 | 427 | 469 | 19 | | | |

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| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 2 | H | 329 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2519 | 1604 | 427 | 469 | 19 | | | |
| 2 | J | 329 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2519 | 1604 | 427 | 469 | 19 | | | |
| 2 | L | 329 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2519 | 1604 | 427 | 469 | 19 | | | |
| 2 | N | 329 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2519 | 1604 | 427 | 469 | 19 | | | |
| 2 | P | 329 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2519 | 1604 | 427 | 469 | 19 | | | |
| 2 | R | 329 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2519 | 1604 | 427 | 469 | 19 | | | |
| 2 | T | 329 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2519 | 1604 | 427 | 469 | 19 | | | |
| 2 | V | 329 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2519 | 1604 | 427 | 469 | 19 | | | |
| 2 | X | 329 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2519 | 1604 | 427 | 469 | 19 | | | |
| 2 | Z | 329 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2519 | 1604 | 427 | 469 | 19 | | | |
| 2 | 2 | 329 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2519 | 1604 | 427 | 469 | 19 | | | |
| 2 | 4 | 329 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2519 | 1604 | 427 | 469 | 19 | | | |
| 2 | 6 | 329 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2519 | 1604 | 427 | 469 | 19 | | | |

- Molecule 3 is POTASSIUM ION (three-letter code: K) (formula: K).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|
| 3 | B | 1 | Total | K | 0 | 0 |
| | | | 1 | 1 | | |
| 3 | D | 1 | Total | K | 0 | 0 |
| | | | 1 | 1 | | |
| 3 | F | 1 | Total | K | 0 | 0 |
| | | | 1 | 1 | | |
| 3 | H | 1 | Total | K | 0 | 0 |
| | | | 1 | 1 | | |
| 3 | J | 1 | Total | K | 0 | 0 |
| | | | 1 | 1 | | |
| 3 | L | 1 | Total | K | 0 | 0 |
| | | | 1 | 1 | | |

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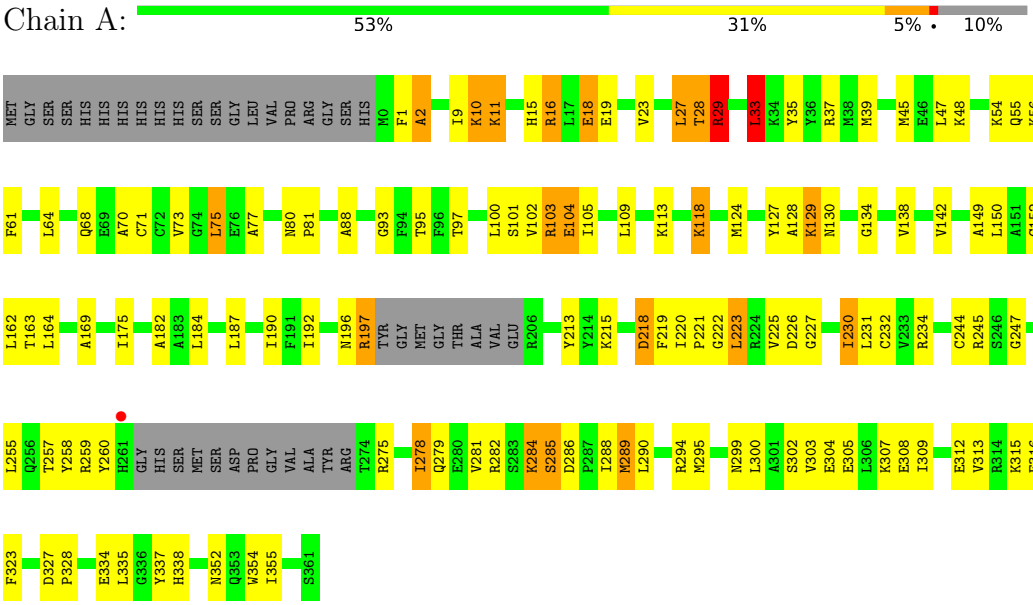
| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 3 | N | 1 | Total K<br>1 1 | 0 | 0 |
| 3 | P | 1 | Total K<br>1 1 | 0 | 0 |
| 3 | R | 1 | Total K<br>1 1 | 0 | 0 |
| 3 | T | 1 | Total K<br>1 1 | 0 | 0 |
| 3 | V | 1 | Total K<br>1 1 | 0 | 0 |
| 3 | X | 1 | Total K<br>1 1 | 0 | 0 |
| 3 | Z | 1 | Total K<br>1 1 | 0 | 0 |
| 3 | 2 | 1 | Total K<br>1 1 | 0 | 0 |
| 3 | 4 | 1 | Total K<br>1 1 | 0 | 0 |
| 3 | 6 | 1 | Total K<br>1 1 | 0 | 0 |

# 3 Residue-property plots (i)

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

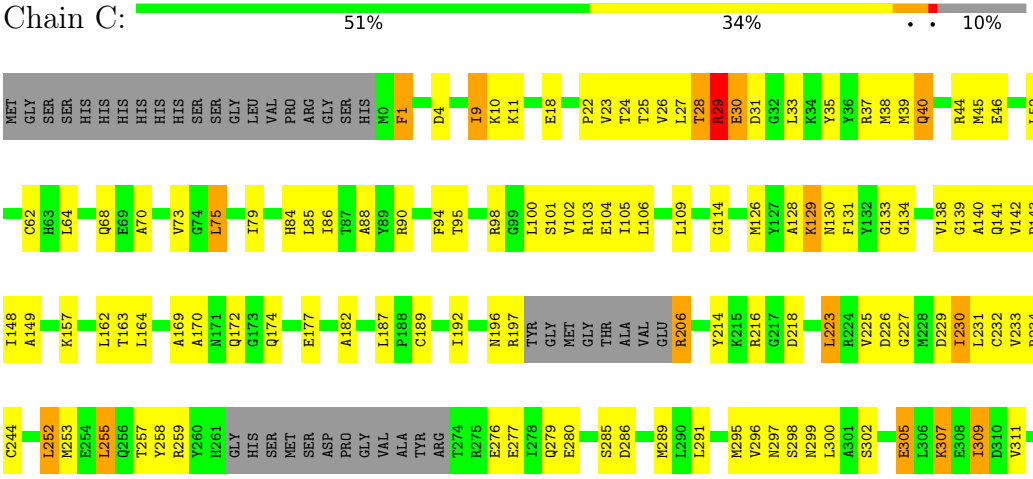
• Molecule 1: Pyruvate dehydrogenase E1 component subunit alpha, somatic form, mitochondrial

Chain A:



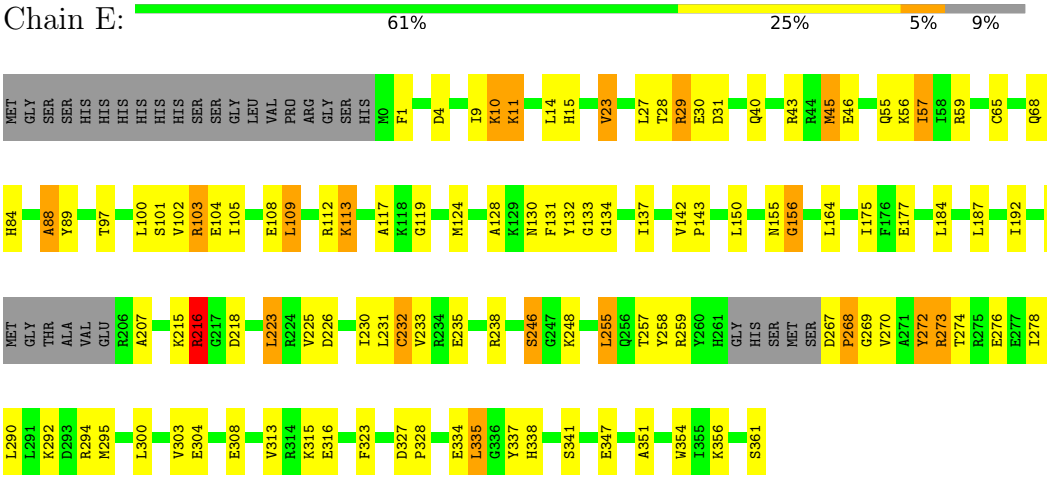

• Molecule 1: Pyruvate dehydrogenase E1 component subunit alpha, somatic form, mitochondrial

Chain C:



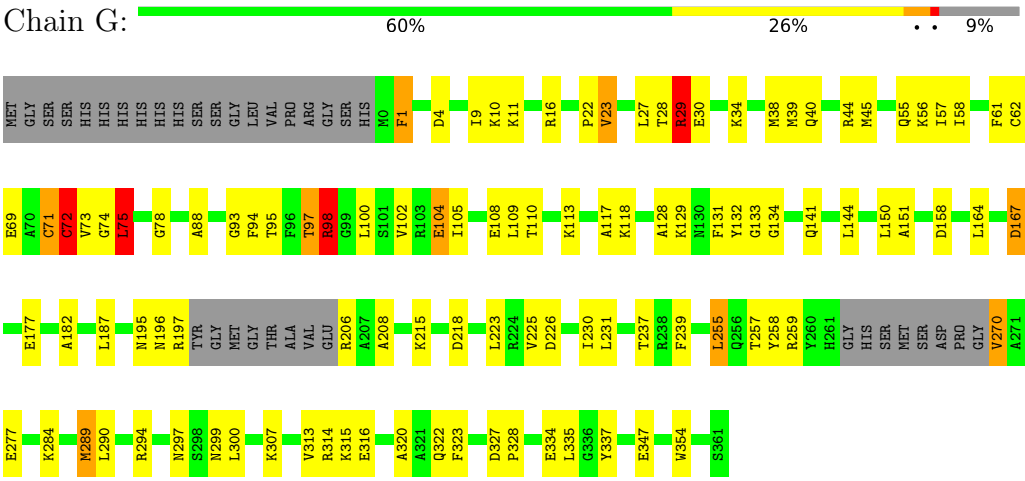
• Molecule 1: Pyruvate dehydrogenase E1 component subunit alpha, somatic form, mitochondrial

Chain E:



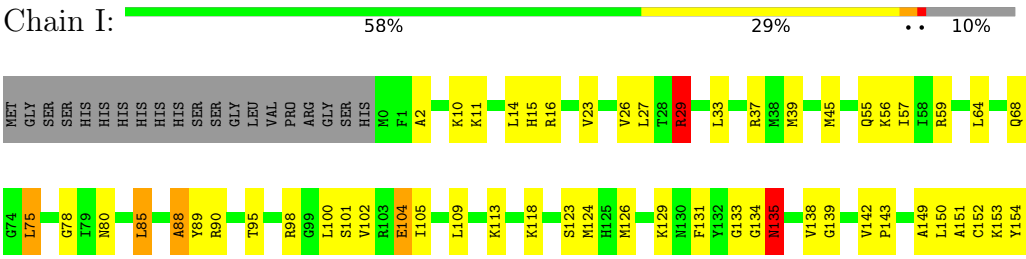

• Molecule 1: Pyruvate dehydrogenase E1 component subunit alpha, somatic form, mitochondrial

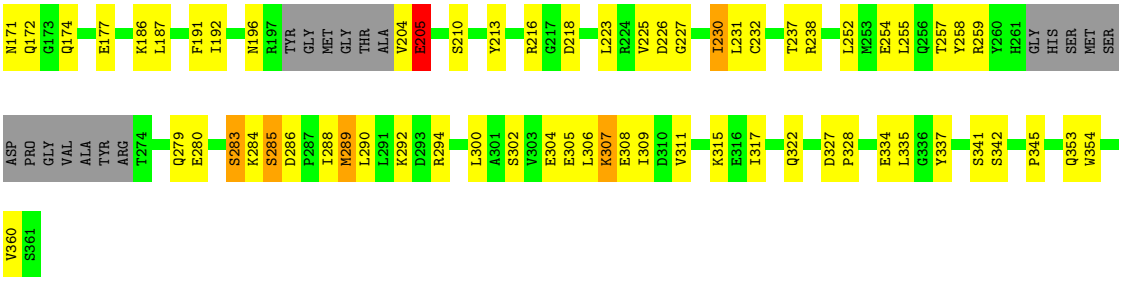
Chain G:




• Molecule 1: Pyruvate dehydrogenase E1 component subunit alpha, somatic form, mitochondrial

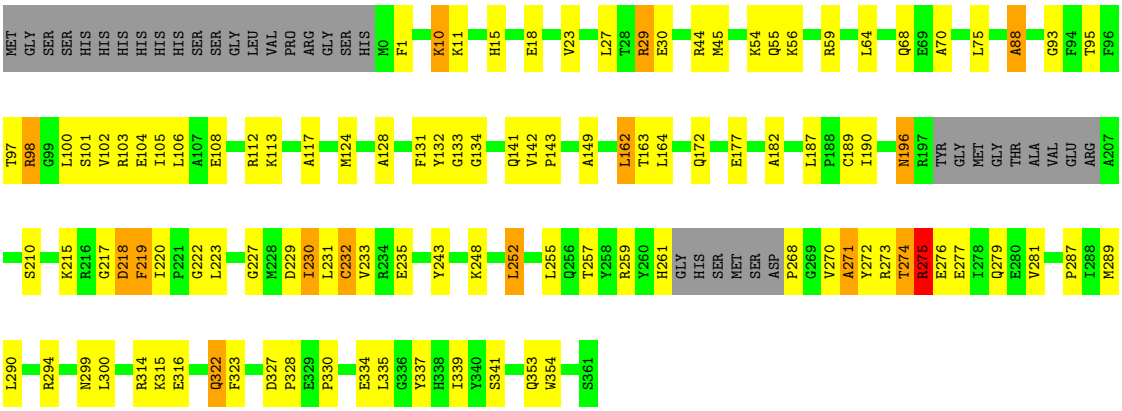
Chain I:





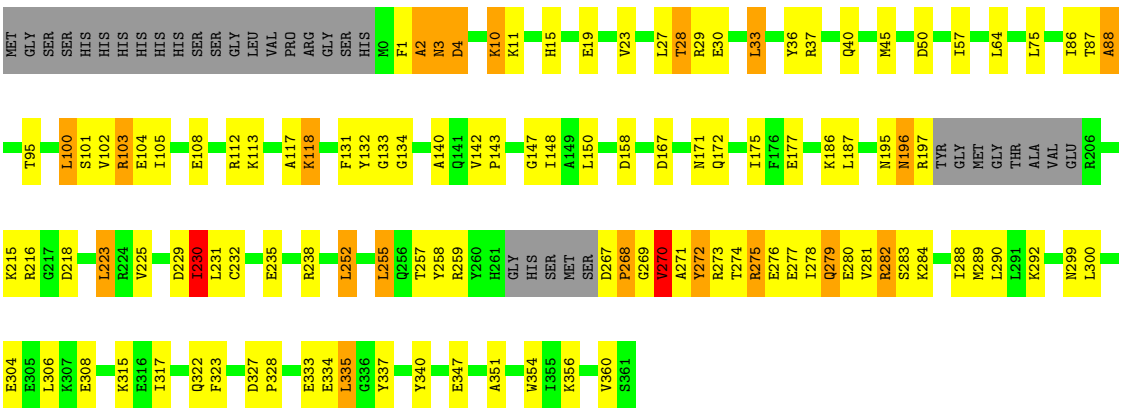
• Molecule 1: Pyruvate dehydrogenase E1 component subunit alpha, somatic form, mitochondrial

Chain K:



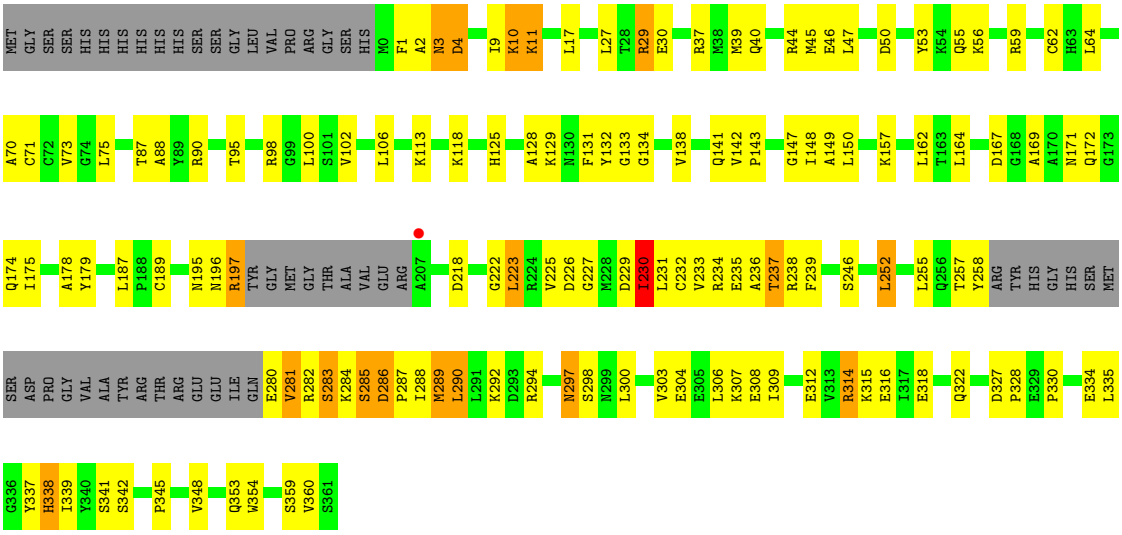
• Molecule 1: Pyruvate dehydrogenase E1 component subunit alpha, somatic form, mitochondrial

Chain M:



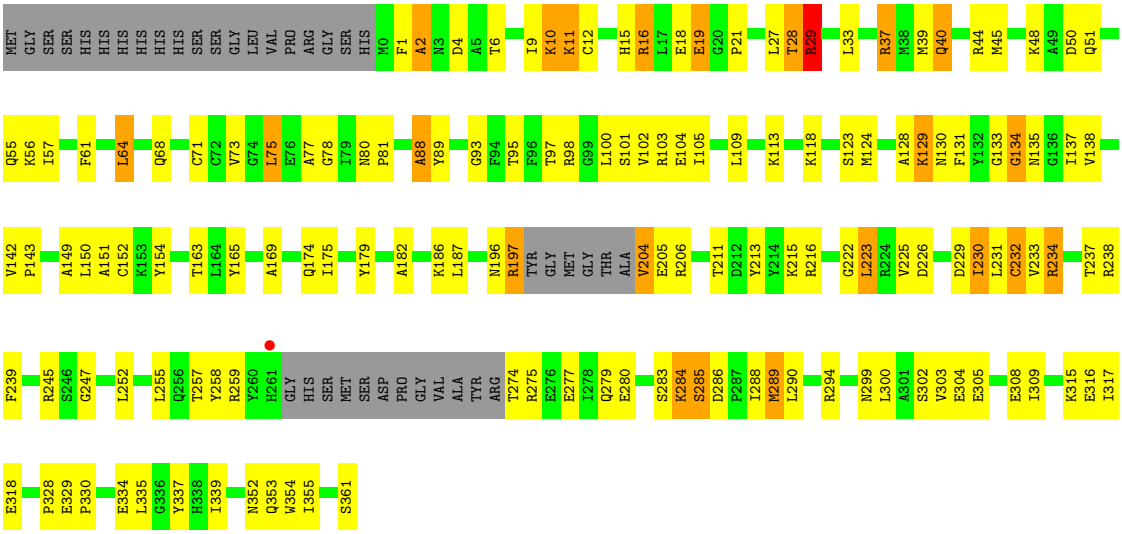
• Molecule 1: Pyruvate dehydrogenase E1 component subunit alpha, somatic form, mitochondrial

Chain O:



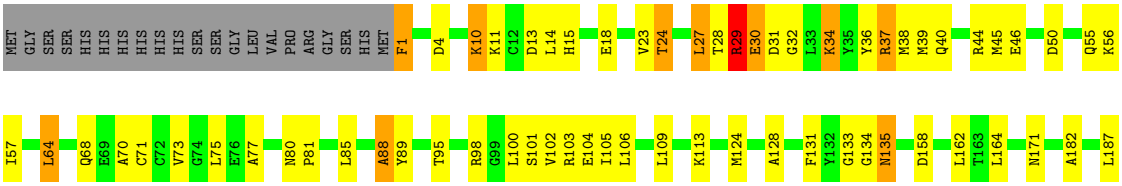
• Molecule 1: Pyruvate dehydrogenase E1 component subunit alpha, somatic form, mitochondrial

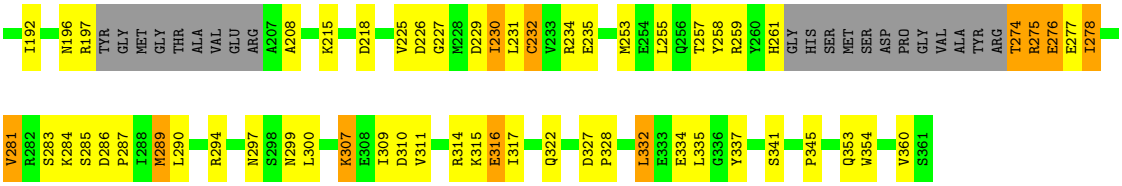
Chain Q:



• Molecule 1: Pyruvate dehydrogenase E1 component subunit alpha, somatic form, mitochondrial

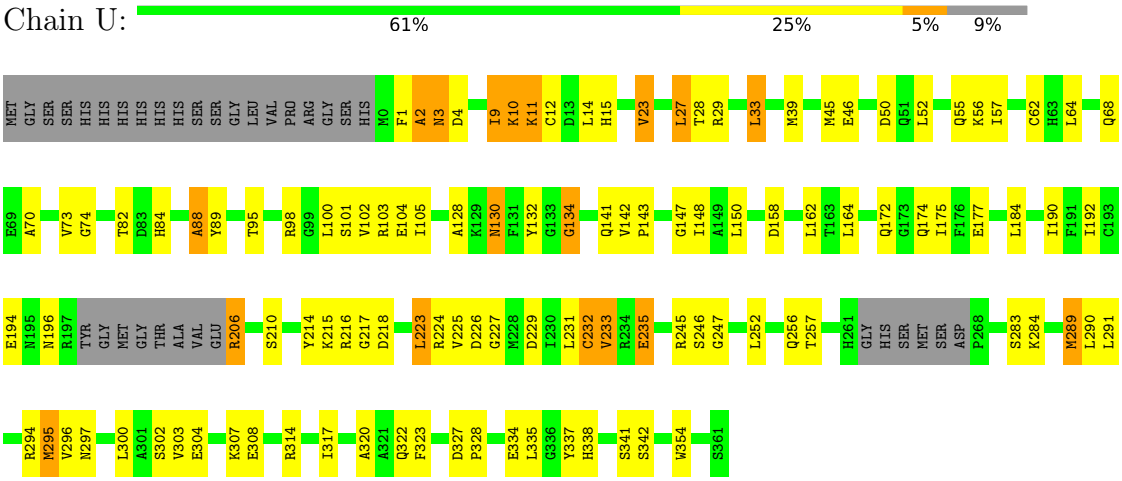
Chain S:





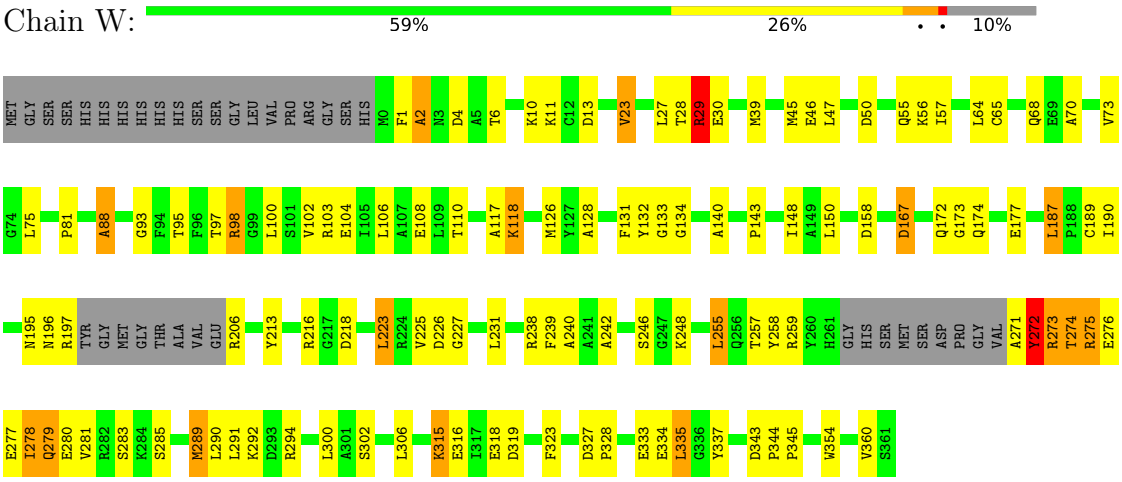
• Molecule 1: Pyruvate dehydrogenase E1 component subunit alpha, somatic form, mitochondrial

Chain U:



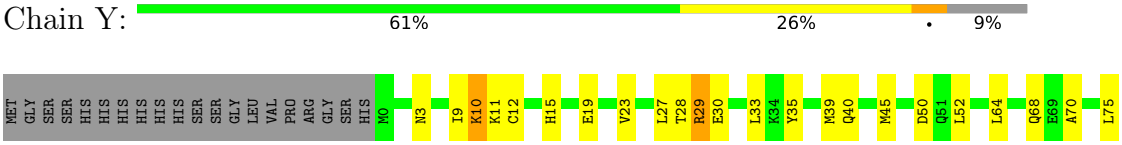

• Molecule 1: Pyruvate dehydrogenase E1 component subunit alpha, somatic form, mitochondrial

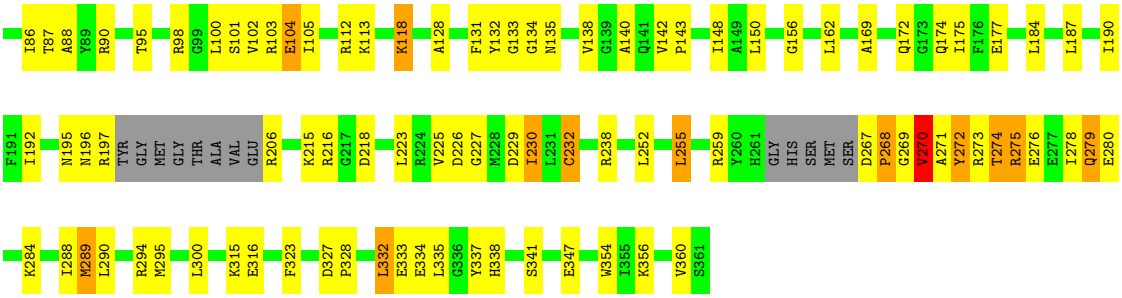
Chain W:




• Molecule 1: Pyruvate dehydrogenase E1 component subunit alpha, somatic form, mitochondrial

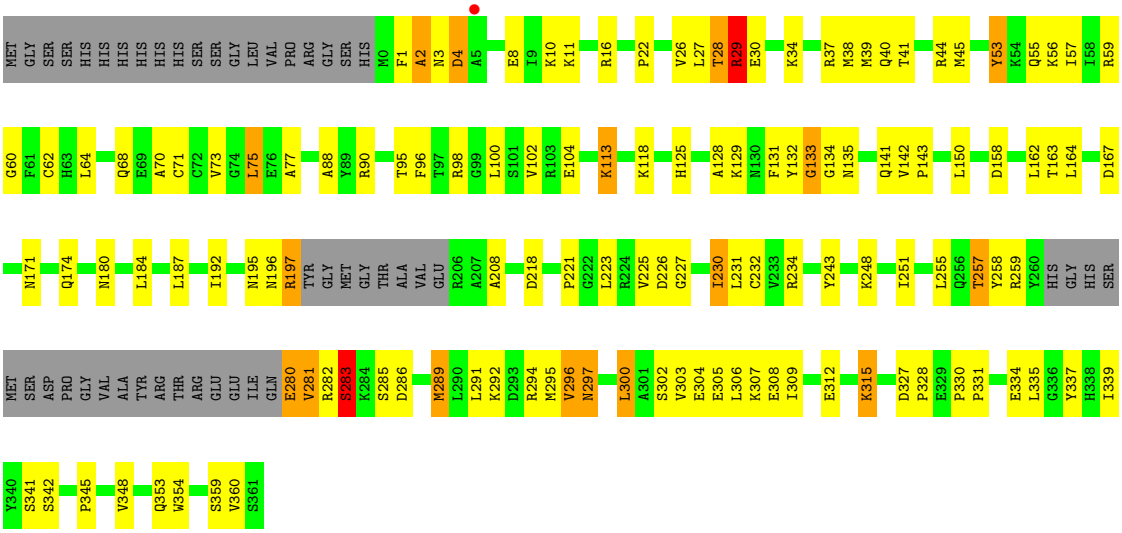
Chain Y:





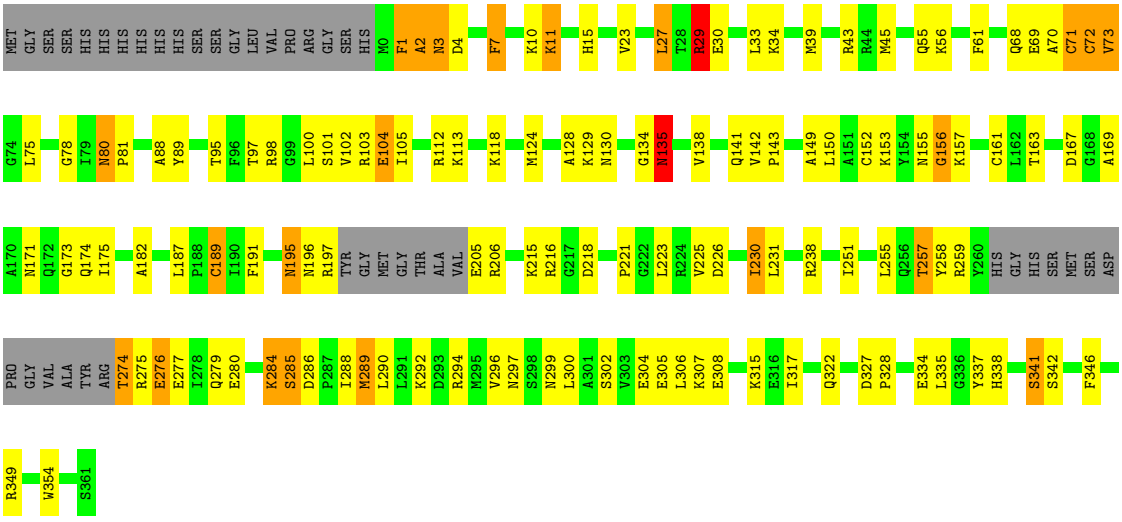
• Molecule 1: Pyruvate dehydrogenase E1 component subunit alpha, somatic form, mitochondrial

Chain 1:



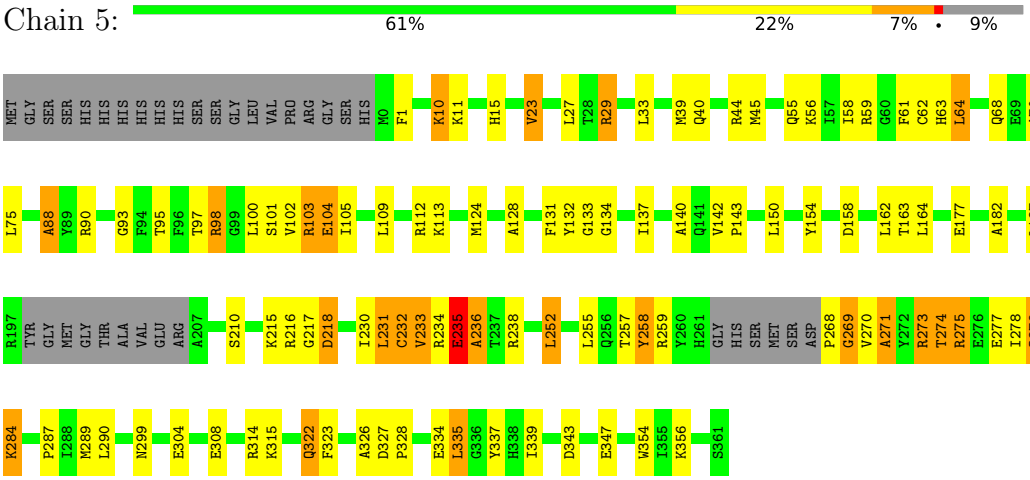
• Molecule 1: Pyruvate dehydrogenase E1 component subunit alpha, somatic form, mitochondrial

Chain 3:



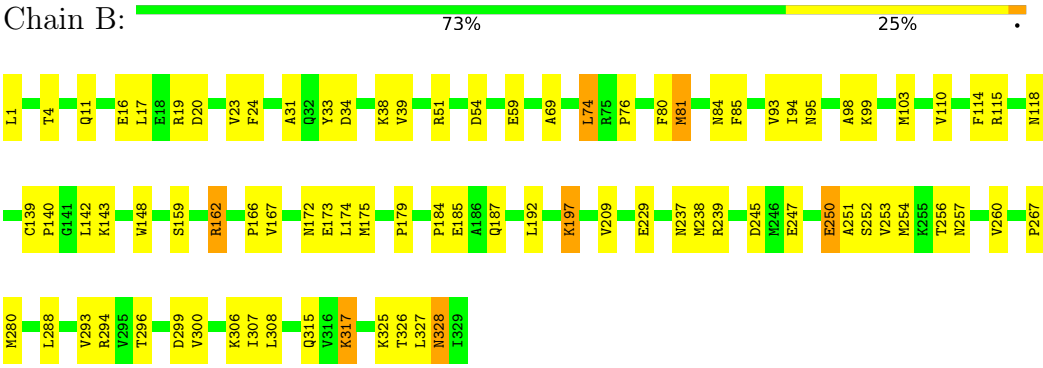
• Molecule 1: Pyruvate dehydrogenase E1 component subunit alpha, somatic form, mitochondrial

Chain 5:



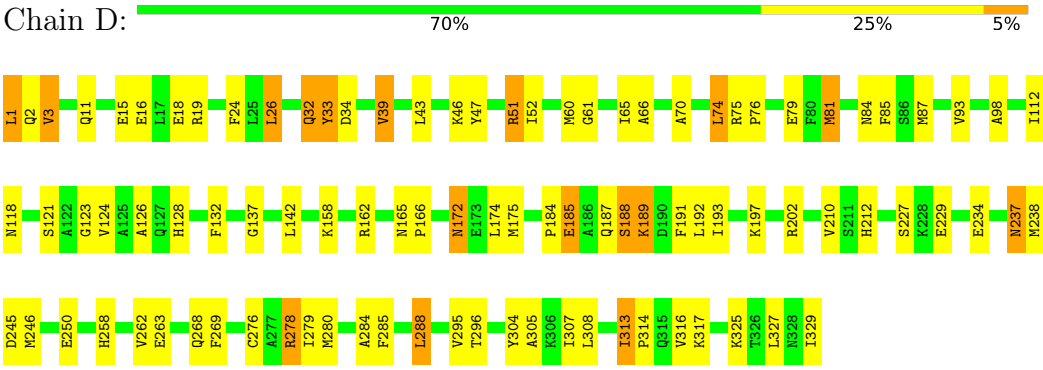

• Molecule 2: Pyruvate dehydrogenase E1 component subunit beta, mitochondrial

Chain B:



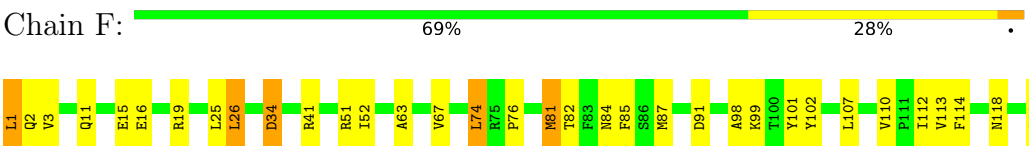

• Molecule 2: Pyruvate dehydrogenase E1 component subunit beta, mitochondrial

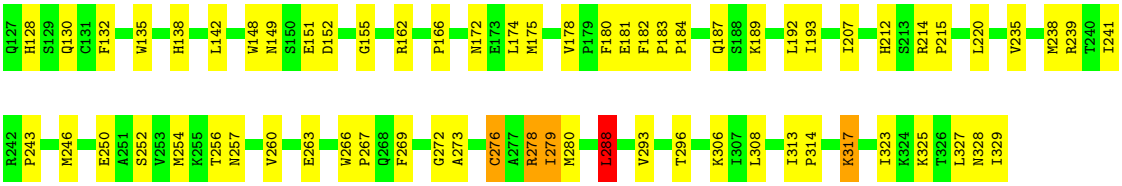
Chain D:




• Molecule 2: Pyruvate dehydrogenase E1 component subunit beta, mitochondrial

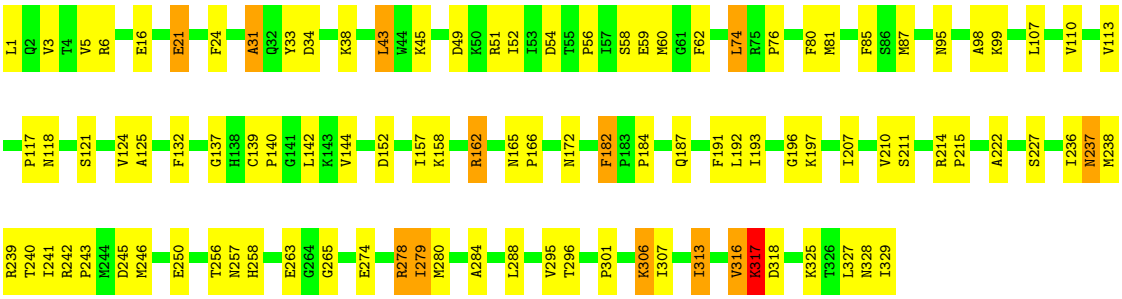
Chain F:





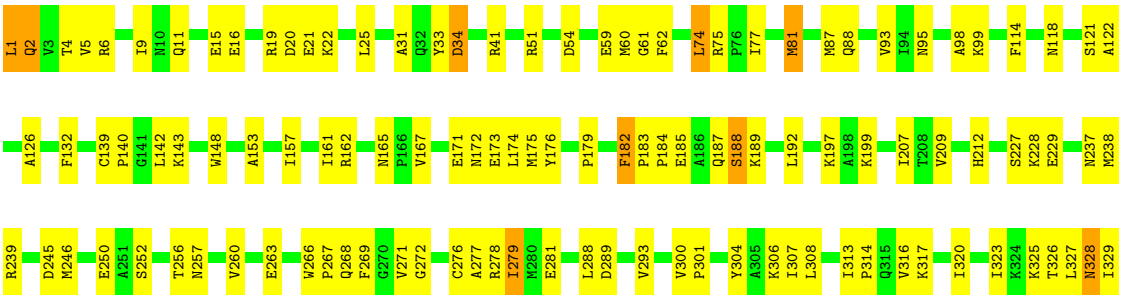

• Molecule 2: Pyruvate dehydrogenase E1 component subunit beta, mitochondrial

Chain H:



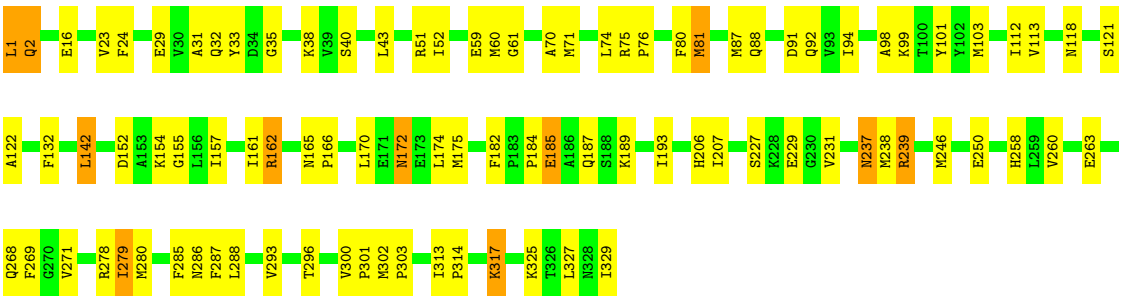

• Molecule 2: Pyruvate dehydrogenase E1 component subunit beta, mitochondrial

Chain J:



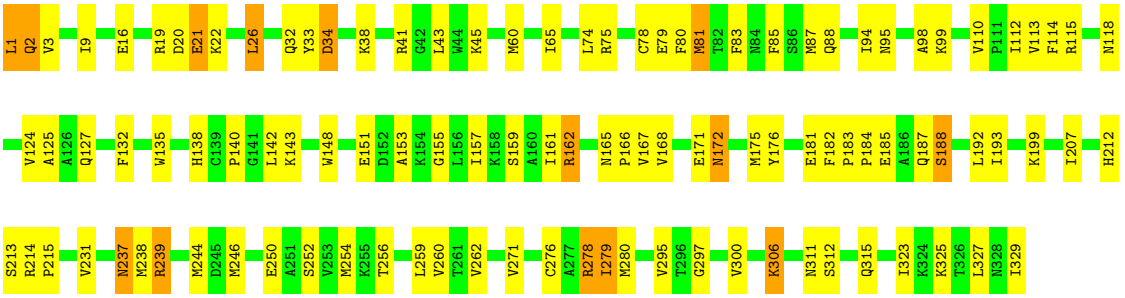

• Molecule 2: Pyruvate dehydrogenase E1 component subunit beta, mitochondrial

Chain L:



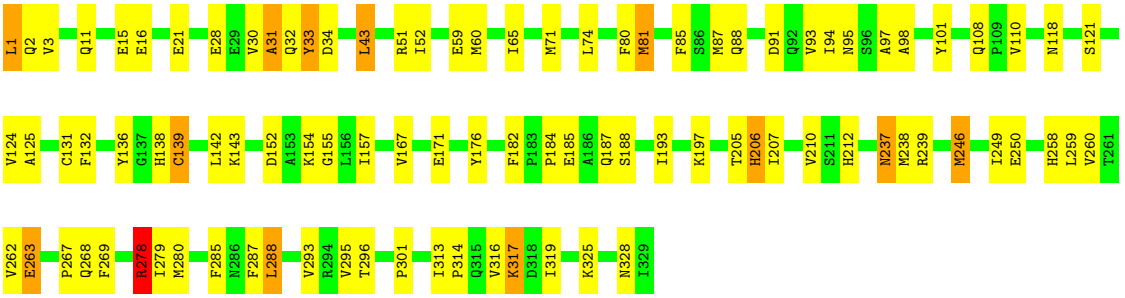

• Molecule 2: Pyruvate dehydrogenase E1 component subunit beta, mitochondrial

Chain N:



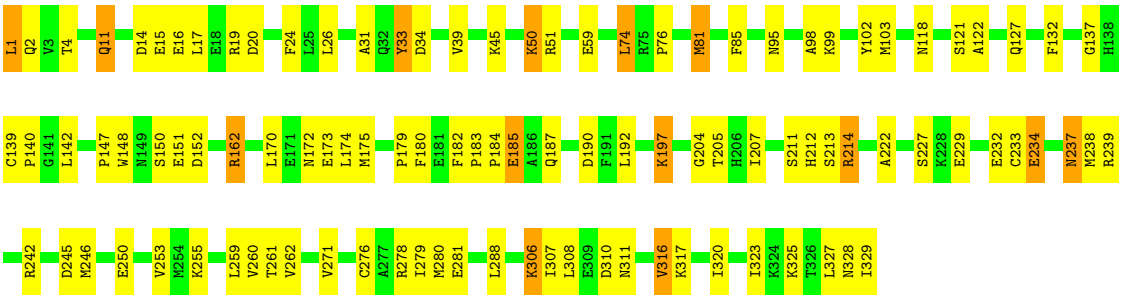

• Molecule 2: Pyruvate dehydrogenase E1 component subunit beta, mitochondrial

Chain P:



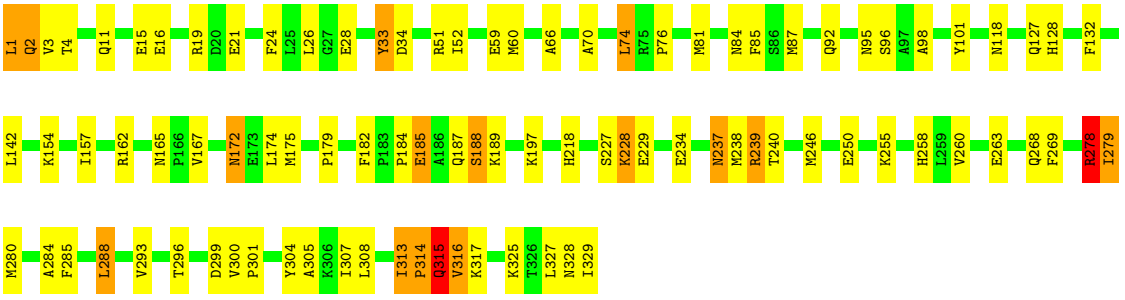

• Molecule 2: Pyruvate dehydrogenase E1 component subunit beta, mitochondrial

Chain R:



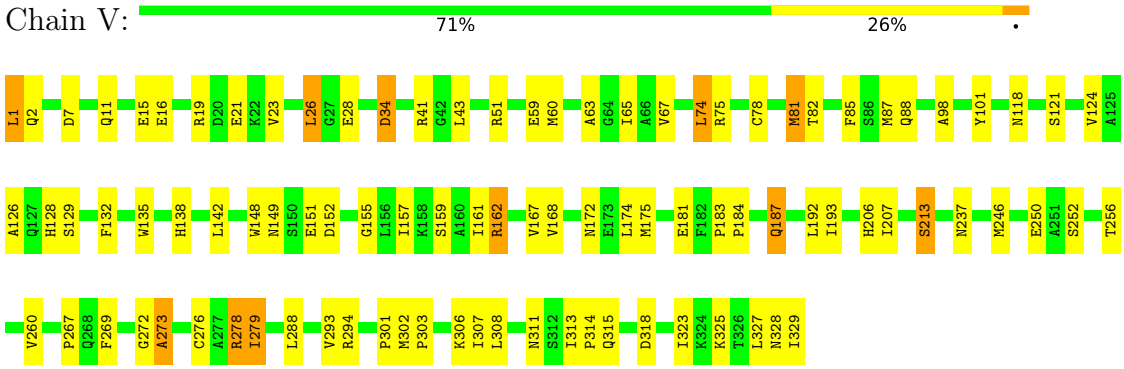

• Molecule 2: Pyruvate dehydrogenase E1 component subunit beta, mitochondrial

Chain T:



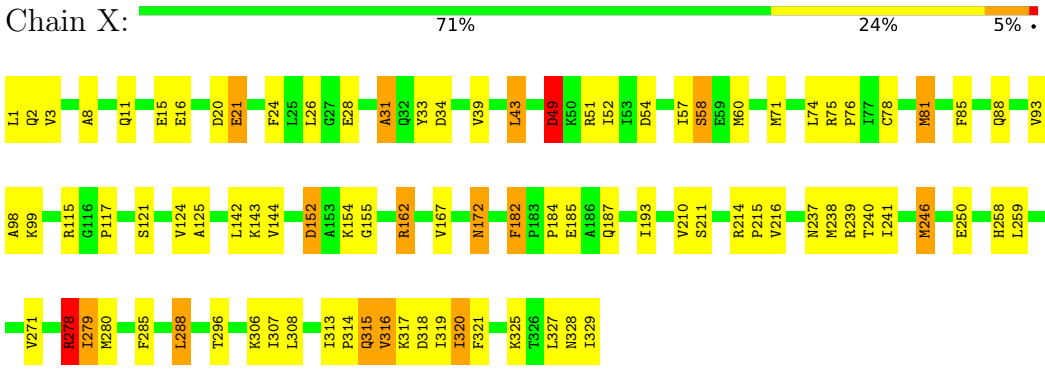

• Molecule 2: Pyruvate dehydrogenase E1 component subunit beta, mitochondrial

Chain V:



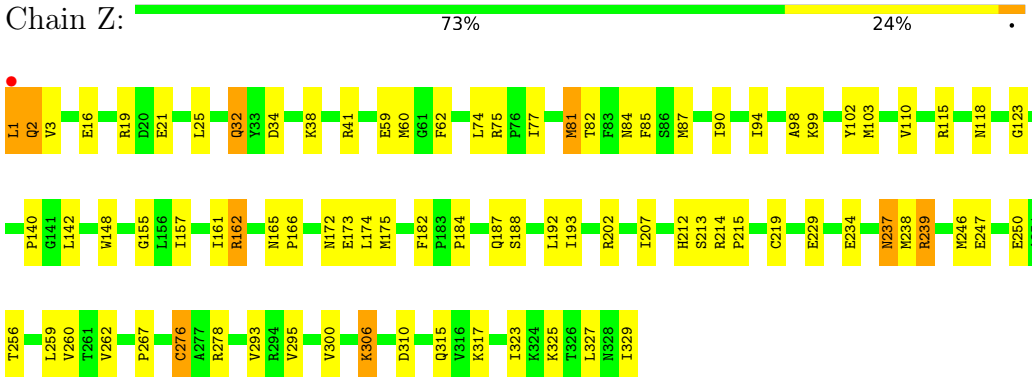

• Molecule 2: Pyruvate dehydrogenase E1 component subunit beta, mitochondrial

Chain X:



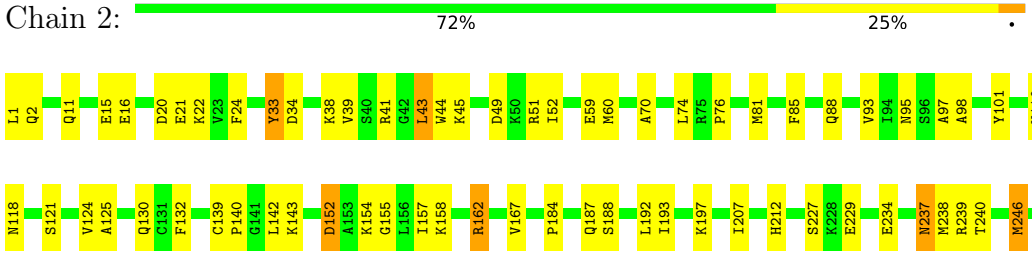

• Molecule 2: Pyruvate dehydrogenase E1 component subunit beta, mitochondrial

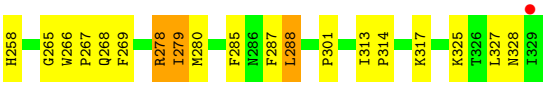
Chain Z:




• Molecule 2: Pyruvate dehydrogenase E1 component subunit beta, mitochondrial

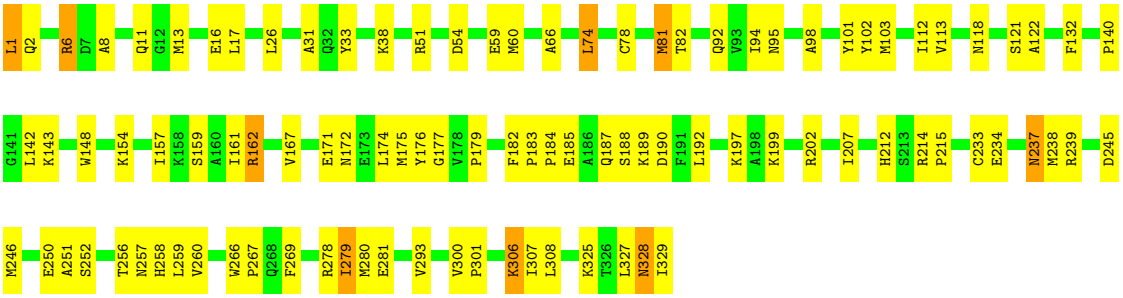
Chain 2:






• Molecule 2: Pyruvate dehydrogenase E1 component subunit beta, mitochondrial

Chain 4:




• Molecule 2: Pyruvate dehydrogenase E1 component subunit beta, mitochondrial

Chain 6:

# 4 Data and refinement statistics (i)

| Property | Value | Source |
|---|---|---|
| Space group | P 1 | Depositor |
| Cell constants<br>a, b, c, $\alpha$, $\beta$, $\gamma$ | 119.28Å 128.29Å 228.41Å<br>90.14° 90.05° 90.02° | Depositor |
| Resolution (Å) | 50.00 – 3.01<br>49.11 – 3.01 | Depositor<br>EDS |
| % Data completeness<br>(in resolution range) | 97.9 (50.00-3.01)<br>97.9 (49.11-3.01) | Depositor<br>EDS |
| $R_{merge}$ | 0.08 | Depositor |
| $R_{sym}$ | (Not available) | Depositor |
| $< I/\sigma(I) >$ [1] | 2.43 (at 3.01Å) | Xtriage |
| Refinement program | REFMAC 5.4.0069 | Depositor |
| R, $R_{free}$ | 0.189 , 0.253<br>0.196 , 0.257 | Depositor<br>DCC |
| $R_{free}$ test set | 13221 reflections (5.04%) | wwPDB-VP |
| Wilson B-factor (Å$^2$) | 56.5 | Xtriage |
| Anisotropy | 0.005 | Xtriage |
| Bulk solvent $k_{sol}$(e/Å$^3$), $B_{sol}$(Å$^2$) | 0.33 , 41.1 | EDS |
| L-test for twinning[2] | $< \|L\| > = 0.53$, $< L^2 > = 0.36$ | Xtriage |
| Estimated twinning fraction | 0.429 for h,-k,-l<br>0.000 for -h,k,-l<br>0.000 for -h,-k,l | Xtriage |
| $F_o$,$F_c$ correlation | 0.95 | EDS |
| Total number of atoms | 83339 | wwPDB-VP |
| Average B, all atoms (Å$^2$) | 55.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 46.55 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.1273e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

# 5 Model quality (i)

## 5.1 Standard geometry (i)

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

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

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | #$\|Z\|$ >5 | RMSZ | #$\|Z\|$ >5 |
| 1 | 1 | 0.79 | 1/2663 (0.0%) | 0.87 | 2/3583 (0.1%) |
| 1 | 3 | 0.87 | 3/2725 (0.1%) | 0.91 | 3/3666 (0.1%) |
| 1 | 5 | 0.78 | 2/2764 (0.1%) | 0.83 | 2/3720 (0.1%) |
| 1 | A | 0.93 | 2/2727 (0.1%) | 0.94 | 3/3669 (0.1%) |
| 1 | C | 0.92 | 3/2727 (0.1%) | 0.92 | 2/3669 (0.1%) |
| 1 | E | 0.91 | 1/2780 (0.0%) | 0.96 | 1/3742 (0.0%) |
| 1 | G | 0.90 | 4/2763 (0.1%) | 0.93 | 3/3718 (0.1%) |
| 1 | I | 0.88 | 1/2743 (0.0%) | 0.90 | 3/3691 (0.1%) |
| 1 | K | 0.81 | 0/2764 | 0.85 | 1/3720 (0.0%) |
| 1 | M | 0.90 | 3/2780 (0.1%) | 0.93 | 2/3742 (0.1%) |
| 1 | O | 0.81 | 0/2628 | 0.89 | 3/3537 (0.1%) |
| 1 | Q | 0.86 | 1/2743 (0.0%) | 0.93 | 5/3691 (0.1%) |
| 1 | S | 0.86 | 0/2711 | 0.92 | 3/3648 (0.1%) |
| 1 | U | 0.94 | 2/2775 (0.1%) | 0.95 | 1/3734 (0.0%) |
| 1 | W | 0.88 | 1/2756 (0.0%) | 0.93 | 3/3708 (0.1%) |
| 1 | Y | 0.93 | 2/2780 (0.1%) | 0.93 | 1/3742 (0.0%) |
| 2 | 2 | 0.90 | 2/2574 (0.1%) | 0.93 | 2/3488 (0.1%) |
| 2 | 4 | 0.87 | 1/2574 (0.0%) | 0.93 | 1/3488 (0.0%) |
| 2 | 6 | 0.90 | 2/2574 (0.1%) | 0.94 | 7/3488 (0.2%) |
| 2 | B | 1.00 | 3/2574 (0.1%) | 0.98 | 3/3488 (0.1%) |
| 2 | D | 0.95 | 0/2574 | 0.99 | 7/3488 (0.2%) |
| 2 | F | 0.95 | 0/2574 | 0.94 | 3/3488 (0.1%) |
| 2 | H | 0.93 | 1/2574 (0.0%) | 0.93 | 1/3488 (0.0%) |
| 2 | J | 0.89 | 1/2574 (0.0%) | 0.92 | 2/3488 (0.1%) |
| 2 | L | 0.90 | 0/2574 | 0.93 | 3/3488 (0.1%) |
| 2 | N | 0.87 | 1/2574 (0.0%) | 0.90 | 4/3488 (0.1%) |
| 2 | P | 0.91 | 1/2574 (0.0%) | 0.95 | 4/3488 (0.1%) |
| 2 | R | 0.95 | 1/2574 (0.0%) | 0.97 | 5/3488 (0.1%) |
| 2 | T | 0.92 | 0/2574 | 0.96 | 5/3488 (0.1%) |
| 2 | V | 0.91 | 1/2574 (0.0%) | 0.94 | 1/3488 (0.0%) |
| 2 | X | 0.90 | 0/2574 | 0.94 | 4/3488 (0.1%) |
| 2 | Z | 0.87 | 2/2574 (0.1%) | 0.88 | 3/3488 (0.1%) |

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | $\#\|Z\| > 5$ | RMSZ | $\#\|Z\| > 5$ |
| All | All | 0.89 | 42/85013 (0.0%) | 0.93 | 93/114788 (0.1%) |

All (42) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | Y | 232 | CYS | CB-SG | -10.74 | 1.64 | 1.82 |
| 1 | 5 | 232 | CYS | CB-SG | -7.94 | 1.68 | 1.82 |
| 1 | M | 232 | CYS | CB-SG | -7.92 | 1.68 | 1.82 |
| 2 | B | 276 | CYS | CB-SG | -7.73 | 1.69 | 1.82 |
| 1 | W | 189 | CYS | CB-SG | -7.02 | 1.70 | 1.82 |
| 1 | I | 283 | SER | CB-OG | 6.91 | 1.51 | 1.42 |
| 1 | U | 232 | CYS | CB-SG | -6.63 | 1.71 | 1.82 |
| 2 | Z | 276 | CYS | CB-SG | -6.60 | 1.71 | 1.82 |
| 2 | N | 276 | CYS | CB-SG | -6.50 | 1.71 | 1.82 |
| 1 | 3 | 71 | CYS | CB-SG | -6.42 | 1.71 | 1.82 |
| 1 | C | 305 | GLU | CD-OE1 | 6.27 | 1.32 | 1.25 |
| 2 | V | 276 | CYS | CB-SG | -6.25 | 1.71 | 1.82 |
| 2 | R | 233 | CYS | CB-SG | -6.24 | 1.71 | 1.82 |
| 1 | M | 276 | GLU | CB-CG | 6.12 | 1.63 | 1.52 |
| 1 | G | 1 | PHE | CE2-CZ | -6.07 | 1.25 | 1.37 |
| 1 | C | 329 | GLU | CG-CD | 6.01 | 1.60 | 1.51 |
| 1 | C | 244 | CYS | CB-SG | -6.00 | 1.72 | 1.82 |
| 2 | 6 | 139 | CYS | CB-SG | -5.88 | 1.72 | 1.81 |
| 1 | Y | 12 | CYS | CB-SG | -5.77 | 1.72 | 1.81 |
| 2 | P | 139 | CYS | CB-SG | -5.75 | 1.72 | 1.81 |
| 2 | 2 | 139 | CYS | CB-SG | -5.69 | 1.72 | 1.81 |
| 2 | Z | 247 | GLU | CG-CD | 5.53 | 1.60 | 1.51 |
| 2 | 6 | 181 | GLU | CG-CD | 5.51 | 1.60 | 1.51 |
| 2 | 2 | 250 | GLU | CG-CD | 5.50 | 1.60 | 1.51 |
| 1 | 5 | 62 | CYS | CB-SG | -5.46 | 1.73 | 1.81 |
| 2 | J | 139 | CYS | CB-SG | -5.45 | 1.73 | 1.81 |
| 1 | E | 232 | CYS | CB-SG | -5.35 | 1.73 | 1.81 |
| 2 | B | 315 | GLN | CG-CD | 5.33 | 1.63 | 1.51 |
| 1 | U | 62 | CYS | CB-SG | -5.32 | 1.73 | 1.81 |
| 1 | G | 71 | CYS | CB-SG | -5.26 | 1.73 | 1.81 |
| 1 | M | 276 | GLU | CG-CD | 5.23 | 1.59 | 1.51 |
| 1 | 1 | 232 | CYS | CB-SG | -5.21 | 1.73 | 1.81 |
| 1 | G | 72 | CYS | CB-SG | -5.21 | 1.73 | 1.81 |
| 1 | Q | 232 | CYS | CB-SG | -5.18 | 1.73 | 1.81 |
| 2 | H | 113 | VAL | CB-CG2 | -5.14 | 1.42 | 1.52 |
| 1 | A | 244 | CYS | CB-SG | -5.12 | 1.73 | 1.81 |
| 1 | G | 1 | PHE | CG-CD1 | -5.12 | 1.31 | 1.38 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | A | 71 | CYS | CB-SG | -5.05 | 1.73 | 1.81 |
| 2 | B | 250 | GLU | CD-OE2 | 5.01 | 1.31 | 1.25 |
| 1 | 3 | 161 | CYS | CB-SG | -5.01 | 1.73 | 1.81 |
| 2 | 4 | 33 | TYR | CE1-CZ | 5.01 | 1.45 | 1.38 |
| 1 | 3 | 189 | CYS | CB-SG | -5.00 | 1.73 | 1.81 |

All (93) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | C | 29 | ARG | NE-CZ-NH1 | 10.01 | 125.31 | 120.30 |
| 2 | P | 278 | ARG | NE-CZ-NH2 | -9.34 | 115.63 | 120.30 |
| 2 | P | 278 | ARG | NE-CZ-NH1 | 9.10 | 124.85 | 120.30 |
| 2 | 2 | 278 | ARG | NE-CZ-NH2 | -8.95 | 115.83 | 120.30 |
| 2 | D | 278 | ARG | NE-CZ-NH2 | -8.14 | 116.23 | 120.30 |
| 2 | X | 278 | ARG | NE-CZ-NH1 | 7.78 | 124.19 | 120.30 |
| 2 | T | 278 | ARG | NE-CZ-NH1 | 7.75 | 124.17 | 120.30 |
| 2 | 6 | 152 | ASP | CB-CG-OD1 | 7.71 | 125.24 | 118.30 |
| 1 | E | 109 | LEU | CB-CG-CD2 | -7.14 | 98.86 | 111.00 |
| 1 | O | 90 | ARG | NE-CZ-NH1 | 7.03 | 123.81 | 120.30 |
| 1 | Y | 294 | ARG | NE-CZ-NH1 | -6.95 | 116.82 | 120.30 |
| 1 | 1 | 29 | ARG | NE-CZ-NH1 | -6.88 | 116.86 | 120.30 |
| 2 | 6 | 152 | ASP | CB-CG-OD2 | -6.87 | 112.11 | 118.30 |
| 2 | N | 239 | ARG | NE-CZ-NH1 | -6.75 | 116.93 | 120.30 |
| 1 | W | 29 | ARG | NE-CZ-NH1 | 6.74 | 123.67 | 120.30 |
| 2 | L | 152 | ASP | CB-CG-OD1 | 6.73 | 124.36 | 118.30 |
| 2 | H | 152 | ASP | CB-CG-OD2 | -6.71 | 112.26 | 118.30 |
| 2 | 4 | 6 | ARG | NE-CZ-NH1 | -6.63 | 116.99 | 120.30 |
| 2 | D | 75 | ARG | NE-CZ-NH1 | -6.45 | 117.08 | 120.30 |
| 2 | F | 26 | LEU | CB-CG-CD1 | -6.42 | 100.08 | 111.00 |
| 2 | J | 289 | ASP | CB-CG-OD1 | 6.39 | 124.05 | 118.30 |
| 2 | N | 276 | CYS | CA-CB-SG | -6.29 | 102.69 | 114.00 |
| 2 | R | 14 | ASP | CB-CG-OD1 | 6.25 | 123.92 | 118.30 |
| 1 | O | 29 | ARG | NE-CZ-NH1 | 6.20 | 123.40 | 120.30 |
| 2 | D | 19 | ARG | NE-CZ-NH1 | 6.19 | 123.39 | 120.30 |
| 1 | C | 29 | ARG | NE-CZ-NH2 | -6.13 | 117.23 | 120.30 |
| 2 | N | 75 | ARG | NE-CZ-NH1 | -6.03 | 117.29 | 120.30 |
| 1 | W | 187 | LEU | CB-CG-CD1 | -5.98 | 100.84 | 111.00 |
| 2 | B | 299 | ASP | CB-CG-OD1 | 5.95 | 123.66 | 118.30 |
| 2 | D | 245 | ASP | CB-CG-OD2 | -5.94 | 112.96 | 118.30 |
| 1 | A | 29 | ARG | NE-CZ-NH1 | 5.88 | 123.24 | 120.30 |
| 2 | 6 | 51 | ARG | NE-CZ-NH1 | -5.82 | 117.39 | 120.30 |
| 2 | D | 242 | ARG | NE-CZ-NH1 | -5.82 | 117.39 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 2 | D | 210 | VAL | CB-CA-C | -5.81 | 100.36 | 111.40 |
| 2 | P | 71 | MET | CG-SD-CE | 5.78 | 109.44 | 100.20 |
| 2 | Z | 239 | ARG | NE-CZ-NH1 | -5.74 | 117.43 | 120.30 |
| 1 | 3 | 135 | ASN | N-CA-C | -5.73 | 95.53 | 111.00 |
| 2 | B | 294 | ARG | NE-CZ-NH2 | 5.72 | 123.16 | 120.30 |
| 2 | 6 | 115 | ARG | NE-CZ-NH1 | -5.72 | 117.44 | 120.30 |
| 1 | Q | 29 | ARG | NE-CZ-NH1 | 5.72 | 123.16 | 120.30 |
| 1 | W | 167 | ASP | CB-CG-OD2 | 5.72 | 123.44 | 118.30 |
| 2 | X | 43 | LEU | CB-CG-CD2 | -5.70 | 101.31 | 111.00 |
| 1 | S | 29 | ARG | NE-CZ-NH1 | -5.66 | 117.47 | 120.30 |
| 1 | O | 90 | ARG | NE-CZ-NH2 | -5.65 | 117.47 | 120.30 |
| 1 | 5 | 64 | LEU | CA-CB-CG | -5.61 | 102.39 | 115.30 |
| 2 | T | 299 | ASP | CB-CG-OD1 | 5.60 | 123.34 | 118.30 |
| 1 | K | 162 | LEU | CB-CG-CD2 | -5.57 | 101.53 | 111.00 |
| 2 | Z | 75 | ARG | NE-CZ-NH1 | -5.57 | 117.52 | 120.30 |
| 1 | I | 29 | ARG | NE-CZ-NH1 | 5.54 | 123.07 | 120.30 |
| 1 | S | 135 | ASN | N-CA-C | -5.53 | 96.08 | 111.00 |
| 1 | 3 | 71 | CYS | CA-CB-SG | -5.53 | 104.05 | 114.00 |
| 2 | T | 314 | PRO | N-CA-C | 5.52 | 126.46 | 112.10 |
| 1 | Q | 234 | ARG | NE-CZ-NH1 | -5.46 | 117.57 | 120.30 |
| 2 | J | 6 | ARG | NE-CZ-NH1 | -5.45 | 117.58 | 120.30 |
| 2 | 2 | 41 | ARG | NE-CZ-NH2 | -5.45 | 117.58 | 120.30 |
| 2 | F | 276 | CYS | CA-CB-SG | -5.38 | 104.31 | 114.00 |
| 2 | T | 19 | ARG | NE-CZ-NH1 | 5.36 | 122.98 | 120.30 |
| 2 | R | 214 | ARG | NE-CZ-NH1 | 5.34 | 122.97 | 120.30 |
| 2 | 6 | 139 | CYS | CA-CB-SG | -5.34 | 104.39 | 114.00 |
| 1 | S | 64 | LEU | CA-CB-CG | -5.33 | 103.03 | 115.30 |
| 2 | L | 239 | ARG | NE-CZ-NH1 | -5.33 | 117.63 | 120.30 |
| 1 | Q | 37 | ARG | NE-CZ-NH1 | -5.32 | 117.64 | 120.30 |
| 2 | F | 288 | LEU | CB-CG-CD2 | -5.32 | 101.96 | 111.00 |
| 2 | V | 288 | LEU | CB-CG-CD2 | -5.31 | 101.97 | 111.00 |
| 1 | Q | 64 | LEU | CA-CB-CG | -5.30 | 103.10 | 115.30 |
| 2 | N | 113 | VAL | CB-CA-C | -5.26 | 101.41 | 111.40 |
| 2 | D | 51 | ARG | NE-CZ-NH1 | -5.24 | 117.68 | 120.30 |
| 1 | U | 134 | GLY | N-CA-C | -5.24 | 100.01 | 113.10 |
| 1 | G | 75 | LEU | CB-CG-CD1 | 5.23 | 119.90 | 111.00 |
| 2 | Z | 276 | CYS | CA-CB-SG | -5.21 | 104.61 | 114.00 |
| 1 | M | 252 | LEU | CB-CG-CD1 | -5.21 | 102.14 | 111.00 |
| 2 | R | 278 | ARG | NE-CZ-NH2 | -5.20 | 117.70 | 120.30 |
| 2 | 6 | 210 | VAL | CB-CA-C | -5.19 | 101.54 | 111.40 |
| 1 | A | 64 | LEU | CA-CB-CG | -5.19 | 103.37 | 115.30 |
| 2 | R | 316 | VAL | CB-CA-C | -5.18 | 101.55 | 111.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 2 | R | 152 | ASP | CB-CG-OD1 | 5.17 | 122.96 | 118.30 |
| 1 | Q | 134 | GLY | N-CA-C | -5.16 | 100.20 | 113.10 |
| 2 | L | 152 | ASP | CB-CG-OD2 | -5.14 | 113.67 | 118.30 |
| 1 | G | 98 | ARG | NE-CZ-NH1 | 5.14 | 122.87 | 120.30 |
| 1 | 5 | 252 | LEU | CB-CG-CD1 | -5.14 | 102.26 | 111.00 |
| 2 | 6 | 279 | ILE | CG1-CB-CG2 | -5.14 | 100.10 | 111.40 |
| 2 | X | 152 | ASP | CB-CG-OD2 | -5.13 | 113.69 | 118.30 |
| 1 | G | 167 | ASP | CB-CG-OD2 | 5.12 | 122.91 | 118.30 |
| 1 | M | 33 | LEU | CB-CG-CD2 | -5.11 | 102.32 | 111.00 |
| 2 | B | 247 | GLU | CA-CB-CG | 5.09 | 124.59 | 113.40 |
| 1 | I | 135 | ASN | N-CA-C | -5.06 | 97.33 | 111.00 |
| 2 | T | 239 | ARG | NE-CZ-NH1 | -5.06 | 117.77 | 120.30 |
| 1 | 1 | 29 | ARG | CD-NE-CZ | 5.06 | 130.68 | 123.60 |
| 2 | P | 210 | VAL | CB-CA-C | -5.05 | 101.80 | 111.40 |
| 1 | A | 33 | LEU | CA-CB-CG | -5.04 | 103.70 | 115.30 |
| 2 | X | 115 | ARG | NE-CZ-NH2 | -5.01 | 117.79 | 120.30 |
| 1 | I | 71 | CYS | CA-CB-SG | -5.01 | 104.98 | 114.00 |
| 1 | 3 | 29 | ARG | NE-CZ-NH1 | 5.00 | 122.80 | 120.30 |

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts (i)

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 1 | 1 | 2614 | 0 | 2587 | 120 | 0 |
| 1 | 3 | 2676 | 0 | 2644 | 123 | 0 |
| 1 | 5 | 2712 | 0 | 2679 | 115 | 0 |
| 1 | A | 2677 | 0 | 2645 | 136 | 0 |
| 1 | C | 2677 | 0 | 2645 | 116 | 0 |
| 1 | E | 2728 | 0 | 2693 | 93 | 0 |
| 1 | G | 2712 | 0 | 2681 | 103 | 0 |
| 1 | I | 2693 | 0 | 2660 | 88 | 0 |
| 1 | K | 2712 | 0 | 2679 | 97 | 0 |
| 1 | M | 2728 | 0 | 2693 | 97 | 0 |
| 1 | O | 2580 | 0 | 2552 | 119 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 1 | Q | 2693 | 0 | 2660 | 122 | 0 |
| 1 | S | 2661 | 0 | 2630 | 130 | 0 |
| 1 | U | 2723 | 0 | 2692 | 87 | 0 |
| 1 | W | 2705 | 0 | 2672 | 95 | 0 |
| 1 | Y | 2728 | 0 | 2693 | 93 | 0 |
| 2 | 2 | 2519 | 0 | 2517 | 72 | 0 |
| 2 | 4 | 2519 | 0 | 2517 | 82 | 0 |
| 2 | 6 | 2519 | 0 | 2517 | 74 | 0 |
| 2 | B | 2519 | 0 | 2517 | 60 | 0 |
| 2 | D | 2519 | 0 | 2517 | 77 | 0 |
| 2 | F | 2519 | 0 | 2517 | 86 | 0 |
| 2 | H | 2519 | 0 | 2517 | 81 | 0 |
| 2 | J | 2519 | 0 | 2517 | 85 | 0 |
| 2 | L | 2519 | 0 | 2517 | 79 | 0 |
| 2 | N | 2519 | 0 | 2517 | 78 | 0 |
| 2 | P | 2519 | 0 | 2517 | 70 | 0 |
| 2 | R | 2519 | 0 | 2517 | 77 | 0 |
| 2 | T | 2519 | 0 | 2517 | 81 | 0 |
| 2 | V | 2519 | 0 | 2517 | 73 | 0 |
| 2 | X | 2519 | 0 | 2517 | 79 | 0 |
| 2 | Z | 2519 | 0 | 2517 | 70 | 0 |
| 3 | 2 | 1 | 0 | 0 | 0 | 0 |
| 3 | 4 | 1 | 0 | 0 | 0 | 0 |
| 3 | 6 | 1 | 0 | 0 | 0 | 0 |
| 3 | B | 1 | 0 | 0 | 0 | 0 |
| 3 | D | 1 | 0 | 0 | 0 | 0 |
| 3 | F | 1 | 0 | 0 | 0 | 0 |
| 3 | H | 1 | 0 | 0 | 0 | 0 |
| 3 | J | 1 | 0 | 0 | 0 | 0 |
| 3 | L | 1 | 0 | 0 | 0 | 0 |
| 3 | N | 1 | 0 | 0 | 0 | 0 |
| 3 | P | 1 | 0 | 0 | 0 | 0 |
| 3 | R | 1 | 0 | 0 | 0 | 0 |
| 3 | T | 1 | 0 | 0 | 0 | 0 |
| 3 | V | 1 | 0 | 0 | 0 | 0 |
| 3 | X | 1 | 0 | 0 | 0 | 0 |
| 3 | Z | 1 | 0 | 0 | 0 | 0 |
| All | All | 83339 | 0 | 82777 | 2778 | 0 |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 17.

All (2778) 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:O:231:LEU:HD12 | 1:O:294:ARG:NH1 | 1.20 | 1.50 |
| 1:A:289:MET:CE | 1:A:290:LEU:HD23 | 1.60 | 1.30 |
| 1:G:270:VAL:HG12 | 1:G:273:ARG:NH2 | 1.51 | 1.22 |
| 1:M:268:PRO:HB2 | 1:M:270:VAL:HG23 | 1.21 | 1.17 |
| 1:1:280:GLU:HG2 | 1:1:281:VAL:N | 1.55 | 1.17 |
| 2:F:246:MET:CE | 2:F:279:ILE:HD13 | 1.73 | 1.16 |
| 1:A:18:GLU:HG2 | 1:A:19:GLU:H | 1.06 | 1.16 |
| 1:S:28:THR:CG2 | 1:S:30:GLU:HB2 | 1.76 | 1.15 |
| 1:5:230:ILE:HG23 | 1:5:231:LEU:HD23 | 1.28 | 1.14 |
| 1:A:289:MET:HE2 | 1:A:290:LEU:HD23 | 1.14 | 1.13 |
| 1:S:28:THR:HG21 | 1:S:30:GLU:CB | 1.77 | 1.13 |
| 1:Q:18:GLU:HG2 | 1:Q:19:GLU:H | 1.10 | 1.13 |
| 1:3:69:GLU:O | 1:3:73:VAL:HG23 | 1.47 | 1.12 |
| 1:S:278:ILE:H | 1:S:278:ILE:CD1 | 1.60 | 1.12 |
| 1:Y:268:PRO:HB2 | 1:Y:270:VAL:HG12 | 1.20 | 1.12 |
| 1:S:278:ILE:H | 1:S:278:ILE:HD12 | 1.07 | 1.11 |
| 1:S:28:THR:CG2 | 1:S:30:GLU:CB | 2.29 | 1.11 |
| 1:O:231:LEU:CD1 | 1:O:294:ARG:NH1 | 2.17 | 1.07 |
| 1:5:275:ARG:HG3 | 1:5:275:ARG:NH1 | 1.58 | 1.07 |
| 1:S:28:THR:HG22 | 1:S:30:GLU:N | 1.68 | 1.07 |
| 1:M:230:ILE:HG13 | 1:M:230:ILE:O | 1.54 | 1.07 |
| 1:M:267:ASP:CB | 1:M:268:PRO:HD2 | 1.84 | 1.06 |
| 1:Y:267:ASP:CB | 1:Y:268:PRO:HD3 | 1.84 | 1.06 |
| 1:5:270:VAL:O | 1:5:274:THR:HG23 | 1.52 | 1.06 |
| 1:1:197:ARG:HB3 | 1:1:197:ARG:HH11 | 1.20 | 1.05 |
| 1:A:289:MET:CE | 1:A:290:LEU:CD2 | 2.34 | 1.05 |
| 1:G:272:TYR:HD1 | 1:G:273:ARG:N | 1.53 | 1.04 |
| 1:U:88:ALA:O | 1:U:134:GLY:HA2 | 1.57 | 1.04 |
| 1:M:268:PRO:HB2 | 1:M:270:VAL:CG2 | 1.87 | 1.03 |
| 2:N:279:ILE:HG22 | 2:N:280:MET:N | 1.73 | 1.03 |
| 1:5:275:ARG:HG3 | 1:5:275:ARG:HH11 | 0.86 | 1.03 |
| 1:5:275:ARG:HH11 | 1:5:275:ARG:CG | 1.71 | 1.01 |
| 1:U:327:ASP:OD1 | 1:U:328:PRO:HD2 | 1.60 | 1.01 |
| 1:A:197:ARG:HB3 | 1:A:197:ARG:HH11 | 1.23 | 1.01 |
| 2:D:313:ILE:HG22 | 2:D:314:PRO:HD2 | 1.44 | 1.00 |
| 1:M:267:ASP:CB | 1:M:268:PRO:CD | 2.39 | 1.00 |
| 2:N:278:ARG:HH11 | 2:N:278:ARG:CG | 1.75 | 1.00 |
| 1:A:289:MET:HE2 | 1:A:290:LEU:CD2 | 1.90 | 0.99 |
| 2:F:246:MET:HE1 | 2:F:279:ILE:HD13 | 1.45 | 0.99 |
| 2:N:278:ARG:HG3 | 2:N:278:ARG:NH1 | 1.75 | 0.99 |
| 1:K:275:ARG:HG2 | 1:K:275:ARG:HH11 | 1.27 | 0.98 |
| 1:K:98:ARG:HG2 | 1:K:131:PHE:HB2 | 1.44 | 0.98 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:284:LYS:O | 1:A:285:SER:HB3 | 1.61 | 0.98 |
| 1:1:196:ASN:HB3 | 1:1:257:THR:HG23 | 1.42 | 0.98 |
| 1:S:278:ILE:HD12 | 1:S:278:ILE:N | 1.70 | 0.98 |
| 2:2:184:PRO:HA | 2:2:187:GLN:HE21 | 1.25 | 0.98 |
| 2:Z:1:LEU:HD13 | 2:Z:2:GLN:H | 1.28 | 0.97 |
| 2:V:313:ILE:HG23 | 2:V:314:PRO:HD2 | 1.46 | 0.97 |
| 1:Q:18:GLU:HG2 | 1:Q:19:GLU:N | 1.80 | 0.97 |
| 1:5:29:ARG:HH11 | 1:5:29:ARG:HG3 | 1.30 | 0.97 |
| 1:G:272:TYR:CD1 | 1:G:273:ARG:N | 2.33 | 0.96 |
| 1:G:327:ASP:OD1 | 1:G:328:PRO:HD2 | 1.65 | 0.96 |
| 1:3:39:MET:HG2 | 1:3:73:VAL:HG21 | 1.45 | 0.96 |
| 1:O:229:ASP:OD1 | 1:O:231:LEU:HB2 | 1.64 | 0.96 |
| 1:Y:267:ASP:CB | 1:Y:268:PRO:CD | 2.44 | 0.96 |
| 1:S:28:THR:HG21 | 1:S:30:GLU:HB3 | 1.43 | 0.95 |
| 1:Q:45:MET:HE3 | 1:Q:102:VAL:HG13 | 1.46 | 0.95 |
| 1:3:68:GLN:HE21 | 1:3:259:ARG:HB3 | 1.30 | 0.95 |
| 1:G:131:PHE:CE2 | 1:G:133:GLY:HA2 | 2.02 | 0.94 |
| 1:A:18:GLU:HG2 | 1:A:19:GLU:N | 1.82 | 0.94 |
| 2:V:278:ARG:HH11 | 2:V:278:ARG:HG3 | 1.32 | 0.94 |
| 1:S:29:ARG:HA | 1:S:300:LEU:HD22 | 1.49 | 0.94 |
| 1:E:216:ARG:HG3 | 1:E:216:ARG:HH11 | 1.30 | 0.93 |
| 1:C:229:ASP:O | 1:C:233:VAL:HG23 | 1.68 | 0.93 |
| 1:C:68:GLN:HE21 | 1:C:259:ARG:HB3 | 1.31 | 0.93 |
| 2:N:278:ARG:HH11 | 2:N:278:ARG:HG3 | 1.31 | 0.92 |
| 2:T:278:ARG:HG3 | 2:T:278:ARG:HH11 | 1.31 | 0.92 |
| 1:K:11:LYS:HB3 | 1:K:23:VAL:HG12 | 1.52 | 0.92 |
| 1:G:270:VAL:HG12 | 1:G:273:ARG:HH22 | 1.10 | 0.91 |
| 1:O:231:LEU:HD12 | 1:O:294:ARG:HH11 | 1.13 | 0.91 |
| 1:A:16:ARG:HG2 | 1:A:16:ARG:HH11 | 1.34 | 0.91 |
| 2:6:98:ALA:HB2 | 2:6:142:LEU:HD13 | 1.52 | 0.91 |
| 1:G:98:ARG:HG2 | 1:G:131:PHE:HB2 | 1.53 | 0.91 |
| 1:G:196:ASN:HB3 | 1:G:257:THR:HG23 | 1.53 | 0.90 |
| 1:3:354:TRP:CZ2 | 2:6:325:LYS:HG2 | 2.07 | 0.90 |
| 1:3:68:GLN:NE2 | 1:3:259:ARG:HB3 | 1.87 | 0.90 |
| 2:X:278:ARG:HH11 | 2:X:278:ARG:HG3 | 1.35 | 0.90 |
| 1:W:68:GLN:HE21 | 1:W:259:ARG:HB3 | 1.36 | 0.90 |
| 2:B:118:ASN:HD21 | 2:B:132:PHE:H | 1.16 | 0.90 |
| 1:E:45:MET:HE1 | 1:E:105:ILE:HD12 | 1.51 | 0.90 |
| 1:C:196:ASN:HB3 | 1:C:257:THR:HG23 | 1.53 | 0.89 |
| 1:S:28:THR:HG22 | 1:S:28:THR:O | 1.70 | 0.89 |
| 1:3:113:LYS:HD2 | 1:3:328:PRO:HG2 | 1.52 | 0.89 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:F:246:MET:CE | 2:F:279:ILE:CD1 | 2.50 | 0.89 |
| 2:R:212:HIS:HB3 | 2:R:238:MET:HE3 | 1.55 | 0.89 |
| 1:S:88:ALA:O | 1:S:134:GLY:HA2 | 1.73 | 0.89 |
| 1:G:272:TYR:CD1 | 1:G:272:TYR:C | 2.47 | 0.88 |
| 1:S:29:ARG:CA | 1:S:300:LEU:HD22 | 2.02 | 0.88 |
| 1:Q:289:MET:CE | 1:Q:290:LEU:HD23 | 2.03 | 0.88 |
| 1:S:274:THR:O | 1:S:278:ILE:HD13 | 1.73 | 0.88 |
| 1:K:45:MET:HE3 | 1:K:102:VAL:HG22 | 1.55 | 0.88 |
| 1:Q:284:LYS:O | 1:Q:285:SER:HB3 | 1.71 | 0.88 |
| 1:M:274:THR:O | 1:M:277:GLU:HB3 | 1.74 | 0.88 |
| 2:4:1:LEU:HD13 | 2:4:2:GLN:H | 1.37 | 0.88 |
| 1:O:197:ARG:HB3 | 1:O:197:ARG:HH11 | 1.37 | 0.88 |
| 1:A:197:ARG:HB3 | 1:A:197:ARG:NH1 | 1.88 | 0.87 |
| 1:K:334:GLU:HG2 | 1:K:337:TYR:CE2 | 2.09 | 0.87 |
| 1:O:231:LEU:HD12 | 1:O:294:ARG:HH12 | 1.35 | 0.87 |
| 2:P:184:PRO:HA | 2:P:187:GLN:HE21 | 1.39 | 0.87 |
| 1:K:88:ALA:O | 1:K:134:GLY:HA2 | 1.74 | 0.87 |
| 1:3:284:LYS:NZ | 1:3:284:LYS:HB3 | 1.89 | 0.87 |
| 1:Y:270:VAL:O | 1:Y:270:VAL:HG22 | 1.74 | 0.86 |
| 1:1:303:VAL:HG13 | 1:1:304:GLU:OE2 | 1.76 | 0.86 |
| 1:O:196:ASN:HB3 | 1:O:257:THR:HG23 | 1.57 | 0.86 |
| 1:A:16:ARG:HH11 | 1:A:16:ARG:CG | 1.89 | 0.86 |
| 1:5:98:ARG:HG2 | 1:5:131:PHE:HB2 | 1.57 | 0.85 |
| 1:S:68:GLN:HE21 | 1:S:259:ARG:HB3 | 1.41 | 0.85 |
| 1:M:268:PRO:CB | 1:M:270:VAL:HG23 | 2.07 | 0.85 |
| 1:M:334:GLU:HG2 | 1:M:337:TYR:CE2 | 2.12 | 0.85 |
| 1:W:131:PHE:CE2 | 1:W:133:GLY:HA2 | 2.10 | 0.85 |
| 2:H:98:ALA:HB2 | 2:H:142:LEU:HD13 | 1.59 | 0.85 |
| 1:5:182:ALA:HA | 1:5:187:LEU:HD12 | 1.59 | 0.84 |
| 1:5:269:GLY:O | 1:5:273:ARG:HD3 | 1.77 | 0.84 |
| 1:E:131:PHE:CE2 | 1:E:133:GLY:HA2 | 2.11 | 0.84 |
| 1:G:55:GLN:O | 1:G:56:LYS:HB2 | 1.75 | 0.84 |
| 1:M:131:PHE:CE2 | 1:M:133:GLY:HA2 | 2.12 | 0.84 |
| 1:S:28:THR:HG21 | 1:S:30:GLU:HB2 | 1.45 | 0.84 |
| 2:2:184:PRO:HA | 2:2:187:GLN:NE2 | 1.91 | 0.83 |
| 2:R:325:LYS:HG2 | 1:S:354:TRP:CZ2 | 2.13 | 0.83 |
| 1:S:277:GLU:O | 1:S:281:VAL:HG23 | 1.77 | 0.83 |
| 1:M:45:MET:HE1 | 1:M:105:ILE:HD12 | 1.59 | 0.83 |
| 1:I:113:LYS:HD3 | 1:I:328:PRO:HG2 | 1.59 | 0.83 |
| 1:5:269:GLY:HA3 | 1:5:273:ARG:NH1 | 1.94 | 0.83 |
| 1:1:88:ALA:O | 1:1:134:GLY:HA2 | 1.78 | 0.83 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:45:MET:HE3 | 1:A:102:VAL:HG13 | 1.59 | 0.83 |
| 1:K:45:MET:HE1 | 1:K:105:ILE:HD12 | 1.61 | 0.83 |
| 1:5:45:MET:HE3 | 1:5:102:VAL:HG22 | 1.61 | 0.83 |
| 2:F:98:ALA:HB2 | 2:F:142:LEU:HD13 | 1.60 | 0.83 |
| 1:U:289:MET:HE2 | 1:U:290:LEU:HD23 | 1.59 | 0.82 |
| 1:Y:334:GLU:HG2 | 1:Y:337:TYR:CE2 | 2.13 | 0.82 |
| 1:E:334:GLU:HG2 | 1:E:337:TYR:CE2 | 2.14 | 0.82 |
| 2:N:118:ASN:HD21 | 2:N:132:PHE:H | 1.26 | 0.82 |
| 2:N:278:ARG:CG | 2:N:278:ARG:NH1 | 2.38 | 0.82 |
| 1:Y:270:VAL:O | 1:Y:270:VAL:CG2 | 2.28 | 0.82 |
| 1:1:68:GLN:HE21 | 1:1:259:ARG:HB3 | 1.44 | 0.82 |
| 1:G:272:TYR:HA | 1:G:275:ARG:HD3 | 1.60 | 0.82 |
| 1:O:229:ASP:C | 1:O:231:LEU:H | 1.82 | 0.81 |
| 1:5:230:ILE:HG23 | 1:5:231:LEU:CD2 | 2.09 | 0.81 |
| 1:U:84:HIS:CE1 | 1:U:130:ASN:ND2 | 2.48 | 0.81 |
| 1:W:98:ARG:HG2 | 1:W:131:PHE:HB2 | 1.62 | 0.81 |
| 2:F:329:ILE:HG13 | 2:F:329:ILE:OXT | 1.80 | 0.81 |
| 2:T:278:ARG:HG3 | 2:T:278:ARG:NH1 | 1.90 | 0.81 |
| 1:1:100:LEU:HD13 | 1:1:128:ALA:HB2 | 1.60 | 0.81 |
| 1:O:230:ILE:HD12 | 1:O:230:ILE:O | 1.79 | 0.81 |
| 2:V:313:ILE:HG23 | 2:V:314:PRO:CD | 2.10 | 0.81 |
| 1:W:196:ASN:HB3 | 1:W:257:THR:HG23 | 1.62 | 0.81 |
| 2:B:280:MET:HE1 | 2:D:276:CYS:HB3 | 1.62 | 0.81 |
| 1:1:231:LEU:HD12 | 1:1:294:ARG:NH1 | 1.95 | 0.81 |
| 1:K:289:MET:CE | 1:K:290:LEU:HD23 | 2.10 | 0.81 |
| 2:F:1:LEU:HD13 | 2:F:2:GLN:H | 1.46 | 0.81 |
| 1:Q:289:MET:HE2 | 1:Q:290:LEU:HD23 | 1.61 | 0.81 |
| 2:F:246:MET:HE3 | 2:F:279:ILE:HD13 | 1.62 | 0.80 |
| 1:K:113:LYS:HD3 | 1:K:328:PRO:HG2 | 1.63 | 0.80 |
| 1:U:101:SER:OG | 1:U:104:GLU:HG3 | 1.81 | 0.80 |
| 1:W:55:GLN:O | 1:W:56:LYS:HB2 | 1.81 | 0.80 |
| 1:3:274:THR:HB | 1:3:276:GLU:HG3 | 1.63 | 0.80 |
| 2:T:313:ILE:HG22 | 2:T:314:PRO:HD2 | 1.62 | 0.80 |
| 1:3:258:TYR:CE2 | 1:3:277:GLU:OE2 | 2.34 | 0.80 |
| 2:P:11:GLN:O | 2:P:15:GLU:HG3 | 1.81 | 0.80 |
| 2:X:184:PRO:HA | 2:X:187:GLN:NE2 | 1.97 | 0.80 |
| 2:V:278:ARG:HG3 | 2:V:278:ARG:NH1 | 1.92 | 0.80 |
| 1:5:269:GLY:C | 1:5:273:ARG:NH1 | 2.35 | 0.80 |
| 2:V:98:ALA:HB2 | 2:V:142:LEU:HD13 | 1.62 | 0.80 |
| 1:K:327:ASP:OD1 | 1:K:328:PRO:HD2 | 1.82 | 0.80 |
| 1:Y:268:PRO:HB2 | 1:Y:270:VAL:CG1 | 2.07 | 0.80 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:354:TRP:CZ2 | 2:D:325:LYS:HG2 | 2.18 | 0.79 |
| 2:N:279:ILE:CG2 | 2:N:280:MET:N | 2.45 | 0.79 |
| 1:U:334:GLU:HG2 | 1:U:337:TYR:CE2 | 2.18 | 0.79 |
| 1:K:131:PHE:CE2 | 1:K:133:GLY:HA2 | 2.18 | 0.79 |
| 1:Q:29:ARG:HH11 | 1:Q:29:ARG:HG3 | 1.48 | 0.79 |
| 1:M:45:MET:HE3 | 1:M:102:VAL:HG13 | 1.64 | 0.79 |
| 1:U:88:ALA:O | 1:U:134:GLY:CA | 2.31 | 0.79 |
| 1:C:88:ALA:O | 1:C:134:GLY:HA2 | 1.83 | 0.79 |
| 1:S:45:MET:HE3 | 1:S:102:VAL:HG13 | 1.63 | 0.79 |
| 1:5:334:GLU:HG2 | 1:5:337:TYR:CE2 | 2.18 | 0.79 |
| 2:L:98:ALA:HB2 | 2:L:142:LEU:CD1 | 2.12 | 0.78 |
| 2:6:184:PRO:HA | 2:6:187:GLN:NE2 | 1.98 | 0.78 |
| 1:O:29:ARG:HB2 | 1:O:300:LEU:HD22 | 1.64 | 0.78 |
| 1:Q:68:GLN:HE21 | 1:Q:259:ARG:HB3 | 1.48 | 0.78 |
| 1:U:289:MET:CE | 1:U:290:LEU:HD23 | 2.13 | 0.78 |
| 1:3:69:GLU:O | 1:3:73:VAL:CG2 | 2.30 | 0.78 |
| 1:O:280:GLU:HG2 | 1:O:281:VAL:N | 1.98 | 0.78 |
| 2:V:207:ILE:HD13 | 2:V:323:ILE:HG23 | 1.64 | 0.78 |
| 1:O:230:ILE:O | 1:O:230:ILE:CD1 | 2.31 | 0.78 |
| 1:W:334:GLU:HG2 | 1:W:337:TYR:CE2 | 2.19 | 0.78 |
| 1:Q:197:ARG:HB3 | 1:Q:197:ARG:HH11 | 1.46 | 0.77 |
| 1:C:234:ARG:NE | 1:C:238:ARG:NH2 | 2.32 | 0.77 |
| 1:Y:230:ILE:O | 1:Y:230:ILE:HG13 | 1.84 | 0.77 |
| 1:5:113:LYS:HD3 | 1:5:328:PRO:HG2 | 1.66 | 0.77 |
| 1:A:289:MET:HE3 | 1:A:290:LEU:HD23 | 1.63 | 0.77 |
| 1:E:57:ILE:HD13 | 1:E:57:ILE:N | 1.98 | 0.77 |
| 2:V:118:ASN:HD21 | 2:V:132:PHE:H | 1.28 | 0.77 |
| 1:5:131:PHE:CE2 | 1:5:133:GLY:HA2 | 2.18 | 0.77 |
| 1:G:270:VAL:CG1 | 1:G:273:ARG:HH22 | 1.95 | 0.77 |
| 1:O:71:CYS:O | 1:O:75:LEU:HB2 | 1.84 | 0.77 |
| 1:I:113:LYS:CD | 1:I:328:PRO:HG2 | 2.13 | 0.77 |
| 1:5:88:ALA:O | 1:5:134:GLY:HA2 | 1.84 | 0.77 |
| 1:U:45:MET:HE1 | 1:U:105:ILE:HD12 | 1.67 | 0.77 |
| 2:N:207:ILE:HD13 | 2:N:323:ILE:HG23 | 1.66 | 0.77 |
| 2:B:280:MET:CE | 2:D:276:CYS:HB3 | 2.15 | 0.77 |
| 1:K:182:ALA:HA | 1:K:187:LEU:HD12 | 1.67 | 0.77 |
| 1:O:230:ILE:O | 1:O:230:ILE:CG1 | 2.32 | 0.77 |
| 2:V:329:ILE:HG13 | 2:V:329:ILE:OXT | 1.83 | 0.77 |
| 2:2:121:SER:HB3 | 2:2:124:VAL:HG21 | 1.65 | 0.77 |
| 1:Q:29:ARG:HH11 | 1:Q:29:ARG:CG | 1.98 | 0.76 |
| 1:S:37:ARG:HH11 | 1:S:37:ARG:CG | 1.98 | 0.76 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:5:196:ASN:HB3 | 1:5:257:THR:HG23 | 1.67 | 0.76 |
| 1:M:223:LEU:N | 1:M:223:LEU:HD23 | 2.00 | 0.76 |
| 1:S:28:THR:HG22 | 1:S:30:GLU:CA | 2.15 | 0.76 |
| 2:P:118:ASN:HD21 | 2:P:132:PHE:H | 1.31 | 0.76 |
| 2:D:11:GLN:O | 2:D:15:GLU:HG3 | 1.86 | 0.76 |
| 2:V:278:ARG:HH11 | 2:V:278:ARG:CG | 1.98 | 0.76 |
| 1:S:196:ASN:HB3 | 1:S:257:THR:HG23 | 1.66 | 0.76 |
| 2:F:327:LEU:O | 2:F:329:ILE:HG23 | 1.86 | 0.76 |
| 1:5:277:GLU:O | 1:5:281:VAL:HG23 | 1.86 | 0.76 |
| 1:G:72:CYS:HB2 | 1:G:97:THR:HG21 | 1.68 | 0.76 |
| 1:E:88:ALA:O | 1:E:134:GLY:HA2 | 1.86 | 0.76 |
| 1:A:29:ARG:HA | 1:A:300:LEU:HD22 | 1.68 | 0.76 |
| 2:B:118:ASN:HD21 | 2:B:132:PHE:N | 1.84 | 0.75 |
| 2:H:184:PRO:HA | 2:H:187:GLN:NE2 | 2.02 | 0.75 |
| 1:W:10:LYS:HG2 | 1:W:11:LYS:N | 2.00 | 0.75 |
| 2:X:11:GLN:O | 2:X:15:GLU:HG3 | 1.87 | 0.75 |
| 1:K:100:LEU:HD13 | 1:K:128:ALA:HB2 | 1.69 | 0.75 |
| 1:A:231:LEU:HD12 | 1:A:294:ARG:NH1 | 2.01 | 0.75 |
| 1:I:204:VAL:HG23 | 1:I:205:GLU:H | 1.50 | 0.75 |
| 1:M:272:TYR:CD1 | 1:M:272:TYR:C | 2.60 | 0.75 |
| 1:C:95:THR:CG2 | 1:C:100:LEU:HD22 | 2.15 | 0.75 |
| 1:A:29:ARG:HH11 | 1:A:29:ARG:CG | 1.99 | 0.75 |
| 1:G:270:VAL:CG1 | 1:G:273:ARG:NH2 | 2.43 | 0.75 |
| 1:O:230:ILE:O | 1:O:230:ILE:HG13 | 1.86 | 0.74 |
| 1:1:280:GLU:CG | 1:1:281:VAL:N | 2.40 | 0.74 |
| 1:C:253:MET:HE3 | 1:C:255:LEU:CD1 | 2.16 | 0.74 |
| 1:O:229:ASP:O | 1:O:231:LEU:N | 2.20 | 0.74 |
| 1:3:196:ASN:HB3 | 1:3:257:THR:HG23 | 1.69 | 0.74 |
| 1:5:269:GLY:CA | 1:5:273:ARG:NH1 | 2.50 | 0.74 |
| 1:C:29:ARG:HD2 | 1:C:300:LEU:O | 1.88 | 0.74 |
| 1:G:88:ALA:O | 1:G:134:GLY:HA2 | 1.88 | 0.74 |
| 1:G:150:LEU:HA | 1:G:187:LEU:HD22 | 1.70 | 0.74 |
| 2:L:238:MET:O | 2:L:239:ARG:HB2 | 1.86 | 0.74 |
| 1:A:10:LYS:HG2 | 1:A:11:LYS:N | 2.02 | 0.73 |
| 1:Q:197:ARG:HB3 | 1:Q:197:ARG:NH1 | 2.02 | 0.73 |
| 1:A:334:GLU:HG2 | 1:A:337:TYR:CE2 | 2.23 | 0.73 |
| 1:I:354:TRP:CZ2 | 2:L:325:LYS:HG2 | 2.23 | 0.73 |
| 2:J:143:LYS:HB2 | 2:J:167:VAL:HG22 | 1.69 | 0.73 |
| 1:5:11:LYS:HB3 | 1:5:23:VAL:HG13 | 1.69 | 0.73 |
| 1:Q:88:ALA:O | 1:Q:134:GLY:HA2 | 1.87 | 0.73 |
| 2:R:207:ILE:HD13 | 2:R:323:ILE:HG23 | 1.70 | 0.73 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:1:3:ASN:O | 1:1:4:ASP:HB3 | 1.89 | 0.73 |
| 1:C:68:GLN:NE2 | 1:C:259:ARG:HB3 | 2.03 | 0.73 |
| 1:K:275:ARG:HG2 | 1:K:275:ARG:NH1 | 2.01 | 0.73 |
| 1:I:55:GLN:O | 1:I:56:LYS:HB2 | 1.88 | 0.73 |
| 2:J:246:MET:O | 2:J:250:GLU:HG3 | 1.89 | 0.73 |
| 2:T:316:VAL:O | 2:T:316:VAL:CG1 | 2.37 | 0.73 |
| 1:K:29:ARG:HH11 | 1:K:29:ARG:HG3 | 1.54 | 0.73 |
| 1:M:327:ASP:OD1 | 1:M:328:PRO:HD2 | 1.89 | 0.73 |
| 1:S:95:THR:CG2 | 1:S:100:LEU:HD22 | 2.18 | 0.73 |
| 2:V:252:SER:O | 2:V:256:THR:HG23 | 1.89 | 0.73 |
| 1:3:29:ARG:HA | 1:3:300:LEU:HD22 | 1.69 | 0.73 |
| 1:M:88:ALA:O | 1:M:134:GLY:HA2 | 1.88 | 0.72 |
| 1:Y:268:PRO:CB | 1:Y:270:VAL:HG12 | 2.10 | 0.72 |
| 1:K:196:ASN:HB3 | 1:K:257:THR:HG23 | 1.69 | 0.72 |
| 1:S:28:THR:CG2 | 1:S:30:GLU:N | 2.48 | 0.72 |
| 1:E:142:VAL:HG21 | 1:E:175:ILE:HG12 | 1.72 | 0.72 |
| 2:D:313:ILE:CG2 | 2:D:314:PRO:HD2 | 2.19 | 0.72 |
| 2:N:110:VAL:O | 2:N:166:PRO:HD3 | 1.88 | 0.72 |
| 1:3:55:GLN:O | 1:3:56:LYS:HB2 | 1.88 | 0.72 |
| 1:U:354:TRP:CZ2 | 2:X:325:LYS:HG2 | 2.25 | 0.72 |
| 1:C:29:ARG:CA | 1:C:300:LEU:HD22 | 2.19 | 0.72 |
| 1:U:74:GLY:HA3 | 1:U:233:VAL:CG1 | 2.19 | 0.72 |
| 1:W:88:ALA:O | 1:W:134:GLY:HA2 | 1.90 | 0.72 |
| 2:R:99:LYS:O | 2:R:103:MET:HG3 | 1.90 | 0.71 |
| 1:5:268:PRO:O | 1:5:271:ALA:HB3 | 1.90 | 0.71 |
| 1:C:45:MET:HE3 | 1:C:102:VAL:HG13 | 1.73 | 0.71 |
| 2:F:1:LEU:HD13 | 2:F:2:GLN:N | 2.03 | 0.71 |
| 1:O:100:LEU:HD13 | 1:O:128:ALA:HB2 | 1.70 | 0.71 |
| 1:3:274:THR:CB | 1:3:276:GLU:HG3 | 2.20 | 0.71 |
| 1:5:269:GLY:HA3 | 1:5:273:ARG:HH12 | 1.56 | 0.71 |
| 1:5:270:VAL:O | 1:5:274:THR:CG2 | 2.35 | 0.71 |
| 1:A:318:GLU:HG2 | 2:P:287:PHE:CE2 | 2.26 | 0.71 |
| 2:F:207:ILE:HD13 | 2:F:323:ILE:HG23 | 1.71 | 0.71 |
| 2:D:39:VAL:HG11 | 2:D:115:ARG:NH2 | 2.05 | 0.71 |
| 1:K:11:LYS:HB3 | 1:K:23:VAL:CG1 | 2.21 | 0.71 |
| 2:Z:212:HIS:HB3 | 2:Z:238:MET:HE3 | 1.73 | 0.71 |
| 2:P:121:SER:HB3 | 2:P:124:VAL:CG2 | 2.21 | 0.71 |
| 1:C:230:ILE:O | 1:C:230:ILE:HG13 | 1.89 | 0.71 |
| 1:S:27:LEU:HD22 | 1:S:28:THR:N | 2.05 | 0.71 |
| 1:O:45:MET:HE3 | 1:O:102:VAL:HG13 | 1.73 | 0.70 |
| 2:R:118:ASN:HD21 | 2:R:132:PHE:H | 1.35 | 0.70 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:3:72:CYS:HB2 | 1:3:97:THR:HG21 | 1.73 | 0.70 |
| 1:G:196:ASN:HD21 | 1:G:259:ARG:HE | 1.39 | 0.70 |
| 2:Z:115:ARG:HD2 | 2:Z:157:ILE:HD11 | 1.73 | 0.70 |
| 1:M:280:GLU:C | 1:M:280:GLU:OE1 | 2.30 | 0.70 |
| 1:A:29:ARG:HH11 | 1:A:29:ARG:HG3 | 1.57 | 0.70 |
| 1:1:29:ARG:HG2 | 1:1:29:ARG:HH11 | 1.56 | 0.70 |
| 1:1:231:LEU:HD12 | 1:1:294:ARG:HH11 | 1.54 | 0.70 |
| 2:F:118:ASN:HD21 | 2:F:132:PHE:H | 1.39 | 0.70 |
| 2:V:34:ASP:OD2 | 2:V:41:ARG:HA | 1.91 | 0.70 |
| 1:O:29:ARG:HB2 | 1:O:300:LEU:CD2 | 2.21 | 0.70 |
| 2:H:16:GLU:OE2 | 2:H:162:ARG:NH1 | 2.25 | 0.70 |
| 2:P:121:SER:HB3 | 2:P:124:VAL:HG21 | 1.72 | 0.70 |
| 1:O:280:GLU:O | 1:O:283:SER:N | 2.25 | 0.70 |
| 2:D:185:GLU:O | 2:D:185:GLU:HG2 | 1.88 | 0.69 |
| 1:M:131:PHE:CZ | 1:M:133:GLY:HA2 | 2.28 | 0.69 |
| 1:M:196:ASN:ND2 | 1:M:259:ARG:HE | 1.89 | 0.69 |
| 2:N:327:LEU:O | 2:N:329:ILE:HG23 | 1.92 | 0.69 |
| 1:Q:354:TRP:CZ2 | 2:T:325:LYS:HG2 | 2.27 | 0.69 |
| 1:1:280:GLU:HG2 | 1:1:281:VAL:H | 1.53 | 0.69 |
| 2:2:193:ILE:HD13 | 2:2:239:ARG:NH2 | 2.07 | 0.69 |
| 2:N:250:GLU:O | 2:N:254:MET:HG3 | 1.91 | 0.69 |
| 1:I:29:ARG:HA | 1:I:300:LEU:HD22 | 1.73 | 0.69 |
| 1:I:335:LEU:HD23 | 1:I:335:LEU:O | 1.92 | 0.69 |
| 2:P:184:PRO:HA | 2:P:187:GLN:NE2 | 2.07 | 0.69 |
| 1:U:11:LYS:HB3 | 1:U:23:VAL:CG1 | 2.23 | 0.69 |
| 2:F:34:ASP:OD2 | 2:F:41:ARG:HA | 1.92 | 0.69 |
| 1:K:101:SER:OG | 1:K:104:GLU:HG2 | 1.93 | 0.69 |
| 1:5:64:LEU:N | 1:5:64:LEU:HD23 | 2.06 | 0.69 |
| 2:D:246:MET:O | 2:D:250:GLU:HG3 | 1.92 | 0.69 |
| 2:H:121:SER:HB3 | 2:H:124:VAL:HG21 | 1.74 | 0.69 |
| 1:S:37:ARG:CZ | 1:S:309:ILE:HG23 | 2.22 | 0.69 |
| 1:1:100:LEU:HD13 | 1:1:128:ALA:CB | 2.22 | 0.69 |
| 2:Z:1:LEU:HD13 | 2:Z:2:GLN:N | 2.06 | 0.69 |
| 2:Z:184:PRO:HA | 2:Z:187:GLN:NE2 | 2.08 | 0.69 |
| 1:I:68:GLN:NE2 | 1:I:259:ARG:HB3 | 2.08 | 0.69 |
| 1:S:28:THR:HG22 | 1:S:30:GLU:H | 1.53 | 0.69 |
| 1:S:28:THR:HG22 | 1:S:30:GLU:CB | 2.21 | 0.69 |
| 1:S:28:THR:O | 1:S:29:ARG:C | 2.29 | 0.69 |
| 2:T:327:LEU:O | 2:T:329:ILE:HG23 | 1.93 | 0.69 |
| 1:3:29:ARG:HG2 | 1:3:29:ARG:HH11 | 1.58 | 0.69 |
| 1:5:29:ARG:HH11 | 1:5:29:ARG:CG | 2.03 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:E:131:PHE:CZ | 1:E:133:GLY:HA2 | 2.28 | 0.69 |
| 1:U:142:VAL:HG21 | 1:U:175:ILE:HG12 | 1.75 | 0.69 |
| 1:Y:131:PHE:CE2 | 1:Y:133:GLY:HA2 | 2.28 | 0.69 |
| 2:N:19:ARG:HG2 | 2:N:19:ARG:HH11 | 1.57 | 0.69 |
| 2:T:316:VAL:O | 2:T:316:VAL:HG13 | 1.92 | 0.69 |
| 2:N:252:SER:O | 2:N:256:THR:HG23 | 1.93 | 0.68 |
| 1:O:286:ASP:OD2 | 1:O:286:ASP:C | 2.31 | 0.68 |
| 1:1:197:ARG:HH11 | 1:1:197:ARG:CB | 2.01 | 0.68 |
| 1:C:131:PHE:CE2 | 1:C:133:GLY:HA2 | 2.28 | 0.68 |
| 1:I:101:SER:OG | 1:I:104:GLU:HG3 | 1.94 | 0.68 |
| 1:K:55:GLN:O | 1:K:56:LYS:HB2 | 1.94 | 0.68 |
| 1:U:1:PHE:CD2 | 1:U:29:ARG:NH2 | 2.62 | 0.68 |
| 2:Z:19:ARG:HG2 | 2:Z:19:ARG:HH11 | 1.57 | 0.68 |
| 1:K:268:PRO:O | 1:K:271:ALA:HB3 | 1.94 | 0.68 |
| 2:L:92:GLN:OE1 | 2:L:92:GLN:HA | 1.93 | 0.68 |
| 1:S:29:ARG:HG3 | 1:S:300:LEU:O | 1.92 | 0.68 |
| 1:I:257:THR:OG1 | 1:I:258:TYR:N | 2.26 | 0.68 |
| 1:Q:334:GLU:HG2 | 1:Q:337:TYR:CE2 | 2.27 | 0.68 |
| 2:V:88:GLN:HG2 | 2:X:60:MET:CE | 2.23 | 0.68 |
| 1:W:118:LYS:HB2 | 1:W:118:LYS:NZ | 2.09 | 0.68 |
| 1:5:10:LYS:HG2 | 1:5:11:LYS:N | 2.07 | 0.68 |
| 1:5:327:ASP:OD1 | 1:5:328:PRO:HD2 | 1.94 | 0.68 |
| 1:W:100:LEU:HD13 | 1:W:128:ALA:HB2 | 1.75 | 0.68 |
| 1:1:297:ASN:N | 1:1:297:ASN:HD22 | 1.88 | 0.68 |
| 1:A:138:VAL:HG13 | 1:A:169:ALA:HB2 | 1.75 | 0.68 |
| 1:A:196:ASN:ND2 | 1:A:259:ARG:HD3 | 2.08 | 0.68 |
| 1:M:113:LYS:HD3 | 1:M:328:PRO:HG2 | 1.76 | 0.68 |
| 2:X:98:ALA:HB2 | 2:X:142:LEU:HD13 | 1.75 | 0.68 |
| 1:S:28:THR:CG2 | 1:S:30:GLU:H | 2.06 | 0.68 |
| 1:O:231:LEU:CD1 | 1:O:294:ARG:HH11 | 1.92 | 0.68 |
| 2:P:237:ASN:HD22 | 2:P:237:ASN:C | 1.96 | 0.68 |
| 1:W:272:TYR:HA | 1:W:275:ARG:HG3 | 1.75 | 0.68 |
| 2:4:199:LYS:HD3 | 2:4:239:ARG:NH2 | 2.08 | 0.68 |
| 1:G:272:TYR:HA | 1:G:275:ARG:CD | 2.24 | 0.67 |
| 1:M:274:THR:O | 1:M:277:GLU:CB | 2.42 | 0.67 |
| 1:S:274:THR:O | 1:S:276:GLU:N | 2.27 | 0.67 |
| 2:F:102:TYR:CD2 | 2:H:301:PRO:HG2 | 2.29 | 0.67 |
| 1:S:274:THR:HB | 1:S:276:GLU:CG | 2.24 | 0.67 |
| 2:V:88:GLN:HG2 | 2:X:60:MET:HE1 | 1.76 | 0.67 |
| 1:K:100:LEU:CD1 | 1:K:128:ALA:HB2 | 2.23 | 0.67 |
| 1:O:286:ASP:OD2 | 1:O:287:PRO:N | 2.27 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:33:TYR:O | 2:B:34:ASP:HB2 | 1.93 | 0.67 |
| 1:S:30:GLU:C | 1:S:30:GLU:OE1 | 2.32 | 0.67 |
| 1:S:88:ALA:O | 1:S:134:GLY:CA | 2.42 | 0.67 |
| 2:T:33:TYR:O | 2:T:34:ASP:HB2 | 1.95 | 0.67 |
| 1:W:327:ASP:OD1 | 1:W:328:PRO:HD2 | 1.94 | 0.67 |
| 1:Y:196:ASN:ND2 | 1:Y:259:ARG:HE | 1.93 | 0.67 |
| 1:1:29:ARG:HA | 1:1:300:LEU:HD22 | 1.75 | 0.67 |
| 1:3:89:TYR:HB2 | 1:3:124:MET:HG2 | 1.76 | 0.67 |
| 2:N:157:ILE:O | 2:N:161:ILE:HG13 | 1.95 | 0.67 |
| 1:O:236:ALA:O | 1:O:237:THR:C | 2.33 | 0.67 |
| 1:U:74:GLY:HA3 | 1:U:233:VAL:HG12 | 1.75 | 0.67 |
| 2:T:118:ASN:HD21 | 2:T:132:PHE:H | 1.43 | 0.67 |
| 1:U:177:GLU:OE2 | 1:W:173:GLY:N | 2.26 | 0.67 |
| 2:X:121:SER:HB3 | 2:X:124:VAL:HG21 | 1.75 | 0.67 |
| 2:6:155:GLY:HA3 | 2:6:193:ILE:HG13 | 1.76 | 0.67 |
| 1:O:284:LYS:O | 1:O:285:SER:HB3 | 1.94 | 0.67 |
| 2:D:238:MET:O | 2:D:239:ARG:HB2 | 1.93 | 0.67 |
| 2:D:263:GLU:O | 2:D:296:THR:HA | 1.95 | 0.67 |
| 2:R:1:LEU:HD13 | 2:R:2:GLN:H | 1.60 | 0.67 |
| 1:3:284:LYS:NZ | 1:3:284:LYS:CB | 2.58 | 0.67 |
| 2:V:327:LEU:O | 2:V:329:ILE:HG23 | 1.96 | 0.66 |
| 1:3:101:SER:OG | 1:3:104:GLU:HG3 | 1.95 | 0.66 |
| 1:K:131:PHE:CZ | 1:K:133:GLY:HA2 | 2.30 | 0.66 |
| 1:M:270:VAL:O | 1:M:273:ARG:N | 2.29 | 0.66 |
| 1:S:28:THR:HG23 | 1:S:30:GLU:HB2 | 1.74 | 0.66 |
| 1:3:11:LYS:HB3 | 1:3:23:VAL:HG12 | 1.77 | 0.66 |
| 1:3:257:THR:OG1 | 1:3:258:TYR:N | 2.28 | 0.66 |
| 1:K:229:ASP:OD1 | 1:K:231:LEU:HB2 | 1.94 | 0.66 |
| 1:W:271:ALA:O | 1:W:272:TYR:C | 2.30 | 0.66 |
| 1:Y:223:LEU:N | 1:Y:223:LEU:HD23 | 2.11 | 0.66 |
| 2:2:1:LEU:HD13 | 2:2:2:GLN:N | 2.11 | 0.66 |
| 2:F:246:MET:HE3 | 2:F:279:ILE:CD1 | 2.19 | 0.66 |
| 1:W:196:ASN:HD21 | 1:W:259:ARG:HE | 1.41 | 0.66 |
| 1:5:289:MET:CE | 1:5:290:LEU:HD23 | 2.26 | 0.66 |
| 2:R:118:ASN:HD21 | 2:R:132:PHE:N | 1.92 | 0.66 |
| 2:T:238:MET:O | 2:T:239:ARG:HB2 | 1.95 | 0.66 |
| 1:G:334:GLU:HG2 | 1:G:337:TYR:CD2 | 2.30 | 0.66 |
| 1:M:45:MET:CE | 1:M:102:VAL:HG13 | 2.26 | 0.66 |
| 1:M:272:TYR:C | 1:M:272:TYR:HD1 | 1.97 | 0.66 |
| 2:N:1:LEU:HD13 | 2:N:2:GLN:H | 1.61 | 0.66 |
| 1:U:100:LEU:HD13 | 1:U:128:ALA:HB2 | 1.76 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:1:292:LYS:HG3 | 1:1:306:LEU:HD13 | 1.77 | 0.66 |
| 2:2:238:MET:O | 2:2:239:ARG:HB2 | 1.96 | 0.66 |
| 1:A:352:ASN:H | 1:A:355:ILE:HD12 | 1.61 | 0.66 |
| 1:C:29:ARG:HA | 1:C:300:LEU:HD22 | 1.75 | 0.66 |
| 1:K:232:CYS:O | 1:K:233:VAL:C | 2.32 | 0.66 |
| 1:C:197:ARG:NH2 | 1:C:277:GLU:OE2 | 2.29 | 0.66 |
| 1:1:327:ASP:OD1 | 1:1:328:PRO:HD2 | 1.96 | 0.66 |
| 1:5:231:LEU:HD23 | 1:5:231:LEU:N | 2.11 | 0.66 |
| 2:B:325:LYS:HG2 | 1:C:354:TRP:CZ2 | 2.31 | 0.65 |
| 1:G:11:LYS:HB3 | 1:G:23:VAL:CG1 | 2.26 | 0.65 |
| 1:O:327:ASP:OD1 | 1:O:328:PRO:HD2 | 1.96 | 0.65 |
| 2:T:185:GLU:O | 2:T:185:GLU:HG2 | 1.93 | 0.65 |
| 1:Y:172:GLN:HE22 | 2:2:88:GLN:HE22 | 1.44 | 0.65 |
| 1:5:233:VAL:O | 1:5:234:ARG:C | 2.33 | 0.65 |
| 1:A:230:ILE:O | 1:A:230:ILE:HG13 | 1.96 | 0.65 |
| 1:K:268:PRO:O | 1:K:271:ALA:CB | 2.45 | 0.65 |
| 1:S:113:LYS:HD3 | 1:S:328:PRO:HG2 | 1.78 | 0.65 |
| 2:4:92:GLN:OE1 | 2:4:92:GLN:HA | 1.96 | 0.65 |
| 1:W:272:TYR:C | 1:W:272:TYR:CD2 | 2.70 | 0.65 |
| 1:Y:29:ARG:NH1 | 1:Y:300:LEU:O | 2.30 | 0.65 |
| 2:6:278:ARG:HG3 | 2:6:278:ARG:NH1 | 2.12 | 0.65 |
| 1:C:55:GLN:O | 1:C:56:LYS:HB2 | 1.97 | 0.65 |
| 1:I:327:ASP:OD1 | 1:I:328:PRO:HD2 | 1.97 | 0.65 |
| 1:K:274:THR:O | 1:K:276:GLU:N | 2.29 | 0.65 |
| 1:Y:195:ASN:C | 1:Y:195:ASN:OD1 | 2.33 | 0.65 |
| 1:Y:327:ASP:OD1 | 1:Y:328:PRO:HD2 | 1.96 | 0.65 |
| 1:1:113:LYS:HE2 | 1:1:331:PRO:HD3 | 1.77 | 0.65 |
| 1:S:274:THR:O | 1:S:278:ILE:CD1 | 2.45 | 0.65 |
| 1:3:11:LYS:HB3 | 1:3:23:VAL:CG1 | 2.27 | 0.65 |
| 2:D:237:ASN:C | 2:D:237:ASN:HD22 | 2.00 | 0.65 |
| 1:E:354:TRP:CZ2 | 2:H:325:LYS:HG2 | 2.32 | 0.65 |
| 2:2:110:VAL:O | 2:2:110:VAL:HG12 | 1.95 | 0.65 |
| 2:6:184:PRO:HA | 2:6:187:GLN:HE21 | 1.62 | 0.65 |
| 1:A:29:ARG:CA | 1:A:300:LEU:HD22 | 2.26 | 0.65 |
| 1:A:286:ASP:OD2 | 1:A:288:ILE:HB | 1.97 | 0.65 |
| 1:W:11:LYS:HB3 | 1:W:23:VAL:HG12 | 1.79 | 0.65 |
| 1:5:270:VAL:O | 1:5:271:ALA:C | 2.35 | 0.65 |
| 1:Q:29:ARG:NH1 | 1:Q:300:LEU:O | 2.30 | 0.64 |
| 2:Z:34:ASP:OD2 | 2:Z:41:ARG:HG3 | 1.96 | 0.64 |
| 1:3:274:THR:HB | 1:3:276:GLU:CG | 2.27 | 0.64 |
| 2:J:16:GLU:OE2 | 2:J:162:ARG:NH1 | 2.30 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:P:154:LYS:O | 2:P:157:ILE:HG22 | 1.98 | 0.64 |
| 1:U:225:VAL:HG12 | 1:U:226:ASP:N | 2.11 | 0.64 |
| 1:1:29:ARG:HH11 | 1:1:29:ARG:CG | 2.09 | 0.64 |
| 1:3:223:LEU:HD23 | 1:3:223:LEU:H | 1.62 | 0.64 |
| 1:3:231:LEU:HD12 | 1:3:294:ARG:NH1 | 2.12 | 0.64 |
| 1:E:225:VAL:HG12 | 1:E:226:ASP:N | 2.11 | 0.64 |
| 2:P:1:LEU:HD13 | 2:P:2:GLN:N | 2.12 | 0.64 |
| 1:Q:204:VAL:HG23 | 1:Q:205:GLU:OE1 | 1.97 | 0.64 |
| 1:1:291:LEU:O | 1:1:295:MET:HG2 | 1.98 | 0.64 |
| 2:J:269:PHE:HE1 | 2:L:271:VAL:HA | 1.63 | 0.64 |
| 1:S:274:THR:C | 1:S:276:GLU:N | 2.47 | 0.64 |
| 1:Y:162:LEU:HG | 1:Y:192:ILE:HD11 | 1.78 | 0.64 |
| 2:2:98:ALA:HB2 | 2:2:142:LEU:HD13 | 1.78 | 0.64 |
| 1:A:18:GLU:CG | 1:A:19:GLU:H | 1.97 | 0.64 |
| 1:G:334:GLU:HG2 | 1:G:337:TYR:CE2 | 2.32 | 0.64 |
| 2:J:184:PRO:HA | 2:J:187:GLN:NE2 | 2.13 | 0.64 |
| 1:O:334:GLU:HG2 | 1:O:337:TYR:CE2 | 2.31 | 0.64 |
| 1:W:271:ALA:O | 1:W:274:THR:N | 2.30 | 0.64 |
| 1:A:100:LEU:HD13 | 1:A:128:ALA:HB2 | 1.79 | 0.64 |
| 1:O:131:PHE:CE2 | 1:O:133:GLY:HA2 | 2.33 | 0.64 |
| 1:Q:289:MET:HE1 | 1:Q:290:LEU:HD23 | 1.77 | 0.64 |
| 2:D:191:PHE:O | 2:D:192:LEU:HD12 | 1.97 | 0.64 |
| 1:K:289:MET:HE3 | 1:K:290:LEU:HD23 | 1.80 | 0.64 |
| 2:Z:19:ARG:HG2 | 2:Z:19:ARG:NH1 | 2.11 | 0.64 |
| 1:1:88:ALA:O | 1:1:134:GLY:CA | 2.46 | 0.64 |
| 1:A:45:MET:HE1 | 1:A:105:ILE:HD12 | 1.80 | 0.64 |
| 2:B:148:TRP:O | 2:B:175:MET:HE2 | 1.97 | 0.64 |
| 1:G:131:PHE:CZ | 1:G:133:GLY:HA2 | 2.32 | 0.64 |
| 2:R:316:VAL:O | 2:R:316:VAL:CG1 | 2.44 | 0.64 |
| 2:V:1:LEU:HD13 | 2:V:2:GLN:N | 2.12 | 0.64 |
| 1:1:71:CYS:O | 1:1:75:LEU:HB2 | 1.97 | 0.64 |
| 1:C:101:SER:OG | 1:C:104:GLU:HG3 | 1.98 | 0.63 |
| 2:N:184:PRO:HA | 2:N:187:GLN:NE2 | 2.12 | 0.63 |
| 1:5:268:PRO:O | 1:5:271:ALA:N | 2.31 | 0.63 |
| 2:D:172:ASN:HD22 | 2:D:175:MET:H | 1.46 | 0.63 |
| 1:K:275:ARG:HH11 | 1:K:275:ARG:CG | 2.06 | 0.63 |
| 2:N:34:ASP:OD2 | 2:N:41:ARG:HG3 | 1.98 | 0.63 |
| 2:V:19:ARG:HG2 | 2:V:19:ARG:HH11 | 1.64 | 0.63 |
| 1:1:225:VAL:HG12 | 1:1:226:ASP:N | 2.14 | 0.63 |
| 1:3:274:THR:HB | 1:3:276:GLU:H | 1.63 | 0.63 |
| 2:R:98:ALA:HB2 | 2:R:142:LEU:HD13 | 1.79 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:S:37:ARG:CG | 1:S:37:ARG:NH1 | 2.59 | 0.63 |
| 1:3:100:LEU:HD13 | 1:3:128:ALA:HB2 | 1.80 | 0.63 |
| 1:E:101:SER:OG | 1:E:104:GLU:HG3 | 1.97 | 0.63 |
| 2:F:181:GLU:O | 2:F:183:PRO:HD3 | 1.99 | 0.63 |
| 2:L:98:ALA:HB2 | 2:L:142:LEU:HD13 | 1.79 | 0.63 |
| 2:L:155:GLY:HA3 | 2:L:193:ILE:HG13 | 1.78 | 0.63 |
| 1:O:297:ASN:HD22 | 1:O:297:ASN:N | 1.97 | 0.63 |
| 2:T:118:ASN:HD21 | 2:T:132:PHE:N | 1.96 | 0.63 |
| 1:U:334:GLU:HG2 | 1:U:337:TYR:CD2 | 2.34 | 0.63 |
| 1:Y:50:ASP:HB2 | 1:Y:64:LEU:CD1 | 2.29 | 0.63 |
| 1:5:11:LYS:HB3 | 1:5:23:VAL:CG1 | 2.29 | 0.63 |
| 1:C:182:ALA:HA | 1:C:187:LEU:HD12 | 1.81 | 0.63 |
| 1:K:270:VAL:HG22 | 1:K:273:ARG:HH12 | 1.64 | 0.63 |
| 2:L:172:ASN:ND2 | 2:L:174:LEU:H | 1.95 | 0.63 |
| 1:C:88:ALA:O | 1:C:134:GLY:CA | 2.46 | 0.63 |
| 1:K:274:THR:O | 1:K:277:GLU:N | 2.31 | 0.63 |
| 1:1:16:ARG:HG2 | 1:1:16:ARG:HH11 | 1.63 | 0.63 |
| 1:W:196:ASN:O | 1:W:197:ARG:HB2 | 1.98 | 0.63 |
| 1:Y:45:MET:HE1 | 1:Y:105:ILE:HD12 | 1.79 | 0.63 |
| 1:3:113:LYS:CD | 1:3:328:PRO:HG2 | 2.28 | 0.63 |
| 1:3:205:GLU:HG3 | 1:3:206:ARG:N | 2.14 | 0.63 |
| 2:4:184:PRO:HA | 2:4:187:GLN:NE2 | 2.14 | 0.63 |
| 1:5:273:ARG:HD3 | 1:5:273:ARG:H | 1.62 | 0.63 |
| 1:A:335:LEU:HD23 | 1:A:335:LEU:C | 2.19 | 0.63 |
| 2:B:172:ASN:HD22 | 2:B:175:MET:H | 1.45 | 0.63 |
| 2:J:118:ASN:HD21 | 2:J:132:PHE:H | 1.45 | 0.63 |
| 2:J:252:SER:O | 2:J:256:THR:HG23 | 1.99 | 0.62 |
| 1:Q:10:LYS:HG2 | 1:Q:11:LYS:N | 2.14 | 0.62 |
| 2:Z:276:CYS:HB3 | 2:2:280:MET:CE | 2.29 | 0.62 |
| 1:C:257:THR:OG1 | 1:C:258:TYR:N | 2.32 | 0.62 |
| 2:N:16:GLU:OE2 | 2:N:162:ARG:NH1 | 2.32 | 0.62 |
| 1:Q:50:ASP:HB2 | 1:Q:64:LEU:HD13 | 1.81 | 0.62 |
| 1:S:37:ARG:NH1 | 1:S:37:ARG:HG3 | 2.13 | 0.62 |
| 1:Y:88:ALA:O | 1:Y:134:GLY:HA2 | 1.99 | 0.62 |
| 2:N:19:ARG:HG2 | 2:N:19:ARG:NH1 | 2.13 | 0.62 |
| 1:W:29:ARG:NH1 | 1:W:300:LEU:O | 2.32 | 0.62 |
| 2:X:259:LEU:CD2 | 2:X:279:ILE:HG13 | 2.29 | 0.62 |
| 2:4:172:ASN:HD22 | 2:4:175:MET:H | 1.47 | 0.62 |
| 2:N:1:LEU:HD13 | 2:N:2:GLN:N | 2.13 | 0.62 |
| 1:G:68:GLN:HE21 | 1:G:259:ARG:HB3 | 1.64 | 0.62 |
| 1:Q:335:LEU:HD23 | 1:Q:335:LEU:O | 2.00 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:T:307:ILE:HG23 | 2:T:308:LEU:N | 2.15 | 0.62 |
| 1:U:84:HIS:CE1 | 1:U:130:ASN:HD21 | 2.15 | 0.62 |
| 1:O:29:ARG:CB | 1:O:300:LEU:HD22 | 2.29 | 0.62 |
| 1:Y:272:TYR:CD1 | 1:Y:272:TYR:C | 2.72 | 0.62 |
| 2:6:246:MET:O | 2:6:250:GLU:HG3 | 1.99 | 0.62 |
| 1:I:196:ASN:HB3 | 1:I:257:THR:HG23 | 1.80 | 0.62 |
| 2:P:316:VAL:O | 2:P:317:LYS:C | 2.35 | 0.62 |
| 1:Q:29:ARG:HA | 1:Q:300:LEU:HD22 | 1.82 | 0.62 |
| 1:S:4:ASP:HA | 1:S:300:LEU:HD21 | 1.82 | 0.62 |
| 1:3:1:PHE:HB3 | 1:3:299:ASN:O | 1.99 | 0.62 |
| 2:H:316:VAL:O | 2:H:317:LYS:C | 2.37 | 0.62 |
| 1:I:231:LEU:HD12 | 1:I:294:ARG:NH1 | 2.15 | 0.62 |
| 2:L:263:GLU:O | 2:L:296:THR:HA | 1.98 | 0.62 |
| 1:O:100:LEU:HD13 | 1:O:128:ALA:CB | 2.29 | 0.62 |
| 1:U:11:LYS:HB3 | 1:U:23:VAL:HG12 | 1.82 | 0.62 |
| 2:Z:172:ASN:HD22 | 2:Z:175:MET:H | 1.47 | 0.62 |
| 1:1:132:TYR:N | 1:1:132:TYR:CD1 | 2.68 | 0.62 |
| 1:5:268:PRO:C | 1:5:270:VAL:N | 2.52 | 0.62 |
| 1:A:196:ASN:HD21 | 1:A:259:ARG:HD3 | 1.64 | 0.62 |
| 2:H:98:ALA:HB2 | 2:H:142:LEU:CD1 | 2.29 | 0.62 |
| 2:J:172:ASN:HD22 | 2:J:175:MET:H | 1.48 | 0.62 |
| 1:O:280:GLU:CG | 1:O:281:VAL:N | 2.62 | 0.62 |
| 1:Q:257:THR:OG1 | 1:Q:258:TYR:N | 2.33 | 0.62 |
| 1:S:27:LEU:HD22 | 1:S:27:LEU:C | 2.19 | 0.62 |
| 2:X:327:LEU:O | 2:X:329:ILE:HG23 | 2.00 | 0.62 |
| 2:2:51:ARG:HH11 | 2:2:51:ARG:HG3 | 1.64 | 0.62 |
| 1:G:223:LEU:N | 1:G:223:LEU:HD23 | 2.15 | 0.62 |
| 1:I:45:MET:HE3 | 1:I:102:VAL:HG13 | 1.81 | 0.62 |
| 1:K:231:LEU:HD12 | 1:K:294:ARG:NH1 | 2.15 | 0.62 |
| 1:Q:274:THR:O | 1:Q:277:GLU:N | 2.33 | 0.62 |
| 1:W:327:ASP:CG | 1:W:328:PRO:HD2 | 2.20 | 0.61 |
| 1:3:150:LEU:HA | 1:3:187:LEU:HD22 | 1.82 | 0.61 |
| 2:6:165:ASN:HB3 | 2:6:166:PRO:HD2 | 1.81 | 0.61 |
| 2:D:1:LEU:HD12 | 2:D:3:VAL:HG12 | 1.82 | 0.61 |
| 2:X:278:ARG:HG3 | 2:X:278:ARG:NH1 | 2.03 | 0.61 |
| 1:3:1:PHE:N | 1:3:1:PHE:CD2 | 2.68 | 0.61 |
| 1:3:205:GLU:HG3 | 1:3:206:ARG:H | 1.65 | 0.61 |
| 2:4:300:VAL:HG12 | 1:5:339:ILE:HD11 | 1.82 | 0.61 |
| 2:6:191:PHE:O | 2:6:192:LEU:HD12 | 2.00 | 0.61 |
| 1:A:1:PHE:HA | 1:A:299:ASN:ND2 | 2.14 | 0.61 |
| 1:O:39:MET:HG2 | 1:O:73:VAL:HG21 | 1.83 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:P:98:ALA:HB2 | 2:P:142:LEU:HD13 | 1.81 | 0.61 |
| 1:Q:80:ASN:HB3 | 1:Q:81:PRO:HD2 | 1.81 | 0.61 |
| 1:Y:196:ASN:O | 1:Y:197:ARG:HB2 | 1.99 | 0.61 |
| 2:Z:300:VAL:HG12 | 1:1:339:ILE:HD11 | 1.81 | 0.61 |
| 1:1:297:ASN:HD22 | 1:1:297:ASN:H | 1.48 | 0.61 |
| 1:3:71:CYS:O | 1:3:72:CYS:C | 2.36 | 0.61 |
| 2:4:308:LEU:HD22 | 1:5:335:LEU:HB2 | 1.83 | 0.61 |
| 1:5:70:ALA:HB2 | 1:5:287:PRO:HB3 | 1.81 | 0.61 |
| 1:O:197:ARG:HB3 | 1:O:197:ARG:NH1 | 2.12 | 0.61 |
| 1:Q:16:ARG:HH11 | 1:Q:16:ARG:CG | 2.14 | 0.61 |
| 2:T:184:PRO:HA | 2:T:187:GLN:NE2 | 2.14 | 0.61 |
| 1:W:271:ALA:O | 1:W:273:ARG:N | 2.33 | 0.61 |
| 2:D:316:VAL:O | 2:D:316:VAL:CG1 | 2.49 | 0.61 |
| 1:E:289:MET:CE | 1:E:290:LEU:HD23 | 2.30 | 0.61 |
| 1:M:195:ASN:C | 1:M:195:ASN:OD1 | 2.37 | 0.61 |
| 1:W:271:ALA:O | 1:W:274:THR:HG23 | 2.01 | 0.61 |
| 1:I:174:GLN:HB3 | 2:J:60:MET:HG2 | 1.83 | 0.61 |
| 1:M:196:ASN:HD22 | 1:M:259:ARG:HE | 1.47 | 0.61 |
| 2:R:1:LEU:CD1 | 2:R:2:GLN:H | 2.13 | 0.61 |
| 2:R:316:VAL:O | 2:R:316:VAL:HG12 | 1.99 | 0.61 |
| 1:E:272:TYR:CE1 | 1:E:276:GLU:OE2 | 2.54 | 0.61 |
| 1:O:286:ASP:OD2 | 1:O:287:PRO:HD2 | 2.01 | 0.61 |
| 1:3:335:LEU:HD23 | 1:3:335:LEU:C | 2.20 | 0.61 |
| 2:D:327:LEU:O | 2:D:329:ILE:HG23 | 2.00 | 0.61 |
| 1:K:229:ASP:O | 1:K:231:LEU:N | 2.33 | 0.61 |
| 1:C:11:LYS:HB3 | 1:C:23:VAL:HG12 | 1.82 | 0.61 |
| 1:S:44:ARG:HB2 | 1:S:317:ILE:HG13 | 1.83 | 0.61 |
| 2:Z:207:ILE:HD13 | 2:Z:323:ILE:HG23 | 1.83 | 0.61 |
| 2:Z:250:GLU:O | 2:Z:254:MET:HG3 | 2.00 | 0.61 |
| 1:I:335:LEU:HD23 | 1:I:335:LEU:C | 2.21 | 0.60 |
| 2:L:278:ARG:NH1 | 2:L:278:ARG:HG3 | 2.15 | 0.60 |
| 1:O:280:GLU:O | 1:O:282:ARG:N | 2.34 | 0.60 |
| 1:S:274:THR:O | 1:S:275:ARG:C | 2.38 | 0.60 |
| 1:3:29:ARG:HH11 | 1:3:29:ARG:CG | 2.13 | 0.60 |
| 1:K:10:LYS:HG2 | 1:K:11:LYS:N | 2.15 | 0.60 |
| 1:O:289:MET:CE | 1:O:290:LEU:HD23 | 2.31 | 0.60 |
| 2:R:95:ASN:ND2 | 2:T:87:MET:CE | 2.64 | 0.60 |
| 2:V:313:ILE:CG2 | 2:V:314:PRO:CD | 2.78 | 0.60 |
| 2:Z:246:MET:O | 2:Z:250:GLU:HG3 | 2.00 | 0.60 |
| 2:H:193:ILE:HD13 | 2:H:239:ARG:NH2 | 2.16 | 0.60 |
| 2:N:278:ARG:HH11 | 2:N:278:ARG:HG2 | 1.65 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:O:286:ASP:OD2 | 1:O:287:PRO:CD | 2.49 | 0.60 |
| 1:Y:45:MET:HE3 | 1:Y:102:VAL:HG13 | 1.83 | 0.60 |
| 1:I:174:GLN:HB3 | 2:J:60:MET:CG | 2.30 | 0.60 |
| 2:P:1:LEU:HD13 | 2:P:2:GLN:H | 1.64 | 0.60 |
| 2:P:110:VAL:HG12 | 2:P:110:VAL:O | 2.00 | 0.60 |
| 2:Z:327:LEU:O | 2:Z:329:ILE:HG23 | 2.00 | 0.60 |
| 1:1:40:GLN:O | 1:1:44:ARG:HG2 | 2.01 | 0.60 |
| 2:4:329:ILE:OXT | 2:4:329:ILE:HG13 | 2.02 | 0.60 |
| 2:H:21:GLU:HG2 | 2:H:21:GLU:O | 2.01 | 0.60 |
| 2:N:325:LYS:HG2 | 1:O:354:TRP:CZ2 | 2.35 | 0.60 |
| 1:O:174:GLN:HB3 | 2:P:60:MET:HG2 | 1.84 | 0.60 |
| 2:2:155:GLY:HA3 | 2:2:193:ILE:HG13 | 1.83 | 0.60 |
| 2:6:98:ALA:HB2 | 2:6:142:LEU:CD1 | 2.28 | 0.60 |
| 1:G:272:TYR:CA | 1:G:275:ARG:HD3 | 2.31 | 0.60 |
| 1:G:274:THR:O | 1:G:277:GLU:N | 2.34 | 0.60 |
| 1:M:270:VAL:O | 1:M:272:TYR:N | 2.35 | 0.60 |
| 1:A:55:GLN:O | 1:A:56:LYS:HB2 | 2.02 | 0.60 |
| 2:B:98:ALA:HB2 | 2:B:142:LEU:HD13 | 1.83 | 0.60 |
| 1:E:45:MET:HE3 | 1:E:102:VAL:HG22 | 1.84 | 0.60 |
| 1:E:177:GLU:OE2 | 1:G:173:GLY:N | 2.35 | 0.60 |
| 1:S:45:MET:CE | 1:S:105:ILE:HD12 | 2.31 | 0.60 |
| 2:T:258:HIS:CD2 | 2:T:327:LEU:HD23 | 2.36 | 0.60 |
| 1:U:70:ALA:HB3 | 1:U:227:GLY:O | 2.01 | 0.60 |
| 1:W:108:GLU:OE1 | 1:W:117:ALA:N | 2.29 | 0.60 |
| 1:3:78:GLY:HA2 | 1:3:238:ARG:HG2 | 1.82 | 0.60 |
| 2:B:238:MET:O | 2:B:239:ARG:HB2 | 2.01 | 0.60 |
| 1:1:53:TYR:CD2 | 1:1:62:CYS:HB3 | 2.36 | 0.60 |
| 1:1:131:PHE:CE2 | 1:1:133:GLY:HA2 | 2.36 | 0.60 |
| 1:1:334:GLU:HG2 | 1:1:337:TYR:CE2 | 2.37 | 0.60 |
| 1:3:7:PHE:CD2 | 1:3:294:ARG:HD3 | 2.37 | 0.60 |
| 1:C:335:LEU:C | 1:C:335:LEU:HD23 | 2.21 | 0.60 |
| 1:Q:335:LEU:HD23 | 1:Q:335:LEU:C | 2.22 | 0.60 |
| 2:4:246:MET:O | 2:4:250:GLU:HG3 | 2.02 | 0.60 |
| 1:M:3:ASN:O | 1:M:3:ASN:ND2 | 2.34 | 0.60 |
| 1:G:10:LYS:HG2 | 1:G:11:LYS:N | 2.16 | 0.59 |
| 1:G:196:ASN:O | 1:G:197:ARG:HB2 | 2.01 | 0.59 |
| 2:X:278:ARG:HH11 | 2:X:278:ARG:CG | 2.12 | 0.59 |
| 2:D:258:HIS:CD2 | 2:D:327:LEU:HD23 | 2.38 | 0.59 |
| 2:J:4:THR:HA | 2:J:179:PRO:HA | 1.84 | 0.59 |
| 2:R:16:GLU:OE2 | 2:R:162:ARG:NH1 | 2.35 | 0.59 |
| 1:S:28:THR:O | 1:S:30:GLU:N | 2.35 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:1:39:MET:HG2 | 1:1:73:VAL:HG21 | 1.83 | 0.59 |
| 1:E:304:GLU:O | 1:E:308:GLU:HG3 | 2.02 | 0.59 |
| 1:I:345:PRO:HB3 | 1:I:360:VAL:HG12 | 1.84 | 0.59 |
| 1:S:257:THR:OG1 | 1:S:258:TYR:N | 2.35 | 0.59 |
| 1:M:15:HIS:CG | 1:M:215:LYS:HG2 | 2.37 | 0.59 |
| 1:Q:61:PHE:HD2 | 1:Q:124:MET:CE | 2.16 | 0.59 |
| 1:Q:61:PHE:HD2 | 1:Q:124:MET:HE2 | 1.68 | 0.59 |
| 1:S:345:PRO:HB3 | 1:S:360:VAL:HG12 | 1.83 | 0.59 |
| 2:H:121:SER:HB3 | 2:H:124:VAL:CG2 | 2.32 | 0.59 |
| 1:M:274:THR:O | 1:M:277:GLU:N | 2.35 | 0.59 |
| 1:O:286:ASP:OD2 | 1:O:288:ILE:N | 2.35 | 0.59 |
| 1:W:174:GLN:HB3 | 2:X:60:MET:HG2 | 1.84 | 0.59 |
| 1:1:280:GLU:O | 1:1:283:SER:N | 2.28 | 0.59 |
| 2:4:98:ALA:HB2 | 2:4:142:LEU:HD13 | 1.83 | 0.59 |
| 2:R:11:GLN:O | 2:R:15:GLU:HG3 | 2.03 | 0.59 |
| 1:W:315:LYS:HB2 | 1:W:315:LYS:NZ | 2.18 | 0.59 |
| 1:Y:15:HIS:CG | 1:Y:215:LYS:HG2 | 2.38 | 0.59 |
| 1:3:284:LYS:HB3 | 1:3:284:LYS:HZ1 | 1.66 | 0.59 |
| 1:A:80:ASN:HB3 | 1:A:81:PRO:HD2 | 1.84 | 0.59 |
| 2:D:84:ASN:ND2 | 2:D:128:HIS:HA | 2.18 | 0.59 |
| 1:O:88:ALA:HB2 | 1:O:141:GLN:NE2 | 2.18 | 0.59 |
| 1:Q:113:LYS:HD3 | 1:Q:328:PRO:HG2 | 1.83 | 0.59 |
| 1:A:281:VAL:O | 1:A:281:VAL:HG12 | 2.03 | 0.59 |
| 1:G:274:THR:O | 1:G:276:GLU:N | 2.35 | 0.59 |
| 1:O:29:ARG:CA | 1:O:300:LEU:HD22 | 2.33 | 0.59 |
| 1:1:280:GLU:O | 1:1:282:ARG:N | 2.35 | 0.59 |
| 1:C:334:GLU:HG2 | 1:C:337:TYR:CE2 | 2.37 | 0.59 |
| 1:S:40:GLN:O | 1:S:44:ARG:HG2 | 2.02 | 0.59 |
| 1:1:285:SER:O | 1:1:286:ASP:C | 2.41 | 0.59 |
| 2:H:81:MET:HB3 | 2:H:85:PHE:CD2 | 2.38 | 0.59 |
| 2:J:11:GLN:O | 2:J:15:GLU:HG3 | 2.03 | 0.59 |
| 1:O:236:ALA:O | 1:O:239:PHE:N | 2.35 | 0.59 |
| 2:P:268:GLN:O | 2:P:269:PHE:HB2 | 2.03 | 0.59 |
| 1:Q:50:ASP:HB2 | 1:Q:64:LEU:CD1 | 2.33 | 0.59 |
| 1:3:102:VAL:HG11 | 1:3:317:ILE:HD12 | 1.85 | 0.59 |
| 2:F:184:PRO:HA | 2:F:187:GLN:NE2 | 2.18 | 0.58 |
| 2:J:1:LEU:CD1 | 2:J:2:GLN:H | 2.16 | 0.58 |
| 1:S:46:GLU:OE1 | 1:S:46:GLU:HA | 2.03 | 0.58 |
| 1:Y:289:MET:CE | 1:Y:290:LEU:HD23 | 2.32 | 0.58 |
| 1:A:16:ARG:CG | 1:A:16:ARG:NH1 | 2.53 | 0.58 |
| 1:A:29:ARG:NH1 | 1:A:300:LEU:O | 2.36 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:4:95:ASN:HD21 | 2:6:87:MET:CE | 2.16 | 0.58 |
| 1:M:132:TYR:CD1 | 1:M:148:ILE:HD13 | 2.38 | 0.58 |
| 1:O:335:LEU:HD23 | 1:O:335:LEU:C | 2.23 | 0.58 |
| 1:5:270:VAL:HG12 | 1:5:271:ALA:N | 2.17 | 0.58 |
| 1:E:108:GLU:OE2 | 1:E:119:GLY:HA2 | 2.04 | 0.58 |
| 1:E:267:ASP:O | 1:E:270:VAL:N | 2.37 | 0.58 |
| 1:E:272:TYR:CD1 | 1:E:272:TYR:C | 2.76 | 0.58 |
| 1:E:272:TYR:HE1 | 1:E:276:GLU:OE2 | 1.87 | 0.58 |
| 1:S:327:ASP:OD1 | 1:S:328:PRO:HD2 | 2.04 | 0.58 |
| 1:W:57:ILE:HG22 | 1:W:110:THR:HG22 | 1.84 | 0.58 |
| 1:3:29:ARG:NH1 | 1:3:300:LEU:O | 2.37 | 0.58 |
| 1:3:206:ARG:NH2 | 2:6:32:GLN:HE22 | 2.00 | 0.58 |
| 1:S:39:MET:HG2 | 1:S:73:VAL:HG21 | 1.86 | 0.58 |
| 1:S:100:LEU:HD13 | 1:S:128:ALA:HB2 | 1.84 | 0.58 |
| 2:X:193:ILE:HD13 | 2:X:239:ARG:NH2 | 2.17 | 0.58 |
| 1:3:223:LEU:HD23 | 1:3:223:LEU:N | 2.18 | 0.58 |
| 2:4:148:TRP:CD1 | 2:4:175:MET:HE2 | 2.38 | 0.58 |
| 1:5:231:LEU:CD2 | 1:5:231:LEU:N | 2.64 | 0.58 |
| 1:I:304:GLU:O | 1:I:308:GLU:HG3 | 2.02 | 0.58 |
| 1:S:29:ARG:HB2 | 1:S:300:LEU:CD2 | 2.33 | 0.58 |
| 1:1:77:ALA:HB3 | 1:1:234:ARG:HG3 | 1.85 | 0.58 |
| 2:4:102:TYR:CG | 2:6:301:PRO:HG2 | 2.38 | 0.58 |
| 1:5:132:TYR:N | 1:5:132:TYR:CD1 | 2.72 | 0.58 |
| 1:M:289:MET:CE | 1:M:290:LEU:HD23 | 2.34 | 0.58 |
| 2:P:143:LYS:HB2 | 2:P:167:VAL:HG22 | 1.86 | 0.58 |
| 1:Q:353:GLN:NE2 | 2:R:281:GLU:HB3 | 2.18 | 0.58 |
| 2:F:276:CYS:HB3 | 2:H:280:MET:CE | 2.33 | 0.58 |
| 1:1:29:ARG:CA | 1:1:300:LEU:HD22 | 2.33 | 0.58 |
| 2:2:237:ASN:C | 2:2:237:ASN:HD22 | 2.07 | 0.58 |
| 1:E:29:ARG:NH1 | 1:E:300:LEU:O | 2.36 | 0.58 |
| 1:E:274:THR:O | 1:E:278:ILE:HG12 | 2.04 | 0.58 |
| 2:F:172:ASN:HD22 | 2:F:175:MET:H | 1.51 | 0.58 |
| 1:Q:165:TYR:HH | 1:Q:179:TYR:HH | 1.51 | 0.58 |
| 2:R:184:PRO:HG2 | 2:R:185:GLU:H | 1.69 | 0.58 |
| 1:S:30:GLU:CA | 1:S:30:GLU:OE1 | 2.50 | 0.58 |
| 1:G:223:LEU:HD23 | 1:G:223:LEU:H | 1.69 | 0.58 |
| 2:H:51:ARG:HH11 | 2:H:51:ARG:HG3 | 1.68 | 0.58 |
| 1:I:78:GLY:HA2 | 1:I:238:ARG:HG2 | 1.84 | 0.58 |
| 2:L:172:ASN:HD22 | 2:L:174:LEU:N | 2.01 | 0.58 |
| 2:N:99:LYS:HG2 | 2:P:301:PRO:HB3 | 1.84 | 0.58 |
| 2:R:95:ASN:ND2 | 2:T:87:MET:HE1 | 2.19 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:V:121:SER:HB3 | 2:V:124:VAL:HG21 | 1.86 | 0.58 |
| 1:W:132:TYR:N | 1:W:132:TYR:CD1 | 2.71 | 0.58 |
| 2:X:121:SER:HB3 | 2:X:124:VAL:CG2 | 2.34 | 0.58 |
| 1:Y:347:GLU:OE1 | 1:Y:356:LYS:HD3 | 2.04 | 0.58 |
| 2:P:278:ARG:HG3 | 2:P:278:ARG:NH1 | 2.18 | 0.57 |
| 1:1:70:ALA:HB3 | 1:1:227:GLY:O | 2.03 | 0.57 |
| 2:4:17:LEU:O | 2:4:51:ARG:NH2 | 2.37 | 0.57 |
| 1:5:289:MET:HE3 | 1:5:290:LEU:HD23 | 1.86 | 0.57 |
| 1:A:45:MET:CE | 1:A:102:VAL:HG13 | 2.31 | 0.57 |
| 1:A:327:ASP:OD1 | 1:A:328:PRO:HD2 | 2.04 | 0.57 |
| 2:H:238:MET:O | 2:H:239:ARG:HB2 | 2.03 | 0.57 |
| 2:P:193:ILE:HD13 | 2:P:239:ARG:NH2 | 2.19 | 0.57 |
| 1:W:150:LEU:HA | 1:W:187:LEU:HD22 | 1.86 | 0.57 |
| 1:3:274:THR:C | 1:3:276:GLU:N | 2.57 | 0.57 |
| 1:A:33:LEU:HD12 | 1:A:295:MET:HE1 | 1.86 | 0.57 |
| 2:F:11:GLN:O | 2:F:15:GLU:HG3 | 2.04 | 0.57 |
| 1:S:286:ASP:HB3 | 1:S:289:MET:HB3 | 1.86 | 0.57 |
| 2:2:16:GLU:OE2 | 2:2:162:ARG:NH1 | 2.37 | 0.57 |
| 2:4:301:PRO:HB3 | 2:6:99:LYS:HG2 | 1.87 | 0.57 |
| 2:D:212:HIS:HB3 | 2:D:238:MET:HE3 | 1.86 | 0.57 |
| 1:G:55:GLN:O | 1:G:56:LYS:CB | 2.47 | 0.57 |
| 2:H:316:VAL:O | 2:H:318:ASP:N | 2.37 | 0.57 |
| 1:Q:88:ALA:O | 1:Q:134:GLY:CA | 2.52 | 0.57 |
| 2:4:143:LYS:HB2 | 2:4:167:VAL:HG22 | 1.86 | 0.57 |
| 1:5:268:PRO:O | 1:5:270:VAL:N | 2.36 | 0.57 |
| 1:A:2:ALA:H | 1:A:299:ASN:HD22 | 1.52 | 0.57 |
| 2:D:237:ASN:C | 2:D:237:ASN:ND2 | 2.57 | 0.57 |
| 1:E:335:LEU:HG | 1:E:335:LEU:O | 2.02 | 0.57 |
| 2:F:102:TYR:CG | 2:H:301:PRO:HG2 | 2.38 | 0.57 |
| 1:G:274:THR:O | 1:G:275:ARG:C | 2.41 | 0.57 |
| 2:L:237:ASN:C | 2:L:237:ASN:HD22 | 2.08 | 0.57 |
| 1:O:234:ARG:HH21 | 1:O:238:ARG:HH22 | 1.51 | 0.57 |
| 1:U:337:TYR:HB3 | 1:U:338:HIS:CD2 | 2.40 | 0.57 |
| 1:3:284:LYS:HB3 | 1:3:284:LYS:HZ2 | 1.65 | 0.57 |
| 1:I:88:ALA:O | 1:I:134:GLY:HA2 | 2.04 | 0.57 |
| 2:P:118:ASN:ND2 | 2:P:132:PHE:H | 2.02 | 0.57 |
| 2:P:155:GLY:HA3 | 2:P:193:ILE:HG13 | 1.85 | 0.57 |
| 1:Y:68:GLN:HE22 | 1:Y:196:ASN:HD22 | 1.53 | 0.57 |
| 2:2:152:ASP:HA | 2:2:193:ILE:HD12 | 1.87 | 0.57 |
| 2:2:268:GLN:O | 2:2:269:PHE:HB2 | 2.05 | 0.57 |
| 2:4:1:LEU:CD1 | 2:4:2:GLN:H | 2.14 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:D:158:LYS:HE3 | 2:D:191:PHE:O | 2.05 | 0.57 |
| 1:E:267:ASP:O | 1:E:269:GLY:N | 2.38 | 0.57 |
| 2:L:157:ILE:O | 2:L:161:ILE:HG13 | 2.04 | 0.57 |
| 1:M:268:PRO:CB | 1:M:270:VAL:CG2 | 2.74 | 0.57 |
| 1:S:101:SER:OG | 1:S:104:GLU:HG3 | 2.05 | 0.57 |
| 2:F:87:MET:CE | 2:H:95:ASN:ND2 | 2.68 | 0.57 |
| 1:G:151:ALA:HB1 | 2:H:74:LEU:HD22 | 1.86 | 0.57 |
| 1:O:3:ASN:O | 1:O:4:ASP:HB3 | 2.05 | 0.57 |
| 1:Q:78:GLY:HA2 | 1:Q:238:ARG:HG2 | 1.85 | 0.57 |
| 2:6:16:GLU:OE2 | 2:6:162:ARG:NH1 | 2.36 | 0.57 |
| 2:6:268:GLN:O | 2:6:269:PHE:HB2 | 2.04 | 0.57 |
| 1:G:151:ALA:CB | 2:H:74:LEU:HD22 | 2.35 | 0.57 |
| 1:K:275:ARG:NH1 | 1:K:275:ARG:CG | 2.66 | 0.57 |
| 2:T:278:ARG:HH11 | 2:T:278:ARG:CG | 2.12 | 0.57 |
| 2:X:16:GLU:OE2 | 2:X:162:ARG:NH1 | 2.38 | 0.57 |
| 2:4:252:SER:O | 2:4:256:THR:HG23 | 2.04 | 0.57 |
| 1:5:322:GLN:HG3 | 1:5:323:PHE:N | 2.20 | 0.57 |
| 1:C:29:ARG:HG3 | 1:C:30:GLU:N | 2.17 | 0.57 |
| 2:L:23:VAL:HG22 | 2:L:75:ARG:HB2 | 1.87 | 0.57 |
| 2:L:172:ASN:ND2 | 2:L:174:LEU:N | 2.53 | 0.57 |
| 1:S:231:LEU:HD12 | 1:S:294:ARG:NH1 | 2.20 | 0.57 |
| 2:2:154:LYS:O | 2:2:157:ILE:HG22 | 2.05 | 0.57 |
| 1:5:162:LEU:CD1 | 1:5:190:ILE:HD12 | 2.35 | 0.57 |
| 2:D:98:ALA:HB2 | 2:D:142:LEU:HD13 | 1.86 | 0.56 |
| 1:O:229:ASP:C | 1:O:231:LEU:N | 2.47 | 0.56 |
| 1:O:345:PRO:HB3 | 1:O:360:VAL:HG12 | 1.85 | 0.56 |
| 2:P:33:TYR:O | 2:P:34:ASP:HB2 | 2.03 | 0.56 |
| 2:P:207:ILE:HG13 | 2:P:258:HIS:HB2 | 1.85 | 0.56 |
| 2:B:19:ARG:HG2 | 2:B:19:ARG:HH11 | 1.70 | 0.56 |
| 1:I:29:ARG:HH11 | 1:I:29:ARG:HG2 | 1.70 | 0.56 |
| 1:Q:225:VAL:HG12 | 1:Q:226:ASP:N | 2.19 | 0.56 |
| 2:V:51:ARG:HH11 | 2:V:51:ARG:HG3 | 1.70 | 0.56 |
| 1:1:45:MET:CE | 1:1:102:VAL:HA | 2.34 | 0.56 |
| 1:A:169:ALA:O | 1:A:175:ILE:HD12 | 2.05 | 0.56 |
| 1:C:100:LEU:HD13 | 1:C:128:ALA:HB2 | 1.87 | 0.56 |
| 1:E:347:GLU:OE1 | 1:E:356:LYS:HD3 | 2.05 | 0.56 |
| 2:F:246:MET:O | 2:F:250:GLU:HG3 | 2.04 | 0.56 |
| 1:G:74:GLY:HA2 | 1:G:230:ILE:HD12 | 1.87 | 0.56 |
| 1:S:334:GLU:HG2 | 1:S:337:TYR:CE2 | 2.40 | 0.56 |
| 1:Y:101:SER:OG | 1:Y:104:GLU:HG3 | 2.06 | 0.56 |
| 2:Z:99:LYS:HG2 | 2:2:301:PRO:HB3 | 1.88 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:196:ASN:ND2 | 1:A:259:ARG:CD | 2.68 | 0.56 |
| 1:K:229:ASP:C | 1:K:231:LEU:H | 2.08 | 0.56 |
| 2:N:118:ASN:HD21 | 2:N:132:PHE:N | 2.00 | 0.56 |
| 1:E:89:TYR:HB2 | 1:E:124:MET:HG2 | 1.88 | 0.56 |
| 2:F:325:LYS:HG2 | 1:G:354:TRP:CZ2 | 2.39 | 0.56 |
| 1:K:272:TYR:CD1 | 1:K:272:TYR:C | 2.79 | 0.56 |
| 2:T:1:LEU:HD13 | 2:T:2:GLN:N | 2.21 | 0.56 |
| 1:Y:29:ARG:HG2 | 1:Y:29:ARG:HH11 | 1.71 | 0.56 |
| 1:1:196:ASN:HD21 | 1:1:259:ARG:NE | 2.04 | 0.56 |
| 2:N:238:MET:O | 2:N:239:ARG:HB2 | 2.06 | 0.56 |
| 1:O:10:LYS:HG2 | 1:O:11:LYS:N | 2.20 | 0.56 |
| 1:Q:204:VAL:HG23 | 1:Q:205:GLU:H | 1.70 | 0.56 |
| 1:S:29:ARG:HB2 | 1:S:300:LEU:HD23 | 1.86 | 0.56 |
| 2:V:19:ARG:HG2 | 2:V:19:ARG:NH1 | 2.21 | 0.56 |
| 2:V:325:LYS:HG2 | 1:W:354:TRP:CZ2 | 2.41 | 0.56 |
| 1:Y:50:ASP:HB2 | 1:Y:64:LEU:HD11 | 1.86 | 0.56 |
| 1:1:141:GLN:N | 1:1:141:GLN:OE1 | 2.37 | 0.56 |
| 2:2:11:GLN:O | 2:2:15:GLU:HG3 | 2.05 | 0.56 |
| 2:J:304:TYR:O | 1:K:59:ARG:NH2 | 2.39 | 0.56 |
| 1:O:45:MET:CE | 1:O:102:VAL:HA | 2.35 | 0.56 |
| 1:5:100:LEU:CD1 | 1:5:128:ALA:HB2 | 2.36 | 0.56 |
| 1:G:196:ASN:HD21 | 1:G:259:ARG:NE | 2.04 | 0.56 |
| 2:J:148:TRP:O | 2:J:175:MET:HE2 | 2.06 | 0.56 |
| 1:K:70:ALA:HB2 | 1:K:287:PRO:HB3 | 1.86 | 0.56 |
| 1:M:304:GLU:O | 1:M:308:GLU:HG3 | 2.06 | 0.56 |
| 1:Q:29:ARG:HG3 | 1:Q:29:ARG:NH1 | 2.21 | 0.56 |
| 1:Q:222:GLY:HA2 | 1:Q:252:LEU:O | 2.06 | 0.56 |
| 2:X:81:MET:HB3 | 2:X:85:PHE:CD2 | 2.41 | 0.56 |
| 1:5:268:PRO:O | 1:5:271:ALA:CB | 2.54 | 0.56 |
| 1:A:284:LYS:O | 1:A:285:SER:CB | 2.42 | 0.56 |
| 1:C:253:MET:CE | 1:C:255:LEU:CD1 | 2.84 | 0.56 |
| 2:J:300:VAL:HG12 | 1:K:339:ILE:HD11 | 1.87 | 0.56 |
| 2:L:98:ALA:HB2 | 2:L:142:LEU:HD12 | 1.87 | 0.56 |
| 2:L:260:VAL:HG22 | 2:L:293:VAL:HG23 | 1.88 | 0.56 |
| 2:V:149:ASN:OD1 | 2:V:151:GLU:HB3 | 2.06 | 0.56 |
| 1:W:95:THR:HG23 | 1:W:100:LEU:HD22 | 1.88 | 0.56 |
| 1:Y:29:ARG:HG3 | 1:Y:300:LEU:O | 2.05 | 0.56 |
| 1:Y:103:ARG:HG2 | 1:Y:323:PHE:CD2 | 2.40 | 0.56 |
| 1:A:275:ARG:HA | 1:A:278:ILE:HD13 | 1.88 | 0.56 |
| 1:G:40:GLN:O | 1:G:44:ARG:HG2 | 2.06 | 0.56 |
| 1:I:68:GLN:HE21 | 1:I:259:ARG:HB3 | 1.70 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:T:11:GLN:O | 2:T:15:GLU:HG3 | 2.06 | 0.56 |
| 1:U:55:GLN:O | 1:U:56:LYS:HB2 | 2.05 | 0.56 |
| 1:U:174:GLN:HB3 | 2:V:60:MET:HG2 | 1.88 | 0.56 |
| 2:V:272:GLY:O | 2:V:273:ALA:C | 2.44 | 0.56 |
| 2:X:320:ILE:HG22 | 2:X:321:PHE:N | 2.20 | 0.56 |
| 2:4:237:ASN:C | 2:4:237:ASN:HD22 | 2.08 | 0.56 |
| 2:6:11:GLN:O | 2:6:15:GLU:HG3 | 2.05 | 0.56 |
| 2:F:155:GLY:HA3 | 2:F:193:ILE:HG13 | 1.88 | 0.55 |
| 1:K:196:ASN:ND2 | 1:K:259:ARG:HE | 2.04 | 0.55 |
| 1:Q:150:LEU:HA | 1:Q:187:LEU:HD22 | 1.88 | 0.55 |
| 2:V:148:TRP:O | 2:V:175:MET:HE2 | 2.05 | 0.55 |
| 1:1:335:LEU:HD23 | 1:1:335:LEU:C | 2.26 | 0.55 |
| 2:6:278:ARG:HG3 | 2:6:278:ARG:HH11 | 1.71 | 0.55 |
| 1:A:196:ASN:HB3 | 1:A:257:THR:HG23 | 1.88 | 0.55 |
| 1:A:225:VAL:HG12 | 1:A:226:ASP:N | 2.20 | 0.55 |
| 1:A:289:MET:HE1 | 1:A:290:LEU:CD2 | 2.34 | 0.55 |
| 2:B:256:THR:O | 2:B:257:ASN:HB2 | 2.04 | 0.55 |
| 1:M:1:PHE:C | 1:M:2:ALA:O | 2.42 | 0.55 |
| 1:O:229:ASP:OD1 | 1:O:231:LEU:CB | 2.48 | 0.55 |
| 1:Q:2:ALA:H | 1:Q:299:ASN:HD22 | 1.54 | 0.55 |
| 1:U:1:PHE:HD2 | 1:U:29:ARG:NH2 | 2.03 | 0.55 |
| 1:E:334:GLU:HG2 | 1:E:337:TYR:CZ | 2.42 | 0.55 |
| 1:O:132:TYR:N | 1:O:132:TYR:CD1 | 2.75 | 0.55 |
| 1:5:45:MET:HE3 | 1:5:102:VAL:HA | 1.87 | 0.55 |
| 1:5:217:GLY:O | 1:5:218:ASP:HB3 | 2.04 | 0.55 |
| 1:C:4:ASP:HA | 1:C:300:LEU:HD21 | 1.89 | 0.55 |
| 1:G:16:ARG:HG2 | 1:G:16:ARG:HH11 | 1.71 | 0.55 |
| 2:H:24:PHE:CZ | 2:H:76:PRO:HB3 | 2.42 | 0.55 |
| 2:J:301:PRO:HB3 | 2:L:99:LYS:HG2 | 1.88 | 0.55 |
| 2:N:279:ILE:HG22 | 2:N:280:MET:H | 1.66 | 0.55 |
| 1:W:196:ASN:HD21 | 1:W:259:ARG:NE | 2.04 | 0.55 |
| 1:3:80:ASN:HB3 | 1:3:81:PRO:HD2 | 1.88 | 0.55 |
| 1:G:94:PHE:O | 1:G:98:ARG:HB2 | 2.06 | 0.55 |
| 1:S:55:GLN:O | 1:S:56:LYS:HB2 | 2.05 | 0.55 |
| 1:S:71:CYS:SG | 1:S:255:LEU:HD23 | 2.47 | 0.55 |
| 2:X:81:MET:O | 2:X:117:PRO:HD2 | 2.07 | 0.55 |
| 2:Z:81:MET:HB3 | 2:Z:85:PHE:CE2 | 2.42 | 0.55 |
| 1:3:45:MET:HE1 | 1:3:105:ILE:HD12 | 1.89 | 0.55 |
| 1:5:93:GLY:O | 1:5:97:THR:HG23 | 2.07 | 0.55 |
| 1:E:1:PHE:CD2 | 1:E:29:ARG:NH2 | 2.75 | 0.55 |
| 1:G:34:LYS:HE3 | 1:G:38:MET:HE1 | 1.89 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:K:1:PHE:HA | 1:K:299:ASN:HD21 | 1.71 | 0.55 |
| 1:O:167:ASP:HB3 | 1:O:195:ASN:HA | 1.89 | 0.55 |
| 1:G:272:TYR:CD1 | 1:G:273:ARG:CA | 2.90 | 0.55 |
| 1:G:272:TYR:O | 1:G:274:THR:N | 2.40 | 0.55 |
| 2:H:210:VAL:HG12 | 2:H:211:SER:N | 2.21 | 0.55 |
| 1:I:223:LEU:HD23 | 1:I:223:LEU:H | 1.72 | 0.55 |
| 2:J:140:PRO:HB2 | 2:L:301:PRO:HD3 | 1.89 | 0.55 |
| 2:N:214:ARG:N | 2:N:215:PRO:HD2 | 2.21 | 0.55 |
| 1:W:167:ASP:HB3 | 1:W:195:ASN:HA | 1.89 | 0.55 |
| 1:W:177:GLU:OE1 | 2:X:58:SER:HB3 | 2.05 | 0.55 |
| 1:W:345:PRO:HB3 | 1:W:360:VAL:HG12 | 1.89 | 0.55 |
| 2:2:118:ASN:HD21 | 2:2:132:PHE:H | 1.53 | 0.55 |
| 1:3:29:ARG:CA | 1:3:300:LEU:HD22 | 2.36 | 0.55 |
| 1:3:45:MET:HE3 | 1:3:102:VAL:HG13 | 1.89 | 0.55 |
| 1:5:112:ARG:HD2 | 1:5:327:ASP:O | 2.06 | 0.55 |
| 1:5:274:THR:O | 1:5:278:ILE:HG13 | 2.06 | 0.55 |
| 1:C:29:ARG:CB | 1:C:300:LEU:HD22 | 2.36 | 0.55 |
| 1:C:253:MET:HE3 | 1:C:255:LEU:HD13 | 1.86 | 0.55 |
| 2:H:237:ASN:HD22 | 2:H:237:ASN:C | 2.11 | 0.55 |
| 1:K:15:HIS:CG | 1:K:215:LYS:HG2 | 2.41 | 0.55 |
| 1:S:253:MET:HE3 | 1:S:255:LEU:HD11 | 1.87 | 0.55 |
| 1:W:11:LYS:HB3 | 1:W:23:VAL:CG1 | 2.35 | 0.55 |
| 2:4:118:ASN:HD21 | 2:4:132:PHE:H | 1.55 | 0.55 |
| 1:K:45:MET:CE | 1:K:102:VAL:HA | 2.36 | 0.55 |
| 2:F:87:MET:HE3 | 2:H:95:ASN:ND2 | 2.22 | 0.55 |
| 1:G:182:ALA:HA | 1:G:187:LEU:HD12 | 1.88 | 0.55 |
| 1:K:272:TYR:CD1 | 1:K:273:ARG:N | 2.75 | 0.55 |
| 2:R:184:PRO:HA | 2:R:187:GLN:NE2 | 2.22 | 0.55 |
| 1:S:182:ALA:HA | 1:S:187:LEU:HD12 | 1.89 | 0.55 |
| 1:U:95:THR:CG2 | 1:U:100:LEU:HD22 | 2.37 | 0.55 |
| 1:C:1:PHE:HA | 1:C:299:ASN:ND2 | 2.22 | 0.54 |
| 1:C:296:VAL:O | 1:C:298:SER:N | 2.40 | 0.54 |
| 1:E:46:GLU:HA | 1:E:46:GLU:OE1 | 2.07 | 0.54 |
| 2:P:171:GLU:OE1 | 2:P:176:TYR:OH | 2.22 | 0.54 |
| 1:S:229:ASP:HB3 | 1:S:232:CYS:SG | 2.46 | 0.54 |
| 2:T:218:HIS:O | 2:T:316:VAL:HG22 | 2.08 | 0.54 |
| 1:Y:150:LEU:HA | 1:Y:187:LEU:HD22 | 1.89 | 0.54 |
| 1:3:274:THR:C | 1:3:276:GLU:H | 2.10 | 0.54 |
| 1:5:100:LEU:HD13 | 1:5:128:ALA:HB2 | 1.90 | 0.54 |
| 1:A:15:HIS:CG | 1:A:215:LYS:HG2 | 2.42 | 0.54 |
| 1:A:260:TYR:OH | 1:A:286:ASP:HA | 2.08 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:334:GLU:HG2 | 1:C:337:TYR:CD2 | 2.42 | 0.54 |
| 1:E:113:LYS:HD3 | 1:E:328:PRO:HG2 | 1.89 | 0.54 |
| 2:H:51:ARG:O | 2:H:52:ILE:HD13 | 2.07 | 0.54 |
| 2:J:87:MET:HE3 | 2:L:91:ASP:HA | 1.89 | 0.54 |
| 1:M:279:GLN:OE1 | 1:M:279:GLN:CA | 2.56 | 0.54 |
| 1:M:354:TRP:CZ2 | 2:P:325:LYS:HG2 | 2.42 | 0.54 |
| 2:R:213:SER:OG | 2:R:214:ARG:N | 2.41 | 0.54 |
| 2:X:155:GLY:HA3 | 2:X:193:ILE:HG13 | 1.90 | 0.54 |
| 1:I:11:LYS:HB3 | 1:I:23:VAL:CG1 | 2.37 | 0.54 |
| 2:N:115:ARG:HD2 | 2:N:157:ILE:HD11 | 1.88 | 0.54 |
| 1:U:74:GLY:HA3 | 1:U:233:VAL:HG11 | 1.88 | 0.54 |
| 2:X:20:ASP:C | 2:X:20:ASP:OD1 | 2.46 | 0.54 |
| 1:Y:269:GLY:C | 1:Y:271:ALA:H | 2.10 | 0.54 |
| 1:3:142:VAL:HB | 1:3:143:PRO:HD3 | 1.88 | 0.54 |
| 2:6:118:ASN:HD21 | 2:6:132:PHE:H | 1.54 | 0.54 |
| 1:M:10:LYS:HG2 | 1:M:11:LYS:N | 2.22 | 0.54 |
| 1:M:167:ASP:OD2 | 1:M:196:ASN:OD1 | 2.24 | 0.54 |
| 1:U:304:GLU:O | 1:U:308:GLU:HG3 | 2.07 | 0.54 |
| 1:A:303:VAL:CG1 | 1:A:304:GLU:OE2 | 2.56 | 0.54 |
| 2:F:126:ALA:HB1 | 2:H:99:LYS:HD3 | 1.89 | 0.54 |
| 1:G:100:LEU:HD13 | 1:G:128:ALA:HB2 | 1.89 | 0.54 |
| 1:U:68:GLN:NE2 | 1:U:196:ASN:HD22 | 2.06 | 0.54 |
| 1:3:88:ALA:O | 1:3:134:GLY:HA2 | 2.06 | 0.54 |
| 1:C:1:PHE:HA | 1:C:299:ASN:HD21 | 1.71 | 0.54 |
| 1:M:40:GLN:HE21 | 1:M:288:ILE:HD13 | 1.72 | 0.54 |
| 1:M:142:VAL:HG21 | 1:M:175:ILE:HG12 | 1.90 | 0.54 |
| 1:M:278:ILE:O | 1:M:279:GLN:C | 2.44 | 0.54 |
| 1:Q:61:PHE:CD2 | 1:Q:124:MET:CE | 2.91 | 0.54 |
| 1:Q:95:THR:HG23 | 1:Q:100:LEU:HD22 | 1.88 | 0.54 |
| 1:Q:138:VAL:HG13 | 1:Q:169:ALA:HB2 | 1.89 | 0.54 |
| 1:Q:182:ALA:HA | 1:Q:187:LEU:HD12 | 1.90 | 0.54 |
| 1:Q:352:ASN:H | 1:Q:355:ILE:HD12 | 1.73 | 0.54 |
| 2:T:92:GLN:OE1 | 2:T:92:GLN:HA | 2.08 | 0.54 |
| 2:X:31:ALA:HB3 | 2:X:54:ASP:CG | 2.27 | 0.54 |
| 1:Y:11:LYS:HG3 | 1:Y:11:LYS:O | 2.06 | 0.54 |
| 2:B:118:ASN:ND2 | 2:B:132:PHE:H | 1.96 | 0.54 |
| 1:C:40:GLN:O | 1:C:44:ARG:HG2 | 2.08 | 0.54 |
| 2:F:278:ARG:HG3 | 2:F:278:ARG:NH1 | 2.22 | 0.54 |
| 2:F:278:ARG:HH11 | 2:F:278:ARG:CG | 2.21 | 0.54 |
| 2:J:325:LYS:HG2 | 1:K:354:TRP:CZ2 | 2.43 | 0.54 |
| 1:O:40:GLN:O | 1:O:44:ARG:HG2 | 2.08 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:U:9:ILE:HB | 1:U:232:CYS:SG | 2.48 | 0.54 |
| 2:V:23:VAL:HG22 | 2:V:75:ARG:HB2 | 1.89 | 0.54 |
| 2:V:313:ILE:CG2 | 2:V:314:PRO:HD2 | 2.26 | 0.54 |
| 2:X:57:ILE:O | 2:X:57:ILE:HG22 | 2.07 | 0.54 |
| 2:4:185:GLU:O | 2:4:188:SER:HB3 | 2.08 | 0.54 |
| 2:B:172:ASN:ND2 | 2:B:174:LEU:H | 2.05 | 0.54 |
| 1:E:289:MET:HE2 | 1:E:290:LEU:HD23 | 1.88 | 0.54 |
| 2:J:269:PHE:CE1 | 2:L:271:VAL:HA | 2.42 | 0.54 |
| 2:L:165:ASN:HB3 | 2:L:166:PRO:HD2 | 1.89 | 0.54 |
| 2:P:118:ASN:HD21 | 2:P:132:PHE:N | 2.01 | 0.54 |
| 2:4:171:GLU:OE1 | 2:4:176:TYR:OH | 2.23 | 0.54 |
| 2:6:23:VAL:HG22 | 2:6:75:ARG:HB2 | 1.89 | 0.54 |
| 1:A:302:SER:OG | 1:A:305:GLU:HG3 | 2.08 | 0.54 |
| 1:K:243:TYR:CE2 | 1:K:248:LYS:HD2 | 2.43 | 0.54 |
| 1:O:147:GLY:HA2 | 2:P:65:ILE:HG23 | 1.89 | 0.54 |
| 2:R:238:MET:O | 2:R:239:ARG:HB2 | 2.08 | 0.54 |
| 1:S:95:THR:HG23 | 1:S:100:LEU:HD22 | 1.89 | 0.54 |
| 1:A:285:SER:C | 1:A:286:ASP:O | 2.42 | 0.54 |
| 1:K:232:CYS:O | 1:K:235:GLU:N | 2.41 | 0.54 |
| 2:L:80:PHE:O | 2:L:81:MET:C | 2.46 | 0.54 |
| 1:M:223:LEU:HD23 | 1:M:223:LEU:H | 1.72 | 0.54 |
| 1:O:88:ALA:O | 1:O:134:GLY:HA2 | 2.08 | 0.54 |
| 2:P:259:LEU:CD2 | 2:P:279:ILE:HG13 | 2.38 | 0.54 |
| 2:R:24:PHE:CZ | 2:R:76:PRO:HB3 | 2.43 | 0.54 |
| 2:R:99:LYS:HG2 | 2:T:301:PRO:HB3 | 1.89 | 0.54 |
| 2:V:63:ALA:O | 2:V:67:VAL:HG23 | 2.08 | 0.54 |
| 1:W:289:MET:CE | 1:W:290:LEU:HD23 | 2.37 | 0.54 |
| 1:W:343:ASP:HB3 | 1:W:344:PRO:HD2 | 1.89 | 0.54 |
| 2:F:63:ALA:O | 2:F:67:VAL:HG23 | 2.08 | 0.53 |
| 1:G:113:LYS:HD3 | 1:G:328:PRO:HG2 | 1.90 | 0.53 |
| 1:I:302:SER:OG | 1:I:305:GLU:HG3 | 2.08 | 0.53 |
| 1:Q:55:GLN:O | 1:Q:56:LYS:HB2 | 2.07 | 0.53 |
| 1:W:68:GLN:NE2 | 1:W:259:ARG:HB3 | 2.15 | 0.53 |
| 2:Z:16:GLU:OE2 | 2:Z:162:ARG:NH1 | 2.40 | 0.53 |
| 1:1:37:ARG:NH2 | 1:1:309:ILE:HG23 | 2.23 | 0.53 |
| 2:D:165:ASN:HB3 | 2:D:166:PRO:HD2 | 1.89 | 0.53 |
| 2:D:227:SER:C | 2:D:229:GLU:H | 2.11 | 0.53 |
| 2:R:172:ASN:HD22 | 2:R:175:MET:H | 1.54 | 0.53 |
| 2:6:172:ASN:ND2 | 2:6:174:LEU:N | 2.56 | 0.53 |
| 1:A:164:LEU:HG | 1:A:192:ILE:HB | 1.90 | 0.53 |
| 2:D:278:ARG:NH1 | 2:D:278:ARG:HG3 | 2.24 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:F:110:VAL:O | 2:F:166:PRO:HD3 | 2.08 | 0.53 |
| 1:G:98:ARG:HG2 | 1:G:131:PHE:CB | 2.33 | 0.53 |
| 1:K:149:ALA:CB | 1:K:189:CYS:HB2 | 2.39 | 0.53 |
| 1:M:347:GLU:OE1 | 1:M:356:LYS:HD3 | 2.08 | 0.53 |
| 1:K:268:PRO:O | 1:K:271:ALA:N | 2.42 | 0.53 |
| 2:R:327:LEU:O | 2:R:329:ILE:HG23 | 2.09 | 0.53 |
| 1:S:45:MET:HE1 | 1:S:105:ILE:HD12 | 1.90 | 0.53 |
| 1:Y:142:VAL:HG21 | 1:Y:175:ILE:HG12 | 1.88 | 0.53 |
| 1:5:268:PRO:O | 1:5:269:GLY:C | 2.44 | 0.53 |
| 1:I:280:GLU:O | 1:I:284:LYS:HB2 | 2.09 | 0.53 |
| 2:L:70:ALA:HA | 2:L:74:LEU:O | 2.09 | 0.53 |
| 1:U:196:ASN:HB3 | 1:U:257:THR:HG23 | 1.90 | 0.53 |
| 1:U:225:VAL:CG1 | 1:U:226:ASP:N | 2.71 | 0.53 |
| 2:V:152:ASP:HA | 2:V:193:ILE:HD12 | 1.89 | 0.53 |
| 2:6:263:GLU:O | 2:6:296:THR:HA | 2.07 | 0.53 |
| 2:D:24:PHE:CZ | 2:D:76:PRO:HB3 | 2.43 | 0.53 |
| 2:D:212:HIS:HB3 | 2:D:238:MET:CE | 2.38 | 0.53 |
| 2:F:16:GLU:OE2 | 2:F:162:ARG:NH1 | 2.42 | 0.53 |
| 1:I:29:ARG:CA | 1:I:300:LEU:HD22 | 2.38 | 0.53 |
| 2:R:51:ARG:HG3 | 2:R:51:ARG:HH11 | 1.73 | 0.53 |
| 1:S:230:ILE:HG13 | 1:S:230:ILE:O | 2.09 | 0.53 |
| 2:D:280:MET:HA | 2:D:285:PHE:CD1 | 2.43 | 0.53 |
| 1:O:223:LEU:HD23 | 1:O:223:LEU:N | 2.24 | 0.53 |
| 1:Q:77:ALA:CB | 1:Q:234:ARG:HG3 | 2.39 | 0.53 |
| 1:Q:232:CYS:O | 1:Q:233:VAL:C | 2.46 | 0.53 |
| 1:S:50:ASP:HB2 | 1:S:64:LEU:HD13 | 1.90 | 0.53 |
| 2:T:98:ALA:HB2 | 2:T:142:LEU:HD13 | 1.90 | 0.53 |
| 1:Y:29:ARG:HH11 | 1:Y:29:ARG:CG | 2.22 | 0.53 |
| 2:B:19:ARG:HG2 | 2:B:19:ARG:NH1 | 2.23 | 0.53 |
| 1:E:10:LYS:HG2 | 1:E:11:LYS:N | 2.24 | 0.53 |
| 1:I:39:MET:HG2 | 1:I:73:VAL:HG21 | 1.91 | 0.53 |
| 2:L:154:LYS:O | 2:L:157:ILE:HG22 | 2.08 | 0.53 |
| 1:M:102:VAL:HG11 | 1:M:317:ILE:HD12 | 1.91 | 0.53 |
| 2:N:124:VAL:O | 2:N:125:ALA:HB3 | 2.08 | 0.53 |
| 1:Q:286:ASP:HB3 | 1:Q:289:MET:HB3 | 1.90 | 0.53 |
| 2:T:84:ASN:ND2 | 2:T:128:HIS:HA | 2.24 | 0.53 |
| 2:N:81:MET:HB3 | 2:N:85:PHE:CE2 | 2.44 | 0.53 |
| 2:R:102:TYR:CD2 | 2:T:301:PRO:HG2 | 2.44 | 0.53 |
| 1:1:171:ASN:HD21 | 1:1:208:ALA:HB2 | 1.73 | 0.53 |
| 1:A:286:ASP:OD2 | 1:A:288:ILE:N | 2.34 | 0.53 |
| 1:G:231:LEU:HD12 | 1:G:294:ARG:NH1 | 2.24 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:H:34:ASP:O | 2:H:38:LYS:HA | 2.08 | 0.53 |
| 2:P:81:MET:HB3 | 2:P:85:PHE:CD2 | 2.44 | 0.53 |
| 1:A:102:VAL:HG11 | 1:A:317:ILE:CD1 | 2.39 | 0.52 |
| 2:B:24:PHE:CZ | 2:B:76:PRO:HB3 | 2.44 | 0.52 |
| 1:C:232:CYS:HA | 1:C:235:GLU:HB2 | 1.90 | 0.52 |
| 1:E:351:ALA:HA | 2:H:296:THR:O | 2.09 | 0.52 |
| 1:Q:29:ARG:CA | 1:Q:300:LEU:HD22 | 2.38 | 0.52 |
| 1:Q:286:ASP:OD2 | 1:Q:288:ILE:HB | 2.08 | 0.52 |
| 2:6:278:ARG:HH11 | 2:6:278:ARG:CG | 2.21 | 0.52 |
| 1:A:35:TYR:O | 1:A:39:MET:HG3 | 2.09 | 0.52 |
| 2:F:152:ASP:HA | 2:F:193:ILE:HD12 | 1.91 | 0.52 |
| 1:I:334:GLU:HG2 | 1:I:337:TYR:CE2 | 2.44 | 0.52 |
| 2:J:1:LEU:HD12 | 2:J:2:GLN:H | 1.74 | 0.52 |
| 1:O:50:ASP:HB2 | 1:O:64:LEU:HD13 | 1.92 | 0.52 |
| 2:P:278:ARG:HG3 | 2:P:278:ARG:HH11 | 1.72 | 0.52 |
| 1:W:93:GLY:O | 1:W:97:THR:HG23 | 2.09 | 0.52 |
| 2:X:20:ASP:OD1 | 2:X:21:GLU:N | 2.42 | 0.52 |
| 2:4:118:ASN:HD21 | 2:4:132:PHE:N | 2.08 | 0.52 |
| 2:4:172:ASN:ND2 | 2:4:174:LEU:H | 2.07 | 0.52 |
| 2:B:184:PRO:HA | 2:B:187:GLN:NE2 | 2.25 | 0.52 |
| 2:R:246:MET:O | 2:R:250:GLU:HG3 | 2.09 | 0.52 |
| 1:S:131:PHE:CE2 | 1:S:133:GLY:HA2 | 2.44 | 0.52 |
| 1:U:150:LEU:O | 1:U:150:LEU:HG | 2.08 | 0.52 |
| 2:Z:118:ASN:HD21 | 2:Z:132:PHE:H | 1.56 | 0.52 |
| 1:1:57:ILE:HD12 | 1:5:326:ALA:HB1 | 1.91 | 0.52 |
| 2:2:33:TYR:O | 2:2:34:ASP:HB2 | 2.08 | 0.52 |
| 1:3:102:VAL:HG11 | 1:3:317:ILE:CD1 | 2.39 | 0.52 |
| 1:A:95:THR:HG22 | 1:A:100:LEU:HB2 | 1.89 | 0.52 |
| 1:E:223:LEU:N | 1:E:223:LEU:HD23 | 2.23 | 0.52 |
| 1:G:16:ARG:HG2 | 1:G:16:ARG:NH1 | 2.25 | 0.52 |
| 1:G:174:GLN:HB3 | 2:H:60:MET:HG2 | 1.90 | 0.52 |
| 2:L:51:ARG:HH11 | 2:L:51:ARG:HG3 | 1.74 | 0.52 |
| 1:O:235:GLU:O | 1:O:236:ALA:C | 2.47 | 0.52 |
| 1:U:46:GLU:HA | 1:U:46:GLU:OE1 | 2.08 | 0.52 |
| 2:X:51:ARG:O | 2:X:52:ILE:HD13 | 2.10 | 0.52 |
| 1:Y:11:LYS:HB3 | 1:Y:23:VAL:CG1 | 2.40 | 0.52 |
| 2:2:1:LEU:HD13 | 2:2:1:LEU:C | 2.30 | 0.52 |
| 2:D:16:GLU:OE2 | 2:D:162:ARG:NH1 | 2.41 | 0.52 |
| 2:F:112:ILE:HD13 | 2:F:114:PHE:CZ | 2.44 | 0.52 |
| 1:G:272:TYR:C | 1:G:274:THR:N | 2.63 | 0.52 |
| 2:H:118:ASN:HD21 | 2:H:132:PHE:H | 1.58 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:I:150:LEU:HA | 1:I:187:LEU:HD22 | 1.92 | 0.52 |
| 2:R:172:ASN:ND2 | 2:R:174:LEU:H | 2.07 | 0.52 |
| 2:R:271:VAL:HA | 2:T:269:PHE:HE1 | 1.72 | 0.52 |
| 2:T:172:ASN:ND2 | 2:T:174:LEU:H | 2.08 | 0.52 |
| 1:W:29:ARG:CA | 1:W:300:LEU:HD22 | 2.39 | 0.52 |
| 2:Z:306:LYS:HG2 | 1:1:59:ARG:CZ | 2.40 | 0.52 |
| 2:6:227:SER:C | 2:6:229:GLU:H | 2.13 | 0.52 |
| 1:A:278:ILE:HD12 | 1:A:278:ILE:N | 2.25 | 0.52 |
| 2:B:84:ASN:ND2 | 2:B:128:HIS:HA | 2.25 | 0.52 |
| 2:F:263:GLU:O | 2:F:296:THR:HA | 2.10 | 0.52 |
| 2:L:263:GLU:O | 2:L:263:GLU:HG3 | 2.10 | 0.52 |
| 1:Q:68:GLN:NE2 | 1:Q:259:ARG:HB3 | 2.21 | 0.52 |
| 1:Q:142:VAL:HA | 1:Q:163:THR:HG21 | 1.91 | 0.52 |
| 2:R:147:PRO:HD2 | 2:R:170:LEU:O | 2.10 | 0.52 |
| 2:X:51:ARG:HH11 | 2:X:51:ARG:HG3 | 1.75 | 0.52 |
| 2:X:246:MET:O | 2:X:250:GLU:HG3 | 2.09 | 0.52 |
| 1:1:55:GLN:O | 1:1:56:LYS:HB2 | 2.09 | 0.52 |
| 1:M:274:THR:OG1 | 1:M:275:ARG:N | 2.42 | 0.52 |
| 2:P:152:ASP:HA | 2:P:193:ILE:HD12 | 1.92 | 0.52 |
| 1:Q:225:VAL:CG1 | 1:Q:226:ASP:N | 2.72 | 0.52 |
| 1:S:307:LYS:O | 1:S:311:VAL:HG23 | 2.10 | 0.52 |
| 1:Y:334:GLU:HG2 | 1:Y:337:TYR:CD2 | 2.44 | 0.52 |
| 1:1:345:PRO:HB3 | 1:1:360:VAL:HG12 | 1.92 | 0.52 |
| 1:E:103:ARG:HG2 | 1:E:323:PHE:CD2 | 2.44 | 0.52 |
| 2:F:279:ILE:HG22 | 2:F:280:MET:N | 2.24 | 0.52 |
| 1:M:272:TYR:CD1 | 1:M:272:TYR:O | 2.63 | 0.52 |
| 1:U:95:THR:O | 1:U:100:LEU:HB2 | 2.09 | 0.52 |
| 1:C:234:ARG:CD | 1:C:238:ARG:NH2 | 2.73 | 0.52 |
| 2:H:327:LEU:O | 2:H:329:ILE:HG23 | 2.10 | 0.52 |
| 1:S:335:LEU:C | 1:S:335:LEU:HD23 | 2.30 | 0.52 |
| 1:1:4:ASP:HA | 1:1:300:LEU:HD21 | 1.92 | 0.52 |
| 2:4:266:TRP:HB3 | 2:4:267:PRO:HD2 | 1.91 | 0.52 |
| 2:6:87:MET:HE2 | 2:6:132:PHE:HZ | 1.75 | 0.52 |
| 1:G:95:THR:HG22 | 1:G:100:LEU:HB2 | 1.91 | 0.52 |
| 1:I:223:LEU:HD23 | 1:I:223:LEU:N | 2.24 | 0.52 |
| 1:O:142:VAL:HG21 | 1:O:175:ILE:HG12 | 1.91 | 0.52 |
| 2:T:154:LYS:O | 2:T:157:ILE:HG22 | 2.09 | 0.52 |
| 1:3:4:ASP:HA | 1:3:300:LEU:HD21 | 1.92 | 0.52 |
| 1:O:225:VAL:HG12 | 1:O:226:ASP:N | 2.25 | 0.51 |
| 1:Q:131:PHE:CE2 | 1:Q:133:GLY:HA2 | 2.45 | 0.51 |
| 2:R:311:ASN:CG | 1:S:332:LEU:HD11 | 2.30 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:S:105:ILE:O | 1:S:109:LEU:HG | 2.10 | 0.51 |
| 1:3:230:ILE:O | 1:3:230:ILE:HG13 | 2.09 | 0.51 |
| 2:H:263:GLU:O | 2:H:296:THR:HA | 2.10 | 0.51 |
| 2:L:278:ARG:HG3 | 2:L:278:ARG:HH11 | 1.74 | 0.51 |
| 1:Q:93:GLY:O | 1:Q:97:THR:HG23 | 2.09 | 0.51 |
| 1:S:38:MET:O | 1:S:39:MET:C | 2.47 | 0.51 |
| 2:T:250:GLU:HB3 | 2:T:284:ALA:HB2 | 1.92 | 0.51 |
| 1:W:177:GLU:CD | 2:X:58:SER:HB3 | 2.30 | 0.51 |
| 2:X:315:GLN:HG3 | 2:X:318:ASP:OD2 | 2.11 | 0.51 |
| 1:Y:177:GLU:HG2 | 1:1:171:ASN:O | 2.11 | 0.51 |
| 1:A:88:ALA:O | 1:A:134:GLY:HA2 | 2.11 | 0.51 |
| 1:E:9:ILE:CD1 | 1:E:235:GLU:HG3 | 2.40 | 0.51 |
| 2:F:76:PRO:HG2 | 2:F:112:ILE:HG13 | 1.92 | 0.51 |
| 1:G:132:TYR:N | 1:G:132:TYR:CD1 | 2.77 | 0.51 |
| 2:H:184:PRO:HA | 2:H:187:GLN:HE22 | 1.75 | 0.51 |
| 2:H:329:ILE:HG13 | 2:H:329:ILE:OXT | 2.09 | 0.51 |
| 2:L:260:VAL:HG22 | 2:L:293:VAL:CG2 | 2.40 | 0.51 |
| 2:N:246:MET:CE | 2:N:279:ILE:HD13 | 2.40 | 0.51 |
| 1:Y:229:ASP:C | 1:Y:229:ASP:OD1 | 2.49 | 0.51 |
| 2:Z:34:ASP:O | 2:Z:38:LYS:HA | 2.10 | 0.51 |
| 2:Z:155:GLY:HA3 | 2:Z:193:ILE:HG13 | 1.92 | 0.51 |
| 2:Z:184:PRO:HA | 2:Z:187:GLN:HE22 | 1.75 | 0.51 |
| 1:5:29:ARG:HG3 | 1:5:29:ARG:NH1 | 2.11 | 0.51 |
| 2:D:33:TYR:O | 2:D:34:ASP:HB2 | 2.10 | 0.51 |
| 1:E:11:LYS:HB3 | 1:E:23:VAL:HG12 | 1.93 | 0.51 |
| 2:H:246:MET:O | 2:H:250:GLU:HG3 | 2.11 | 0.51 |
| 2:J:260:VAL:HG22 | 2:J:293:VAL:CG2 | 2.40 | 0.51 |
| 1:M:267:ASP:CB | 1:M:268:PRO:HD3 | 2.37 | 0.51 |
| 1:1:95:THR:HG23 | 1:1:100:LEU:HD22 | 1.92 | 0.51 |
| 2:2:121:SER:HB3 | 2:2:124:VAL:CG2 | 2.36 | 0.51 |
| 1:3:45:MET:CE | 1:3:102:VAL:HG13 | 2.41 | 0.51 |
| 1:A:9:ILE:HB | 1:A:232:CYS:SG | 2.50 | 0.51 |
| 2:J:238:MET:O | 2:J:239:ARG:HB2 | 2.11 | 0.51 |
| 1:S:253:MET:CE | 1:S:255:LEU:HD11 | 2.39 | 0.51 |
| 1:5:269:GLY:O | 1:5:273:ARG:CD | 2.55 | 0.51 |
| 1:A:222:GLY:HA2 | 1:A:252:LEU:O | 2.11 | 0.51 |
| 2:D:285:PHE:O | 2:D:288:LEU:HB2 | 2.11 | 0.51 |
| 1:E:11:LYS:O | 1:E:11:LYS:HG3 | 2.11 | 0.51 |
| 2:N:98:ALA:HB2 | 2:N:142:LEU:HD13 | 1.92 | 0.51 |
| 1:Q:11:LYS:HG3 | 1:Q:11:LYS:O | 2.09 | 0.51 |
| 2:T:24:PHE:CZ | 2:T:76:PRO:HB3 | 2.46 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:X:315:GLN:O | 2:X:316:VAL:C | 2.48 | 0.51 |
| 2:2:143:LYS:HB2 | 2:2:167:VAL:HG22 | 1.91 | 0.51 |
| 1:3:95:THR:HG23 | 1:3:100:LEU:HD22 | 1.92 | 0.51 |
| 2:4:140:PRO:HB2 | 2:6:301:PRO:HD3 | 1.93 | 0.51 |
| 1:5:269:GLY:C | 1:5:273:ARG:HH11 | 2.12 | 0.51 |
| 1:C:28:THR:O | 1:C:29:ARG:C | 2.48 | 0.51 |
| 1:C:307:LYS:O | 1:C:311:VAL:HG23 | 2.11 | 0.51 |
| 1:C:322:GLN:HG3 | 1:C:323:PHE:N | 2.25 | 0.51 |
| 2:F:135:TRP:O | 2:F:138:HIS:HB3 | 2.10 | 0.51 |
| 1:M:172:GLN:HE22 | 2:P:88:GLN:HE22 | 1.58 | 0.51 |
| 1:Q:230:ILE:O | 1:Q:230:ILE:HG13 | 2.10 | 0.51 |
| 2:R:20:ASP:C | 2:R:20:ASP:OD1 | 2.48 | 0.51 |
| 2:R:184:PRO:HA | 2:R:187:GLN:HE21 | 1.76 | 0.51 |
| 1:S:259:ARG:NH1 | 1:S:261:HIS:O | 2.44 | 0.51 |
| 2:V:16:GLU:OE2 | 2:V:162:ARG:NH1 | 2.43 | 0.51 |
| 1:Y:275:ARG:HB2 | 1:Y:275:ARG:HH11 | 1.75 | 0.51 |
| 2:2:98:ALA:HB2 | 2:2:142:LEU:CD1 | 2.40 | 0.51 |
| 1:G:1:PHE:HA | 1:G:299:ASN:HD21 | 1.76 | 0.51 |
| 1:I:353:GLN:NE2 | 2:J:281:GLU:HB3 | 2.25 | 0.51 |
| 2:J:19:ARG:NH1 | 2:J:19:ARG:HG2 | 2.26 | 0.51 |
| 1:M:171:ASN:OD1 | 1:M:216:ARG:NH2 | 2.31 | 0.51 |
| 1:O:55:GLN:O | 1:O:56:LYS:HB2 | 2.10 | 0.51 |
| 1:S:232:CYS:HA | 1:S:235:GLU:HB2 | 1.93 | 0.51 |
| 1:Y:10:LYS:HG2 | 1:Y:11:LYS:N | 2.26 | 0.51 |
| 1:Y:272:TYR:C | 1:Y:272:TYR:HD1 | 2.11 | 0.51 |
| 1:G:289:MET:CE | 1:G:290:LEU:HD23 | 2.41 | 0.51 |
| 1:K:277:GLU:O | 1:K:281:VAL:HG23 | 2.10 | 0.51 |
| 1:Q:302:SER:OG | 1:Q:305:GLU:HG3 | 2.11 | 0.51 |
| 2:V:87:MET:CE | 2:X:95:ASN:ND2 | 2.74 | 0.51 |
| 2:2:234:GLU:OE1 | 2:2:255:LYS:NZ | 2.44 | 0.51 |
| 1:3:88:ALA:HB2 | 1:3:141:GLN:NE2 | 2.25 | 0.51 |
| 1:5:40:GLN:O | 1:5:44:ARG:HG2 | 2.11 | 0.51 |
| 1:A:182:ALA:HA | 1:A:187:LEU:HD12 | 1.93 | 0.51 |
| 2:H:144:VAL:HG12 | 2:H:241:ILE:HB | 1.92 | 0.51 |
| 1:I:286:ASP:OD2 | 1:I:288:ILE:HB | 2.11 | 0.51 |
| 1:K:196:ASN:HD21 | 1:K:259:ARG:HE | 1.59 | 0.51 |
| 2:N:329:ILE:HG13 | 2:N:329:ILE:OXT | 2.10 | 0.51 |
| 2:Z:173:GLU:O | 2:Z:173:GLU:HG2 | 2.11 | 0.51 |
| 1:1:280:GLU:CG | 1:1:281:VAL:H | 2.18 | 0.51 |
| 1:A:68:GLN:HE21 | 1:A:259:ARG:HB3 | 1.75 | 0.50 |
| 1:A:313:VAL:O | 1:A:316:GLU:HB3 | 2.11 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:110:VAL:O | 2:B:166:PRO:HD3 | 2.11 | 0.50 |
| 2:H:81:MET:HB3 | 2:H:85:PHE:HD2 | 1.74 | 0.50 |
| 1:I:29:ARG:HH11 | 1:I:29:ARG:CG | 2.24 | 0.50 |
| 2:J:98:ALA:HB2 | 2:J:142:LEU:HD13 | 1.92 | 0.50 |
| 2:N:118:ASN:ND2 | 2:N:132:PHE:H | 2.03 | 0.50 |
| 2:N:171:GLU:OE1 | 2:N:176:TYR:OH | 2.23 | 0.50 |
| 1:Q:29:ARG:HB2 | 1:Q:300:LEU:HD22 | 1.92 | 0.50 |
| 1:U:1:PHE:C | 1:U:2:ALA:O | 2.48 | 0.50 |
| 1:W:100:LEU:HD13 | 1:W:128:ALA:CB | 2.41 | 0.50 |
| 1:Y:225:VAL:HB | 1:Y:255:LEU:HD12 | 1.92 | 0.50 |
| 2:Z:21:GLU:N | 2:Z:21:GLU:OE1 | 2.44 | 0.50 |
| 2:Z:127:GLN:OE1 | 1:1:125:HIS:HE1 | 1.94 | 0.50 |
| 1:3:15:HIS:CG | 1:3:215:LYS:HG2 | 2.46 | 0.50 |
| 1:5:150:LEU:HA | 1:5:187:LEU:HD22 | 1.92 | 0.50 |
| 2:D:18:GLU:OE2 | 1:E:272:TYR:CE2 | 2.63 | 0.50 |
| 1:G:58:ILE:HD13 | 1:G:109:LEU:HB3 | 1.92 | 0.50 |
| 1:K:70:ALA:HB3 | 1:K:227:GLY:O | 2.09 | 0.50 |
| 1:K:93:GLY:O | 1:K:97:THR:HG23 | 2.12 | 0.50 |
| 2:P:238:MET:O | 2:P:239:ARG:HB2 | 2.10 | 0.50 |
| 1:Q:15:HIS:CG | 1:Q:215:LYS:HG2 | 2.46 | 0.50 |
| 1:S:316:GLU:OE1 | 1:S:316:GLU:HA | 2.10 | 0.50 |
| 2:T:314:PRO:O | 2:T:315:GLN:HB2 | 2.11 | 0.50 |
| 1:1:29:ARG:HB2 | 1:1:300:LEU:CD2 | 2.41 | 0.50 |
| 1:3:302:SER:OG | 1:3:305:GLU:HG3 | 2.11 | 0.50 |
| 1:O:223:LEU:HD23 | 1:O:223:LEU:H | 1.76 | 0.50 |
| 1:S:27:LEU:CD2 | 1:S:28:THR:N | 2.73 | 0.50 |
| 1:U:132:TYR:CD1 | 1:U:148:ILE:HD13 | 2.47 | 0.50 |
| 1:W:103:ARG:HG2 | 1:W:323:PHE:CD2 | 2.46 | 0.50 |
| 1:W:140:ALA:O | 1:W:143:PRO:HD2 | 2.11 | 0.50 |
| 1:5:29:ARG:CG | 1:5:29:ARG:NH1 | 2.70 | 0.50 |
| 1:A:196:ASN:HD21 | 1:A:259:ARG:CD | 2.24 | 0.50 |
| 1:C:286:ASP:HB3 | 1:C:289:MET:HB2 | 1.92 | 0.50 |
| 2:D:227:SER:C | 2:D:229:GLU:N | 2.64 | 0.50 |
| 1:E:313:VAL:O | 1:E:316:GLU:HB3 | 2.11 | 0.50 |
| 1:G:71:CYS:O | 1:G:75:LEU:HB2 | 2.11 | 0.50 |
| 2:J:276:CYS:HB3 | 2:L:280:MET:CE | 2.42 | 0.50 |
| 1:Q:100:LEU:HD13 | 1:Q:128:ALA:HB2 | 1.94 | 0.50 |
| 2:V:28:GLU:OE2 | 2:V:59:GLU:OE2 | 2.28 | 0.50 |
| 1:Y:40:GLN:HE21 | 1:Y:288:ILE:HD13 | 1.77 | 0.50 |
| 1:1:308:GLU:O | 1:1:312:GLU:HG3 | 2.11 | 0.50 |
| 1:3:167:ASP:HB3 | 1:3:195:ASN:HA | 1.94 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:6:172:ASN:HD21 | 2:6:174:LEU:HB2 | 1.75 | 0.50 |
| 2:F:51:ARG:O | 2:F:52:ILE:HD13 | 2.11 | 0.50 |
| 1:G:11:LYS:HB3 | 1:G:23:VAL:HG12 | 1.94 | 0.50 |
| 2:J:9:ILE:HG13 | 2:J:153:ALA:HB1 | 1.93 | 0.50 |
| 2:J:31:ALA:HB3 | 2:J:54:ASP:OD2 | 2.12 | 0.50 |
| 2:P:118:ASN:HD21 | 2:P:131:CYS:HA | 1.75 | 0.50 |
| 1:U:33:LEU:HD12 | 1:U:295:MET:HE1 | 1.93 | 0.50 |
| 1:W:225:VAL:HG12 | 1:W:226:ASP:N | 2.27 | 0.50 |
| 1:Y:275:ARG:HB2 | 1:Y:275:ARG:NH1 | 2.26 | 0.50 |
| 1:3:10:LYS:HG2 | 1:3:11:LYS:N | 2.26 | 0.50 |
| 2:4:95:ASN:HD21 | 2:6:87:MET:HE3 | 1.77 | 0.50 |
| 2:6:1:LEU:HD13 | 2:6:2:GLN:N | 2.26 | 0.50 |
| 2:F:19:ARG:HG2 | 2:F:19:ARG:HH11 | 1.76 | 0.50 |
| 1:I:230:ILE:O | 1:I:230:ILE:HG13 | 2.12 | 0.50 |
| 2:L:121:SER:OG | 2:L:122:ALA:N | 2.44 | 0.50 |
| 1:U:320:ALA:O | 1:U:323:PHE:HB3 | 2.12 | 0.50 |
| 2:Z:262:VAL:HA | 2:Z:295:VAL:O | 2.11 | 0.50 |
| 1:3:149:ALA:CB | 1:3:189:CYS:HB2 | 2.41 | 0.50 |
| 1:E:225:VAL:CG1 | 1:E:226:ASP:N | 2.74 | 0.50 |
| 1:G:289:MET:HE2 | 1:G:290:LEU:HD23 | 1.93 | 0.50 |
| 2:J:172:ASN:HD22 | 2:J:175:MET:N | 2.09 | 0.50 |
| 2:L:112:ILE:CG1 | 2:L:113:VAL:N | 2.75 | 0.50 |
| 2:V:155:GLY:HA3 | 2:V:193:ILE:HG13 | 1.93 | 0.50 |
| 1:W:95:THR:HG22 | 1:W:100:LEU:HB2 | 1.93 | 0.50 |
| 1:1:3:ASN:O | 1:1:4:ASP:CB | 2.59 | 0.50 |
| 1:5:95:THR:HG22 | 1:5:100:LEU:HB2 | 1.94 | 0.50 |
| 1:A:225:VAL:CG1 | 1:A:226:ASP:N | 2.75 | 0.50 |
| 1:G:29:ARG:NH1 | 1:G:300:LEU:O | 2.45 | 0.50 |
| 1:M:335:LEU:O | 1:M:335:LEU:HG | 2.11 | 0.50 |
| 2:N:231:VAL:HG21 | 2:N:329:ILE:HD11 | 1.93 | 0.50 |
| 2:T:263:GLU:O | 2:T:296:THR:HA | 2.11 | 0.50 |
| 2:2:124:VAL:O | 2:2:125:ALA:HB3 | 2.12 | 0.50 |
| 1:3:138:VAL:HG13 | 1:3:169:ALA:CB | 2.42 | 0.50 |
| 1:5:335:LEU:HG | 1:5:335:LEU:O | 2.11 | 0.50 |
| 1:C:39:MET:HG2 | 1:C:73:VAL:HG21 | 1.94 | 0.50 |
| 1:C:214:TYR:HA | 1:C:252:LEU:HD22 | 1.94 | 0.50 |
| 1:E:257:THR:OG1 | 1:E:258:TYR:N | 2.44 | 0.50 |
| 1:I:57:ILE:HD13 | 1:I:57:ILE:N | 2.27 | 0.50 |
| 1:S:50:ASP:HB2 | 1:S:64:LEU:CD1 | 2.41 | 0.50 |
| 1:S:277:GLU:O | 1:S:277:GLU:HG2 | 2.06 | 0.50 |
| 1:W:55:GLN:O | 1:W:56:LYS:CB | 2.54 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:Y:88:ALA:O | 1:Y:134:GLY:CA | 2.60 | 0.50 |
| 1:A:281:VAL:O | 1:A:281:VAL:CG1 | 2.60 | 0.49 |
| 2:B:103:MET:SD | 2:D:126:ALA:HB3 | 2.51 | 0.49 |
| 1:E:15:HIS:CG | 1:E:215:LYS:HG2 | 2.47 | 0.49 |
| 1:Q:45:MET:HE1 | 1:Q:105:ILE:HD12 | 1.94 | 0.49 |
| 1:Q:113:LYS:CD | 1:Q:328:PRO:HG2 | 2.42 | 0.49 |
| 2:R:204:GLY:O | 2:R:234:GLU:OE1 | 2.30 | 0.49 |
| 1:S:1:PHE:HA | 1:S:299:ASN:HD21 | 1.76 | 0.49 |
| 1:W:29:ARG:CG | 1:W:29:ARG:HH11 | 2.25 | 0.49 |
| 1:Y:278:ILE:O | 1:Y:279:GLN:C | 2.50 | 0.49 |
| 2:Z:59:GLU:HA | 2:Z:62:PHE:CE2 | 2.47 | 0.49 |
| 1:1:29:ARG:CG | 1:1:29:ARG:NH1 | 2.74 | 0.49 |
| 1:C:1:PHE:CE1 | 1:C:299:ASN:OD1 | 2.66 | 0.49 |
| 1:C:35:TYR:O | 1:C:39:MET:HG3 | 2.12 | 0.49 |
| 1:I:138:VAL:HG13 | 1:I:169:ALA:HB2 | 1.94 | 0.49 |
| 2:J:118:ASN:HD21 | 2:J:132:PHE:N | 2.09 | 0.49 |
| 1:K:270:VAL:O | 1:K:271:ALA:C | 2.50 | 0.49 |
| 2:N:181:GLU:O | 2:N:183:PRO:HD3 | 2.12 | 0.49 |
| 2:N:237:ASN:C | 2:N:237:ASN:ND2 | 2.65 | 0.49 |
| 2:P:280:MET:HA | 2:P:285:PHE:CD1 | 2.47 | 0.49 |
| 1:Q:289:MET:HE1 | 1:Q:290:LEU:CD2 | 2.42 | 0.49 |
| 2:R:329:ILE:OXT | 2:R:329:ILE:HG13 | 2.10 | 0.49 |
| 1:3:284:LYS:O | 1:3:285:SER:HB3 | 2.12 | 0.49 |
| 2:6:24:PHE:CZ | 2:6:76:PRO:HB3 | 2.47 | 0.49 |
| 2:6:51:ARG:O | 2:6:52:ILE:HD13 | 2.13 | 0.49 |
| 1:C:138:VAL:HG13 | 1:C:169:ALA:HB2 | 1.94 | 0.49 |
| 2:F:238:MET:O | 2:F:239:ARG:HB2 | 2.12 | 0.49 |
| 1:I:307:LYS:O | 1:I:311:VAL:HG23 | 2.12 | 0.49 |
| 1:Q:129:LYS:O | 1:Q:130:ASN:HB2 | 2.12 | 0.49 |
| 2:R:102:TYR:CG | 2:T:301:PRO:HG2 | 2.47 | 0.49 |
| 1:G:274:THR:C | 1:G:276:GLU:N | 2.63 | 0.49 |
| 1:I:113:LYS:HG2 | 1:I:328:PRO:O | 2.12 | 0.49 |
| 2:P:246:MET:O | 2:P:250:GLU:HG3 | 2.12 | 0.49 |
| 2:T:172:ASN:ND2 | 2:T:172:ASN:C | 2.65 | 0.49 |
| 1:U:147:GLY:HA2 | 2:V:65:ILE:HG23 | 1.95 | 0.49 |
| 2:V:181:GLU:O | 2:V:183:PRO:HD3 | 2.13 | 0.49 |
| 1:3:43:ARG:HG2 | 1:3:43:ARG:HH11 | 1.76 | 0.49 |
| 1:C:29:ARG:CB | 1:C:300:LEU:CD2 | 2.90 | 0.49 |
| 1:C:318:GLU:O | 1:C:322:GLN:HB3 | 2.13 | 0.49 |
| 1:I:55:GLN:O | 1:I:56:LYS:CB | 2.56 | 0.49 |
| 2:L:1:LEU:HD13 | 2:L:2:GLN:N | 2.28 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:O:29:ARG:HA | 1:O:300:LEU:HD22 | 1.95 | 0.49 |
| 1:Q:231:LEU:HD12 | 1:Q:294:ARG:NH1 | 2.28 | 0.49 |
| 1:U:12:CYS:HB3 | 1:U:224:ARG:O | 2.12 | 0.49 |
| 2:V:273:ALA:N | 2:V:294:ARG:HD3 | 2.28 | 0.49 |
| 1:3:78:GLY:CA | 1:3:238:ARG:HG2 | 2.43 | 0.49 |
| 2:6:238:MET:O | 2:6:239:ARG:HB2 | 2.12 | 0.49 |
| 1:C:302:SER:OG | 1:C:305:GLU:HG3 | 2.13 | 0.49 |
| 1:G:196:ASN:ND2 | 1:G:259:ARG:HE | 2.09 | 0.49 |
| 1:I:139:GLY:HA3 | 1:I:172:GLN:HG3 | 1.94 | 0.49 |
| 2:J:99:LYS:HG2 | 2:L:301:PRO:HB3 | 1.94 | 0.49 |
| 1:M:103:ARG:HG2 | 1:M:323:PHE:CD2 | 2.47 | 0.49 |
| 2:N:212:HIS:HB3 | 2:N:238:MET:CE | 2.42 | 0.49 |
| 1:Q:18:GLU:CG | 1:Q:19:GLU:N | 2.63 | 0.49 |
| 1:S:95:THR:HG22 | 1:S:100:LEU:HB2 | 1.94 | 0.49 |
| 1:Y:132:TYR:CD1 | 1:Y:148:ILE:HD13 | 2.48 | 0.49 |
| 2:4:1:LEU:HD13 | 2:4:2:GLN:N | 2.15 | 0.49 |
| 2:6:92:GLN:OE1 | 2:6:92:GLN:HA | 2.12 | 0.49 |
| 1:A:100:LEU:HD13 | 1:A:128:ALA:CB | 2.43 | 0.49 |
| 2:B:99:LYS:O | 2:B:103:MET:HG3 | 2.13 | 0.49 |
| 2:B:250:GLU:O | 2:B:254:MET:HG3 | 2.13 | 0.49 |
| 1:E:270:VAL:O | 1:E:274:THR:HG23 | 2.13 | 0.49 |
| 1:I:11:LYS:O | 1:I:11:LYS:HG3 | 2.12 | 0.49 |
| 1:Q:101:SER:OG | 1:Q:104:GLU:HG3 | 2.13 | 0.49 |
| 2:R:325:LYS:HG2 | 1:S:354:TRP:CE2 | 2.46 | 0.49 |
| 1:S:27:LEU:C | 1:S:27:LEU:CD2 | 2.77 | 0.49 |
| 2:Z:84:ASN:ND2 | 2:Z:128:HIS:HA | 2.27 | 0.49 |
| 1:1:225:VAL:CG1 | 1:1:226:ASP:N | 2.75 | 0.49 |
| 1:1:230:ILE:O | 1:1:230:ILE:HG13 | 2.11 | 0.49 |
| 2:4:256:THR:O | 2:4:257:ASN:HB2 | 2.11 | 0.49 |
| 2:6:185:GLU:O | 2:6:185:GLU:HG2 | 2.12 | 0.49 |
| 2:6:227:SER:C | 2:6:229:GLU:N | 2.65 | 0.49 |
| 2:D:304:TYR:O | 2:D:305:ALA:C | 2.49 | 0.49 |
| 1:E:84:HIS:CE1 | 1:E:130:ASN:ND2 | 2.80 | 0.49 |
| 1:E:351:ALA:O | 2:H:295:VAL:HG13 | 2.12 | 0.49 |
| 1:K:229:ASP:C | 1:K:231:LEU:N | 2.65 | 0.49 |
| 2:P:313:ILE:HG23 | 2:P:314:PRO:HD2 | 1.94 | 0.49 |
| 1:S:24:THR:HG23 | 1:S:24:THR:O | 2.12 | 0.49 |
| 1:S:68:GLN:NE2 | 1:S:259:ARG:HB3 | 2.19 | 0.49 |
| 2:V:126:ALA:HB1 | 2:X:99:LYS:HD3 | 1.94 | 0.49 |
| 1:1:29:ARG:CB | 1:1:300:LEU:HD22 | 2.43 | 0.49 |
| 1:1:88:ALA:HB2 | 1:1:141:GLN:NE2 | 2.28 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:5:154:TYR:CD1 | 2:6:74:LEU:HD21 | 2.47 | 0.49 |
| 2:N:246:MET:O | 2:N:250:GLU:HG3 | 2.12 | 0.49 |
| 1:O:113:LYS:HB3 | 1:O:330:PRO:HA | 1.95 | 0.49 |
| 2:P:285:PHE:O | 2:P:288:LEU:HB2 | 2.13 | 0.49 |
| 2:R:137:GLY:O | 2:R:242:ARG:HD2 | 2.13 | 0.49 |
| 1:U:229:ASP:OD1 | 1:U:229:ASP:C | 2.51 | 0.49 |
| 2:Z:87:MET:HE3 | 2:2:95:ASN:ND2 | 2.28 | 0.49 |
| 1:3:1:PHE:O | 1:3:2:ALA:O | 2.30 | 0.49 |
| 1:5:103:ARG:HG2 | 1:5:323:PHE:CD2 | 2.47 | 0.49 |
| 1:A:18:GLU:CG | 1:A:19:GLU:N | 2.60 | 0.49 |
| 2:D:112:ILE:O | 2:D:166:PRO:HA | 2.12 | 0.49 |
| 2:D:118:ASN:HD21 | 2:D:132:PHE:H | 1.60 | 0.49 |
| 1:E:75:LEU:HD11 | 1:E:255:LEU:HD21 | 1.94 | 0.49 |
| 1:E:128:ALA:HB3 | 1:E:131:PHE:HB3 | 1.94 | 0.49 |
| 1:K:322:GLN:HG3 | 1:K:323:PHE:N | 2.27 | 0.49 |
| 1:U:27:LEU:HD12 | 1:U:300:LEU:HD13 | 1.95 | 0.49 |
| 1:W:45:MET:HE3 | 1:W:102:VAL:HG22 | 1.95 | 0.49 |
| 1:W:223:LEU:HD23 | 1:W:223:LEU:N | 2.27 | 0.49 |
| 1:W:278:ILE:HG22 | 1:W:279:GLN:N | 2.27 | 0.49 |
| 2:X:24:PHE:CZ | 2:X:76:PRO:HB3 | 2.48 | 0.49 |
| 2:X:214:ARG:HB3 | 2:X:215:PRO:HD3 | 1.94 | 0.49 |
| 1:Y:289:MET:HE2 | 1:Y:290:LEU:HD23 | 1.93 | 0.49 |
| 1:5:131:PHE:CZ | 1:5:133:GLY:HA2 | 2.47 | 0.49 |
| 1:A:162:LEU:HD12 | 1:A:162:LEU:N | 2.28 | 0.48 |
| 1:A:257:THR:OG1 | 1:A:258:TYR:N | 2.45 | 0.48 |
| 1:A:289:MET:CE | 1:A:290:LEU:HD21 | 2.37 | 0.48 |
| 1:C:258:TYR:CD1 | 1:C:258:TYR:C | 2.86 | 0.48 |
| 1:C:340:TYR:HB3 | 2:D:165:ASN:ND2 | 2.27 | 0.48 |
| 1:I:45:MET:HE1 | 1:I:105:ILE:HD12 | 1.95 | 0.48 |
| 2:J:157:ILE:O | 2:J:161:ILE:HG13 | 2.14 | 0.48 |
| 1:K:182:ALA:HA | 1:K:187:LEU:CD1 | 2.38 | 0.48 |
| 1:M:269:GLY:O | 1:M:270:VAL:C | 2.50 | 0.48 |
| 1:U:68:GLN:HE22 | 1:U:196:ASN:HD22 | 1.60 | 0.48 |
| 1:U:100:LEU:HD13 | 1:U:128:ALA:CB | 2.43 | 0.48 |
| 1:Y:45:MET:CE | 1:Y:102:VAL:HG13 | 2.42 | 0.48 |
| 1:Y:95:THR:HG22 | 1:Y:100:LEU:HB2 | 1.96 | 0.48 |
| 2:Z:87:MET:CE | 2:2:95:ASN:ND2 | 2.77 | 0.48 |
| 2:Z:202:ARG:O | 2:Z:234:GLU:HA | 2.13 | 0.48 |
| 1:1:243:TYR:CE2 | 1:1:248:LYS:HD2 | 2.48 | 0.48 |
| 1:3:231:LEU:HD12 | 1:3:294:ARG:HH11 | 1.78 | 0.48 |
| 1:5:71:CYS:SG | 1:5:255:LEU:HD23 | 2.53 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:6:182:PHE:O | 2:6:183:PRO:C | 2.51 | 0.48 |
| 2:B:253:VAL:HG11 | 2:B:288:LEU:HD13 | 1.94 | 0.48 |
| 1:I:89:TYR:HB2 | 1:I:124:MET:HG2 | 1.94 | 0.48 |
| 1:W:10:LYS:HG2 | 1:W:11:LYS:H | 1.78 | 0.48 |
| 2:Z:214:ARG:N | 2:Z:215:PRO:HD2 | 2.28 | 0.48 |
| 2:Z:237:ASN:ND2 | 2:Z:237:ASN:C | 2.67 | 0.48 |
| 1:1:68:GLN:NE2 | 1:1:259:ARG:HB3 | 2.23 | 0.48 |
| 2:2:93:VAL:O | 2:2:97:ALA:HB3 | 2.13 | 0.48 |
| 1:3:100:LEU:HD13 | 1:3:128:ALA:CB | 2.42 | 0.48 |
| 1:3:286:ASP:OD2 | 1:3:288:ILE:HB | 2.13 | 0.48 |
| 1:3:338:HIS:O | 2:4:102:TYR:HA | 2.12 | 0.48 |
| 2:4:238:MET:O | 2:4:239:ARG:HB2 | 2.14 | 0.48 |
| 1:M:281:VAL:HG12 | 1:M:282:ARG:N | 2.27 | 0.48 |
| 2:V:313:ILE:CG2 | 2:V:314:PRO:N | 2.77 | 0.48 |
| 1:3:289:MET:HE3 | 1:3:290:LEU:HD23 | 1.95 | 0.48 |
| 1:A:223:LEU:HD23 | 1:A:223:LEU:N | 2.27 | 0.48 |
| 2:F:172:ASN:ND2 | 2:F:174:LEU:H | 2.11 | 0.48 |
| 2:J:207:ILE:HD13 | 2:J:323:ILE:HG23 | 1.95 | 0.48 |
| 2:L:51:ARG:O | 2:L:52:ILE:HD13 | 2.13 | 0.48 |
| 1:M:50:ASP:HB2 | 1:M:64:LEU:CD1 | 2.43 | 0.48 |
| 1:Q:9:ILE:HB | 1:Q:232:CYS:SG | 2.53 | 0.48 |
| 1:Q:39:MET:HG2 | 1:Q:73:VAL:HG21 | 1.95 | 0.48 |
| 1:Q:149:ALA:O | 1:Q:152:CYS:HB2 | 2.14 | 0.48 |
| 2:R:197:LYS:HA | 2:R:245:ASP:OD2 | 2.13 | 0.48 |
| 1:S:171:ASN:HD21 | 1:S:208:ALA:HB2 | 1.79 | 0.48 |
| 2:T:268:GLN:O | 2:T:269:PHE:HB2 | 2.14 | 0.48 |
| 1:1:4:ASP:HB3 | 1:1:28:THR:HA | 1.95 | 0.48 |
| 1:1:29:ARG:NH1 | 1:1:300:LEU:O | 2.46 | 0.48 |
| 2:H:238:MET:O | 2:H:240:THR:N | 2.45 | 0.48 |
| 1:I:11:LYS:HE3 | 1:I:11:LYS:HB2 | 1.71 | 0.48 |
| 2:J:329:ILE:OXT | 2:J:329:ILE:HG13 | 2.12 | 0.48 |
| 2:N:9:ILE:HG12 | 2:N:153:ALA:HB1 | 1.95 | 0.48 |
| 2:Z:259:LEU:HD12 | 2:Z:260:VAL:N | 2.28 | 0.48 |
| 1:1:16:ARG:HG2 | 1:1:16:ARG:NH1 | 2.26 | 0.48 |
| 1:1:174:GLN:HB3 | 2:2:60:MET:HG2 | 1.94 | 0.48 |
| 1:1:302:SER:OG | 1:1:305:GLU:HG3 | 2.12 | 0.48 |
| 1:3:182:ALA:HA | 1:3:187:LEU:HD12 | 1.95 | 0.48 |
| 1:5:142:VAL:HA | 1:5:163:THR:HG21 | 1.96 | 0.48 |
| 1:C:105:ILE:O | 1:C:109:LEU:HG | 2.14 | 0.48 |
| 1:E:108:GLU:OE1 | 1:E:117:ALA:N | 2.44 | 0.48 |
| 1:M:229:ASP:O | 1:M:231:LEU:N | 2.46 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:Q:77:ALA:HB3 | 1:Q:234:ARG:HG3 | 1.96 | 0.48 |
| 1:S:28:THR:C | 1:S:30:GLU:N | 2.66 | 0.48 |
| 2:T:184:PRO:HA | 2:T:187:GLN:HE21 | 1.75 | 0.48 |
| 1:Y:70:ALA:HB3 | 1:Y:227:GLY:O | 2.12 | 0.48 |
| 1:1:95:THR:CG2 | 1:1:100:LEU:HD22 | 2.43 | 0.48 |
| 1:1:113:LYS:HB3 | 1:1:330:PRO:HA | 1.95 | 0.48 |
| 1:1:257:THR:OG1 | 1:1:258:TYR:N | 2.47 | 0.48 |
| 2:2:51:ARG:HG3 | 2:2:51:ARG:NH1 | 2.27 | 0.48 |
| 1:5:45:MET:CE | 1:5:102:VAL:HA | 2.44 | 0.48 |
| 1:C:162:LEU:N | 1:C:162:LEU:HD12 | 2.29 | 0.48 |
| 2:H:182:PHE:HD2 | 2:H:187:GLN:HG3 | 1.79 | 0.48 |
| 2:J:313:ILE:HG23 | 2:J:314:PRO:HD2 | 1.95 | 0.48 |
| 2:L:246:MET:O | 2:L:250:GLU:HG3 | 2.13 | 0.48 |
| 1:O:39:MET:HE3 | 1:O:288:ILE:HG12 | 1.95 | 0.48 |
| 1:Q:196:ASN:ND2 | 1:Q:259:ARG:HD3 | 2.28 | 0.48 |
| 2:X:28:GLU:HB2 | 2:X:81:MET:HE3 | 1.95 | 0.48 |
| 2:X:39:VAL:O | 2:X:39:VAL:HG12 | 2.13 | 0.48 |
| 2:X:285:PHE:O | 2:X:288:LEU:HB2 | 2.14 | 0.48 |
| 1:Y:354:TRP:CZ2 | 2:2:325:LYS:HG2 | 2.48 | 0.48 |
| 1:3:171:ASN:OD1 | 1:3:216:ARG:NH2 | 2.46 | 0.48 |
| 1:G:177:GLU:CD | 2:H:58:SER:HB3 | 2.34 | 0.48 |
| 1:K:44:ARG:HH21 | 1:K:314:ARG:HE | 1.62 | 0.48 |
| 1:Q:258:TYR:CD1 | 1:Q:258:TYR:C | 2.87 | 0.48 |
| 1:S:278:ILE:H | 1:S:278:ILE:HD13 | 1.65 | 0.48 |
| 2:H:98:ALA:CB | 2:H:142:LEU:HD13 | 2.39 | 0.48 |
| 1:I:10:LYS:HG2 | 1:I:11:LYS:N | 2.28 | 0.48 |
| 1:K:124:MET:O | 1:K:134:GLY:HA3 | 2.14 | 0.48 |
| 2:L:118:ASN:HD21 | 2:L:132:PHE:H | 1.61 | 0.48 |
| 1:M:101:SER:OG | 1:M:104:GLU:HG3 | 2.13 | 0.48 |
| 1:Q:335:LEU:HB2 | 2:T:308:LEU:HD22 | 1.96 | 0.48 |
| 2:V:88:GLN:HG2 | 2:X:60:MET:HE3 | 1.94 | 0.48 |
| 2:Z:98:ALA:HB2 | 2:Z:142:LEU:HD13 | 1.96 | 0.48 |
| 2:4:260:VAL:HG22 | 2:4:293:VAL:CG2 | 2.44 | 0.48 |
| 1:A:352:ASN:HB3 | 2:D:295:VAL:HG22 | 1.94 | 0.48 |
| 2:F:267:PRO:HA | 2:F:296:THR:HG21 | 1.96 | 0.48 |
| 1:M:177:GLU:HG2 | 1:O:171:ASN:O | 2.14 | 0.48 |
| 2:R:140:PRO:HA | 2:R:242:ARG:HH21 | 1.79 | 0.48 |
| 2:R:259:LEU:HD12 | 2:R:260:VAL:N | 2.29 | 0.48 |
| 1:3:292:LYS:HG3 | 1:3:306:LEU:HD13 | 1.95 | 0.48 |
| 2:D:250:GLU:HB3 | 2:D:284:ALA:HB2 | 1.96 | 0.47 |
| 1:G:196:ASN:HB3 | 1:G:257:THR:CG2 | 2.36 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:I:102:VAL:HG11 | 1:I:317:ILE:CD1 | 2.43 | 0.47 |
| 2:L:94:ILE:HD13 | 2:L:94:ILE:HA | 1.64 | 0.47 |
| 1:Q:229:ASP:OD1 | 1:Q:231:LEU:HB2 | 2.14 | 0.47 |
| 2:R:127:GLN:NE2 | 2:T:95:ASN:O | 2.46 | 0.47 |
| 1:S:37:ARG:HH11 | 1:S:37:ARG:HG3 | 1.72 | 0.47 |
| 2:V:308:LEU:HD22 | 1:W:335:LEU:HB2 | 1.96 | 0.47 |
| 1:W:45:MET:HE3 | 1:W:102:VAL:HG13 | 1.96 | 0.47 |
| 2:J:34:ASP:OD2 | 2:J:41:ARG:HA | 2.15 | 0.47 |
| 1:M:15:HIS:ND1 | 1:M:215:LYS:HG2 | 2.30 | 0.47 |
| 2:N:81:MET:HB3 | 2:N:85:PHE:CD2 | 2.48 | 0.47 |
| 1:Q:75:LEU:HD12 | 1:Q:237:THR:OG1 | 2.13 | 0.47 |
| 2:R:327:LEU:HD23 | 2:R:327:LEU:HA | 1.72 | 0.47 |
| 1:S:70:ALA:HB3 | 1:S:227:GLY:O | 2.13 | 0.47 |
| 1:S:164:LEU:N | 1:S:164:LEU:HD12 | 2.29 | 0.47 |
| 1:U:45:MET:CE | 1:U:102:VAL:HG13 | 2.44 | 0.47 |
| 1:U:89:TYR:CD1 | 1:U:89:TYR:C | 2.87 | 0.47 |
| 1:U:95:THR:HG23 | 1:U:100:LEU:HD22 | 1.96 | 0.47 |
| 2:V:21:GLU:OE1 | 2:V:21:GLU:N | 2.47 | 0.47 |
| 2:Z:127:GLN:HE21 | 2:2:95:ASN:HB3 | 1.79 | 0.47 |
| 1:3:334:GLU:HG2 | 1:3:337:TYR:CE2 | 2.48 | 0.47 |
| 2:4:31:ALA:HB3 | 2:4:54:ASP:OD2 | 2.15 | 0.47 |
| 1:A:102:VAL:HG11 | 1:A:317:ILE:HD13 | 1.97 | 0.47 |
| 1:C:164:LEU:HA | 1:C:192:ILE:O | 2.15 | 0.47 |
| 1:C:328:PRO:C | 1:C:329:GLU:O | 2.50 | 0.47 |
| 1:E:100:LEU:HD13 | 1:E:128:ALA:HB2 | 1.96 | 0.47 |
| 2:F:81:MET:HB3 | 2:F:85:PHE:CE2 | 2.49 | 0.47 |
| 1:G:141:GLN:HA | 1:G:144:LEU:HD12 | 1.97 | 0.47 |
| 1:I:29:ARG:NH1 | 1:I:300:LEU:O | 2.47 | 0.47 |
| 1:I:353:GLN:HE22 | 2:J:281:GLU:HB3 | 1.79 | 0.47 |
| 1:M:197:ARG:HG2 | 1:M:257:THR:O | 2.13 | 0.47 |
| 2:N:185:GLU:O | 2:N:188:SER:HB3 | 2.14 | 0.47 |
| 2:R:4:THR:HA | 2:R:179:PRO:HA | 1.96 | 0.47 |
| 2:V:184:PRO:HA | 2:V:187:GLN:HE22 | 1.78 | 0.47 |
| 1:A:279:GLN:HE22 | 1:A:282:ARG:HH21 | 1.63 | 0.47 |
| 1:A:323:PHE:O | 1:A:327:ASP:HB2 | 2.15 | 0.47 |
| 1:E:337:TYR:HB3 | 1:E:338:HIS:CD2 | 2.49 | 0.47 |
| 2:F:15:GLU:OE1 | 2:F:189:LYS:HA | 2.14 | 0.47 |
| 2:F:220:LEU:HD23 | 2:F:235:VAL:HG21 | 1.95 | 0.47 |
| 2:H:214:ARG:HB3 | 2:H:215:PRO:HD3 | 1.96 | 0.47 |
| 1:I:95:THR:HG23 | 1:I:100:LEU:HD22 | 1.95 | 0.47 |
| 2:J:256:THR:O | 2:J:257:ASN:HB2 | 2.15 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:K:45:MET:HE1 | 1:K:105:ILE:CD1 | 2.38 | 0.47 |
| 1:M:11:LYS:HE3 | 1:M:11:LYS:HB2 | 1.63 | 0.47 |
| 2:P:80:PHE:O | 2:P:81:MET:C | 2.49 | 0.47 |
| 2:P:182:PHE:HD2 | 2:P:187:GLN:HG2 | 1.79 | 0.47 |
| 1:U:1:PHE:O | 1:U:2:ALA:O | 2.32 | 0.47 |
| 2:V:87:MET:HE1 | 2:X:95:ASN:ND2 | 2.30 | 0.47 |
| 1:Y:196:ASN:ND2 | 1:Y:259:ARG:NE | 2.61 | 0.47 |
| 1:Y:197:ARG:HA | 1:Y:197:ARG:HD3 | 1.41 | 0.47 |
| 2:6:263:GLU:O | 2:6:263:GLU:HG3 | 2.14 | 0.47 |
| 1:A:29:ARG:HG3 | 1:A:29:ARG:NH1 | 2.28 | 0.47 |
| 2:B:17:LEU:HD23 | 2:B:23:VAL:HG12 | 1.96 | 0.47 |
| 1:C:95:THR:HG23 | 1:C:100:LEU:HD22 | 1.92 | 0.47 |
| 1:C:216:ARG:HH11 | 1:C:216:ARG:HG3 | 1.79 | 0.47 |
| 1:C:223:LEU:N | 1:C:223:LEU:HD23 | 2.29 | 0.47 |
| 2:D:313:ILE:HG22 | 2:D:314:PRO:CD | 2.29 | 0.47 |
| 1:G:74:GLY:CA | 1:G:230:ILE:HD12 | 2.45 | 0.47 |
| 1:I:284:LYS:O | 1:I:285:SER:HB3 | 2.14 | 0.47 |
| 1:O:95:THR:HG23 | 1:O:100:LEU:HD22 | 1.96 | 0.47 |
| 1:O:233:VAL:O | 1:O:234:ARG:C | 2.49 | 0.47 |
| 2:T:172:ASN:HD22 | 2:T:175:MET:H | 1.62 | 0.47 |
| 2:T:182:PHE:CD2 | 2:T:187:GLN:HG3 | 2.50 | 0.47 |
| 1:W:39:MET:HG2 | 1:W:73:VAL:HG21 | 1.94 | 0.47 |
| 2:B:81:MET:HB3 | 2:B:85:PHE:CD2 | 2.50 | 0.47 |
| 1:C:234:ARG:CZ | 1:C:238:ARG:NH2 | 2.78 | 0.47 |
| 1:C:345:PRO:HB3 | 1:C:360:VAL:HG12 | 1.95 | 0.47 |
| 2:J:185:GLU:O | 2:J:188:SER:HB3 | 2.14 | 0.47 |
| 2:N:306:LYS:HG2 | 1:O:59:ARG:CZ | 2.45 | 0.47 |
| 2:P:212:HIS:HB3 | 2:P:238:MET:CE | 2.43 | 0.47 |
| 2:T:307:ILE:CG2 | 2:T:308:LEU:N | 2.77 | 0.47 |
| 1:W:289:MET:HE2 | 1:W:290:LEU:HD23 | 1.97 | 0.47 |
| 1:1:113:LYS:HD2 | 1:1:328:PRO:HG2 | 1.97 | 0.47 |
| 2:B:172:ASN:HD21 | 2:B:174:LEU:HB2 | 1.78 | 0.47 |
| 1:G:45:MET:HE1 | 1:G:105:ILE:HD12 | 1.97 | 0.47 |
| 1:G:272:TYR:CD1 | 1:G:273:ARG:HA | 2.50 | 0.47 |
| 1:G:272:TYR:C | 1:G:274:THR:H | 2.18 | 0.47 |
| 2:H:110:VAL:HG12 | 2:H:110:VAL:O | 2.14 | 0.47 |
| 1:I:70:ALA:HB3 | 1:I:227:GLY:O | 2.14 | 0.47 |
| 1:I:335:LEU:HD21 | 2:L:300:VAL:HG21 | 1.97 | 0.47 |
| 2:N:43:LEU:HD12 | 2:N:43:LEU:N | 2.30 | 0.47 |
| 2:N:212:HIS:HB3 | 2:N:238:MET:HE3 | 1.97 | 0.47 |
| 1:O:44:ARG:NH1 | 1:O:47:LEU:HD12 | 2.29 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:Q:45:MET:HE2 | 1:Q:105:ILE:HB | 1.97 | 0.47 |
| 1:S:10:LYS:HG2 | 1:S:11:LYS:N | 2.30 | 0.47 |
| 1:S:45:MET:HE2 | 1:S:105:ILE:HB | 1.96 | 0.47 |
| 1:U:296:VAL:HG12 | 1:U:297:ASN:HD22 | 1.79 | 0.47 |
| 1:W:95:THR:CG2 | 1:W:100:LEU:HD22 | 2.44 | 0.47 |
| 2:X:1:LEU:C | 2:X:1:LEU:HD13 | 2.35 | 0.47 |
| 1:3:327:ASP:OD1 | 1:3:328:PRO:HD2 | 2.15 | 0.47 |
| 1:3:335:LEU:HD23 | 1:3:335:LEU:O | 2.13 | 0.47 |
| 1:5:45:MET:HE1 | 1:5:105:ILE:HD12 | 1.96 | 0.47 |
| 1:5:162:LEU:HD11 | 1:5:190:ILE:HD12 | 1.97 | 0.47 |
| 1:A:129:LYS:O | 1:A:130:ASN:HB2 | 2.14 | 0.47 |
| 1:A:213:TYR:HB2 | 1:A:254:GLU:OE1 | 2.15 | 0.47 |
| 1:A:308:GLU:O | 1:A:312:GLU:HG3 | 2.14 | 0.47 |
| 1:G:9:ILE:HD11 | 1:G:22:PRO:O | 2.14 | 0.47 |
| 1:G:171:ASN:HD21 | 1:G:208:ALA:HB2 | 1.79 | 0.47 |
| 2:H:33:TYR:O | 2:H:34:ASP:HB2 | 2.15 | 0.47 |
| 2:H:87:MET:HE2 | 2:H:132:PHE:HZ | 1.80 | 0.47 |
| 1:I:177:GLU:OE1 | 2:J:61:GLY:N | 2.47 | 0.47 |
| 2:J:326:THR:C | 2:J:328:ASN:H | 2.16 | 0.47 |
| 1:K:341:SER:HB2 | 2:L:101:TYR:CZ | 2.49 | 0.47 |
| 1:O:257:THR:OG1 | 1:O:258:TYR:N | 2.46 | 0.47 |
| 2:R:237:ASN:C | 2:R:237:ASN:HD22 | 2.17 | 0.47 |
| 2:4:172:ASN:HD22 | 2:4:175:MET:N | 2.13 | 0.47 |
| 1:5:196:ASN:OD1 | 1:5:196:ASN:N | 2.48 | 0.47 |
| 2:6:182:PHE:HA | 2:6:183:PRO:HD2 | 1.64 | 0.47 |
| 2:6:313:ILE:HG23 | 2:6:314:PRO:HD2 | 1.96 | 0.47 |
| 1:A:286:ASP:O | 1:A:290:LEU:HG | 2.14 | 0.47 |
| 1:C:225:VAL:CG1 | 1:C:226:ASP:N | 2.78 | 0.47 |
| 1:C:253:MET:CE | 1:C:255:LEU:HD13 | 2.44 | 0.47 |
| 2:F:263:GLU:HG2 | 2:F:296:THR:HG22 | 1.97 | 0.47 |
| 1:G:225:VAL:HG12 | 1:G:226:ASP:N | 2.30 | 0.47 |
| 2:H:137:GLY:HA2 | 2:H:144:VAL:HG21 | 1.97 | 0.47 |
| 1:K:112:ARG:HD2 | 1:K:327:ASP:O | 2.15 | 0.47 |
| 2:L:258:HIS:CD2 | 2:L:327:LEU:HD23 | 2.49 | 0.47 |
| 1:M:28:THR:O | 1:M:29:ARG:C | 2.53 | 0.47 |
| 2:R:184:PRO:CG | 2:R:185:GLU:H | 2.28 | 0.47 |
| 1:W:29:ARG:HA | 1:W:300:LEU:HD22 | 1.97 | 0.47 |
| 2:X:214:ARG:N | 2:X:215:PRO:HD2 | 2.30 | 0.47 |
| 1:1:45:MET:HE3 | 1:1:102:VAL:HG22 | 1.97 | 0.47 |
| 1:5:304:GLU:O | 1:5:308:GLU:HG3 | 2.14 | 0.47 |
| 1:A:150:LEU:HA | 1:A:187:LEU:HD22 | 1.97 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:316:GLU:OE1 | 1:C:316:GLU:HA | 2.15 | 0.47 |
| 1:E:55:GLN:O | 1:E:56:LYS:HB2 | 2.15 | 0.47 |
| 1:E:272:TYR:CD1 | 1:E:272:TYR:O | 2.68 | 0.47 |
| 1:K:217:GLY:O | 1:K:218:ASP:HB3 | 2.15 | 0.47 |
| 1:M:229:ASP:OD1 | 1:M:231:LEU:HB2 | 2.15 | 0.47 |
| 1:Q:196:ASN:HB3 | 1:Q:257:THR:HG23 | 1.97 | 0.47 |
| 1:S:45:MET:HE2 | 1:S:105:ILE:HD12 | 1.96 | 0.47 |
| 1:U:141:GLN:OE1 | 1:U:141:GLN:N | 2.42 | 0.47 |
| 2:V:260:VAL:HG22 | 2:V:293:VAL:CG2 | 2.44 | 0.47 |
| 1:W:190:ILE:HD13 | 1:W:240:ALA:HB1 | 1.97 | 0.47 |
| 2:X:184:PRO:HA | 2:X:187:GLN:HE22 | 1.76 | 0.47 |
| 2:4:95:ASN:HD21 | 2:6:87:MET:HE1 | 1.80 | 0.47 |
| 1:5:1:PHE:HA | 1:5:299:ASN:HD21 | 1.80 | 0.47 |
| 1:5:269:GLY:CA | 1:5:273:ARG:HH11 | 2.27 | 0.47 |
| 1:A:286:ASP:HB3 | 1:A:289:MET:HB3 | 1.97 | 0.46 |
| 2:F:278:ARG:NH1 | 2:F:278:ARG:CG | 2.77 | 0.46 |
| 1:G:45:MET:HE3 | 1:G:102:VAL:HG22 | 1.96 | 0.46 |
| 1:I:102:VAL:HG11 | 1:I:317:ILE:HD12 | 1.96 | 0.46 |
| 1:M:108:GLU:OE1 | 1:M:117:ALA:N | 2.47 | 0.46 |
| 2:R:276:CYS:HB3 | 2:T:280:MET:CE | 2.45 | 0.46 |
| 1:S:89:TYR:HB2 | 1:S:124:MET:HG2 | 1.96 | 0.46 |
| 1:W:70:ALA:HB3 | 1:W:227:GLY:O | 2.15 | 0.46 |
| 2:Z:238:MET:O | 2:Z:239:ARG:HB2 | 2.13 | 0.46 |
| 1:3:225:VAL:HG12 | 1:3:226:ASP:N | 2.30 | 0.46 |
| 2:6:88:GLN:HE21 | 2:6:88:GLN:HB3 | 1.49 | 0.46 |
| 2:B:148:TRP:CD1 | 2:B:175:MET:HE2 | 2.50 | 0.46 |
| 1:C:11:LYS:CB | 1:C:23:VAL:HG12 | 2.46 | 0.46 |
| 1:E:231:LEU:HD12 | 1:E:294:ARG:NH1 | 2.31 | 0.46 |
| 2:H:237:ASN:C | 2:H:237:ASN:ND2 | 2.68 | 0.46 |
| 2:J:171:GLU:OE1 | 2:J:176:TYR:OH | 2.26 | 0.46 |
| 2:J:271:VAL:HA | 2:L:269:PHE:HE1 | 1.80 | 0.46 |
| 1:K:164:LEU:N | 1:K:164:LEU:HD12 | 2.31 | 0.46 |
| 2:L:285:PHE:C | 2:L:287:PHE:H | 2.18 | 0.46 |
| 1:Q:231:LEU:HA | 1:Q:231:LEU:HD23 | 1.43 | 0.46 |
| 2:Z:94:ILE:HA | 2:Z:94:ILE:HD13 | 1.70 | 0.46 |
| 1:3:138:VAL:HG13 | 1:3:169:ALA:HB2 | 1.97 | 0.46 |
| 2:4:16:GLU:OE2 | 2:4:162:ARG:NH1 | 2.47 | 0.46 |
| 2:B:59:GLU:N | 2:B:59:GLU:OE1 | 2.49 | 0.46 |
| 2:D:118:ASN:HD21 | 2:D:132:PHE:N | 2.13 | 0.46 |
| 1:E:292:LYS:NZ | 1:E:303:VAL:HG23 | 2.31 | 0.46 |
| 2:F:250:GLU:O | 2:F:254:MET:HG3 | 2.15 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:F:313:ILE:HG23 | 2:F:314:PRO:N | 2.28 | 0.46 |
| 2:H:222:ALA:HB2 | 2:H:316:VAL:HG12 | 1.96 | 0.46 |
| 2:H:238:MET:C | 2:H:240:THR:H | 2.18 | 0.46 |
| 1:I:85:LEU:HD23 | 1:I:131:PHE:CD1 | 2.50 | 0.46 |
| 1:K:29:ARG:HH11 | 1:K:29:ARG:CG | 2.25 | 0.46 |
| 2:L:285:PHE:C | 2:L:287:PHE:N | 2.68 | 0.46 |
| 2:P:237:ASN:C | 2:P:237:ASN:ND2 | 2.67 | 0.46 |
| 1:Q:29:ARG:CG | 1:Q:29:ARG:NH1 | 2.66 | 0.46 |
| 1:S:164:LEU:HA | 1:S:192:ILE:O | 2.15 | 0.46 |
| 2:V:26:LEU:HD23 | 2:V:78:CYS:HA | 1.97 | 0.46 |
| 2:X:93:VAL:O | 2:X:97:ALA:HB3 | 2.16 | 0.46 |
| 1:Y:68:GLN:NE2 | 1:Y:196:ASN:HD22 | 2.13 | 0.46 |
| 1:Y:113:LYS:HD3 | 1:Y:328:PRO:HG2 | 1.97 | 0.46 |
| 1:1:4:ASP:CB | 1:1:28:THR:HA | 2.45 | 0.46 |
| 2:2:81:MET:HE3 | 2:2:81:MET:HB2 | 1.85 | 0.46 |
| 1:3:1:PHE:C | 1:3:2:ALA:O | 2.53 | 0.46 |
| 2:F:279:ILE:HD12 | 2:F:279:ILE:HA | 1.67 | 0.46 |
| 1:I:37:ARG:NH2 | 1:I:309:ILE:HG23 | 2.30 | 0.46 |
| 2:J:21:GLU:HA | 2:J:51:ARG:NH2 | 2.30 | 0.46 |
| 1:K:230:ILE:O | 1:K:230:ILE:CG1 | 2.63 | 0.46 |
| 2:L:16:GLU:HG3 | 2:L:161:ILE:HD12 | 1.96 | 0.46 |
| 2:N:87:MET:CE | 2:P:95:ASN:ND2 | 2.79 | 0.46 |
| 1:O:164:LEU:H | 1:O:164:LEU:HD12 | 1.80 | 0.46 |
| 2:R:271:VAL:HA | 2:T:269:PHE:CE1 | 2.50 | 0.46 |
| 1:S:106:LEU:HD23 | 1:S:106:LEU:HA | 1.81 | 0.46 |
| 1:1:286:ASP:HB3 | 1:1:289:MET:HB3 | 1.97 | 0.46 |
| 1:3:29:ARG:CG | 1:3:29:ARG:NH1 | 2.79 | 0.46 |
| 1:3:258:TYR:CZ | 1:3:277:GLU:OE2 | 2.67 | 0.46 |
| 1:5:140:ALA:O | 1:5:143:PRO:HD2 | 2.15 | 0.46 |
| 1:C:174:GLN:HB3 | 2:D:60:MET:HG3 | 1.95 | 0.46 |
| 1:C:296:VAL:C | 1:C:298:SER:H | 2.18 | 0.46 |
| 1:E:29:ARG:HG2 | 1:E:300:LEU:O | 2.16 | 0.46 |
| 1:E:142:VAL:HB | 1:E:143:PRO:HD3 | 1.97 | 0.46 |
| 1:I:45:MET:HE3 | 1:I:102:VAL:HG22 | 1.97 | 0.46 |
| 2:J:121:SER:OG | 2:J:122:ALA:N | 2.48 | 0.46 |
| 1:K:222:GLY:HA2 | 1:K:252:LEU:O | 2.16 | 0.46 |
| 2:N:311:ASN:HA | 2:N:315:GLN:HE21 | 1.81 | 0.46 |
| 1:O:37:ARG:NH2 | 1:O:309:ILE:HG23 | 2.29 | 0.46 |
| 2:R:39:VAL:O | 2:R:39:VAL:HG12 | 2.13 | 0.46 |
| 1:U:39:MET:HG2 | 1:U:73:VAL:HG21 | 1.98 | 0.46 |
| 1:U:231:LEU:HD12 | 1:U:294:ARG:NH1 | 2.30 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:Y:28:THR:O | 1:Y:29:ARG:C | 2.53 | 0.46 |
| 2:Z:25:LEU:HD12 | 2:Z:77:ILE:O | 2.15 | 0.46 |
| 1:1:223:LEU:HD23 | 1:1:223:LEU:H | 1.79 | 0.46 |
| 1:3:55:GLN:O | 1:3:56:LYS:CB | 2.59 | 0.46 |
| 1:C:147:GLY:HA2 | 2:D:65:ILE:HG23 | 1.96 | 0.46 |
| 2:D:172:ASN:ND2 | 2:D:175:MET:H | 2.12 | 0.46 |
| 2:F:313:ILE:HG13 | 2:F:314:PRO:HD2 | 1.98 | 0.46 |
| 1:M:118:LYS:HE2 | 1:M:118:LYS:HB2 | 1.80 | 0.46 |
| 1:O:234:ARG:HE | 1:O:238:ARG:HH12 | 1.63 | 0.46 |
| 1:O:234:ARG:HE | 1:O:238:ARG:NH1 | 2.13 | 0.46 |
| 1:O:348:VAL:HG23 | 1:O:359:SER:HB2 | 1.97 | 0.46 |
| 2:P:16:GLU:OE1 | 2:P:16:GLU:HA | 2.15 | 0.46 |
| 2:V:135:TRP:O | 2:V:138:HIS:HB3 | 2.15 | 0.46 |
| 1:W:275:ARG:HH11 | 1:W:275:ARG:CG | 2.29 | 0.46 |
| 1:W:277:GLU:O | 1:W:281:VAL:HG23 | 2.15 | 0.46 |
| 2:X:263:GLU:O | 2:X:296:THR:HA | 2.16 | 0.46 |
| 2:2:81:MET:HB3 | 2:2:85:PHE:CD2 | 2.51 | 0.46 |
| 1:A:95:THR:HG23 | 1:A:100:LEU:HD22 | 1.97 | 0.46 |
| 1:C:145:GLY:HA2 | 1:C:148:ILE:HD12 | 1.98 | 0.46 |
| 2:F:142:LEU:HA | 2:F:142:LEU:HD12 | 1.59 | 0.46 |
| 1:M:29:ARG:HG3 | 1:M:300:LEU:O | 2.15 | 0.46 |
| 2:R:205:THR:HG22 | 2:R:255:LYS:HD3 | 1.98 | 0.46 |
| 1:U:334:GLU:HG2 | 1:U:337:TYR:CZ | 2.50 | 0.46 |
| 2:V:81:MET:HB3 | 2:V:85:PHE:CD2 | 2.51 | 0.46 |
| 1:5:142:VAL:HA | 1:5:163:THR:CG2 | 2.45 | 0.46 |
| 2:L:279:ILE:HD13 | 2:L:279:ILE:HA | 1.63 | 0.46 |
| 1:M:140:ALA:O | 1:M:143:PRO:HD2 | 2.16 | 0.46 |
| 1:S:225:VAL:HG12 | 1:S:226:ASP:N | 2.30 | 0.46 |
| 2:T:279:ILE:HD12 | 2:T:279:ILE:HG23 | 1.64 | 0.46 |
| 1:U:39:MET:HE2 | 1:U:291:LEU:HD22 | 1.98 | 0.46 |
| 1:U:337:TYR:O | 1:U:338:HIS:HB2 | 2.15 | 0.46 |
| 2:X:280:MET:HA | 2:X:285:PHE:CD1 | 2.51 | 0.46 |
| 1:Y:118:LYS:HE2 | 1:Y:118:LYS:HB2 | 1.83 | 0.46 |
| 1:1:162:LEU:HD12 | 1:1:162:LEU:N | 2.30 | 0.46 |
| 1:3:142:VAL:HG21 | 1:3:175:ILE:HG12 | 1.97 | 0.46 |
| 1:5:162:LEU:HD12 | 1:5:190:ILE:HD12 | 1.97 | 0.46 |
| 1:5:282:ARG:HG2 | 1:5:283:SER:N | 2.31 | 0.46 |
| 1:A:61:PHE:HD2 | 1:A:124:MET:CE | 2.29 | 0.46 |
| 2:D:262:VAL:HG22 | 2:D:295:VAL:HB | 1.98 | 0.46 |
| 1:E:57:ILE:HD13 | 1:E:57:ILE:H | 1.74 | 0.46 |
| 1:E:101:SER:O | 1:E:105:ILE:HG13 | 2.16 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:E:155:ASN:O | 1:E:156:GLY:C | 2.54 | 0.46 |
| 2:F:124:VAL:HB | 2:F:128:HIS:HB2 | 1.98 | 0.46 |
| 1:I:138:VAL:HG13 | 1:I:169:ALA:CB | 2.46 | 0.46 |
| 2:L:184:PRO:HA | 2:L:187:GLN:NE2 | 2.31 | 0.46 |
| 2:L:237:ASN:C | 2:L:237:ASN:ND2 | 2.70 | 0.46 |
| 1:M:101:SER:O | 1:M:105:ILE:HG13 | 2.15 | 0.46 |
| 1:Q:1:PHE:C | 1:Q:2:ALA:O | 2.54 | 0.46 |
| 1:Q:279:GLN:O | 1:Q:280:GLU:C | 2.53 | 0.46 |
| 1:S:85:LEU:HD23 | 1:S:131:PHE:CD1 | 2.50 | 0.46 |
| 1:U:10:LYS:HG2 | 1:U:11:LYS:N | 2.31 | 0.46 |
| 1:W:118:LYS:HB2 | 1:W:118:LYS:HZ2 | 1.78 | 0.46 |
| 1:1:150:LEU:HA | 1:1:187:LEU:HD22 | 1.98 | 0.46 |
| 2:2:20:ASP:OD1 | 2:2:22:LYS:HB2 | 2.15 | 0.46 |
| 2:2:21:GLU:HA | 2:2:51:ARG:NH2 | 2.30 | 0.46 |
| 2:2:212:HIS:HB3 | 2:2:238:MET:HE3 | 1.98 | 0.46 |
| 1:3:149:ALA:HB1 | 1:3:189:CYS:HB2 | 1.98 | 0.46 |
| 1:3:279:GLN:O | 1:3:280:GLU:C | 2.54 | 0.46 |
| 1:A:37:ARG:CZ | 1:A:309:ILE:HG23 | 2.46 | 0.46 |
| 1:A:118:LYS:HE2 | 1:A:118:LYS:HB2 | 1.43 | 0.46 |
| 1:A:164:LEU:N | 1:A:164:LEU:HD12 | 2.31 | 0.46 |
| 1:C:9:ILE:HD11 | 1:C:22:PRO:O | 2.16 | 0.46 |
| 2:F:19:ARG:HG2 | 2:F:19:ARG:NH1 | 2.31 | 0.46 |
| 2:F:214:ARG:N | 2:F:215:PRO:HD2 | 2.31 | 0.46 |
| 2:H:74:LEU:HD12 | 2:H:74:LEU:HA | 1.71 | 0.46 |
| 1:M:11:LYS:O | 1:M:11:LYS:HG3 | 2.14 | 0.46 |
| 2:P:51:ARG:O | 2:P:52:ILE:HD13 | 2.16 | 0.46 |
| 2:P:124:VAL:O | 2:P:125:ALA:HB3 | 2.16 | 0.46 |
| 1:Q:284:LYS:HE3 | 1:Q:284:LYS:HB2 | 1.61 | 0.46 |
| 1:U:29:ARG:HA | 1:U:300:LEU:HD22 | 1.99 | 0.46 |
| 2:Z:252:SER:O | 2:Z:256:THR:HG23 | 2.16 | 0.46 |
| 1:1:221:PRO:HG3 | 1:1:243:TYR:OH | 2.16 | 0.46 |
| 2:4:197:LYS:HA | 2:4:245:ASP:OD2 | 2.16 | 0.46 |
| 2:4:325:LYS:HG2 | 1:5:354:TRP:CZ2 | 2.51 | 0.46 |
| 2:B:16:GLU:OE2 | 2:B:162:ARG:NH1 | 2.48 | 0.45 |
| 2:B:252:SER:O | 2:B:256:THR:HG23 | 2.16 | 0.45 |
| 1:C:1:PHE:CD1 | 1:C:299:ASN:OD1 | 2.68 | 0.45 |
| 1:C:95:THR:HG22 | 1:C:100:LEU:HB2 | 1.97 | 0.45 |
| 2:D:172:ASN:ND2 | 2:D:174:LEU:H | 2.14 | 0.45 |
| 2:F:148:TRP:O | 2:F:175:MET:HE2 | 2.16 | 0.45 |
| 1:M:112:ARG:HD2 | 1:M:327:ASP:O | 2.16 | 0.45 |
| 2:P:206:HIS:ND1 | 2:P:206:HIS:N | 2.63 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:T:26:LEU:HD21 | 2:T:66:ALA:HB2 | 1.97 | 0.45 |
| 2:X:307:ILE:HG23 | 2:X:308:LEU:N | 2.31 | 0.45 |
| 2:2:268:GLN:O | 2:2:269:PHE:CB | 2.62 | 0.45 |
| 2:B:143:LYS:HB2 | 2:B:167:VAL:HG22 | 1.97 | 0.45 |
| 1:C:38:MET:O | 1:C:39:MET:C | 2.54 | 0.45 |
| 1:C:131:PHE:CZ | 1:C:133:GLY:HA2 | 2.51 | 0.45 |
| 2:D:26:LEU:HD21 | 2:D:66:ALA:HB2 | 1.98 | 0.45 |
| 2:F:149:ASN:OD1 | 2:F:151:GLU:HB3 | 2.17 | 0.45 |
| 1:G:61:PHE:HB3 | 1:G:63:HIS:CE1 | 2.50 | 0.45 |
| 2:J:266:TRP:HB3 | 2:J:267:PRO:HD2 | 1.97 | 0.45 |
| 1:Q:37:ARG:NH2 | 1:Q:309:ILE:HG23 | 2.32 | 0.45 |
| 1:U:327:ASP:OD1 | 1:U:328:PRO:CD | 2.50 | 0.45 |
| 1:W:29:ARG:HH11 | 1:W:29:ARG:HG2 | 1.81 | 0.45 |
| 1:W:39:MET:CE | 1:W:291:LEU:HD22 | 2.47 | 0.45 |
| 2:X:81:MET:HB3 | 2:X:85:PHE:HD2 | 1.78 | 0.45 |
| 2:Z:140:PRO:HB2 | 2:2:301:PRO:HD3 | 1.99 | 0.45 |
| 1:1:297:ASN:N | 1:1:297:ASN:ND2 | 2.61 | 0.45 |
| 2:4:148:TRP:O | 2:4:175:MET:HE2 | 2.17 | 0.45 |
| 2:4:269:PHE:CE1 | 2:6:271:VAL:HA | 2.52 | 0.45 |
| 1:5:259:ARG:HH11 | 1:5:259:ARG:HG3 | 1.82 | 0.45 |
| 1:C:231:LEU:HA | 1:C:231:LEU:HD23 | 1.48 | 0.45 |
| 2:H:144:VAL:CG1 | 2:H:241:ILE:HB | 2.47 | 0.45 |
| 2:J:31:ALA:HB3 | 2:J:54:ASP:CG | 2.37 | 0.45 |
| 1:K:108:GLU:OE1 | 1:K:117:ALA:N | 2.41 | 0.45 |
| 2:L:227:SER:C | 2:L:229:GLU:H | 2.19 | 0.45 |
| 2:N:127:GLN:OE1 | 1:O:125:HIS:HE1 | 2.00 | 0.45 |
| 2:N:199:LYS:HD3 | 2:N:239:ARG:NH2 | 2.30 | 0.45 |
| 1:O:95:THR:HG22 | 1:O:100:LEU:HB2 | 1.99 | 0.45 |
| 1:O:314:ARG:HA | 1:O:314:ARG:HD3 | 1.86 | 0.45 |
| 2:P:28:GLU:HB2 | 2:P:81:MET:HE3 | 1.98 | 0.45 |
| 1:S:30:GLU:OE1 | 1:S:30:GLU:O | 2.33 | 0.45 |
| 2:T:70:ALA:HA | 2:T:74:LEU:O | 2.17 | 0.45 |
| 2:T:237:ASN:C | 2:T:237:ASN:HD22 | 2.18 | 0.45 |
| 2:X:238:MET:C | 2:X:240:THR:H | 2.20 | 0.45 |
| 2:X:313:ILE:HG23 | 2:X:314:PRO:HD2 | 1.98 | 0.45 |
| 1:Y:274:THR:O | 1:Y:278:ILE:HD13 | 2.16 | 0.45 |
| 2:Z:325:LYS:HG2 | 1:1:354:TRP:CZ2 | 2.51 | 0.45 |
| 1:1:77:ALA:CB | 1:1:234:ARG:HG3 | 2.46 | 0.45 |
| 1:5:55:GLN:O | 1:5:56:LYS:HB2 | 2.16 | 0.45 |
| 2:6:20:ASP:C | 2:6:20:ASP:OD1 | 2.55 | 0.45 |
| 1:A:138:VAL:HG13 | 1:A:169:ALA:CB | 2.45 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:250:GLU:O | 2:B:251:ALA:C | 2.55 | 0.45 |
| 2:F:25:LEU:HD23 | 2:F:52:ILE:HG23 | 1.98 | 0.45 |
| 2:F:278:ARG:HG3 | 2:F:278:ARG:HH11 | 1.82 | 0.45 |
| 1:G:272:TYR:CE1 | 1:G:273:ARG:HA | 2.52 | 0.45 |
| 1:I:129:LYS:HD3 | 1:I:129:LYS:HA | 1.77 | 0.45 |
| 2:J:74:LEU:HD12 | 2:J:74:LEU:HA | 1.62 | 0.45 |
| 2:J:95:ASN:ND2 | 2:L:87:MET:CE | 2.79 | 0.45 |
| 2:L:59:GLU:O | 2:L:60:MET:C | 2.54 | 0.45 |
| 1:M:75:LEU:HD11 | 1:M:255:LEU:HD21 | 1.97 | 0.45 |
| 2:N:19:ARG:HH11 | 2:N:19:ARG:CG | 2.27 | 0.45 |
| 1:O:149:ALA:CB | 1:O:189:CYS:HB2 | 2.46 | 0.45 |
| 1:O:236:ALA:O | 1:O:237:THR:O | 2.33 | 0.45 |
| 1:Q:21:PRO:HB3 | 1:Q:239:PHE:HB2 | 1.99 | 0.45 |
| 1:S:11:LYS:HB3 | 1:S:23:VAL:HG12 | 1.99 | 0.45 |
| 1:S:314:ARG:HG2 | 1:S:314:ARG:HH11 | 1.81 | 0.45 |
| 2:T:28:GLU:HB2 | 2:T:81:MET:HE3 | 1.99 | 0.45 |
| 2:T:172:ASN:C | 2:T:172:ASN:HD22 | 2.19 | 0.45 |
| 2:T:314:PRO:O | 2:T:315:GLN:CB | 2.61 | 0.45 |
| 2:V:308:LEU:HD23 | 2:V:308:LEU:HA | 1.67 | 0.45 |
| 2:X:152:ASP:HA | 2:X:193:ILE:HD12 | 1.97 | 0.45 |
| 2:X:214:ARG:O | 2:X:216:VAL:N | 2.50 | 0.45 |
| 2:4:306:LYS:HG2 | 1:5:59:ARG:CZ | 2.47 | 0.45 |
| 1:A:129:LYS:HA | 1:A:129:LYS:HD2 | 1.69 | 0.45 |
| 2:D:32:GLN:HE21 | 2:D:32:GLN:HB2 | 1.58 | 0.45 |
| 1:E:65:CYS:O | 1:E:68:GLN:HB2 | 2.16 | 0.45 |
| 1:G:10:LYS:CG | 1:G:11:LYS:N | 2.79 | 0.45 |
| 1:G:167:ASP:HB3 | 1:G:195:ASN:HA | 1.97 | 0.45 |
| 1:G:272:TYR:HD1 | 1:G:273:ARG:CA | 2.26 | 0.45 |
| 2:L:302:MET:HA | 2:L:303:PRO:HD2 | 1.87 | 0.45 |
| 1:O:162:LEU:HD12 | 1:O:162:LEU:N | 2.32 | 0.45 |
| 1:Q:95:THR:CG2 | 1:Q:100:LEU:HD22 | 2.47 | 0.45 |
| 1:W:271:ALA:C | 1:W:273:ARG:N | 2.69 | 0.45 |
| 2:4:214:ARG:N | 2:4:215:PRO:HD2 | 2.32 | 0.45 |
| 2:D:172:ASN:ND2 | 2:D:172:ASN:C | 2.70 | 0.45 |
| 2:F:87:MET:HE1 | 2:H:95:ASN:ND2 | 2.31 | 0.45 |
| 1:G:72:CYS:HB2 | 1:G:97:THR:CG2 | 2.43 | 0.45 |
| 2:H:191:PHE:O | 2:H:192:LEU:HD12 | 2.16 | 0.45 |
| 2:J:260:VAL:HG22 | 2:J:293:VAL:HG22 | 1.98 | 0.45 |
| 2:L:285:PHE:O | 2:L:287:PHE:N | 2.49 | 0.45 |
| 2:P:94:ILE:HD12 | 2:P:139:CYS:SG | 2.57 | 0.45 |
| 1:S:225:VAL:CG1 | 1:S:226:ASP:N | 2.79 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:U:14:LEU:HA | 1:U:14:LEU:HD23 | 1.57 | 0.45 |
| 1:W:258:TYR:OH | 1:W:278:ILE:HD12 | 2.16 | 0.45 |
| 1:C:75:LEU:O | 1:C:79:ILE:HG12 | 2.16 | 0.45 |
| 2:F:172:ASN:ND2 | 2:F:174:LEU:N | 2.65 | 0.45 |
| 2:H:31:ALA:HB3 | 2:H:54:ASP:OD2 | 2.17 | 0.45 |
| 2:J:182:PHE:O | 2:J:183:PRO:C | 2.54 | 0.45 |
| 1:K:272:TYR:O | 1:K:273:ARG:C | 2.55 | 0.45 |
| 2:N:135:TRP:O | 2:N:138:HIS:HB3 | 2.17 | 0.45 |
| 2:R:33:TYR:O | 2:R:34:ASP:HB2 | 2.15 | 0.45 |
| 2:R:148:TRP:O | 2:R:175:MET:HE2 | 2.16 | 0.45 |
| 1:U:223:LEU:N | 1:U:223:LEU:HD23 | 2.32 | 0.45 |
| 2:X:124:VAL:O | 2:X:125:ALA:HB3 | 2.17 | 0.45 |
| 2:X:172:ASN:C | 2:X:172:ASN:HD22 | 2.20 | 0.45 |
| 1:1:29:ARG:HB2 | 1:1:300:LEU:HD22 | 1.99 | 0.45 |
| 1:A:335:LEU:HD23 | 1:A:335:LEU:O | 2.17 | 0.45 |
| 2:D:316:VAL:O | 2:D:316:VAL:HG12 | 2.17 | 0.45 |
| 1:E:196:ASN:ND2 | 1:E:259:ARG:HE | 2.15 | 0.45 |
| 1:E:337:TYR:O | 1:E:338:HIS:HB2 | 2.16 | 0.45 |
| 2:F:124:VAL:O | 2:F:125:ALA:HB3 | 2.16 | 0.45 |
| 1:I:174:GLN:HB3 | 2:J:60:MET:HG3 | 1.97 | 0.45 |
| 1:K:64:LEU:HD12 | 1:K:261:HIS:CD2 | 2.52 | 0.45 |
| 1:K:100:LEU:CD1 | 1:K:128:ALA:CB | 2.94 | 0.45 |
| 2:L:268:GLN:O | 2:L:269:PHE:HB2 | 2.16 | 0.45 |
| 1:O:303:VAL:CG1 | 1:O:304:GLU:OE2 | 2.65 | 0.45 |
| 2:R:95:ASN:ND2 | 2:T:87:MET:HE3 | 2.31 | 0.45 |
| 2:T:227:SER:C | 2:T:229:GLU:N | 2.70 | 0.45 |
| 1:W:106:LEU:HD23 | 1:W:106:LEU:HA | 1.79 | 0.45 |
| 1:W:292:LYS:HG3 | 1:W:306:LEU:HD13 | 1.99 | 0.45 |
| 2:X:182:PHE:HD2 | 2:X:187:GLN:HG3 | 1.81 | 0.45 |
| 1:Y:272:TYR:CD1 | 1:Y:272:TYR:O | 2.70 | 0.45 |
| 1:1:302:SER:O | 1:1:305:GLU:HB2 | 2.17 | 0.45 |
| 2:2:70:ALA:HB1 | 2:2:111:PRO:HD2 | 1.99 | 0.45 |
| 1:3:112:ARG:HD3 | 1:3:112:ARG:HA | 1.73 | 0.45 |
| 1:3:221:PRO:O | 1:3:251:ILE:HG13 | 2.15 | 0.45 |
| 2:B:325:LYS:HG2 | 1:C:354:TRP:CE2 | 2.52 | 0.45 |
| 2:L:51:ARG:HG3 | 2:L:51:ARG:NH1 | 2.31 | 0.45 |
| 2:P:268:GLN:O | 2:P:269:PHE:CB | 2.60 | 0.45 |
| 1:Q:154:TYR:O | 2:R:50:LYS:NZ | 2.50 | 0.45 |
| 2:R:211:SER:HB2 | 2:R:262:VAL:HB | 1.98 | 0.45 |
| 2:R:259:LEU:CD2 | 2:R:279:ILE:HG13 | 2.46 | 0.45 |
| 1:Y:9:ILE:HB | 1:Y:232:CYS:SG | 2.57 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:Y:142:VAL:HB | 1:Y:143:PRO:HD3 | 1.99 | 0.45 |
| 1:5:63:HIS:C | 1:5:64:LEU:HD23 | 2.38 | 0.45 |
| 2:6:32:GLN:HE21 | 2:6:32:GLN:HB2 | 1.51 | 0.45 |
| 1:A:303:VAL:HG13 | 1:A:304:GLU:OE2 | 2.17 | 0.45 |
| 1:C:88:ALA:HB2 | 1:C:141:GLN:NE2 | 2.32 | 0.45 |
| 1:K:142:VAL:HA | 1:K:163:THR:HG21 | 1.98 | 0.45 |
| 2:L:23:VAL:CG2 | 2:L:75:ARG:HB2 | 2.47 | 0.45 |
| 2:N:143:LYS:HB2 | 2:N:167:VAL:HG22 | 1.98 | 0.45 |
| 1:O:308:GLU:O | 1:O:312:GLU:HG3 | 2.16 | 0.45 |
| 1:Q:353:GLN:HE22 | 2:R:281:GLU:HB3 | 1.82 | 0.45 |
| 2:R:81:MET:HE3 | 2:R:81:MET:HB2 | 1.76 | 0.45 |
| 1:S:29:ARG:CB | 1:S:300:LEU:HD22 | 2.45 | 0.45 |
| 1:S:196:ASN:ND2 | 1:S:259:ARG:HD3 | 2.32 | 0.45 |
| 1:U:57:ILE:HD11 | 2:4:328:ASN:ND2 | 2.32 | 0.45 |
| 1:U:341:SER:HB2 | 2:V:101:TYR:CZ | 2.52 | 0.45 |
| 2:V:279:ILE:HA | 2:V:279:ILE:HD13 | 1.71 | 0.45 |
| 1:W:47:LEU:HA | 1:W:47:LEU:HD23 | 1.79 | 0.45 |
| 2:X:21:GLU:HA | 2:X:51:ARG:NH2 | 2.32 | 0.45 |
| 1:1:221:PRO:O | 1:1:251:ILE:HG13 | 2.17 | 0.45 |
| 2:2:237:ASN:HD22 | 2:2:238:MET:N | 2.13 | 0.45 |
| 1:3:296:VAL:HG12 | 1:3:297:ASN:ND2 | 2.32 | 0.45 |
| 2:4:207:ILE:HG13 | 2:4:258:HIS:HB2 | 1.97 | 0.45 |
| 1:5:282:ARG:O | 1:5:284:LYS:N | 2.49 | 0.45 |
| 1:5:289:MET:HE2 | 1:5:290:LEU:HD23 | 1.98 | 0.45 |
| 2:6:191:PHE:C | 2:6:192:LEU:HD12 | 2.36 | 0.45 |
| 1:G:320:ALA:O | 1:G:323:PHE:HB3 | 2.18 | 0.44 |
| 1:I:15:HIS:O | 1:I:16:ARG:HB2 | 2.17 | 0.44 |
| 1:M:1:PHE:HA | 1:M:299:ASN:HD21 | 1.82 | 0.44 |
| 2:N:26:LEU:HD23 | 2:N:78:CYS:HA | 1.98 | 0.44 |
| 1:O:70:ALA:HB3 | 1:O:227:GLY:O | 2.17 | 0.44 |
| 1:O:95:THR:CG2 | 1:O:100:LEU:HD22 | 2.47 | 0.44 |
| 1:S:28:THR:CG2 | 1:S:31:ASP:H | 2.30 | 0.44 |
| 1:U:45:MET:CE | 1:U:102:VAL:HA | 2.48 | 0.44 |
| 1:W:246:SER:OG | 1:W:248:LYS:HG3 | 2.18 | 0.44 |
| 2:Z:99:LYS:O | 2:Z:103:MET:HG3 | 2.17 | 0.44 |
| 2:Z:207:ILE:CD1 | 2:Z:323:ILE:HG23 | 2.46 | 0.44 |
| 1:3:335:LEU:HD21 | 2:6:300:VAL:HG21 | 1.98 | 0.44 |
| 1:A:285:SER:O | 1:A:286:ASP:C | 2.51 | 0.44 |
| 2:B:267:PRO:HA | 2:B:296:THR:HG21 | 1.99 | 0.44 |
| 2:B:317:LYS:HA | 2:B:317:LYS:HD3 | 1.86 | 0.44 |
| 1:C:164:LEU:N | 1:C:164:LEU:HD12 | 2.32 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:D:268:GLN:O | 2:D:269:PHE:HB2 | 2.18 | 0.44 |
| 1:G:57:ILE:HG22 | 1:G:110:THR:HG22 | 1.99 | 0.44 |
| 1:I:126:MET:O | 1:I:133:GLY:HA2 | 2.17 | 0.44 |
| 2:J:20:ASP:C | 2:J:20:ASP:OD1 | 2.56 | 0.44 |
| 1:M:1:PHE:O | 1:M:2:ALA:O | 2.35 | 0.44 |
| 1:S:36:TYR:OH | 1:S:310:ASP:OD1 | 2.19 | 0.44 |
| 1:S:162:LEU:N | 1:S:162:LEU:HD12 | 2.32 | 0.44 |
| 2:V:11:GLN:O | 2:V:15:GLU:HG3 | 2.18 | 0.44 |
| 2:Z:84:ASN:HD21 | 2:Z:128:HIS:C | 2.20 | 0.44 |
| 2:4:94:ILE:HA | 2:4:94:ILE:HD13 | 1.70 | 0.44 |
| 2:4:269:PHE:HE1 | 2:6:271:VAL:HA | 1.82 | 0.44 |
| 1:5:347:GLU:OE1 | 1:5:356:LYS:HD3 | 2.17 | 0.44 |
| 1:A:70:ALA:HB3 | 1:A:227:GLY:O | 2.17 | 0.44 |
| 1:A:286:ASP:OD2 | 1:A:288:ILE:CB | 2.65 | 0.44 |
| 2:D:193:ILE:HD13 | 2:D:239:ARG:NH2 | 2.32 | 0.44 |
| 1:E:29:ARG:CG | 1:E:300:LEU:O | 2.66 | 0.44 |
| 1:E:273:ARG:HE | 1:E:273:ARG:HB3 | 1.57 | 0.44 |
| 1:G:29:ARG:CA | 1:G:300:LEU:HD22 | 2.48 | 0.44 |
| 1:G:45:MET:CE | 1:G:102:VAL:HA | 2.47 | 0.44 |
| 1:K:289:MET:HE2 | 1:K:290:LEU:HD23 | 1.93 | 0.44 |
| 1:M:270:VAL:O | 1:M:273:ARG:HB3 | 2.17 | 0.44 |
| 2:N:112:ILE:HD13 | 2:N:114:PHE:CZ | 2.51 | 0.44 |
| 1:O:150:LEU:HA | 1:O:187:LEU:HD22 | 1.99 | 0.44 |
| 2:T:237:ASN:C | 2:T:237:ASN:ND2 | 2.70 | 0.44 |
| 2:T:279:ILE:HA | 2:T:279:ILE:HD13 | 1.59 | 0.44 |
| 1:W:132:TYR:HB3 | 2:X:71:MET:HE1 | 1.99 | 0.44 |
| 1:Y:112:ARG:HD2 | 1:Y:327:ASP:O | 2.17 | 0.44 |
| 2:Z:123:GLY:O | 1:1:60:GLY:HA3 | 2.17 | 0.44 |
| 2:Z:172:ASN:ND2 | 2:Z:174:LEU:H | 2.15 | 0.44 |
| 1:1:53:TYR:CD2 | 1:1:62:CYS:CB | 2.99 | 0.44 |
| 1:1:223:LEU:HD23 | 1:1:223:LEU:N | 2.32 | 0.44 |
| 2:2:207:ILE:HG13 | 2:2:258:HIS:HB2 | 1.99 | 0.44 |
| 2:2:313:ILE:HG22 | 2:2:314:PRO:N | 2.33 | 0.44 |
| 1:3:173:GLY:N | 1:5:177:GLU:OE2 | 2.40 | 0.44 |
| 1:3:189:CYS:SG | 1:3:191:PHE:CE1 | 3.11 | 0.44 |
| 1:5:101:SER:OG | 1:5:104:GLU:HG3 | 2.17 | 0.44 |
| 2:6:1:LEU:HD22 | 2:6:1:LEU:HA | 1.76 | 0.44 |
| 2:6:316:VAL:O | 2:6:317:LYS:C | 2.55 | 0.44 |
| 1:A:29:ARG:CB | 1:A:300:LEU:HD22 | 2.48 | 0.44 |
| 1:C:84:HIS:CE1 | 1:C:130:ASN:ND2 | 2.85 | 0.44 |
| 1:E:15:HIS:ND1 | 1:E:215:LYS:HG2 | 2.33 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:G:4:ASP:HA | 1:G:300:LEU:HD21 | 1.99 | 0.44 |
| 2:N:148:TRP:O | 2:N:175:MET:HE2 | 2.17 | 0.44 |
| 1:Q:40:GLN:O | 1:Q:44:ARG:HG2 | 2.17 | 0.44 |
| 2:R:59:GLU:OE1 | 2:R:59:GLU:N | 2.49 | 0.44 |
| 1:S:80:ASN:HB3 | 1:S:81:PRO:HD2 | 1.99 | 0.44 |
| 1:Y:184:LEU:HD12 | 1:Y:184:LEU:HA | 1.73 | 0.44 |
| 1:1:1:PHE:O | 1:1:2:ALA:O | 2.35 | 0.44 |
| 1:1:37:ARG:HH21 | 1:1:309:ILE:HG23 | 1.82 | 0.44 |
| 1:3:157:LYS:HA | 1:3:157:LYS:HD3 | 1.79 | 0.44 |
| 2:4:202:ARG:O | 2:4:234:GLU:HA | 2.18 | 0.44 |
| 1:A:184:LEU:HD21 | 1:C:206:ARG:O | 2.18 | 0.44 |
| 2:B:31:ALA:HB3 | 2:B:54:ASP:OD2 | 2.17 | 0.44 |
| 1:C:55:GLN:O | 1:C:56:LYS:CB | 2.64 | 0.44 |
| 1:C:106:LEU:HD23 | 1:C:106:LEU:HA | 1.84 | 0.44 |
| 1:C:149:ALA:CB | 1:C:189:CYS:HB2 | 2.47 | 0.44 |
| 2:D:279:ILE:HG23 | 2:D:279:ILE:HD12 | 1.75 | 0.44 |
| 1:E:334:GLU:HG2 | 1:E:337:TYR:CD2 | 2.49 | 0.44 |
| 2:H:278:ARG:HG3 | 2:H:278:ARG:NH1 | 2.31 | 0.44 |
| 1:I:64:LEU:O | 1:I:90:ARG:NH1 | 2.50 | 0.44 |
| 2:J:199:LYS:HD2 | 2:J:239:ARG:NH2 | 2.32 | 0.44 |
| 2:J:288:LEU:HD12 | 2:J:288:LEU:HA | 1.74 | 0.44 |
| 2:J:316:VAL:O | 2:J:320:ILE:HG13 | 2.18 | 0.44 |
| 1:K:29:ARG:HB2 | 1:K:300:LEU:HD22 | 2.00 | 0.44 |
| 1:O:341:SER:HB2 | 2:P:101:TYR:CZ | 2.52 | 0.44 |
| 2:T:1:LEU:HD13 | 2:T:2:GLN:H | 1.81 | 0.44 |
| 1:W:50:ASP:HB2 | 1:W:64:LEU:CD1 | 2.48 | 0.44 |
| 1:W:225:VAL:HB | 1:W:255:LEU:HD12 | 1.99 | 0.44 |
| 1:W:239:PHE:O | 1:W:242:ALA:HB3 | 2.16 | 0.44 |
| 2:X:31:ALA:HB3 | 2:X:54:ASP:OD2 | 2.17 | 0.44 |
| 1:3:286:ASP:HB3 | 1:3:289:MET:HB3 | 2.00 | 0.44 |
| 1:5:39:MET:HG2 | 1:5:73:VAL:HG21 | 1.99 | 0.44 |
| 1:5:231:LEU:HA | 1:5:231:LEU:HD22 | 1.58 | 0.44 |
| 2:6:24:PHE:CE1 | 2:6:76:PRO:HB3 | 2.52 | 0.44 |
| 1:A:109:LEU:HD23 | 1:A:109:LEU:HA | 1.87 | 0.44 |
| 1:C:11:LYS:HB3 | 1:C:23:VAL:CG1 | 2.46 | 0.44 |
| 1:C:33:LEU:HA | 1:C:33:LEU:HD12 | 1.84 | 0.44 |
| 1:C:253:MET:CE | 1:C:255:LEU:HD11 | 2.48 | 0.44 |
| 1:C:328:PRO:O | 1:C:329:GLU:O | 2.36 | 0.44 |
| 1:I:196:ASN:HD21 | 1:I:259:ARG:HE | 1.63 | 0.44 |
| 2:J:209:VAL:HG21 | 2:J:323:ILE:HD11 | 2.00 | 0.44 |
| 2:N:33:TYR:O | 2:N:34:ASP:HB2 | 2.17 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:N:213:SER:O | 2:N:214:ARG:C | 2.55 | 0.44 |
| 1:Q:223:LEU:N | 1:Q:223:LEU:HD23 | 2.33 | 0.44 |
| 2:R:51:ARG:HG3 | 2:R:51:ARG:NH1 | 2.33 | 0.44 |
| 2:R:227:SER:HB2 | 2:R:232:GLU:OE2 | 2.17 | 0.44 |
| 2:T:227:SER:C | 2:T:229:GLU:H | 2.21 | 0.44 |
| 2:V:43:LEU:HD12 | 2:V:43:LEU:N | 2.33 | 0.44 |
| 2:X:313:ILE:CG2 | 2:X:314:PRO:HD2 | 2.47 | 0.44 |
| 2:Z:102:TYR:CD2 | 2:2:301:PRO:HG2 | 2.52 | 0.44 |
| 1:3:129:LYS:O | 1:3:130:ASN:HB2 | 2.17 | 0.44 |
| 1:3:289:MET:CE | 1:3:290:LEU:HD23 | 2.48 | 0.44 |
| 2:B:17:LEU:O | 2:B:51:ARG:NH2 | 2.47 | 0.44 |
| 1:C:139:GLY:HA3 | 1:C:172:GLN:HG3 | 1.99 | 0.44 |
| 2:D:279:ILE:HD13 | 2:D:279:ILE:HA | 1.67 | 0.44 |
| 1:E:150:LEU:O | 1:E:150:LEU:HG | 2.17 | 0.44 |
| 1:K:29:ARG:HB2 | 1:K:300:LEU:CD2 | 2.48 | 0.44 |
| 1:K:132:TYR:CD1 | 1:K:132:TYR:N | 2.86 | 0.44 |
| 1:K:142:VAL:HA | 1:K:163:THR:CG2 | 2.48 | 0.44 |
| 1:M:147:GLY:HA2 | 2:N:65:ILE:HG23 | 2.00 | 0.44 |
| 2:P:81:MET:HB3 | 2:P:85:PHE:HD2 | 1.80 | 0.44 |
| 1:Q:109:LEU:CD2 | 1:Q:123:SER:HB2 | 2.47 | 0.44 |
| 1:S:37:ARG:HH11 | 1:S:37:ARG:HG2 | 1.78 | 0.44 |
| 1:S:341:SER:HB3 | 2:T:101:TYR:CE1 | 2.53 | 0.44 |
| 1:U:303:VAL:HG12 | 1:U:304:GLU:OE2 | 2.18 | 0.44 |
| 2:V:1:LEU:HD13 | 2:V:2:GLN:H | 1.79 | 0.44 |
| 2:X:49:ASP:OD1 | 2:X:49:ASP:N | 2.50 | 0.44 |
| 2:X:258:HIS:CD2 | 2:X:327:LEU:HD23 | 2.52 | 0.44 |
| 1:1:71:CYS:SG | 1:1:255:LEU:HD23 | 2.57 | 0.44 |
| 1:3:196:ASN:HD21 | 1:3:259:ARG:NE | 2.16 | 0.44 |
| 2:4:8:ALA:O | 2:4:154:LYS:HB2 | 2.18 | 0.44 |
| 2:4:172:ASN:ND2 | 2:4:174:LEU:N | 2.65 | 0.44 |
| 2:6:136:TYR:C | 2:6:138:HIS:H | 2.21 | 0.44 |
| 2:D:79:GLU:HG3 | 2:D:115:ARG:NH1 | 2.33 | 0.44 |
| 1:E:59:ARG:NH1 | 2:H:306:LYS:HG2 | 2.33 | 0.44 |
| 1:E:150:LEU:HA | 1:E:187:LEU:HD22 | 1.99 | 0.44 |
| 1:E:164:LEU:HG | 1:E:192:ILE:HB | 1.99 | 0.44 |
| 2:F:212:HIS:HB3 | 2:F:238:MET:HE3 | 1.99 | 0.44 |
| 2:F:279:ILE:CG2 | 2:F:280:MET:N | 2.80 | 0.44 |
| 1:I:142:VAL:HA | 1:I:163:THR:HG21 | 1.99 | 0.44 |
| 1:M:29:ARG:HA | 1:M:300:LEU:HD22 | 2.00 | 0.44 |
| 1:M:229:ASP:C | 1:M:231:LEU:H | 2.21 | 0.44 |
| 2:P:121:SER:HB3 | 2:P:124:VAL:HG22 | 1.96 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:R:1:LEU:CD1 | 2:R:2:GLN:N | 2.80 | 0.44 |
| 1:1:142:VAL:HA | 1:1:163:THR:HG21 | 1.99 | 0.44 |
| 2:2:118:ASN:HD21 | 2:2:132:PHE:N | 2.14 | 0.44 |
| 2:4:74:LEU:HD12 | 2:4:74:LEU:HA | 1.76 | 0.44 |
| 1:A:1:PHE:C | 1:A:2:ALA:O | 2.54 | 0.44 |
| 1:A:101:SER:OG | 1:A:104:GLU:HG3 | 2.18 | 0.44 |
| 1:A:245:ARG:C | 1:A:247:GLY:H | 2.21 | 0.44 |
| 1:A:278:ILE:CD1 | 1:A:278:ILE:H | 2.31 | 0.44 |
| 2:B:4:THR:HA | 2:B:179:PRO:HA | 1.99 | 0.44 |
| 1:C:9:ILE:HB | 1:C:232:CYS:HB3 | 1.99 | 0.44 |
| 2:F:256:THR:O | 2:F:257:ASN:HB2 | 2.18 | 0.44 |
| 2:F:260:VAL:HG22 | 2:F:293:VAL:HG22 | 2.00 | 0.44 |
| 2:H:279:ILE:HD13 | 2:H:279:ILE:HA | 1.71 | 0.44 |
| 2:H:313:ILE:H | 2:H:313:ILE:HG13 | 1.75 | 0.44 |
| 1:I:14:LEU:HA | 1:I:14:LEU:HD23 | 1.66 | 0.44 |
| 2:J:308:LEU:HD23 | 2:J:308:LEU:HA | 1.62 | 0.44 |
| 2:L:317:LYS:HA | 2:L:317:LYS:HD3 | 1.45 | 0.44 |
| 1:M:334:GLU:HG2 | 1:M:337:TYR:CD2 | 2.53 | 0.44 |
| 1:O:286:ASP:CG | 1:O:287:PRO:HD2 | 2.38 | 0.44 |
| 1:W:1:PHE:HZ | 1:W:302:SER:HB3 | 1.83 | 0.44 |
| 1:W:231:LEU:HD12 | 1:W:294:ARG:NH1 | 2.33 | 0.44 |
| 1:Y:174:GLN:HB3 | 2:Z:60:MET:HG2 | 1.99 | 0.44 |
| 2:Z:276:CYS:HB3 | 2:2:280:MET:HE2 | 2.00 | 0.44 |
| 1:1:280:GLU:C | 1:1:282:ARG:N | 2.71 | 0.44 |
| 1:3:304:GLU:O | 1:3:308:GLU:HG3 | 2.17 | 0.44 |
| 2:4:103:MET:SD | 2:6:126:ALA:HB3 | 2.58 | 0.44 |
| 1:5:258:TYR:CD1 | 1:5:258:TYR:C | 2.92 | 0.44 |
| 1:5:268:PRO:C | 1:5:270:VAL:H | 2.20 | 0.44 |
| 2:6:25:LEU:HD12 | 2:6:77:ILE:O | 2.18 | 0.44 |
| 1:C:126:MET:HB2 | 1:C:126:MET:HE3 | 1.86 | 0.43 |
| 1:C:128:ALA:HB3 | 1:C:131:PHE:HB3 | 2.00 | 0.43 |
| 1:C:142:VAL:HA | 1:C:163:THR:CG2 | 2.48 | 0.43 |
| 2:F:172:ASN:HD22 | 2:F:175:MET:N | 2.16 | 0.43 |
| 2:F:212:HIS:HB3 | 2:F:238:MET:CE | 2.47 | 0.43 |
| 2:F:288:LEU:HD12 | 2:F:288:LEU:HA | 1.83 | 0.43 |
| 1:G:239:PHE:CD1 | 1:G:239:PHE:C | 2.91 | 0.43 |
| 1:I:33:LEU:HD12 | 1:I:33:LEU:HA | 1.78 | 0.43 |
| 2:J:126:ALA:HB3 | 2:L:103:MET:SD | 2.58 | 0.43 |
| 2:N:300:VAL:HG12 | 1:O:339:ILE:HD11 | 2.00 | 0.43 |
| 1:Q:102:VAL:HG11 | 1:Q:317:ILE:CD1 | 2.48 | 0.43 |
| 1:Q:274:THR:O | 1:Q:277:GLU:HB2 | 2.18 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:S:77:ALA:CB | 1:S:234:ARG:HG3 | 2.48 | 0.43 |
| 1:Y:150:LEU:O | 1:Y:150:LEU:HG | 2.18 | 0.43 |
| 1:1:53:TYR:CE2 | 1:1:62:CYS:HB3 | 2.53 | 0.43 |
| 2:2:59:GLU:O | 2:2:60:MET:C | 2.55 | 0.43 |
| 2:2:246:MET:O | 2:2:250:GLU:HG3 | 2.18 | 0.43 |
| 1:3:34:LYS:HB3 | 1:3:34:LYS:HE3 | 1.86 | 0.43 |
| 2:4:81:MET:HE3 | 2:4:81:MET:HB2 | 1.91 | 0.43 |
| 2:4:202:ARG:NH1 | 2:4:233:CYS:O | 2.47 | 0.43 |
| 2:4:327:LEU:O | 2:4:329:ILE:HG23 | 2.18 | 0.43 |
| 1:5:279:GLN:O | 1:5:280:GLU:C | 2.56 | 0.43 |
| 1:C:28:THR:O | 1:C:30:GLU:N | 2.51 | 0.43 |
| 2:D:142:LEU:HA | 2:D:142:LEU:HD12 | 1.72 | 0.43 |
| 2:F:130:GLN:HG3 | 2:F:266:TRP:CH2 | 2.53 | 0.43 |
| 2:F:269:PHE:CD1 | 2:H:274:GLU:HB2 | 2.53 | 0.43 |
| 1:G:108:GLU:OE1 | 1:G:117:ALA:N | 2.45 | 0.43 |
| 1:G:225:VAL:HB | 1:G:255:LEU:HD12 | 2.00 | 0.43 |
| 2:H:81:MET:O | 2:H:117:PRO:HD2 | 2.19 | 0.43 |
| 1:K:113:LYS:HB3 | 1:K:330:PRO:HA | 2.00 | 0.43 |
| 2:N:88:GLN:HE22 | 1:O:172:GLN:HE22 | 1.66 | 0.43 |
| 1:Q:89:TYR:HB2 | 1:Q:124:MET:HG2 | 2.00 | 0.43 |
| 1:U:184:LEU:HD12 | 1:U:184:LEU:HA | 1.82 | 0.43 |
| 2:V:184:PRO:HA | 2:V:187:GLN:NE2 | 2.33 | 0.43 |
| 1:Y:29:ARG:HB2 | 1:Y:300:LEU:CD2 | 2.48 | 0.43 |
| 1:Y:138:VAL:HG13 | 1:Y:169:ALA:HB2 | 2.00 | 0.43 |
| 2:2:51:ARG:O | 2:2:52:ILE:HD13 | 2.18 | 0.43 |
| 1:5:234:ARG:CZ | 1:5:238:ARG:HH22 | 2.31 | 0.43 |
| 1:E:272:TYR:C | 1:E:272:TYR:HD1 | 2.18 | 0.43 |
| 2:F:112:ILE:HG12 | 2:F:113:VAL:N | 2.33 | 0.43 |
| 1:G:93:GLY:O | 1:G:97:THR:HG23 | 2.18 | 0.43 |
| 1:I:292:LYS:HG3 | 1:I:306:LEU:CD1 | 2.48 | 0.43 |
| 1:K:274:THR:O | 1:K:275:ARG:C | 2.56 | 0.43 |
| 2:P:108:GLN:HG3 | 2:P:108:GLN:O | 2.18 | 0.43 |
| 2:R:121:SER:OG | 2:R:122:ALA:N | 2.51 | 0.43 |
| 2:T:238:MET:C | 2:T:240:THR:H | 2.22 | 0.43 |
| 1:U:84:HIS:ND1 | 1:U:130:ASN:ND2 | 2.64 | 0.43 |
| 2:V:172:ASN:HD21 | 2:V:174:LEU:HB2 | 1.82 | 0.43 |
| 2:V:307:ILE:O | 2:V:311:ASN:ND2 | 2.43 | 0.43 |
| 2:X:26:LEU:HD23 | 2:X:78:CYS:HA | 1.98 | 0.43 |
| 1:1:55:GLN:O | 1:1:56:LYS:CB | 2.66 | 0.43 |
| 2:2:238:MET:C | 2:2:240:THR:H | 2.21 | 0.43 |
| 2:2:278:ARG:HA | 2:2:278:ARG:HD2 | 1.74 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:D:46:LYS:HE2 | 2:D:47:TYR:CZ | 2.53 | 0.43 |
| 1:E:29:ARG:HB2 | 1:E:300:LEU:HD23 | 2.01 | 0.43 |
| 1:E:216:ARG:HG3 | 1:E:216:ARG:NH1 | 2.09 | 0.43 |
| 2:F:317:LYS:H | 2:F:317:LYS:HG3 | 1.51 | 0.43 |
| 2:J:88:GLN:HE22 | 1:K:172:GLN:HE22 | 1.66 | 0.43 |
| 2:L:118:ASN:HD21 | 2:L:132:PHE:N | 2.17 | 0.43 |
| 1:M:340:TYR:HB3 | 2:N:165:ASN:ND2 | 2.34 | 0.43 |
| 1:Q:16:ARG:HH11 | 1:Q:16:ARG:HG2 | 1.84 | 0.43 |
| 1:Q:213:TYR:HA | 1:Q:216:ARG:HG2 | 2.00 | 0.43 |
| 1:S:27:LEU:HD11 | 1:S:32:GLY:HA3 | 1.99 | 0.43 |
| 2:V:43:LEU:N | 2:V:43:LEU:CD1 | 2.81 | 0.43 |
| 2:V:246:MET:O | 2:V:250:GLU:HG3 | 2.18 | 0.43 |
| 1:3:72:CYS:HB2 | 1:3:97:THR:CG2 | 2.45 | 0.43 |
| 2:D:70:ALA:HA | 2:D:74:LEU:O | 2.18 | 0.43 |
| 2:J:212:HIS:HB3 | 2:J:238:MET:CE | 2.48 | 0.43 |
| 1:K:177:GLU:OE1 | 2:L:61:GLY:N | 2.52 | 0.43 |
| 2:P:260:VAL:HG22 | 2:P:293:VAL:HG23 | 2.00 | 0.43 |
| 1:Q:142:VAL:HG21 | 1:Q:175:ILE:HG12 | 2.00 | 0.43 |
| 1:S:27:LEU:HD23 | 1:S:27:LEU:HA | 1.64 | 0.43 |
| 2:T:172:ASN:ND2 | 2:T:174:LEU:N | 2.66 | 0.43 |
| 2:T:182:PHE:HD2 | 2:T:187:GLN:HG3 | 1.84 | 0.43 |
| 2:T:246:MET:O | 2:T:250:GLU:HG3 | 2.19 | 0.43 |
| 1:W:46:GLU:OE2 | 1:W:65:CYS:N | 2.51 | 0.43 |
| 2:4:148:TRP:CD1 | 2:4:175:MET:CE | 3.02 | 0.43 |
| 2:6:268:GLN:O | 2:6:269:PHE:CB | 2.63 | 0.43 |
| 2:6:313:ILE:CG2 | 2:6:314:PRO:HD2 | 2.48 | 0.43 |
| 1:A:1:PHE:O | 1:A:2:ALA:O | 2.36 | 0.43 |
| 1:A:149:ALA:O | 1:A:152:CYS:HB2 | 2.19 | 0.43 |
| 2:B:74:LEU:N | 2:B:74:LEU:CD1 | 2.81 | 0.43 |
| 1:E:223:LEU:HD23 | 1:E:223:LEU:H | 1.84 | 0.43 |
| 2:F:252:SER:O | 2:F:256:THR:HG23 | 2.18 | 0.43 |
| 2:H:80:PHE:O | 2:H:81:MET:C | 2.55 | 0.43 |
| 2:H:250:GLU:HB3 | 2:H:284:ALA:HB2 | 2.00 | 0.43 |
| 2:H:258:HIS:CD2 | 2:H:327:LEU:HD23 | 2.53 | 0.43 |
| 1:I:151:ALA:O | 1:I:154:TYR:HB3 | 2.19 | 0.43 |
| 2:J:271:VAL:O | 2:J:272:GLY:C | 2.56 | 0.43 |
| 2:L:29:GLU:O | 2:L:35:GLY:HA2 | 2.19 | 0.43 |
| 1:Q:196:ASN:ND2 | 1:Q:259:ARG:CD | 2.81 | 0.43 |
| 1:Q:339:ILE:HD11 | 2:T:300:VAL:HG12 | 2.01 | 0.43 |
| 2:T:260:VAL:HG22 | 2:T:293:VAL:HG22 | 2.00 | 0.43 |
| 2:X:1:LEU:HD13 | 2:X:2:GLN:N | 2.33 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:X:321:PHE:O | 2:X:325:LYS:HB2 | 2.18 | 0.43 |
| 1:Y:337:TYR:HB3 | 1:Y:338:HIS:CD2 | 2.53 | 0.43 |
| 2:2:44:TRP:HA | 2:2:52:ILE:HG13 | 2.01 | 0.43 |
| 2:4:121:SER:OG | 2:4:122:ALA:N | 2.49 | 0.43 |
| 1:5:68:GLN:NE2 | 1:5:196:ASN:HD22 | 2.16 | 0.43 |
| 2:6:182:PHE:O | 2:6:183:PRO:O | 2.36 | 0.43 |
| 2:B:209:VAL:HA | 2:B:260:VAL:O | 2.19 | 0.43 |
| 2:B:260:VAL:HG22 | 2:B:293:VAL:HG23 | 1.99 | 0.43 |
| 1:C:37:ARG:NH2 | 1:C:309:ILE:HG23 | 2.33 | 0.43 |
| 1:M:95:THR:HG23 | 1:M:100:LEU:HD22 | 2.00 | 0.43 |
| 1:M:150:LEU:HA | 1:M:187:LEU:HD22 | 2.00 | 0.43 |
| 1:M:223:LEU:N | 1:M:223:LEU:CD2 | 2.73 | 0.43 |
| 1:M:279:GLN:OE1 | 1:M:279:GLN:O | 2.36 | 0.43 |
| 2:P:59:GLU:O | 2:P:60:MET:C | 2.56 | 0.43 |
| 1:Q:129:LYS:HA | 1:Q:129:LYS:HD2 | 1.81 | 0.43 |
| 2:T:51:ARG:O | 2:T:52:ILE:HD13 | 2.18 | 0.43 |
| 1:U:74:GLY:CA | 1:U:233:VAL:HG12 | 2.47 | 0.43 |
| 1:U:245:ARG:C | 1:U:247:GLY:H | 2.22 | 0.43 |
| 1:W:128:ALA:HB3 | 1:W:131:PHE:HB3 | 1.99 | 0.43 |
| 2:2:285:PHE:O | 2:2:288:LEU:HB2 | 2.18 | 0.43 |
| 1:3:142:VAL:HA | 1:3:163:THR:CG2 | 2.48 | 0.43 |
| 1:5:314:ARG:HA | 1:5:314:ARG:HD2 | 1.76 | 0.43 |
| 2:6:172:ASN:ND2 | 2:6:174:LEU:H | 2.15 | 0.43 |
| 1:A:29:ARG:CG | 1:A:29:ARG:NH1 | 2.68 | 0.43 |
| 1:A:29:ARG:HB2 | 1:A:300:LEU:HD22 | 2.00 | 0.43 |
| 1:E:112:ARG:HD2 | 1:E:327:ASP:O | 2.18 | 0.43 |
| 1:K:196:ASN:ND2 | 1:K:259:ARG:NE | 2.66 | 0.43 |
| 1:M:3:ASN:O | 1:M:4:ASP:HB3 | 2.19 | 0.43 |
| 1:O:87:THR:OG1 | 1:O:88:ALA:N | 2.52 | 0.43 |
| 1:Q:143:PRO:CG | 1:Q:174:GLN:HB2 | 2.49 | 0.43 |
| 2:X:210:VAL:HG12 | 2:X:211:SER:N | 2.34 | 0.43 |
| 2:Z:172:ASN:HD22 | 2:Z:175:MET:N | 2.13 | 0.43 |
| 2:4:95:ASN:ND2 | 2:6:87:MET:CE | 2.80 | 0.43 |
| 1:5:45:MET:HE3 | 1:5:102:VAL:CG2 | 2.40 | 0.43 |
| 1:A:61:PHE:CD2 | 1:A:124:MET:CE | 3.02 | 0.43 |
| 1:G:196:ASN:ND2 | 1:G:259:ARG:NE | 2.65 | 0.43 |
| 2:L:38:LYS:HD3 | 2:L:38:LYS:HA | 1.90 | 0.43 |
| 2:N:155:GLY:HA3 | 2:N:193:ILE:HG13 | 1.99 | 0.43 |
| 2:N:207:ILE:CD1 | 2:N:323:ILE:HG23 | 2.43 | 0.43 |
| 1:O:337:TYR:O | 1:O:338:HIS:HB2 | 2.19 | 0.43 |
| 1:W:118:LYS:HB2 | 1:W:118:LYS:HZ3 | 1.82 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:Y:341:SER:H | 2:Z:165:ASN:HD21 | 1.66 | 0.43 |
| 2:Z:157:ILE:O | 2:Z:161:ILE:HG13 | 2.18 | 0.43 |
| 2:2:81:MET:O | 2:2:117:PRO:HD2 | 2.18 | 0.43 |
| 1:3:174:GLN:HB3 | 2:4:60:MET:CG | 2.49 | 0.43 |
| 2:4:279:ILE:HA | 2:4:279:ILE:HD13 | 1.68 | 0.43 |
| 1:5:279:GLN:O | 1:5:280:GLU:O | 2.36 | 0.43 |
| 1:A:39:MET:HE3 | 1:A:288:ILE:HA | 2.00 | 0.43 |
| 1:A:190:ILE:HG23 | 1:A:251:ILE:HG23 | 2.00 | 0.43 |
| 1:E:267:ASP:HA | 1:E:268:PRO:HD2 | 1.66 | 0.43 |
| 1:E:289:MET:HE1 | 1:E:290:LEU:HD23 | 1.99 | 0.43 |
| 2:H:210:VAL:CG1 | 2:H:211:SER:N | 2.81 | 0.43 |
| 2:L:16:GLU:OE2 | 2:L:162:ARG:NH1 | 2.51 | 0.43 |
| 2:L:227:SER:C | 2:L:229:GLU:N | 2.72 | 0.43 |
| 2:L:313:ILE:HG23 | 2:L:314:PRO:HD2 | 2.00 | 0.43 |
| 2:L:327:LEU:O | 2:L:329:ILE:HG23 | 2.19 | 0.43 |
| 1:Q:1:PHE:O | 1:Q:2:ALA:O | 2.37 | 0.43 |
| 1:Q:229:ASP:C | 1:Q:231:LEU:N | 2.72 | 0.43 |
| 2:R:74:LEU:HD12 | 2:R:74:LEU:HA | 1.83 | 0.43 |
| 1:U:45:MET:HE3 | 1:U:102:VAL:HG13 | 2.01 | 0.43 |
| 1:U:172:GLN:HE22 | 2:X:88:GLN:HE22 | 1.67 | 0.43 |
| 2:V:167:VAL:HG12 | 2:V:168:VAL:N | 2.33 | 0.43 |
| 1:Y:64:LEU:O | 1:Y:90:ARG:NH1 | 2.52 | 0.43 |
| 2:Z:102:TYR:CG | 2:2:301:PRO:HG2 | 2.54 | 0.43 |
| 2:Z:148:TRP:O | 2:Z:175:MET:HE2 | 2.19 | 0.43 |
| 1:3:349:ARG:HH12 | 2:4:281:GLU:CD | 2.22 | 0.43 |
| 2:4:177:GLY:O | 2:4:179:PRO:HD3 | 2.18 | 0.43 |
| 1:5:58:ILE:HD13 | 1:5:109:LEU:HB3 | 2.01 | 0.43 |
| 2:B:34:ASP:O | 2:B:38:LYS:HA | 2.18 | 0.42 |
| 2:D:188:SER:OG | 2:D:189:LYS:N | 2.52 | 0.42 |
| 1:E:75:LEU:HD12 | 1:E:233:VAL:CG1 | 2.49 | 0.42 |
| 2:H:31:ALA:HB3 | 2:H:54:ASP:CG | 2.39 | 0.42 |
| 2:J:279:ILE:HD13 | 2:J:279:ILE:HA | 1.62 | 0.42 |
| 1:Q:118:LYS:HE2 | 1:Q:118:LYS:HB2 | 1.62 | 0.42 |
| 1:Q:245:ARG:C | 1:Q:247:GLY:H | 2.21 | 0.42 |
| 1:S:13:ASP:O | 1:S:14:LEU:HD23 | 2.19 | 0.42 |
| 1:W:289:MET:HE1 | 1:W:290:LEU:HD23 | 2.00 | 0.42 |
| 1:Y:226:ASP:C | 1:Y:226:ASP:OD1 | 2.56 | 0.42 |
| 2:Z:32:GLN:HE21 | 2:Z:32:GLN:HB3 | 1.49 | 0.42 |
| 2:Z:87:MET:CE | 2:2:95:ASN:HD21 | 2.32 | 0.42 |
| 1:3:174:GLN:HB3 | 2:4:60:MET:HG2 | 2.00 | 0.42 |
| 2:B:80:PHE:O | 2:B:81:MET:C | 2.57 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:70:ALA:HB3 | 1:C:227:GLY:O | 2.18 | 0.42 |
| 1:C:140:ALA:O | 1:C:143:PRO:HD2 | 2.18 | 0.42 |
| 1:C:291:LEU:O | 1:C:295:MET:HG2 | 2.19 | 0.42 |
| 2:F:74:LEU:HD12 | 2:F:74:LEU:HA | 1.65 | 0.42 |
| 2:J:148:TRP:CD1 | 2:J:175:MET:HE2 | 2.54 | 0.42 |
| 1:K:314:ARG:HA | 1:K:314:ARG:HD2 | 1.82 | 0.42 |
| 2:L:88:GLN:HE21 | 2:L:88:GLN:HB3 | 1.39 | 0.42 |
| 2:L:278:ARG:HH11 | 2:L:278:ARG:CG | 2.31 | 0.42 |
| 2:L:286:ASN:H | 2:L:286:ASN:ND2 | 2.16 | 0.42 |
| 1:M:258:TYR:CE1 | 1:M:259:ARG:O | 2.72 | 0.42 |
| 2:N:151:GLU:OE1 | 2:N:183:PRO:HG2 | 2.18 | 0.42 |
| 1:O:162:LEU:N | 1:O:162:LEU:CD1 | 2.82 | 0.42 |
| 2:T:59:GLU:O | 2:T:60:MET:C | 2.57 | 0.42 |
| 1:U:1:PHE:HZ | 1:U:302:SER:HB3 | 1.85 | 0.42 |
| 1:U:55:GLN:O | 1:U:56:LYS:CB | 2.67 | 0.42 |
| 2:Z:2:GLN:HE21 | 2:Z:2:GLN:HB3 | 1.42 | 0.42 |
| 1:1:341:SER:HB2 | 2:2:101:TYR:CZ | 2.54 | 0.42 |
| 2:2:34:ASP:O | 2:2:38:LYS:HA | 2.19 | 0.42 |
| 2:6:59:GLU:O | 2:6:60:MET:C | 2.57 | 0.42 |
| 1:A:45:MET:CE | 1:A:105:ILE:HD12 | 2.49 | 0.42 |
| 1:A:303:VAL:HG12 | 1:A:304:GLU:OE2 | 2.19 | 0.42 |
| 2:H:59:GLU:HA | 2:H:62:PHE:CE2 | 2.54 | 0.42 |
| 1:I:191:PHE:O | 1:I:252:LEU:HA | 2.19 | 0.42 |
| 1:O:157:LYS:HD3 | 1:O:157:LYS:HA | 1.89 | 0.42 |
| 1:O:178:ALA:O | 1:O:179:TYR:C | 2.56 | 0.42 |
| 2:P:279:ILE:HD13 | 2:P:279:ILE:HA | 1.86 | 0.42 |
| 1:Q:234:ARG:O | 1:Q:238:ARG:HG3 | 2.20 | 0.42 |
| 1:S:29:ARG:N | 1:S:300:LEU:HD22 | 2.33 | 0.42 |
| 1:U:15:HIS:CG | 1:U:215:LYS:HG2 | 2.54 | 0.42 |
| 1:U:215:LYS:O | 1:U:217:GLY:N | 2.52 | 0.42 |
| 2:Z:237:ASN:C | 2:Z:237:ASN:HD22 | 2.23 | 0.42 |
| 1:3:346:PHE:N | 1:3:346:PHE:CD1 | 2.87 | 0.42 |
| 2:4:6:ARG:HD3 | 2:4:38:LYS:O | 2.19 | 0.42 |
| 1:C:177:GLU:OE1 | 2:D:61:GLY:N | 2.50 | 0.42 |
| 1:G:307:LYS:HA | 1:G:307:LYS:HD2 | 1.94 | 0.42 |
| 2:H:165:ASN:HB3 | 2:H:166:PRO:HD2 | 2.02 | 0.42 |
| 1:I:75:LEU:HD21 | 1:I:192:ILE:HD13 | 2.00 | 0.42 |
| 1:I:171:ASN:OD1 | 1:I:216:ARG:NH2 | 2.48 | 0.42 |
| 1:O:334:GLU:HG2 | 1:O:337:TYR:CD2 | 2.54 | 0.42 |
| 1:S:15:HIS:CG | 1:S:215:LYS:HG2 | 2.54 | 0.42 |
| 2:X:262:VAL:HG21 | 2:X:319:ILE:HD13 | 2.01 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:Y:289:MET:HE2 | 1:Y:290:LEU:CD2 | 2.49 | 0.42 |
| 2:4:95:ASN:ND2 | 2:6:87:MET:HE1 | 2.35 | 0.42 |
| 2:4:212:HIS:HB3 | 2:4:238:MET:CE | 2.50 | 0.42 |
| 1:5:33:LEU:HD12 | 1:5:33:LEU:HA | 1.92 | 0.42 |
| 2:6:121:SER:HB3 | 2:6:124:VAL:CG2 | 2.49 | 0.42 |
| 2:6:259:LEU:HD12 | 2:6:260:VAL:N | 2.34 | 0.42 |
| 2:6:260:VAL:HG22 | 2:6:293:VAL:HG23 | 2.00 | 0.42 |
| 1:A:93:GLY:O | 1:A:97:THR:HG23 | 2.19 | 0.42 |
| 2:B:307:ILE:CG2 | 2:B:308:LEU:N | 2.83 | 0.42 |
| 2:D:307:ILE:HG23 | 2:D:308:LEU:N | 2.34 | 0.42 |
| 1:E:207:ALA:HB1 | 2:H:56:PRO:HB3 | 2.01 | 0.42 |
| 1:G:11:LYS:HB3 | 1:G:23:VAL:HG13 | 2.00 | 0.42 |
| 1:I:75:LEU:HD12 | 1:I:237:THR:OG1 | 2.20 | 0.42 |
| 1:I:95:THR:HG22 | 1:I:100:LEU:HB2 | 2.02 | 0.42 |
| 1:I:142:VAL:HB | 1:I:143:PRO:HD3 | 2.00 | 0.42 |
| 1:K:113:LYS:HG2 | 1:K:328:PRO:O | 2.20 | 0.42 |
| 1:M:229:ASP:C | 1:M:231:LEU:N | 2.72 | 0.42 |
| 1:Q:16:ARG:CG | 1:Q:16:ARG:NH1 | 2.77 | 0.42 |
| 1:Q:29:ARG:HG3 | 1:Q:300:LEU:O | 2.19 | 0.42 |
| 1:W:88:ALA:O | 1:W:134:GLY:CA | 2.65 | 0.42 |
| 2:X:143:LYS:HB2 | 2:X:167:VAL:HG22 | 2.01 | 0.42 |
| 2:4:17:LEU:HA | 2:4:17:LEU:HD23 | 1.77 | 0.42 |
| 1:A:60:GLY:HA3 | 2:D:123:GLY:O | 2.20 | 0.42 |
| 1:C:85:LEU:HD23 | 1:C:131:PHE:CD1 | 2.55 | 0.42 |
| 1:C:85:LEU:HD21 | 1:C:94:PHE:CD1 | 2.54 | 0.42 |
| 2:F:241:ILE:HG23 | 2:F:241:ILE:HD12 | 1.79 | 0.42 |
| 1:G:104:GLU:H | 1:G:104:GLU:HG3 | 1.50 | 0.42 |
| 2:H:51:ARG:HG3 | 2:H:51:ARG:NH1 | 2.33 | 0.42 |
| 2:J:59:GLU:HA | 2:J:62:PHE:CE2 | 2.55 | 0.42 |
| 2:J:59:GLU:O | 2:J:60:MET:C | 2.56 | 0.42 |
| 1:K:68:GLN:NE2 | 1:K:196:ASN:HD22 | 2.18 | 0.42 |
| 1:M:282:ARG:HG2 | 1:M:283:SER:N | 2.34 | 0.42 |
| 1:M:292:LYS:HG3 | 1:M:306:LEU:CD1 | 2.49 | 0.42 |
| 1:O:106:LEU:HA | 1:O:106:LEU:HD23 | 1.79 | 0.42 |
| 1:Q:151:ALA:O | 1:Q:154:TYR:HB3 | 2.19 | 0.42 |
| 1:S:274:THR:HB | 1:S:276:GLU:HG3 | 1.98 | 0.42 |
| 2:T:188:SER:OG | 2:T:189:LYS:N | 2.52 | 0.42 |
| 1:W:1:PHE:O | 1:W:2:ALA:O | 2.37 | 0.42 |
| 2:Z:84:ASN:ND2 | 2:Z:128:HIS:C | 2.73 | 0.42 |
| 2:Z:259:LEU:HD12 | 2:Z:260:VAL:H | 1.83 | 0.42 |
| 1:1:315:LYS:NZ | 1:1:315:LYS:HB2 | 2.34 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:3:33:LEU:HD12 | 1:3:33:LEU:HA | 1.84 | 0.42 |
| 1:3:112:ARG:HD2 | 1:3:327:ASP:O | 2.19 | 0.42 |
| 1:3:284:LYS:O | 1:3:285:SER:CB | 2.68 | 0.42 |
| 2:4:59:GLU:OE1 | 2:4:59:GLU:N | 2.50 | 0.42 |
| 2:4:250:GLU:O | 2:4:251:ALA:C | 2.57 | 0.42 |
| 1:5:64:LEU:N | 1:5:64:LEU:CD2 | 2.68 | 0.42 |
| 2:B:139:CYS:HA | 2:B:140:PRO:HD2 | 1.86 | 0.42 |
| 2:B:307:ILE:HG21 | 2:B:307:ILE:HD13 | 1.79 | 0.42 |
| 1:C:11:LYS:HB2 | 1:C:11:LYS:HE3 | 1.79 | 0.42 |
| 1:C:45:MET:HE3 | 1:C:102:VAL:HG22 | 2.01 | 0.42 |
| 1:C:53:TYR:CD2 | 1:C:62:CYS:HB2 | 2.55 | 0.42 |
| 2:D:191:PHE:C | 2:D:192:LEU:HD12 | 2.39 | 0.42 |
| 1:G:215:LYS:HB2 | 1:G:215:LYS:HE3 | 1.92 | 0.42 |
| 2:H:43:LEU:HA | 2:H:43:LEU:HD12 | 1.75 | 0.42 |
| 1:I:196:ASN:ND2 | 1:I:259:ARG:CD | 2.82 | 0.42 |
| 2:N:21:GLU:OE1 | 2:N:21:GLU:N | 2.49 | 0.42 |
| 2:P:262:VAL:HA | 2:P:295:VAL:O | 2.20 | 0.42 |
| 2:R:81:MET:HB3 | 2:R:85:PHE:HD2 | 1.84 | 0.42 |
| 1:S:196:ASN:ND2 | 1:S:259:ARG:CD | 2.83 | 0.42 |
| 1:S:289:MET:HE3 | 1:S:290:LEU:HD23 | 2.00 | 0.42 |
| 1:U:3:ASN:O | 1:U:4:ASP:HB3 | 2.20 | 0.42 |
| 2:X:8:ALA:HB1 | 2:X:154:LYS:HB2 | 2.02 | 0.42 |
| 2:X:98:ALA:HB2 | 2:X:142:LEU:CD1 | 2.48 | 0.42 |
| 2:X:238:MET:O | 2:X:240:THR:N | 2.47 | 0.42 |
| 1:Y:52:LEU:HD23 | 1:Y:52:LEU:HA | 1.86 | 0.42 |
| 2:Z:310:ASP:O | 2:Z:315:GLN:NE2 | 2.52 | 0.42 |
| 1:1:164:LEU:HA | 1:1:192:ILE:O | 2.19 | 0.42 |
| 2:2:24:PHE:CZ | 2:2:76:PRO:HB3 | 2.54 | 0.42 |
| 2:2:227:SER:C | 2:2:229:GLU:H | 2.23 | 0.42 |
| 1:5:235:GLU:O | 1:5:236:ALA:C | 2.57 | 0.42 |
| 2:B:300:VAL:HG12 | 1:C:339:ILE:HD11 | 2.01 | 0.42 |
| 1:C:129:LYS:HD2 | 1:C:129:LYS:HA | 1.46 | 0.42 |
| 2:H:5:VAL:O | 2:H:6:ARG:C | 2.58 | 0.42 |
| 2:J:197:LYS:HA | 2:J:245:ASP:OD2 | 2.20 | 0.42 |
| 2:N:140:PRO:HB2 | 2:P:301:PRO:HD3 | 2.02 | 0.42 |
| 1:O:9:ILE:CD1 | 1:O:235:GLU:HG3 | 2.50 | 0.42 |
| 2:P:278:ARG:HH11 | 2:P:278:ARG:CG | 2.31 | 0.42 |
| 1:Q:329:GLU:HB3 | 1:Q:330:PRO:HD2 | 2.01 | 0.42 |
| 2:R:17:LEU:HD23 | 2:R:17:LEU:HA | 1.78 | 0.42 |
| 2:T:4:THR:HA | 2:T:179:PRO:HA | 2.01 | 0.42 |
| 2:T:280:MET:HA | 2:T:285:PHE:CD1 | 2.55 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:V:88:GLN:HE22 | 1:W:172:GLN:HE22 | 1.66 | 0.42 |
| 2:V:269:PHE:CE1 | 2:X:271:VAL:HA | 2.55 | 0.42 |
| 2:V:315:GLN:O | 2:V:318:ASP:N | 2.52 | 0.42 |
| 1:1:100:LEU:CD1 | 1:1:128:ALA:HB2 | 2.41 | 0.42 |
| 2:4:26:LEU:HD21 | 2:4:66:ALA:HB2 | 2.01 | 0.42 |
| 2:4:142:LEU:HA | 2:4:142:LEU:HD12 | 1.84 | 0.42 |
| 2:4:279:ILE:HG22 | 2:4:280:MET:N | 2.35 | 0.42 |
| 1:5:137:ILE:HD13 | 1:5:137:ILE:HA | 1.74 | 0.42 |
| 1:5:281:VAL:O | 1:5:282:ARG:O | 2.37 | 0.42 |
| 1:A:218:ASP:C | 1:A:218:ASP:OD1 | 2.58 | 0.42 |
| 2:B:173:GLU:O | 2:B:173:GLU:HG2 | 2.19 | 0.42 |
| 2:D:93:VAL:HG22 | 2:D:114:PHE:CZ | 2.55 | 0.42 |
| 2:D:172:ASN:ND2 | 2:D:174:LEU:N | 2.68 | 0.42 |
| 1:G:45:MET:HE3 | 1:G:102:VAL:HG13 | 2.00 | 0.42 |
| 2:H:51:ARG:C | 2:H:52:ILE:HD13 | 2.39 | 0.42 |
| 2:J:75:ARG:HG2 | 2:J:75:ARG:HH11 | 1.85 | 0.42 |
| 1:K:132:TYR:HB3 | 2:L:71:MET:HE1 | 2.02 | 0.42 |
| 2:N:259:LEU:HD12 | 2:N:260:VAL:N | 2.34 | 0.42 |
| 1:O:222:GLY:HA2 | 1:O:252:LEU:O | 2.20 | 0.42 |
| 1:S:70:ALA:HB2 | 1:S:287:PRO:HB3 | 2.02 | 0.42 |
| 2:T:329:ILE:OXT | 2:T:329:ILE:HG13 | 2.19 | 0.42 |
| 1:Y:50:ASP:HB2 | 1:Y:64:LEU:HD13 | 2.00 | 0.42 |
| 1:Y:75:LEU:HD11 | 1:Y:255:LEU:HD21 | 2.00 | 0.42 |
| 1:A:48:LYS:HB2 | 1:A:48:LYS:HE2 | 1.83 | 0.42 |
| 1:C:234:ARG:NE | 1:C:238:ARG:HH21 | 2.15 | 0.42 |
| 2:D:121:SER:HB3 | 2:D:124:VAL:CG2 | 2.50 | 0.42 |
| 1:E:4:ASP:HA | 1:E:300:LEU:HD21 | 2.01 | 0.42 |
| 2:H:157:ILE:HG23 | 2:H:158:LYS:N | 2.35 | 0.42 |
| 2:H:256:THR:O | 2:H:257:ASN:HB2 | 2.19 | 0.42 |
| 2:J:165:ASN:O | 2:J:167:VAL:HG23 | 2.20 | 0.42 |
| 1:K:196:ASN:OD1 | 1:K:196:ASN:N | 2.52 | 0.42 |
| 1:K:231:LEU:HB2 | 1:K:294:ARG:HH12 | 1.84 | 0.42 |
| 2:N:262:VAL:HA | 2:N:295:VAL:O | 2.20 | 0.42 |
| 1:Q:68:GLN:O | 1:Q:71:CYS:HB2 | 2.20 | 0.42 |
| 1:S:274:THR:HB | 1:S:276:GLU:CB | 2.49 | 0.42 |
| 2:T:16:GLU:OE2 | 2:T:162:ARG:NH1 | 2.52 | 0.42 |
| 2:X:144:VAL:CG1 | 2:X:241:ILE:HB | 2.50 | 0.42 |
| 1:Y:267:ASP:O | 1:Y:268:PRO:O | 2.37 | 0.42 |
| 1:1:34:LYS:HG2 | 1:1:38:MET:CE | 2.50 | 0.42 |
| 1:1:64:LEU:O | 1:1:90:ARG:HD3 | 2.20 | 0.42 |
| 1:1:142:VAL:HB | 1:1:143:PRO:HD3 | 2.00 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:221:PRO:O | 1:A:251:ILE:HG13 | 2.20 | 0.41 |
| 1:G:94:PHE:CZ | 1:G:164:LEU:HD22 | 2.54 | 0.41 |
| 1:I:225:VAL:HG12 | 1:I:226:ASP:N | 2.35 | 0.41 |
| 2:J:277:ALA:O | 2:J:281:GLU:HG3 | 2.19 | 0.41 |
| 1:K:162:LEU:HD11 | 1:K:190:ILE:HD12 | 2.02 | 0.41 |
| 1:M:86:ILE:HG12 | 1:M:87:THR:N | 2.35 | 0.41 |
| 2:N:237:ASN:C | 2:N:237:ASN:HD22 | 2.24 | 0.41 |
| 1:O:229:ASP:OD1 | 1:O:231:LEU:N | 2.53 | 0.41 |
| 1:Q:12:CYS:SG | 1:Q:225:VAL:HG22 | 2.60 | 0.41 |
| 1:Q:29:ARG:HB2 | 1:Q:300:LEU:CD2 | 2.49 | 0.41 |
| 1:Q:137:ILE:HD13 | 2:T:85:PHE:HE1 | 1.85 | 0.41 |
| 1:Q:304:GLU:O | 1:Q:308:GLU:HG3 | 2.20 | 0.41 |
| 2:R:95:ASN:HD21 | 2:T:87:MET:CE | 2.32 | 0.41 |
| 2:R:139:CYS:HA | 2:R:140:PRO:HD2 | 1.91 | 0.41 |
| 2:R:253:VAL:HG11 | 2:R:288:LEU:HD13 | 2.02 | 0.41 |
| 2:R:306:LYS:HD3 | 2:R:310:ASP:OD2 | 2.20 | 0.41 |
| 1:W:272:TYR:CD2 | 1:W:273:ARG:N | 2.88 | 0.41 |
| 1:Y:35:TYR:O | 1:Y:39:MET:HG3 | 2.20 | 0.41 |
| 1:Y:332:LEU:O | 1:Y:332:LEU:HG | 2.20 | 0.41 |
| 1:1:142:VAL:HA | 1:1:163:THR:CG2 | 2.50 | 0.41 |
| 2:2:76:PRO:HG2 | 2:2:112:ILE:HG13 | 2.01 | 0.41 |
| 2:2:238:MET:O | 2:2:240:THR:N | 2.51 | 0.41 |
| 2:4:307:ILE:CG2 | 2:4:308:LEU:N | 2.83 | 0.41 |
| 1:A:127:TYR:CD1 | 1:A:127:TYR:N | 2.88 | 0.41 |
| 1:A:219:PHE:CD1 | 1:A:220:ILE:HG13 | 2.55 | 0.41 |
| 2:F:121:SER:HB3 | 2:F:124:VAL:HG21 | 2.02 | 0.41 |
| 2:J:268:GLN:O | 2:J:269:PHE:HB2 | 2.20 | 0.41 |
| 1:M:50:ASP:HB2 | 1:M:64:LEU:HD11 | 2.01 | 0.41 |
| 1:O:234:ARG:HE | 1:O:238:ARG:NH2 | 2.17 | 0.41 |
| 2:P:30:VAL:HG23 | 2:P:31:ALA:N | 2.36 | 0.41 |
| 1:S:34:LYS:HE2 | 1:S:34:LYS:HB3 | 1.67 | 0.41 |
| 2:X:75:ARG:HG2 | 2:X:75:ARG:HH11 | 1.86 | 0.41 |
| 2:4:157:ILE:O | 2:4:161:ILE:HG13 | 2.21 | 0.41 |
| 2:6:212:HIS:HB3 | 2:6:238:MET:CE | 2.51 | 0.41 |
| 1:A:278:ILE:N | 1:A:278:ILE:CD1 | 2.83 | 0.41 |
| 2:B:20:ASP:C | 2:B:20:ASP:OD1 | 2.59 | 0.41 |
| 1:G:313:VAL:O | 1:G:316:GLU:HB3 | 2.19 | 0.41 |
| 1:I:113:LYS:HD2 | 1:I:328:PRO:HG2 | 2.01 | 0.41 |
| 1:K:141:GLN:OE1 | 1:K:141:GLN:N | 2.44 | 0.41 |
| 1:M:29:ARG:CA | 1:M:300:LEU:HD22 | 2.51 | 0.41 |
| 2:R:81:MET:HB3 | 2:R:85:PHE:CD2 | 2.55 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:S:37:ARG:NH1 | 1:S:309:ILE:HG23 | 2.35 | 0.41 |
| 2:T:165:ASN:O | 2:T:167:VAL:HG23 | 2.20 | 0.41 |
| 1:U:104:GLU:HG3 | 1:U:104:GLU:H | 1.65 | 0.41 |
| 1:W:213:TYR:HA | 1:W:216:ARG:HG2 | 2.02 | 0.41 |
| 2:Z:81:MET:HB3 | 2:Z:85:PHE:CD2 | 2.56 | 0.41 |
| 2:Z:278:ARG:HD2 | 2:Z:278:ARG:HA | 1.75 | 0.41 |
| 2:Z:278:ARG:HG3 | 2:Z:278:ARG:NH1 | 2.35 | 0.41 |
| 1:1:297:ASN:H | 1:1:297:ASN:ND2 | 2.17 | 0.41 |
| 1:3:152:CYS:O | 1:3:153:LYS:C | 2.57 | 0.41 |
| 2:4:307:ILE:HG23 | 2:4:308:LEU:N | 2.35 | 0.41 |
| 1:5:238:ARG:HH11 | 1:5:238:ARG:HD3 | 1.73 | 0.41 |
| 2:6:172:ASN:HD22 | 2:6:175:MET:H | 1.67 | 0.41 |
| 1:A:29:ARG:HB2 | 1:A:300:LEU:CD2 | 2.50 | 0.41 |
| 1:A:75:LEU:HD12 | 1:A:75:LEU:HA | 1.88 | 0.41 |
| 1:C:276:GLU:HA | 1:C:279:GLN:HB2 | 2.03 | 0.41 |
| 1:E:43:ARG:NE | 1:E:69:GLU:OE2 | 2.46 | 0.41 |
| 1:G:66:ASP:HA | 1:G:69:GLU:OE2 | 2.19 | 0.41 |
| 2:H:124:VAL:O | 2:H:125:ALA:HB3 | 2.20 | 0.41 |
| 1:I:213:TYR:HB2 | 1:I:254:GLU:OE1 | 2.20 | 0.41 |
| 1:I:289:MET:CE | 1:I:290:LEU:HD23 | 2.51 | 0.41 |
| 2:L:172:ASN:HB3 | 2:L:175:MET:HG2 | 2.01 | 0.41 |
| 2:L:207:ILE:HG13 | 2:L:258:HIS:HB2 | 2.02 | 0.41 |
| 1:O:197:ARG:HH11 | 1:O:197:ARG:CB | 2.20 | 0.41 |
| 2:T:285:PHE:O | 2:T:288:LEU:HB2 | 2.20 | 0.41 |
| 1:Y:335:LEU:O | 1:Y:335:LEU:HG | 2.18 | 0.41 |
| 2:B:256:THR:O | 2:B:257:ASN:CB | 2.68 | 0.41 |
| 2:F:313:ILE:HG13 | 2:F:314:PRO:CD | 2.50 | 0.41 |
| 1:G:128:ALA:HB3 | 1:G:131:PHE:HB3 | 2.02 | 0.41 |
| 1:I:149:ALA:O | 1:I:152:CYS:HB2 | 2.21 | 0.41 |
| 2:J:22:LYS:HD2 | 2:J:74:LEU:HD12 | 2.02 | 0.41 |
| 2:J:93:VAL:HG22 | 2:J:114:PHE:CZ | 2.55 | 0.41 |
| 2:J:327:LEU:O | 2:J:329:ILE:N | 2.54 | 0.41 |
| 1:M:36:TYR:O | 1:M:37:ARG:C | 2.58 | 0.41 |
| 2:N:34:ASP:O | 2:N:38:LYS:HA | 2.21 | 0.41 |
| 2:P:263:GLU:O | 2:P:296:THR:HA | 2.21 | 0.41 |
| 2:R:279:ILE:HD13 | 2:R:279:ILE:HA | 1.98 | 0.41 |
| 2:T:313:ILE:CG2 | 2:T:314:PRO:HD2 | 2.43 | 0.41 |
| 1:1:95:THR:HG22 | 1:1:100:LEU:HB2 | 2.01 | 0.41 |
| 1:1:184:LEU:HA | 1:1:184:LEU:HD12 | 1.73 | 0.41 |
| 1:1:280:GLU:O | 1:1:283:SER:OG | 2.37 | 0.41 |
| 2:4:31:ALA:HB3 | 2:4:54:ASP:CG | 2.40 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:52:LEU:HD23 | 1:C:52:LEU:HA | 1.84 | 0.41 |
| 1:E:9:ILE:HB | 1:E:232:CYS:SG | 2.61 | 0.41 |
| 1:E:14:LEU:HA | 1:E:14:LEU:HD23 | 1.77 | 0.41 |
| 2:J:25:LEU:HD12 | 2:J:77:ILE:O | 2.20 | 0.41 |
| 2:J:329:ILE:OXT | 2:J:329:ILE:CG1 | 2.68 | 0.41 |
| 2:L:24:PHE:CZ | 2:L:76:PRO:HB3 | 2.56 | 0.41 |
| 2:L:170:LEU:HA | 2:L:170:LEU:HD23 | 1.88 | 0.41 |
| 2:N:172:ASN:ND2 | 2:N:172:ASN:C | 2.73 | 0.41 |
| 1:O:55:GLN:O | 1:O:56:LYS:CB | 2.69 | 0.41 |
| 1:O:234:ARG:NH2 | 1:O:238:ARG:HH22 | 2.18 | 0.41 |
| 1:O:292:LYS:HG3 | 1:O:306:LEU:HD13 | 2.01 | 0.41 |
| 1:U:317:ILE:HD13 | 1:U:317:ILE:HA | 1.81 | 0.41 |
| 2:X:75:ARG:HG2 | 2:X:75:ARG:NH1 | 2.36 | 0.41 |
| 2:X:237:ASN:C | 2:X:237:ASN:ND2 | 2.74 | 0.41 |
| 1:1:225:VAL:CG1 | 1:1:226:ASP:H | 2.33 | 0.41 |
| 1:3:3:ASN:O | 1:3:4:ASP:HB3 | 2.21 | 0.41 |
| 2:4:112:ILE:CG1 | 2:4:113:VAL:N | 2.83 | 0.41 |
| 2:4:182:PHE:O | 2:4:183:PRO:C | 2.58 | 0.41 |
| 1:5:234:ARG:NE | 1:5:238:ARG:NH2 | 2.68 | 0.41 |
| 2:6:81:MET:HE3 | 2:6:81:MET:HB2 | 1.97 | 0.41 |
| 2:B:95:ASN:ND2 | 2:D:87:MET:CE | 2.84 | 0.41 |
| 2:B:197:LYS:HA | 2:B:245:ASP:OD2 | 2.20 | 0.41 |
| 2:B:326:THR:C | 2:B:328:ASN:H | 2.22 | 0.41 |
| 1:C:53:TYR:CE2 | 1:C:62:CYS:HB2 | 2.56 | 0.41 |
| 2:D:81:MET:HB3 | 2:D:85:PHE:CD2 | 2.55 | 0.41 |
| 1:K:95:THR:HG22 | 1:K:105:ILE:HD11 | 2.02 | 0.41 |
| 2:N:271:VAL:HA | 2:P:269:PHE:HE1 | 1.85 | 0.41 |
| 1:Q:4:ASP:HB3 | 1:Q:28:THR:HA | 2.03 | 0.41 |
| 2:V:142:LEU:HD12 | 2:V:142:LEU:HA | 1.89 | 0.41 |
| 1:Y:100:LEU:HD13 | 1:Y:128:ALA:HB2 | 2.01 | 0.41 |
| 1:Y:269:GLY:O | 1:Y:272:TYR:HB3 | 2.20 | 0.41 |
| 2:2:130:GLN:HG3 | 2:2:266:TRP:CH2 | 2.55 | 0.41 |
| 1:3:187:LEU:O | 1:3:189:CYS:N | 2.54 | 0.41 |
| 1:5:61:PHE:CD2 | 1:5:124:MET:SD | 3.13 | 0.41 |
| 2:6:28:GLU:OE2 | 2:6:59:GLU:OE2 | 2.39 | 0.41 |
| 1:A:39:MET:HG2 | 1:A:73:VAL:HG21 | 2.02 | 0.41 |
| 1:A:55:GLN:O | 1:A:56:LYS:CB | 2.65 | 0.41 |
| 1:A:337:TYR:O | 1:A:338:HIS:HB2 | 2.21 | 0.41 |
| 2:D:278:ARG:HG3 | 2:D:278:ARG:HH11 | 1.85 | 0.41 |
| 2:F:99:LYS:HG2 | 2:H:301:PRO:HB3 | 2.02 | 0.41 |
| 2:F:266:TRP:HB3 | 2:F:267:PRO:HD2 | 2.03 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:I:78:GLY:HA2 | 1:I:238:ARG:CG | 2.51 | 0.41 |
| 2:J:81:MET:HE3 | 2:J:81:MET:HB2 | 1.80 | 0.41 |
| 2:J:118:ASN:ND2 | 2:J:132:PHE:H | 2.17 | 0.41 |
| 1:K:142:VAL:HB | 1:K:143:PRO:HD3 | 2.01 | 0.41 |
| 2:L:59:GLU:OE1 | 2:L:59:GLU:N | 2.51 | 0.41 |
| 2:L:206:HIS:HD2 | 2:L:231:VAL:HA | 1.86 | 0.41 |
| 1:M:225:VAL:HB | 1:M:255:LEU:HD12 | 2.02 | 0.41 |
| 2:N:83:PHE:CZ | 2:N:168:VAL:HG13 | 2.56 | 0.41 |
| 2:N:95:ASN:ND2 | 2:P:87:MET:CE | 2.84 | 0.41 |
| 1:S:289:MET:CE | 1:S:290:LEU:HD23 | 2.51 | 0.41 |
| 1:U:9:ILE:H | 1:U:9:ILE:HG12 | 1.69 | 0.41 |
| 2:Z:110:VAL:O | 2:Z:166:PRO:HD3 | 2.21 | 0.41 |
| 1:1:2:ALA:HB3 | 1:1:300:LEU:HD23 | 2.02 | 0.41 |
| 1:1:57:ILE:HD12 | 1:5:326:ALA:CB | 2.50 | 0.41 |
| 1:1:162:LEU:N | 1:1:162:LEU:CD1 | 2.84 | 0.41 |
| 2:2:39:VAL:O | 2:2:39:VAL:CG1 | 2.68 | 0.41 |
| 2:2:157:ILE:HG23 | 2:2:158:LYS:N | 2.34 | 0.41 |
| 1:5:15:HIS:CG | 1:5:215:LYS:HG2 | 2.56 | 0.41 |
| 2:6:237:ASN:C | 2:6:237:ASN:ND2 | 2.74 | 0.41 |
| 1:A:29:ARG:HH11 | 1:A:29:ARG:HG2 | 1.83 | 0.41 |
| 1:A:80:ASN:HB3 | 1:A:81:PRO:CD | 2.50 | 0.41 |
| 2:B:94:ILE:HA | 2:B:94:ILE:HD13 | 1.80 | 0.41 |
| 2:B:172:ASN:HD22 | 2:B:175:MET:N | 2.13 | 0.41 |
| 2:B:327:LEU:HA | 2:B:327:LEU:HD23 | 1.80 | 0.41 |
| 1:C:25:THR:OG1 | 1:C:26:VAL:N | 2.53 | 0.41 |
| 1:C:64:LEU:O | 1:C:90:ARG:NH1 | 2.48 | 0.41 |
| 1:C:114:GLY:N | 1:C:327:ASP:OD2 | 2.52 | 0.41 |
| 1:C:157:LYS:HD3 | 1:C:157:LYS:HA | 1.89 | 0.41 |
| 1:C:337:TYR:O | 1:C:338:HIS:HB2 | 2.21 | 0.41 |
| 2:D:16:GLU:OE2 | 2:D:158:LYS:NZ | 2.53 | 0.41 |
| 2:D:172:ASN:HD22 | 2:D:172:ASN:C | 2.24 | 0.41 |
| 2:D:184:PRO:HA | 2:D:187:GLN:NE2 | 2.36 | 0.41 |
| 1:E:40:GLN:HE21 | 1:E:288:ILE:HD13 | 1.86 | 0.41 |
| 1:E:137:ILE:HD13 | 1:E:137:ILE:HA | 1.82 | 0.41 |
| 1:E:246:SER:OG | 1:E:248:LYS:HG3 | 2.21 | 0.41 |
| 2:H:139:CYS:HA | 2:H:140:PRO:HD2 | 1.65 | 0.41 |
| 1:I:152:CYS:O | 1:I:153:LYS:C | 2.58 | 0.41 |
| 2:J:9:ILE:CG1 | 2:J:153:ALA:HB1 | 2.51 | 0.41 |
| 1:K:230:ILE:O | 1:K:230:ILE:HG12 | 2.20 | 0.41 |
| 1:K:232:CYS:HA | 1:K:235:GLU:HB2 | 2.03 | 0.41 |
| 2:L:51:ARG:C | 2:L:52:ILE:HD13 | 2.41 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:M:57:ILE:N | 1:M:57:ILE:HD13 | 2.35 | 0.41 |
| 1:M:269:GLY:O | 1:M:272:TYR:HB3 | 2.21 | 0.41 |
| 1:M:279:GLN:OE1 | 1:M:279:GLN:HA | 2.20 | 0.41 |
| 2:N:20:ASP:OD1 | 2:N:22:LYS:HB2 | 2.21 | 0.41 |
| 2:N:297:GLY:HA2 | 2:N:312:SER:O | 2.21 | 0.41 |
| 1:O:196:ASN:CB | 1:O:257:THR:HG23 | 2.39 | 0.41 |
| 1:Q:29:ARG:CB | 1:Q:300:LEU:HD22 | 2.49 | 0.41 |
| 1:Q:258:TYR:C | 1:Q:258:TYR:HD1 | 2.24 | 0.41 |
| 2:V:124:VAL:HB | 2:V:128:HIS:HB2 | 2.03 | 0.41 |
| 2:V:269:PHE:HE1 | 2:X:271:VAL:HA | 1.85 | 0.41 |
| 2:V:313:ILE:HG22 | 2:V:314:PRO:N | 2.36 | 0.41 |
| 1:Y:276:GLU:O | 1:Y:280:GLU:HB2 | 2.20 | 0.41 |
| 2:Z:219:CYS:SG | 2:Z:262:VAL:HG21 | 2.61 | 0.41 |
| 1:1:45:MET:HE2 | 1:1:102:VAL:HG13 | 2.02 | 0.41 |
| 1:1:180:ASN:O | 1:1:184:LEU:HB2 | 2.21 | 0.41 |
| 1:1:348:VAL:HG23 | 1:1:359:SER:HB2 | 2.03 | 0.41 |
| 1:3:43:ARG:HG2 | 1:3:43:ARG:NH1 | 2.36 | 0.41 |
| 1:3:69:GLU:O | 1:3:70:ALA:C | 2.57 | 0.41 |
| 1:3:129:LYS:HA | 1:3:129:LYS:HD2 | 1.67 | 0.41 |
| 1:5:234:ARG:O | 1:5:235:GLU:C | 2.58 | 0.41 |
| 2:6:182:PHE:CD2 | 2:6:187:GLN:HG3 | 2.56 | 0.41 |
| 2:6:260:VAL:HG22 | 2:6:293:VAL:CG2 | 2.51 | 0.41 |
| 1:A:27:LEU:HD22 | 1:A:28:THR:O | 2.20 | 0.41 |
| 1:A:142:VAL:HA | 1:A:163:THR:CG2 | 2.51 | 0.41 |
| 1:E:132:TYR:CD1 | 1:E:132:TYR:N | 2.88 | 0.41 |
| 2:F:178:VAL:HG12 | 2:F:180:PHE:CE1 | 2.56 | 0.41 |
| 2:F:272:GLY:O | 2:F:273:ALA:C | 2.60 | 0.41 |
| 2:F:308:LEU:HA | 2:F:308:LEU:HD23 | 1.84 | 0.41 |
| 1:K:106:LEU:HD23 | 1:K:106:LEU:HA | 1.88 | 0.41 |
| 1:K:112:ARG:HA | 1:K:112:ARG:HD3 | 1.94 | 0.41 |
| 2:L:185:GLU:O | 2:L:185:GLU:HG2 | 2.20 | 0.41 |
| 2:N:79:GLU:HG2 | 2:N:80:PHE:N | 2.35 | 0.41 |
| 1:O:53:TYR:CD2 | 1:O:62:CYS:HB2 | 2.56 | 0.41 |
| 1:O:142:VAL:HB | 1:O:143:PRO:HD3 | 2.03 | 0.41 |
| 2:T:218:HIS:HB3 | 2:T:316:VAL:HG23 | 2.03 | 0.41 |
| 2:T:268:GLN:O | 2:T:269:PHE:CB | 2.69 | 0.41 |
| 1:U:50:ASP:HB2 | 1:U:64:LEU:CD1 | 2.51 | 0.41 |
| 2:X:279:ILE:HD12 | 2:X:279:ILE:HG23 | 1.82 | 0.41 |
| 1:Y:29:ARG:CG | 1:Y:300:LEU:O | 2.69 | 0.41 |
| 1:Y:196:ASN:OD1 | 1:Y:196:ASN:N | 2.48 | 0.41 |
| 1:1:41:THR:HG21 | 1:1:96:PHE:CZ | 2.56 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:4:278:ARG:NH1 | 2:4:278:ARG:HG3 | 2.36 | 0.41 |
| 1:A:103:ARG:HG2 | 1:A:103:ARG:HH11 | 1.86 | 0.40 |
| 2:D:51:ARG:O | 2:D:52:ILE:HD13 | 2.21 | 0.40 |
| 1:G:196:ASN:ND2 | 1:G:259:ARG:CD | 2.84 | 0.40 |
| 1:G:197:ARG:HG3 | 1:G:258:TYR:HD2 | 1.85 | 0.40 |
| 2:H:207:ILE:HG13 | 2:H:258:HIS:HB2 | 2.02 | 0.40 |
| 1:I:135:ASN:N | 1:I:135:ASN:ND2 | 2.69 | 0.40 |
| 2:P:249:ILE:HD13 | 2:P:249:ILE:HG21 | 1.89 | 0.40 |
| 2:T:304:TYR:O | 2:T:305:ALA:C | 2.59 | 0.40 |
| 1:U:206:ARG:HH11 | 1:U:206:ARG:HB3 | 1.86 | 0.40 |
| 1:W:4:ASP:HA | 1:W:300:LEU:HD21 | 2.02 | 0.40 |
| 1:W:45:MET:CE | 1:W:102:VAL:HA | 2.51 | 0.40 |
| 1:W:126:MET:HB2 | 1:W:126:MET:HE3 | 1.82 | 0.40 |
| 1:W:196:ASN:ND2 | 1:W:259:ARG:NE | 2.68 | 0.40 |
| 1:Y:29:ARG:HB2 | 1:Y:300:LEU:HD22 | 2.03 | 0.40 |
| 1:3:27:LEU:HG | 1:3:231:LEU:HD21 | 2.02 | 0.40 |
| 1:3:155:ASN:O | 1:3:156:GLY:C | 2.58 | 0.40 |
| 1:3:197:ARG:HD2 | 1:3:257:THR:O | 2.22 | 0.40 |
| 1:3:341:SER:HB2 | 2:4:101:TYR:CZ | 2.56 | 0.40 |
| 2:4:26:LEU:HD23 | 2:4:78:CYS:HA | 2.03 | 0.40 |
| 2:4:237:ASN:C | 2:4:237:ASN:ND2 | 2.74 | 0.40 |
| 2:6:258:HIS:CD2 | 2:6:327:LEU:HD23 | 2.56 | 0.40 |
| 1:A:47:LEU:HD23 | 1:A:47:LEU:HA | 1.89 | 0.40 |
| 1:A:77:ALA:CB | 1:A:234:ARG:HG3 | 2.51 | 0.40 |
| 1:A:95:THR:CG2 | 1:A:100:LEU:HD22 | 2.52 | 0.40 |
| 2:B:307:ILE:HG23 | 2:B:308:LEU:N | 2.37 | 0.40 |
| 1:E:341:SER:HB2 | 2:F:101:TYR:CE1 | 2.56 | 0.40 |
| 1:M:351:ALA:O | 2:P:295:VAL:HG13 | 2.22 | 0.40 |
| 1:O:17:LEU:HD23 | 1:O:17:LEU:HA | 1.86 | 0.40 |
| 1:O:46:GLU:HA | 1:O:46:GLU:OE1 | 2.22 | 0.40 |
| 1:Q:204:VAL:HB | 1:Q:211:THR:CG2 | 2.51 | 0.40 |
| 1:Q:318:GLU:HG2 | 2:2:287:PHE:CE2 | 2.57 | 0.40 |
| 2:R:19:ARG:NH1 | 2:R:19:ARG:HG2 | 2.36 | 0.40 |
| 2:R:150:SER:HB2 | 2:R:180:PHE:HB2 | 2.03 | 0.40 |
| 2:V:157:ILE:O | 2:V:161:ILE:HG13 | 2.20 | 0.40 |
| 1:Y:33:LEU:HD12 | 1:Y:295:MET:HE1 | 2.03 | 0.40 |
| 1:Y:162:LEU:CD1 | 1:Y:190:ILE:HD12 | 2.52 | 0.40 |
| 1:1:167:ASP:HB3 | 1:1:195:ASN:HA | 2.03 | 0.40 |
| 2:2:118:ASN:ND2 | 2:2:132:PHE:H | 2.19 | 0.40 |
| 2:2:237:ASN:C | 2:2:237:ASN:ND2 | 2.74 | 0.40 |
| 2:2:279:ILE:HD13 | 2:2:279:ILE:HA | 1.83 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:4:259:LEU:HD22 | 2:4:279:ILE:HG13 | 2.02 | 0.40 |
| 1:5:45:MET:HE1 | 1:5:105:ILE:CD1 | 2.51 | 0.40 |
| 1:5:63:HIS:HB3 | 1:5:90:ARG:HG3 | 2.03 | 0.40 |
| 2:B:39:VAL:HG11 | 2:B:115:ARG:NH2 | 2.37 | 0.40 |
| 2:B:95:ASN:ND2 | 2:D:87:MET:HE1 | 2.37 | 0.40 |
| 1:E:109:LEU:HA | 1:E:109:LEU:HD23 | 1.60 | 0.40 |
| 2:H:196:GLY:O | 2:H:245:ASP:HB2 | 2.21 | 0.40 |
| 1:I:109:LEU:HA | 1:I:109:LEU:HD23 | 1.85 | 0.40 |
| 1:I:109:LEU:CD2 | 1:I:123:SER:HB2 | 2.50 | 0.40 |
| 2:J:118:ASN:N | 2:J:171:GLU:O | 2.49 | 0.40 |
| 2:J:172:ASN:ND2 | 2:J:174:LEU:N | 2.69 | 0.40 |
| 2:L:286:ASN:H | 2:L:286:ASN:HD22 | 1.68 | 0.40 |
| 1:O:113:LYS:HB2 | 1:O:113:LYS:HE2 | 1.92 | 0.40 |
| 1:O:138:VAL:HG13 | 1:O:169:ALA:HB2 | 2.04 | 0.40 |
| 1:O:231:LEU:O | 1:O:232:CYS:C | 2.56 | 0.40 |
| 1:O:234:ARG:HE | 1:O:238:ARG:HH22 | 1.69 | 0.40 |
| 2:P:118:ASN:ND2 | 2:P:131:CYS:HA | 2.36 | 0.40 |
| 2:P:136:TYR:C | 2:P:138:HIS:H | 2.25 | 0.40 |
| 2:R:151:GLU:OE1 | 2:R:183:PRO:HG3 | 2.21 | 0.40 |
| 1:S:34:LYS:HD2 | 1:S:38:MET:HE2 | 2.02 | 0.40 |
| 2:V:74:LEU:HD12 | 2:V:74:LEU:HA | 1.83 | 0.40 |
| 2:V:172:ASN:ND2 | 2:V:172:ASN:C | 2.74 | 0.40 |
| 1:W:81:PRO:HA | 1:W:98:ARG:NH2 | 2.36 | 0.40 |
| 2:Z:260:VAL:HG22 | 2:Z:293:VAL:HG23 | 2.03 | 0.40 |
| 2:6:157:ILE:HG23 | 2:6:158:LYS:N | 2.37 | 0.40 |
| 1:A:285:SER:HA | 1:A:290:LEU:HD21 | 2.04 | 0.40 |
| 1:C:46:GLU:HA | 1:C:46:GLU:OE1 | 2.21 | 0.40 |
| 1:C:86:ILE:O | 1:C:86:ILE:HG23 | 2.21 | 0.40 |
| 2:D:202:ARG:O | 2:D:234:GLU:HA | 2.20 | 0.40 |
| 1:E:108:GLU:OE2 | 1:E:119:GLY:CA | 2.69 | 0.40 |
| 1:E:184:LEU:HD12 | 1:E:184:LEU:HA | 1.91 | 0.40 |
| 1:E:341:SER:HB2 | 2:F:101:TYR:CZ | 2.56 | 0.40 |
| 1:G:39:MET:HG2 | 1:G:73:VAL:HG21 | 2.04 | 0.40 |
| 2:J:278:ARG:NH1 | 2:J:278:ARG:HG3 | 2.36 | 0.40 |
| 1:K:219:PHE:CD1 | 1:K:220:ILE:HG13 | 2.56 | 0.40 |
| 1:M:258:TYR:CD1 | 1:M:258:TYR:C | 2.95 | 0.40 |
| 2:P:93:VAL:O | 2:P:97:ALA:HB3 | 2.21 | 0.40 |
| 2:R:307:ILE:CG2 | 2:R:308:LEU:N | 2.84 | 0.40 |
| 1:U:4:ASP:HA | 1:U:300:LEU:HD21 | 2.03 | 0.40 |
| 1:U:162:LEU:HD12 | 1:U:190:ILE:HD12 | 2.03 | 0.40 |
| 1:U:164:LEU:HG | 1:U:192:ILE:HB | 2.03 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:V:43:LEU:CD1 | 2:V:43:LEU:H | 2.34 | 0.40 |
| 2:V:302:MET:HA | 2:V:303:PRO:HD2 | 1.96 | 0.40 |
| 1:W:132:TYR:CD1 | 1:W:148:ILE:HD13 | 2.57 | 0.40 |
| 1:W:315:LYS:HB2 | 1:W:315:LYS:HZ3 | 1.86 | 0.40 |
| 1:Y:86:ILE:HG12 | 1:Y:87:THR:N | 2.37 | 0.40 |
| 1:Y:225:VAL:HG12 | 1:Y:226:ASP:N | 2.36 | 0.40 |
| 2:Z:278:ARG:HG3 | 2:Z:278:ARG:HH11 | 1.86 | 0.40 |
| 1:1:296:VAL:HG12 | 1:1:297:ASN:HD22 | 1.84 | 0.40 |
| 1:5:10:LYS:HG2 | 1:5:11:LYS:H | 1.84 | 0.40 |
| 2:6:172:ASN:HD22 | 2:6:174:LEU:N | 2.18 | 0.40 |
| 2:B:93:VAL:HG22 | 2:B:114:PHE:CZ | 2.57 | 0.40 |
| 2:F:84:ASN:ND2 | 2:F:128:HIS:HA | 2.36 | 0.40 |
| 1:G:78:GLY:HA3 | 1:G:237:THR:CG2 | 2.52 | 0.40 |
| 2:H:242:ARG:HA | 2:H:243:PRO:HA | 1.93 | 0.40 |
| 2:J:5:VAL:HB | 2:J:175:MET:O | 2.22 | 0.40 |
| 1:O:132:TYR:CD1 | 1:O:148:ILE:HD13 | 2.55 | 0.40 |
| 1:O:141:GLN:OE1 | 1:O:141:GLN:N | 2.52 | 0.40 |
| 2:R:222:ALA:HB1 | 2:R:320:ILE:HG13 | 2.03 | 0.40 |
| 1:S:341:SER:HB3 | 2:T:101:TYR:CZ | 2.57 | 0.40 |
| 2:T:234:GLU:OE1 | 2:T:255:LYS:NZ | 2.47 | 0.40 |
| 1:U:52:LEU:HD23 | 1:U:52:LEU:HA | 1.94 | 0.40 |
| 1:U:142:VAL:HB | 1:U:143:PRO:HD3 | 2.03 | 0.40 |
| 2:V:121:SER:HB3 | 2:V:124:VAL:CG2 | 2.50 | 0.40 |
| 2:V:301:PRO:HB3 | 2:X:99:LYS:HG2 | 2.04 | 0.40 |
| 1:W:57:ILE:N | 1:W:57:ILE:HD13 | 2.35 | 0.40 |
| 1:1:53:TYR:C | 1:1:55:GLN:N | 2.74 | 0.40 |
| 2:2:327:LEU:HD23 | 2:2:327:LEU:HA | 1.87 | 0.40 |
| 1:3:1:PHE:H | 1:3:1:PHE:HD2 | 1.69 | 0.40 |
| 1:3:61:PHE:HD2 | 1:3:124:MET:CE | 2.35 | 0.40 |
| 1:3:135:ASN:ND2 | 1:3:135:ASN:N | 2.70 | 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 X-ray entries followed by that with respect to entries of similar resolution.

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles |
|---|---|---|---|---|---|---|
| 1 | 1 | 329/382 (86%) | 295 (90%) | 25 (8%) | 9 (3%) | 5 25 |
| 1 | 3 | 336/382 (88%) | 305 (91%) | 25 (7%) | 6 (2%) | 8 35 |
| 1 | 5 | 341/382 (89%) | 306 (90%) | 22 (6%) | 13 (4%) | 3 17 |
| 1 | A | 336/382 (88%) | 311 (93%) | 20 (6%) | 5 (2%) | 10 40 |
| 1 | C | 336/382 (88%) | 303 (90%) | 28 (8%) | 5 (2%) | 10 40 |
| 1 | E | 343/382 (90%) | 313 (91%) | 23 (7%) | 7 (2%) | 7 32 |
| 1 | G | 340/382 (89%) | 305 (90%) | 29 (8%) | 6 (2%) | 8 35 |
| 1 | I | 338/382 (88%) | 309 (91%) | 24 (7%) | 5 (2%) | 10 40 |
| 1 | K | 341/382 (89%) | 304 (89%) | 31 (9%) | 6 (2%) | 8 35 |
| 1 | M | 343/382 (90%) | 311 (91%) | 24 (7%) | 8 (2%) | 6 29 |
| 1 | O | 326/382 (85%) | 286 (88%) | 32 (10%) | 8 (2%) | 5 26 |
| 1 | Q | 338/382 (88%) | 314 (93%) | 19 (6%) | 5 (2%) | 10 40 |
| 1 | S | 334/382 (87%) | 301 (90%) | 25 (8%) | 8 (2%) | 6 28 |
| 1 | U | 342/382 (90%) | 313 (92%) | 23 (7%) | 6 (2%) | 8 35 |
| 1 | W | 339/382 (89%) | 312 (92%) | 22 (6%) | 5 (2%) | 10 40 |
| 1 | Y | 343/382 (90%) | 319 (93%) | 19 (6%) | 5 (2%) | 10 40 |
| 2 | 2 | 327/329 (99%) | 297 (91%) | 26 (8%) | 4 (1%) | 13 46 |
| 2 | 4 | 327/329 (99%) | 304 (93%) | 23 (7%) | 0 | 100 100 |
| 2 | 6 | 327/329 (99%) | 300 (92%) | 24 (7%) | 3 (1%) | 17 53 |
| 2 | B | 327/329 (99%) | 307 (94%) | 19 (6%) | 1 (0%) | 41 75 |
| 2 | D | 327/329 (99%) | 306 (94%) | 19 (6%) | 2 (1%) | 25 62 |
| 2 | F | 327/329 (99%) | 304 (93%) | 22 (7%) | 1 (0%) | 41 75 |
| 2 | H | 327/329 (99%) | 300 (92%) | 24 (7%) | 3 (1%) | 17 53 |
| 2 | J | 327/329 (99%) | 302 (92%) | 25 (8%) | 0 | 100 100 |
| 2 | L | 327/329 (99%) | 302 (92%) | 24 (7%) | 1 (0%) | 41 75 |
| 2 | N | 327/329 (99%) | 307 (94%) | 20 (6%) | 0 | 100 100 |
| 2 | P | 327/329 (99%) | 292 (89%) | 30 (9%) | 5 (2%) | 10 40 |
| 2 | R | 327/329 (99%) | 310 (95%) | 16 (5%) | 1 (0%) | 41 75 |
| 2 | T | 327/329 (99%) | 308 (94%) | 16 (5%) | 3 (1%) | 17 53 |
| 2 | V | 327/329 (99%) | 294 (90%) | 30 (9%) | 3 (1%) | 17 53 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles |
|---|---|---|---|---|---|---|
| 2 | X | 327/329 (99%) | 294 (90%) | 30 (9%) | 3 (1%) | 17 53 |
| 2 | Z | 327/329 (99%) | 306 (94%) | 20 (6%) | 1 (0%) | 41 75 |
| All | All | 10637/11376 (94%) | 9740 (92%) | 759 (7%) | 138 (1%) | 12 43 |

All (138) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 2 | ALA |
| 1 | A | 285 | SER |
| 1 | E | 268 | PRO |
| 1 | I | 2 | ALA |
| 1 | K | 274 | THR |
| 1 | K | 275 | ARG |
| 1 | M | 268 | PRO |
| 1 | M | 270 | VAL |
| 1 | M | 271 | ALA |
| 1 | O | 230 | ILE |
| 1 | O | 281 | VAL |
| 1 | O | 285 | SER |
| 2 | P | 43 | LEU |
| 1 | Q | 285 | SER |
| 1 | S | 275 | ARG |
| 2 | T | 188 | SER |
| 1 | U | 2 | ALA |
| 1 | U | 216 | ARG |
| 1 | W | 2 | ALA |
| 1 | Y | 268 | PRO |
| 1 | 1 | 2 | ALA |
| 1 | 1 | 4 | ASP |
| 1 | 1 | 281 | VAL |
| 1 | 1 | 283 | SER |
| 2 | 2 | 43 | LEU |
| 1 | 3 | 2 | ALA |
| 1 | 3 | 285 | SER |
| 1 | 5 | 235 | GLU |
| 1 | 5 | 280 | GLU |
| 1 | 5 | 282 | ARG |
| 1 | 5 | 283 | SER |
| 1 | C | 285 | SER |
| 1 | C | 297 | ASN |
| 2 | D | 137 | GLY |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | D | 188 | SER |
| 1 | G | 29 | ARG |
| 1 | G | 275 | ARG |
| 2 | H | 317 | LYS |
| 1 | I | 205 | GLU |
| 1 | I | 285 | SER |
| 1 | K | 218 | ASP |
| 1 | K | 230 | ILE |
| 1 | M | 2 | ALA |
| 1 | Q | 2 | ALA |
| 1 | Q | 275 | ARG |
| 1 | S | 285 | SER |
| 2 | T | 315 | GLN |
| 1 | U | 130 | ASN |
| 1 | U | 235 | GLU |
| 1 | W | 272 | TYR |
| 1 | Y | 270 | VAL |
| 1 | 5 | 88 | ALA |
| 1 | 5 | 218 | ASP |
| 1 | 5 | 236 | ALA |
| 1 | A | 129 | LYS |
| 1 | A | 156 | GLY |
| 1 | E | 88 | ALA |
| 1 | E | 97 | THR |
| 1 | G | 273 | ARG |
| 1 | K | 88 | ALA |
| 1 | K | 271 | ALA |
| 1 | M | 88 | ALA |
| 1 | O | 237 | THR |
| 2 | P | 31 | ALA |
| 1 | Q | 129 | LYS |
| 1 | S | 88 | ALA |
| 1 | S | 297 | ASN |
| 2 | V | 273 | ALA |
| 1 | W | 88 | ALA |
| 1 | W | 218 | ASP |
| 2 | X | 49 | ASP |
| 1 | 1 | 133 | GLY |
| 1 | 1 | 230 | ILE |
| 1 | 5 | 216 | ARG |
| 1 | 5 | 258 | TYR |
| 1 | 5 | 271 | ALA |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | 6 | 181 | GLU |
| 2 | 6 | 183 | PRO |
| 1 | C | 170 | ALA |
| 1 | C | 218 | ASP |
| 1 | E | 218 | ASP |
| 2 | H | 31 | ALA |
| 2 | L | 31 | ALA |
| 1 | M | 4 | ASP |
| 1 | M | 218 | ASP |
| 1 | O | 4 | ASP |
| 1 | O | 218 | ASP |
| 1 | O | 338 | HIS |
| 2 | P | 32 | GLN |
| 2 | P | 317 | LYS |
| 1 | S | 29 | ARG |
| 1 | S | 218 | ASP |
| 1 | S | 276 | GLU |
| 1 | S | 281 | VAL |
| 2 | T | 228 | LYS |
| 1 | U | 218 | ASP |
| 1 | W | 285 | SER |
| 2 | X | 31 | ALA |
| 1 | Y | 218 | ASP |
| 1 | 1 | 218 | ASP |
| 1 | 3 | 218 | ASP |
| 1 | 3 | 275 | ARG |
| 1 | 5 | 233 | VAL |
| 1 | 5 | 269 | GLY |
| 1 | 5 | 281 | VAL |
| 1 | A | 218 | ASP |
| 2 | B | 69 | ALA |
| 1 | E | 216 | ARG |
| 1 | G | 62 | CYS |
| 1 | G | 218 | ASP |
| 1 | I | 88 | ALA |
| 1 | I | 218 | ASP |
| 1 | Q | 88 | ALA |
| 1 | U | 88 | ALA |
| 2 | V | 213 | SER |
| 1 | Y | 140 | ALA |
| 1 | 1 | 22 | PRO |
| 1 | 3 | 276 | GLU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | 6 | 31 | ALA |
| 1 | E | 230 | ILE |
| 1 | G | 297 | ASN |
| 1 | O | 2 | ALA |
| 2 | R | 31 | ALA |
| 2 | V | 267 | PRO |
| 1 | Y | 156 | GLY |
| 1 | 1 | 296 | VAL |
| 2 | 2 | 45 | LYS |
| 2 | 2 | 267 | PRO |
| 1 | 3 | 156 | GLY |
| 2 | P | 267 | PRO |
| 1 | C | 329 | GLU |
| 1 | E | 156 | GLY |
| 1 | M | 230 | ILE |
| 2 | X | 267 | PRO |
| 2 | Z | 267 | PRO |
| 2 | 2 | 265 | GLY |
| 2 | H | 265 | GLY |
| 2 | F | 243 | PRO |

### 5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles |
|---|---|---|---|---|---|
| 1 | 1 | 271/310 (87%) | 243 (90%) | 28 (10%) | 7 26 |
| 1 | 3 | 278/310 (90%) | 250 (90%) | 28 (10%) | 7 27 |
| 1 | 5 | 281/310 (91%) | 254 (90%) | 27 (10%) | 8 30 |
| 1 | A | 278/310 (90%) | 250 (90%) | 28 (10%) | 7 27 |
| 1 | C | 278/310 (90%) | 249 (90%) | 29 (10%) | 7 26 |
| 1 | E | 282/310 (91%) | 258 (92%) | 24 (8%) | 10 36 |
| 1 | G | 281/310 (91%) | 255 (91%) | 26 (9%) | 9 32 |
| 1 | I | 280/310 (90%) | 255 (91%) | 25 (9%) | 9 34 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles |
|---|---|---|---|---|---|
| 1 | K | 281/310 (91%) | 258 (92%) | 23 (8%) | 11 38 |
| 1 | M | 282/310 (91%) | 251 (89%) | 31 (11%) | 6 24 |
| 1 | O | 268/310 (86%) | 239 (89%) | 29 (11%) | 6 24 |
| 1 | Q | 280/310 (90%) | 249 (89%) | 31 (11%) | 6 23 |
| 1 | S | 277/310 (89%) | 249 (90%) | 28 (10%) | 7 27 |
| 1 | U | 282/310 (91%) | 251 (89%) | 31 (11%) | 6 24 |
| 1 | W | 280/310 (90%) | 248 (89%) | 32 (11%) | 5 22 |
| 1 | Y | 282/310 (91%) | 253 (90%) | 29 (10%) | 7 26 |
| 2 | 2 | 268/268 (100%) | 252 (94%) | 16 (6%) | 19 51 |
| 2 | 4 | 268/268 (100%) | 253 (94%) | 15 (6%) | 21 54 |
| 2 | 6 | 268/268 (100%) | 251 (94%) | 17 (6%) | 18 49 |
| 2 | B | 268/268 (100%) | 253 (94%) | 15 (6%) | 21 54 |
| 2 | D | 268/268 (100%) | 249 (93%) | 19 (7%) | 14 44 |
| 2 | F | 268/268 (100%) | 251 (94%) | 17 (6%) | 18 49 |
| 2 | H | 268/268 (100%) | 244 (91%) | 24 (9%) | 9 33 |
| 2 | J | 268/268 (100%) | 247 (92%) | 21 (8%) | 12 40 |
| 2 | L | 268/268 (100%) | 251 (94%) | 17 (6%) | 18 49 |
| 2 | N | 268/268 (100%) | 245 (91%) | 23 (9%) | 10 36 |
| 2 | P | 268/268 (100%) | 248 (92%) | 20 (8%) | 13 42 |
| 2 | R | 268/268 (100%) | 245 (91%) | 23 (9%) | 10 36 |
| 2 | T | 268/268 (100%) | 247 (92%) | 21 (8%) | 12 40 |
| 2 | V | 268/268 (100%) | 249 (93%) | 19 (7%) | 14 44 |
| 2 | X | 268/268 (100%) | 245 (91%) | 23 (9%) | 10 36 |
| 2 | Z | 268/268 (100%) | 251 (94%) | 17 (6%) | 18 49 |
| All | All | 8749/9248 (95%) | 7993 (91%) | 756 (9%) | 10 36 |

All (756) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 10 | LYS |
| 1 | A | 11 | LYS |
| 1 | A | 16 | ARG |
| 1 | A | 18 | GLU |
| 1 | A | 23 | VAL |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 27 | LEU |
| 1 | A | 28 | THR |
| 1 | A | 29 | ARG |
| 1 | A | 33 | LEU |
| 1 | A | 54 | LYS |
| 1 | A | 57 | ILE |
| 1 | A | 59 | ARG |
| 1 | A | 75 | LEU |
| 1 | A | 103 | ARG |
| 1 | A | 104 | GLU |
| 1 | A | 113 | LYS |
| 1 | A | 118 | LYS |
| 1 | A | 155 | ASN |
| 1 | A | 197 | ARG |
| 1 | A | 223 | LEU |
| 1 | A | 230 | ILE |
| 1 | A | 255 | LEU |
| 1 | A | 278 | ILE |
| 1 | A | 284 | LYS |
| 1 | A | 289 | MET |
| 1 | A | 307 | LYS |
| 1 | A | 315 | LYS |
| 1 | A | 322 | GLN |
| 2 | B | 1 | LEU |
| 2 | B | 11 | GLN |
| 2 | B | 74 | LEU |
| 2 | B | 81 | MET |
| 2 | B | 159 | SER |
| 2 | B | 162 | ARG |
| 2 | B | 185 | GLU |
| 2 | B | 192 | LEU |
| 2 | B | 197 | LYS |
| 2 | B | 229 | GLU |
| 2 | B | 237 | ASN |
| 2 | B | 279 | ILE |
| 2 | B | 306 | LYS |
| 2 | B | 317 | LYS |
| 2 | B | 328 | ASN |
| 1 | C | 1 | PHE |
| 1 | C | 9 | ILE |
| 1 | C | 10 | LYS |
| 1 | C | 18 | GLU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | C | 24 | THR |
| 1 | C | 27 | LEU |
| 1 | C | 28 | THR |
| 1 | C | 29 | ARG |
| 1 | C | 30 | GLU |
| 1 | C | 31 | ASP |
| 1 | C | 40 | GLN |
| 1 | C | 75 | LEU |
| 1 | C | 98 | ARG |
| 1 | C | 103 | ARG |
| 1 | C | 129 | LYS |
| 1 | C | 206 | ARG |
| 1 | C | 223 | LEU |
| 1 | C | 230 | ILE |
| 1 | C | 252 | LEU |
| 1 | C | 255 | LEU |
| 1 | C | 280 | GLU |
| 1 | C | 307 | LYS |
| 1 | C | 309 | ILE |
| 1 | C | 314 | ARG |
| 1 | C | 315 | LYS |
| 1 | C | 316 | GLU |
| 1 | C | 322 | GLN |
| 1 | C | 333 | GLU |
| 1 | C | 353 | GLN |
| 2 | D | 1 | LEU |
| 2 | D | 2 | GLN |
| 2 | D | 3 | VAL |
| 2 | D | 26 | LEU |
| 2 | D | 32 | GLN |
| 2 | D | 33 | TYR |
| 2 | D | 39 | VAL |
| 2 | D | 43 | LEU |
| 2 | D | 74 | LEU |
| 2 | D | 81 | MET |
| 2 | D | 172 | ASN |
| 2 | D | 185 | GLU |
| 2 | D | 189 | LYS |
| 2 | D | 197 | LYS |
| 2 | D | 237 | ASN |
| 2 | D | 239 | ARG |
| 2 | D | 288 | LEU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | D | 313 | ILE |
| 2 | D | 317 | LYS |
| 1 | E | 10 | LYS |
| 1 | E | 11 | LYS |
| 1 | E | 23 | VAL |
| 1 | E | 27 | LEU |
| 1 | E | 28 | THR |
| 1 | E | 29 | ARG |
| 1 | E | 30 | GLU |
| 1 | E | 31 | ASP |
| 1 | E | 45 | MET |
| 1 | E | 57 | ILE |
| 1 | E | 103 | ARG |
| 1 | E | 113 | LYS |
| 1 | E | 216 | ARG |
| 1 | E | 223 | LEU |
| 1 | E | 238 | ARG |
| 1 | E | 246 | SER |
| 1 | E | 255 | LEU |
| 1 | E | 272 | TYR |
| 1 | E | 273 | ARG |
| 1 | E | 279 | GLN |
| 1 | E | 295 | MET |
| 1 | E | 315 | LYS |
| 1 | E | 335 | LEU |
| 1 | E | 361 | SER |
| 2 | F | 1 | LEU |
| 2 | F | 3 | VAL |
| 2 | F | 26 | LEU |
| 2 | F | 34 | ASP |
| 2 | F | 74 | LEU |
| 2 | F | 81 | MET |
| 2 | F | 82 | THR |
| 2 | F | 91 | ASP |
| 2 | F | 107 | LEU |
| 2 | F | 182 | PHE |
| 2 | F | 192 | LEU |
| 2 | F | 278 | ARG |
| 2 | F | 279 | ILE |
| 2 | F | 288 | LEU |
| 2 | F | 306 | LYS |
| 2 | F | 317 | LYS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | F | 328 | ASN |
| 1 | G | 23 | VAL |
| 1 | G | 27 | LEU |
| 1 | G | 28 | THR |
| 1 | G | 29 | ARG |
| 1 | G | 30 | GLU |
| 1 | G | 72 | CYS |
| 1 | G | 75 | LEU |
| 1 | G | 97 | THR |
| 1 | G | 98 | ARG |
| 1 | G | 104 | GLU |
| 1 | G | 118 | LYS |
| 1 | G | 129 | LYS |
| 1 | G | 158 | ASP |
| 1 | G | 206 | ARG |
| 1 | G | 255 | LEU |
| 1 | G | 270 | VAL |
| 1 | G | 272 | TYR |
| 1 | G | 275 | ARG |
| 1 | G | 276 | GLU |
| 1 | G | 284 | LYS |
| 1 | G | 289 | MET |
| 1 | G | 314 | ARG |
| 1 | G | 315 | LYS |
| 1 | G | 322 | GLN |
| 1 | G | 335 | LEU |
| 1 | G | 347 | GLU |
| 2 | H | 1 | LEU |
| 2 | H | 3 | VAL |
| 2 | H | 21 | GLU |
| 2 | H | 43 | LEU |
| 2 | H | 45 | LYS |
| 2 | H | 49 | ASP |
| 2 | H | 74 | LEU |
| 2 | H | 107 | LEU |
| 2 | H | 162 | ARG |
| 2 | H | 172 | ASN |
| 2 | H | 182 | PHE |
| 2 | H | 197 | LYS |
| 2 | H | 227 | SER |
| 2 | H | 236 | ILE |
| 2 | H | 237 | ASN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | H | 278 | ARG |
| 2 | H | 279 | ILE |
| 2 | H | 288 | LEU |
| 2 | H | 306 | LYS |
| 2 | H | 307 | ILE |
| 2 | H | 313 | ILE |
| 2 | H | 316 | VAL |
| 2 | H | 317 | LYS |
| 2 | H | 328 | ASN |
| 1 | I | 26 | VAL |
| 1 | I | 27 | LEU |
| 1 | I | 29 | ARG |
| 1 | I | 59 | ARG |
| 1 | I | 75 | LEU |
| 1 | I | 80 | ASN |
| 1 | I | 85 | LEU |
| 1 | I | 98 | ARG |
| 1 | I | 104 | GLU |
| 1 | I | 118 | LYS |
| 1 | I | 135 | ASN |
| 1 | I | 186 | LYS |
| 1 | I | 205 | GLU |
| 1 | I | 210 | SER |
| 1 | I | 230 | ILE |
| 1 | I | 232 | CYS |
| 1 | I | 255 | LEU |
| 1 | I | 279 | GLN |
| 1 | I | 283 | SER |
| 1 | I | 289 | MET |
| 1 | I | 307 | LYS |
| 1 | I | 315 | LYS |
| 1 | I | 322 | GLN |
| 1 | I | 341 | SER |
| 1 | I | 342 | SER |
| 2 | J | 1 | LEU |
| 2 | J | 2 | GLN |
| 2 | J | 33 | TYR |
| 2 | J | 34 | ASP |
| 2 | J | 74 | LEU |
| 2 | J | 81 | MET |
| 2 | J | 173 | GLU |
| 2 | J | 182 | PHE |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | J | 188 | SER |
| 2 | J | 189 | LYS |
| 2 | J | 192 | LEU |
| 2 | J | 227 | SER |
| 2 | J | 228 | LYS |
| 2 | J | 229 | GLU |
| 2 | J | 237 | ASN |
| 2 | J | 263 | GLU |
| 2 | J | 279 | ILE |
| 2 | J | 306 | LYS |
| 2 | J | 307 | ILE |
| 2 | J | 317 | LYS |
| 2 | J | 328 | ASN |
| 1 | K | 10 | LYS |
| 1 | K | 18 | GLU |
| 1 | K | 27 | LEU |
| 1 | K | 29 | ARG |
| 1 | K | 30 | GLU |
| 1 | K | 54 | LYS |
| 1 | K | 75 | LEU |
| 1 | K | 98 | ARG |
| 1 | K | 103 | ARG |
| 1 | K | 196 | ASN |
| 1 | K | 210 | SER |
| 1 | K | 219 | PHE |
| 1 | K | 223 | LEU |
| 1 | K | 232 | CYS |
| 1 | K | 252 | LEU |
| 1 | K | 255 | LEU |
| 1 | K | 275 | ARG |
| 1 | K | 279 | GLN |
| 1 | K | 315 | LYS |
| 1 | K | 316 | GLU |
| 1 | K | 322 | GLN |
| 1 | K | 335 | LEU |
| 1 | K | 353 | GLN |
| 2 | L | 1 | LEU |
| 2 | L | 2 | GLN |
| 2 | L | 32 | GLN |
| 2 | L | 33 | TYR |
| 2 | L | 40 | SER |
| 2 | L | 43 | LEU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | L | 81 | MET |
| 2 | L | 142 | LEU |
| 2 | L | 162 | ARG |
| 2 | L | 172 | ASN |
| 2 | L | 182 | PHE |
| 2 | L | 185 | GLU |
| 2 | L | 189 | LYS |
| 2 | L | 237 | ASN |
| 2 | L | 279 | ILE |
| 2 | L | 288 | LEU |
| 2 | L | 317 | LYS |
| 1 | M | 3 | ASN |
| 1 | M | 10 | LYS |
| 1 | M | 19 | GLU |
| 1 | M | 23 | VAL |
| 1 | M | 27 | LEU |
| 1 | M | 28 | THR |
| 1 | M | 30 | GLU |
| 1 | M | 33 | LEU |
| 1 | M | 100 | LEU |
| 1 | M | 103 | ARG |
| 1 | M | 118 | LYS |
| 1 | M | 158 | ASP |
| 1 | M | 186 | LYS |
| 1 | M | 196 | ASN |
| 1 | M | 223 | LEU |
| 1 | M | 230 | ILE |
| 1 | M | 235 | GLU |
| 1 | M | 238 | ARG |
| 1 | M | 252 | LEU |
| 1 | M | 255 | LEU |
| 1 | M | 270 | VAL |
| 1 | M | 272 | TYR |
| 1 | M | 275 | ARG |
| 1 | M | 279 | GLN |
| 1 | M | 282 | ARG |
| 1 | M | 284 | LYS |
| 1 | M | 315 | LYS |
| 1 | M | 322 | GLN |
| 1 | M | 333 | GLU |
| 1 | M | 335 | LEU |
| 1 | M | 360 | VAL |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | N | 1 | LEU |
| 2 | N | 2 | GLN |
| 2 | N | 3 | VAL |
| 2 | N | 21 | GLU |
| 2 | N | 26 | LEU |
| 2 | N | 32 | GLN |
| 2 | N | 34 | ASP |
| 2 | N | 45 | LYS |
| 2 | N | 60 | MET |
| 2 | N | 74 | LEU |
| 2 | N | 81 | MET |
| 2 | N | 94 | ILE |
| 2 | N | 159 | SER |
| 2 | N | 162 | ARG |
| 2 | N | 172 | ASN |
| 2 | N | 182 | PHE |
| 2 | N | 188 | SER |
| 2 | N | 192 | LEU |
| 2 | N | 237 | ASN |
| 2 | N | 244 | MET |
| 2 | N | 278 | ARG |
| 2 | N | 279 | ILE |
| 2 | N | 306 | LYS |
| 1 | O | 1 | PHE |
| 1 | O | 3 | ASN |
| 1 | O | 10 | LYS |
| 1 | O | 11 | LYS |
| 1 | O | 27 | LEU |
| 1 | O | 30 | GLU |
| 1 | O | 98 | ARG |
| 1 | O | 118 | LYS |
| 1 | O | 129 | LYS |
| 1 | O | 197 | ARG |
| 1 | O | 223 | LEU |
| 1 | O | 230 | ILE |
| 1 | O | 246 | SER |
| 1 | O | 252 | LEU |
| 1 | O | 255 | LEU |
| 1 | O | 283 | SER |
| 1 | O | 286 | ASP |
| 1 | O | 289 | MET |
| 1 | O | 290 | LEU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | O | 297 | ASN |
| 1 | O | 298 | SER |
| 1 | O | 307 | LYS |
| 1 | O | 314 | ARG |
| 1 | O | 315 | LYS |
| 1 | O | 316 | GLU |
| 1 | O | 318 | GLU |
| 1 | O | 322 | GLN |
| 1 | O | 342 | SER |
| 1 | O | 353 | GLN |
| 2 | P | 1 | LEU |
| 2 | P | 3 | VAL |
| 2 | P | 21 | GLU |
| 2 | P | 33 | TYR |
| 2 | P | 43 | LEU |
| 2 | P | 74 | LEU |
| 2 | P | 81 | MET |
| 2 | P | 91 | ASP |
| 2 | P | 185 | GLU |
| 2 | P | 188 | SER |
| 2 | P | 197 | LYS |
| 2 | P | 205 | THR |
| 2 | P | 206 | HIS |
| 2 | P | 237 | ASN |
| 2 | P | 246 | MET |
| 2 | P | 263 | GLU |
| 2 | P | 278 | ARG |
| 2 | P | 288 | LEU |
| 2 | P | 319 | ILE |
| 2 | P | 328 | ASN |
| 1 | Q | 6 | THR |
| 1 | Q | 10 | LYS |
| 1 | Q | 11 | LYS |
| 1 | Q | 16 | ARG |
| 1 | Q | 19 | GLU |
| 1 | Q | 27 | LEU |
| 1 | Q | 28 | THR |
| 1 | Q | 29 | ARG |
| 1 | Q | 33 | LEU |
| 1 | Q | 40 | GLN |
| 1 | Q | 48 | LYS |
| 1 | Q | 51 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | Q | 57 | ILE |
| 1 | Q | 75 | LEU |
| 1 | Q | 98 | ARG |
| 1 | Q | 103 | ARG |
| 1 | Q | 135 | ASN |
| 1 | Q | 186 | LYS |
| 1 | Q | 197 | ARG |
| 1 | Q | 204 | VAL |
| 1 | Q | 206 | ARG |
| 1 | Q | 223 | LEU |
| 1 | Q | 230 | ILE |
| 1 | Q | 255 | LEU |
| 1 | Q | 283 | SER |
| 1 | Q | 284 | LYS |
| 1 | Q | 289 | MET |
| 1 | Q | 303 | VAL |
| 1 | Q | 315 | LYS |
| 1 | Q | 316 | GLU |
| 1 | Q | 361 | SER |
| 2 | R | 1 | LEU |
| 2 | R | 11 | GLN |
| 2 | R | 26 | LEU |
| 2 | R | 33 | TYR |
| 2 | R | 45 | LYS |
| 2 | R | 50 | LYS |
| 2 | R | 74 | LEU |
| 2 | R | 81 | MET |
| 2 | R | 162 | ARG |
| 2 | R | 173 | GLU |
| 2 | R | 182 | PHE |
| 2 | R | 185 | GLU |
| 2 | R | 190 | ASP |
| 2 | R | 192 | LEU |
| 2 | R | 197 | LYS |
| 2 | R | 229 | GLU |
| 2 | R | 234 | GLU |
| 2 | R | 237 | ASN |
| 2 | R | 261 | THR |
| 2 | R | 280 | MET |
| 2 | R | 306 | LYS |
| 2 | R | 317 | LYS |
| 2 | R | 328 | ASN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | S | 1 | PHE |
| 1 | S | 10 | LYS |
| 1 | S | 18 | GLU |
| 1 | S | 24 | THR |
| 1 | S | 27 | LEU |
| 1 | S | 30 | GLU |
| 1 | S | 34 | LYS |
| 1 | S | 37 | ARG |
| 1 | S | 57 | ILE |
| 1 | S | 75 | LEU |
| 1 | S | 98 | ARG |
| 1 | S | 103 | ARG |
| 1 | S | 135 | ASN |
| 1 | S | 158 | ASP |
| 1 | S | 197 | ARG |
| 1 | S | 230 | ILE |
| 1 | S | 232 | CYS |
| 1 | S | 274 | THR |
| 1 | S | 278 | ILE |
| 1 | S | 283 | SER |
| 1 | S | 284 | LYS |
| 1 | S | 289 | MET |
| 1 | S | 307 | LYS |
| 1 | S | 315 | LYS |
| 1 | S | 316 | GLU |
| 1 | S | 322 | GLN |
| 1 | S | 332 | LEU |
| 1 | S | 353 | GLN |
| 2 | T | 1 | LEU |
| 2 | T | 2 | GLN |
| 2 | T | 3 | VAL |
| 2 | T | 21 | GLU |
| 2 | T | 33 | TYR |
| 2 | T | 74 | LEU |
| 2 | T | 96 | SER |
| 2 | T | 127 | GLN |
| 2 | T | 172 | ASN |
| 2 | T | 185 | GLU |
| 2 | T | 197 | LYS |
| 2 | T | 228 | LYS |
| 2 | T | 237 | ASN |
| 2 | T | 278 | ARG |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | T | 279 | ILE |
| 2 | T | 288 | LEU |
| 2 | T | 313 | ILE |
| 2 | T | 315 | GLN |
| 2 | T | 316 | VAL |
| 2 | T | 317 | LYS |
| 2 | T | 328 | ASN |
| 1 | U | 3 | ASN |
| 1 | U | 9 | ILE |
| 1 | U | 10 | LYS |
| 1 | U | 11 | LYS |
| 1 | U | 23 | VAL |
| 1 | U | 27 | LEU |
| 1 | U | 28 | THR |
| 1 | U | 33 | LEU |
| 1 | U | 82 | THR |
| 1 | U | 98 | ARG |
| 1 | U | 103 | ARG |
| 1 | U | 158 | ASP |
| 1 | U | 194 | GLU |
| 1 | U | 206 | ARG |
| 1 | U | 210 | SER |
| 1 | U | 214 | TYR |
| 1 | U | 223 | LEU |
| 1 | U | 233 | VAL |
| 1 | U | 235 | GLU |
| 1 | U | 246 | SER |
| 1 | U | 252 | LEU |
| 1 | U | 256 | GLN |
| 1 | U | 283 | SER |
| 1 | U | 284 | LYS |
| 1 | U | 289 | MET |
| 1 | U | 295 | MET |
| 1 | U | 307 | LYS |
| 1 | U | 314 | ARG |
| 1 | U | 322 | GLN |
| 1 | U | 335 | LEU |
| 1 | U | 342 | SER |
| 2 | V | 1 | LEU |
| 2 | V | 7 | ASP |
| 2 | V | 26 | LEU |
| 2 | V | 34 | ASP |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | V | 74 | LEU |
| 2 | V | 81 | MET |
| 2 | V | 82 | THR |
| 2 | V | 129 | SER |
| 2 | V | 159 | SER |
| 2 | V | 162 | ARG |
| 2 | V | 187 | GLN |
| 2 | V | 192 | LEU |
| 2 | V | 206 | HIS |
| 2 | V | 213 | SER |
| 2 | V | 237 | ASN |
| 2 | V | 278 | ARG |
| 2 | V | 279 | ILE |
| 2 | V | 306 | LYS |
| 2 | V | 328 | ASN |
| 1 | W | 6 | THR |
| 1 | W | 13 | ASP |
| 1 | W | 23 | VAL |
| 1 | W | 27 | LEU |
| 1 | W | 28 | THR |
| 1 | W | 29 | ARG |
| 1 | W | 30 | GLU |
| 1 | W | 75 | LEU |
| 1 | W | 98 | ARG |
| 1 | W | 104 | GLU |
| 1 | W | 118 | LYS |
| 1 | W | 158 | ASP |
| 1 | W | 206 | ARG |
| 1 | W | 223 | LEU |
| 1 | W | 238 | ARG |
| 1 | W | 255 | LEU |
| 1 | W | 272 | TYR |
| 1 | W | 273 | ARG |
| 1 | W | 274 | THR |
| 1 | W | 275 | ARG |
| 1 | W | 276 | GLU |
| 1 | W | 278 | ILE |
| 1 | W | 279 | GLN |
| 1 | W | 280 | GLU |
| 1 | W | 283 | SER |
| 1 | W | 289 | MET |
| 1 | W | 315 | LYS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | W | 316 | GLU |
| 1 | W | 318 | GLU |
| 1 | W | 319 | ASP |
| 1 | W | 333 | GLU |
| 1 | W | 335 | LEU |
| 2 | X | 3 | VAL |
| 2 | X | 21 | GLU |
| 2 | X | 33 | TYR |
| 2 | X | 34 | ASP |
| 2 | X | 43 | LEU |
| 2 | X | 49 | ASP |
| 2 | X | 58 | SER |
| 2 | X | 74 | LEU |
| 2 | X | 81 | MET |
| 2 | X | 162 | ARG |
| 2 | X | 172 | ASN |
| 2 | X | 182 | PHE |
| 2 | X | 185 | GLU |
| 2 | X | 246 | MET |
| 2 | X | 278 | ARG |
| 2 | X | 279 | ILE |
| 2 | X | 288 | LEU |
| 2 | X | 306 | LYS |
| 2 | X | 315 | GLN |
| 2 | X | 316 | VAL |
| 2 | X | 317 | LYS |
| 2 | X | 320 | ILE |
| 2 | X | 328 | ASN |
| 1 | Y | 3 | ASN |
| 1 | Y | 10 | LYS |
| 1 | Y | 19 | GLU |
| 1 | Y | 27 | LEU |
| 1 | Y | 29 | ARG |
| 1 | Y | 30 | GLU |
| 1 | Y | 98 | ARG |
| 1 | Y | 104 | GLU |
| 1 | Y | 118 | LYS |
| 1 | Y | 135 | ASN |
| 1 | Y | 206 | ARG |
| 1 | Y | 216 | ARG |
| 1 | Y | 230 | ILE |
| 1 | Y | 238 | ARG |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | Y | 252 | LEU |
| 1 | Y | 255 | LEU |
| 1 | Y | 270 | VAL |
| 1 | Y | 272 | TYR |
| 1 | Y | 273 | ARG |
| 1 | Y | 274 | THR |
| 1 | Y | 275 | ARG |
| 1 | Y | 279 | GLN |
| 1 | Y | 284 | LYS |
| 1 | Y | 289 | MET |
| 1 | Y | 315 | LYS |
| 1 | Y | 316 | GLU |
| 1 | Y | 332 | LEU |
| 1 | Y | 333 | GLU |
| 1 | Y | 360 | VAL |
| 2 | Z | 1 | LEU |
| 2 | Z | 2 | GLN |
| 2 | Z | 3 | VAL |
| 2 | Z | 32 | GLN |
| 2 | Z | 74 | LEU |
| 2 | Z | 81 | MET |
| 2 | Z | 82 | THR |
| 2 | Z | 90 | ILE |
| 2 | Z | 162 | ARG |
| 2 | Z | 182 | PHE |
| 2 | Z | 188 | SER |
| 2 | Z | 192 | LEU |
| 2 | Z | 213 | SER |
| 2 | Z | 229 | GLU |
| 2 | Z | 237 | ASN |
| 2 | Z | 306 | LYS |
| 2 | Z | 317 | LYS |
| 1 | 1 | 8 | GLU |
| 1 | 1 | 10 | LYS |
| 1 | 1 | 11 | LYS |
| 1 | 1 | 26 | VAL |
| 1 | 1 | 27 | LEU |
| 1 | 1 | 28 | THR |
| 1 | 1 | 29 | ARG |
| 1 | 1 | 30 | GLU |
| 1 | 1 | 53 | TYR |
| 1 | 1 | 75 | LEU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 1 | 98 | ARG |
| 1 | 1 | 104 | GLU |
| 1 | 1 | 113 | LYS |
| 1 | 1 | 118 | LYS |
| 1 | 1 | 129 | LYS |
| 1 | 1 | 135 | ASN |
| 1 | 1 | 158 | ASP |
| 1 | 1 | 197 | ARG |
| 1 | 1 | 257 | THR |
| 1 | 1 | 280 | GLU |
| 1 | 1 | 283 | SER |
| 1 | 1 | 289 | MET |
| 1 | 1 | 297 | ASN |
| 1 | 1 | 300 | LEU |
| 1 | 1 | 307 | LYS |
| 1 | 1 | 315 | LYS |
| 1 | 1 | 342 | SER |
| 1 | 1 | 353 | GLN |
| 2 | 2 | 33 | TYR |
| 2 | 2 | 43 | LEU |
| 2 | 2 | 49 | ASP |
| 2 | 2 | 74 | LEU |
| 2 | 2 | 140 | PRO |
| 2 | 2 | 152 | ASP |
| 2 | 2 | 162 | ARG |
| 2 | 2 | 188 | SER |
| 2 | 2 | 192 | LEU |
| 2 | 2 | 197 | LYS |
| 2 | 2 | 237 | ASN |
| 2 | 2 | 246 | MET |
| 2 | 2 | 279 | ILE |
| 2 | 2 | 288 | LEU |
| 2 | 2 | 317 | LYS |
| 2 | 2 | 328 | ASN |
| 1 | 3 | 1 | PHE |
| 1 | 3 | 3 | ASN |
| 1 | 3 | 7 | PHE |
| 1 | 3 | 11 | LYS |
| 1 | 3 | 27 | LEU |
| 1 | 3 | 29 | ARG |
| 1 | 3 | 30 | GLU |
| 1 | 3 | 72 | CYS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 3 | 73 | VAL |
| 1 | 3 | 75 | LEU |
| 1 | 3 | 80 | ASN |
| 1 | 3 | 98 | ARG |
| 1 | 3 | 103 | ARG |
| 1 | 3 | 104 | GLU |
| 1 | 3 | 118 | LYS |
| 1 | 3 | 135 | ASN |
| 1 | 3 | 195 | ASN |
| 1 | 3 | 230 | ILE |
| 1 | 3 | 255 | LEU |
| 1 | 3 | 257 | THR |
| 1 | 3 | 274 | THR |
| 1 | 3 | 284 | LYS |
| 1 | 3 | 289 | MET |
| 1 | 3 | 307 | LYS |
| 1 | 3 | 315 | LYS |
| 1 | 3 | 322 | GLN |
| 1 | 3 | 341 | SER |
| 1 | 3 | 342 | SER |
| 2 | 4 | 1 | LEU |
| 2 | 4 | 11 | GLN |
| 2 | 4 | 13 | MET |
| 2 | 4 | 74 | LEU |
| 2 | 4 | 81 | MET |
| 2 | 4 | 82 | THR |
| 2 | 4 | 159 | SER |
| 2 | 4 | 162 | ARG |
| 2 | 4 | 189 | LYS |
| 2 | 4 | 190 | ASP |
| 2 | 4 | 192 | LEU |
| 2 | 4 | 237 | ASN |
| 2 | 4 | 279 | ILE |
| 2 | 4 | 306 | LYS |
| 2 | 4 | 328 | ASN |
| 1 | 5 | 10 | LYS |
| 1 | 5 | 23 | VAL |
| 1 | 5 | 27 | LEU |
| 1 | 5 | 29 | ARG |
| 1 | 5 | 75 | LEU |
| 1 | 5 | 98 | ARG |
| 1 | 5 | 103 | ARG |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 5 | 104 | GLU |
| 1 | 5 | 158 | ASP |
| 1 | 5 | 164 | LEU |
| 1 | 5 | 196 | ASN |
| 1 | 5 | 210 | SER |
| 1 | 5 | 231 | LEU |
| 1 | 5 | 232 | CYS |
| 1 | 5 | 235 | GLU |
| 1 | 5 | 252 | LEU |
| 1 | 5 | 273 | ARG |
| 1 | 5 | 274 | THR |
| 1 | 5 | 275 | ARG |
| 1 | 5 | 279 | GLN |
| 1 | 5 | 280 | GLU |
| 1 | 5 | 281 | VAL |
| 1 | 5 | 284 | LYS |
| 1 | 5 | 315 | LYS |
| 1 | 5 | 322 | GLN |
| 1 | 5 | 335 | LEU |
| 1 | 5 | 343 | ASP |
| 2 | 6 | 1 | LEU |
| 2 | 6 | 2 | GLN |
| 2 | 6 | 32 | GLN |
| 2 | 6 | 33 | TYR |
| 2 | 6 | 81 | MET |
| 2 | 6 | 162 | ARG |
| 2 | 6 | 172 | ASN |
| 2 | 6 | 185 | GLU |
| 2 | 6 | 189 | LYS |
| 2 | 6 | 206 | HIS |
| 2 | 6 | 213 | SER |
| 2 | 6 | 237 | ASN |
| 2 | 6 | 278 | ARG |
| 2 | 6 | 279 | ILE |
| 2 | 6 | 300 | VAL |
| 2 | 6 | 317 | LYS |
| 2 | 6 | 328 | ASN |

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

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 55 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 68 | GLN |
| 1 | A | 125 | HIS |
| 1 | A | 135 | ASN |
| 1 | A | 196 | ASN |
| 1 | A | 279 | GLN |
| 1 | A | 297 | ASN |
| 1 | A | 299 | ASN |
| 2 | B | 32 | GLN |
| 2 | B | 84 | ASN |
| 2 | B | 118 | ASN |
| 2 | B | 172 | ASN |
| 2 | B | 187 | GLN |
| 2 | B | 237 | ASN |
| 1 | C | 68 | GLN |
| 1 | C | 92 | HIS |
| 1 | C | 130 | ASN |
| 1 | C | 297 | ASN |
| 2 | D | 32 | GLN |
| 2 | D | 88 | GLN |
| 2 | D | 118 | ASN |
| 2 | D | 172 | ASN |
| 2 | D | 237 | ASN |
| 2 | D | 328 | ASN |
| 1 | E | 40 | GLN |
| 1 | E | 55 | GLN |
| 1 | E | 68 | GLN |
| 1 | E | 125 | HIS |
| 1 | E | 130 | ASN |
| 1 | E | 297 | ASN |
| 1 | E | 299 | ASN |
| 1 | E | 338 | HIS |
| 2 | F | 32 | GLN |
| 2 | F | 88 | GLN |
| 2 | F | 118 | ASN |
| 2 | F | 172 | ASN |
| 2 | F | 187 | GLN |
| 2 | F | 237 | ASN |
| 2 | F | 315 | GLN |
| 1 | G | 55 | GLN |
| 1 | G | 68 | GLN |
| 1 | G | 80 | ASN |
| 1 | G | 125 | HIS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | G | 196 | ASN |
| 1 | G | 297 | ASN |
| 1 | G | 299 | ASN |
| 2 | H | 2 | GLN |
| 2 | H | 32 | GLN |
| 2 | H | 88 | GLN |
| 2 | H | 118 | ASN |
| 2 | H | 172 | ASN |
| 2 | H | 187 | GLN |
| 2 | H | 206 | HIS |
| 2 | H | 237 | ASN |
| 1 | I | 40 | GLN |
| 1 | I | 68 | GLN |
| 1 | I | 125 | HIS |
| 1 | I | 135 | ASN |
| 1 | I | 297 | ASN |
| 1 | I | 299 | ASN |
| 1 | I | 353 | GLN |
| 2 | J | 10 | ASN |
| 2 | J | 88 | GLN |
| 2 | J | 118 | ASN |
| 2 | J | 172 | ASN |
| 2 | J | 187 | GLN |
| 2 | J | 237 | ASN |
| 2 | J | 268 | GLN |
| 1 | K | 40 | GLN |
| 1 | K | 55 | GLN |
| 1 | K | 63 | HIS |
| 1 | K | 68 | GLN |
| 1 | K | 80 | ASN |
| 1 | K | 92 | HIS |
| 1 | K | 125 | HIS |
| 1 | K | 130 | ASN |
| 1 | K | 297 | ASN |
| 1 | K | 299 | ASN |
| 2 | L | 88 | GLN |
| 2 | L | 118 | ASN |
| 2 | L | 172 | ASN |
| 2 | L | 187 | GLN |
| 2 | L | 206 | HIS |
| 2 | L | 237 | ASN |
| 2 | L | 286 | ASN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | L | 328 | ASN |
| 1 | M | 40 | GLN |
| 1 | M | 51 | GLN |
| 1 | M | 55 | GLN |
| 1 | M | 297 | ASN |
| 1 | M | 299 | ASN |
| 2 | N | 2 | GLN |
| 2 | N | 32 | GLN |
| 2 | N | 88 | GLN |
| 2 | N | 118 | ASN |
| 2 | N | 172 | ASN |
| 2 | N | 187 | GLN |
| 2 | N | 237 | ASN |
| 2 | N | 315 | GLN |
| 1 | O | 63 | HIS |
| 1 | O | 80 | ASN |
| 1 | O | 125 | HIS |
| 1 | O | 297 | ASN |
| 2 | P | 2 | GLN |
| 2 | P | 88 | GLN |
| 2 | P | 118 | ASN |
| 2 | P | 172 | ASN |
| 2 | P | 187 | GLN |
| 2 | P | 237 | ASN |
| 2 | P | 328 | ASN |
| 1 | Q | 51 | GLN |
| 1 | Q | 55 | GLN |
| 1 | Q | 68 | GLN |
| 1 | Q | 125 | HIS |
| 1 | Q | 135 | ASN |
| 1 | Q | 279 | GLN |
| 1 | Q | 297 | ASN |
| 1 | Q | 299 | ASN |
| 1 | Q | 353 | GLN |
| 2 | R | 10 | ASN |
| 2 | R | 32 | GLN |
| 2 | R | 88 | GLN |
| 2 | R | 95 | ASN |
| 2 | R | 118 | ASN |
| 2 | R | 172 | ASN |
| 2 | R | 187 | GLN |
| 2 | R | 237 | ASN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | R | 268 | GLN |
| 1 | S | 68 | GLN |
| 1 | S | 80 | ASN |
| 1 | S | 84 | HIS |
| 1 | S | 196 | ASN |
| 1 | S | 279 | GLN |
| 1 | S | 297 | ASN |
| 1 | S | 299 | ASN |
| 2 | T | 118 | ASN |
| 2 | T | 172 | ASN |
| 2 | T | 187 | GLN |
| 2 | T | 237 | ASN |
| 2 | T | 286 | ASN |
| 2 | T | 328 | ASN |
| 1 | U | 40 | GLN |
| 1 | U | 51 | GLN |
| 1 | U | 55 | GLN |
| 1 | U | 63 | HIS |
| 1 | U | 68 | GLN |
| 1 | U | 125 | HIS |
| 1 | U | 130 | ASN |
| 1 | U | 297 | ASN |
| 2 | V | 2 | GLN |
| 2 | V | 32 | GLN |
| 2 | V | 88 | GLN |
| 2 | V | 118 | ASN |
| 2 | V | 172 | ASN |
| 2 | V | 187 | GLN |
| 2 | V | 237 | ASN |
| 2 | V | 257 | ASN |
| 1 | W | 40 | GLN |
| 1 | W | 55 | GLN |
| 1 | W | 68 | GLN |
| 1 | W | 125 | HIS |
| 1 | W | 196 | ASN |
| 1 | W | 279 | GLN |
| 1 | W | 297 | ASN |
| 2 | X | 2 | GLN |
| 2 | X | 32 | GLN |
| 2 | X | 88 | GLN |
| 2 | X | 118 | ASN |
| 2 | X | 172 | ASN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | X | 187 | GLN |
| 2 | X | 237 | ASN |
| 2 | X | 268 | GLN |
| 2 | X | 328 | ASN |
| 1 | Y | 40 | GLN |
| 1 | Y | 68 | GLN |
| 1 | Y | 80 | ASN |
| 1 | Y | 125 | HIS |
| 1 | Y | 135 | ASN |
| 1 | Y | 297 | ASN |
| 1 | Y | 299 | ASN |
| 1 | Y | 338 | HIS |
| 2 | Z | 2 | GLN |
| 2 | Z | 32 | GLN |
| 2 | Z | 88 | GLN |
| 2 | Z | 118 | ASN |
| 2 | Z | 172 | ASN |
| 2 | Z | 187 | GLN |
| 2 | Z | 237 | ASN |
| 1 | 1 | 68 | GLN |
| 1 | 1 | 125 | HIS |
| 1 | 1 | 135 | ASN |
| 1 | 1 | 196 | ASN |
| 1 | 1 | 297 | ASN |
| 1 | 1 | 353 | GLN |
| 2 | 2 | 2 | GLN |
| 2 | 2 | 88 | GLN |
| 2 | 2 | 95 | ASN |
| 2 | 2 | 118 | ASN |
| 2 | 2 | 172 | ASN |
| 2 | 2 | 187 | GLN |
| 2 | 2 | 237 | ASN |
| 2 | 2 | 315 | GLN |
| 2 | 2 | 328 | ASN |
| 1 | 3 | 40 | GLN |
| 1 | 3 | 68 | GLN |
| 1 | 3 | 125 | HIS |
| 1 | 3 | 135 | ASN |
| 1 | 3 | 279 | GLN |
| 1 | 3 | 297 | ASN |
| 1 | 3 | 299 | ASN |
| 2 | 4 | 2 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | 4 | 32 | GLN |
| 2 | 4 | 88 | GLN |
| 2 | 4 | 95 | ASN |
| 2 | 4 | 118 | ASN |
| 2 | 4 | 172 | ASN |
| 2 | 4 | 187 | GLN |
| 2 | 4 | 237 | ASN |
| 2 | 4 | 328 | ASN |
| 1 | 5 | 55 | GLN |
| 1 | 5 | 68 | GLN |
| 1 | 5 | 125 | HIS |
| 1 | 5 | 297 | ASN |
| 1 | 5 | 299 | ASN |
| 2 | 6 | 32 | GLN |
| 2 | 6 | 88 | GLN |
| 2 | 6 | 118 | ASN |
| 2 | 6 | 172 | ASN |
| 2 | 6 | 187 | GLN |
| 2 | 6 | 237 | ASN |
| 2 | 6 | 328 | ASN |

#### 5.3.3 RNA

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates

There are no monosaccharides in this entry.

### 5.6 Ligand geometry

Of 16 ligands modelled in this entry, 16 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers (i)

There are no such residues in this entry.

## 5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

# 6 Fit of model and data

## 6.1 Protein, DNA and RNA chains

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

| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|
| 1 | 1 | 335/382 (87%) | -0.29 | 1 (0%) 94 83 | 46, 56, 67, 88 | 0 |
| 1 | 3 | 342/382 (89%) | -0.37 | 0 100 100 | 45, 55, 72, 101 | 0 |
| 1 | 5 | 347/382 (90%) | -0.39 | 0 100 100 | 45, 56, 69, 92 | 0 |
| 1 | A | 342/382 (89%) | -0.41 | 1 (0%) 94 83 | 44, 55, 70, 101 | 0 |
| 1 | C | 342/382 (89%) | -0.33 | 0 100 100 | 47, 56, 72, 100 | 0 |
| 1 | E | 349/382 (91%) | -0.47 | 0 100 100 | 45, 55, 67, 86 | 0 |
| 1 | G | 346/382 (90%) | -0.40 | 0 100 100 | 42, 55, 69, 86 | 0 |
| 1 | I | 344/382 (90%) | -0.36 | 0 100 100 | 44, 56, 75, 103 | 0 |
| 1 | K | 347/382 (90%) | -0.39 | 0 100 100 | 45, 56, 69, 86 | 0 |
| 1 | M | 349/382 (91%) | -0.48 | 0 100 100 | 45, 55, 66, 85 | 0 |
| 1 | O | 332/382 (86%) | -0.32 | 1 (0%) 94 83 | 45, 57, 66, 86 | 0 |
| 1 | Q | 344/382 (90%) | -0.42 | 1 (0%) 94 83 | 43, 56, 74, 98 | 0 |
| 1 | S | 340/382 (89%) | -0.34 | 0 100 100 | 47, 55, 73, 105 | 0 |
| 1 | U | 348/382 (91%) | -0.47 | 0 100 100 | 42, 55, 66, 84 | 0 |
| 1 | W | 345/382 (90%) | -0.43 | 0 100 100 | 43, 55, 70, 84 | 0 |
| 1 | Y | 349/382 (91%) | -0.44 | 0 100 100 | 46, 55, 66, 87 | 0 |
| 2 | 2 | 329/329 (100%) | -0.51 | 1 (0%) 94 83 | 45, 54, 63, 73 | 0 |
| 2 | 4 | 329/329 (100%) | -0.45 | 0 100 100 | 44, 54, 63, 73 | 0 |
| 2 | 6 | 329/329 (100%) | -0.48 | 0 100 100 | 45, 53, 63, 73 | 0 |
| 2 | B | 329/329 (100%) | -0.51 | 0 100 100 | 46, 53, 62, 72 | 0 |
| 2 | D | 329/329 (100%) | -0.50 | 0 100 100 | 44, 53, 61, 73 | 0 |
| 2 | F | 329/329 (100%) | -0.48 | 0 100 100 | 45, 54, 64, 76 | 0 |
| 2 | H | 329/329 (100%) | -0.47 | 0 100 100 | 45, 53, 63, 75 | 0 |
| 2 | J | 329/329 (100%) | -0.49 | 0 100 100 | 46, 54, 63, 71 | 0 |

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | | | OWAB(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 2 | L | 329/329 (100%) | -0.47 | 0 | 100 | 100 | 45, 53, 62, 72 | 0 |
| 2 | N | 329/329 (100%) | -0.48 | 0 | 100 | 100 | 47, 54, 63, 73 | 0 |
| 2 | P | 329/329 (100%) | -0.52 | 0 | 100 | 100 | 44, 53, 63, 74 | 0 |
| 2 | R | 329/329 (100%) | -0.50 | 0 | 100 | 100 | 45, 53, 62, 71 | 0 |
| 2 | T | 329/329 (100%) | -0.50 | 0 | 100 | 100 | 45, 53, 62, 73 | 0 |
| 2 | V | 329/329 (100%) | -0.48 | 0 | 100 | 100 | 47, 54, 64, 77 | 0 |
| 2 | X | 329/329 (100%) | -0.47 | 0 | 100 | 100 | 45, 54, 63, 75 | 0 |
| 2 | Z | 329/329 (100%) | -0.45 | 1 (0%) | 94 | 83 | 45, 54, 62, 73 | 0 |
| All | All | 10765/11376 (94%) | -0.44 | 6 (0%) | 95 | 89 | 42, 54, 65, 105 | 0 |

All (6) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | Q | 261 | HIS | 4.1 |
| 1 | 1 | 5 | ALA | 3.4 |
| 1 | A | 261 | HIS | 3.3 |
| 2 | 2 | 329 | ILE | 2.9 |
| 2 | Z | 1 | LEU | 2.3 |
| 1 | O | 207 | ALA | 2.1 |

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

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

## 6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

## 6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95$^{th}$ percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 3 | K | T | 1006 | 1/1 | 0.90 | 0.08 | 76,76,76,76 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 3 | K | H | 1013 | 1/1 | 0.93 | 0.07 | 79,79,79,79 | 0 |
| 3 | K | V | 1004 | 1/1 | 0.93 | 0.07 | 70,70,70,70 | 0 |
| 3 | K | D | 1002 | 1/1 | 0.95 | 0.05 | 72,72,72,72 | 0 |
| 3 | K | R | 1001 | 1/1 | 0.95 | 0.06 | 70,70,70,70 | 0 |
| 3 | K | J | 1014 | 1/1 | 0.96 | 0.10 | 78,78,78,78 | 0 |
| 3 | K | F | 1008 | 1/1 | 0.96 | 0.06 | 75,75,75,75 | 0 |
| 3 | K | Z | 1010 | 1/1 | 0.96 | 0.07 | 75,75,75,75 | 0 |
| 3 | K | 2 | 1015 | 1/1 | 0.96 | 0.06 | 88,88,88,88 | 0 |
| 3 | K | P | 1012 | 1/1 | 0.97 | 0.05 | 84,84,84,84 | 0 |
| 3 | K | X | 1005 | 1/1 | 0.97 | 0.10 | 67,67,67,67 | 0 |
| 3 | K | B | 1003 | 1/1 | 0.97 | 0.06 | 65,65,65,65 | 0 |
| 3 | K | N | 1009 | 1/1 | 0.97 | 0.07 | 79,79,79,79 | 0 |
| 3 | K | 4 | 1016 | 1/1 | 0.97 | 0.18 | 80,80,80,80 | 0 |
| 3 | K | 6 | 1007 | 1/1 | 0.97 | 0.09 | 69,69,69,69 | 0 |
| 3 | K | L | 1011 | 1/1 | 0.98 | 0.06 | 69,69,69,69 | 0 |

## 6.5 Other polymers (i)

There are no such residues in this entry.