# Full wwPDB EM Validation Report

Jul 13, 2026 – 11:05 PM EDT

| | | |
|---|---|---|
| PDB ID | : | 8TRZ / pdb_00008trz |
| EMDB ID | : | EMD-41586 |
| Title | : | Cryo-EM structure of N-glycosylated Pomacea canaliculata hemocyanin |
| Authors | : | Brola, T.R.; Chiumiento, I.R.; Gragera, M.; Carazo, J.M.; Heras, H.; Dreon, M.S.; Otero, L.H. |
| Deposited on | : | 2023-08-10 |
| Resolution | : | 4.40 Å(reported) |
| Based on initial model | : | . |

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

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

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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The following versions of software and data (see references (1)) were used in the production of this report:

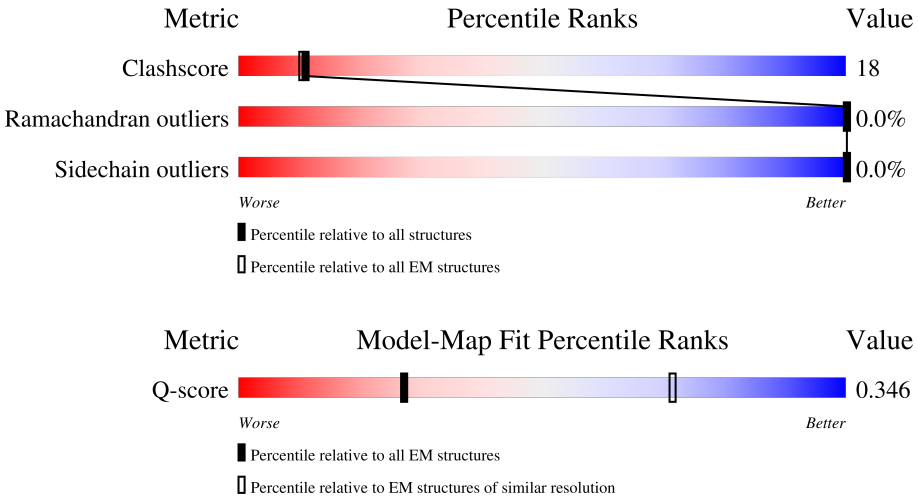
| | | |
|---|---|---|
| EMDB validation analysis | : | 0.0.1.dev133 |
| Mogul | : | 2022.3.0, CSD as543be (2022) |
| MolProbity | : | 4-5-2 with Phenix2.0 |
| Buster-report | : | wwPDB partial adaption of 1.1.7 (2018) |
| Percentile statistics | : | 20250101.v01 (using entries in the PDB archive January 1st 2025) |
| EM percentile statistics | : | 202505.v01 (Using data in the EMDB archive up until May 2025) |
| MapQ | : | 1.9.13 |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | 2.50 |

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
*ELECTRON MICROSCOPY*

The reported resolution of this entry is 4.40 Å.

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







| Metric | Whole archive (#Entries) | EM structures (#Entries) | Similar EM resolution (#Entries, resolution range(Å)) |
|---|---|---|---|
| Clashscore | 229148 | 23984 | - |
| Ramachandran outliers | 224038 | 23583 | - |
| Sidechain outliers | 223484 | 23102 | - |
| Q-score | - | 25397 | 3132 ( 3.91 - 4.90 ) |

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

| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | A | 3408 | 60% 39% |
| 1 | B | 3408 | 61% 38% |
| 1 | C | 3408 | 62% 38% |
| 1 | D | 3408 | 61% 38% |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | E | 3408 | 61% 39% |
| 1 | F | 3408 | 60% 39% |
| 1 | G | 3408 | 60% 40% |
| 1 | H | 3408 | 59% 40% |
| 1 | I | 3408 | 61% 39% |
| 1 | J | 3408 | 61% 39% |
| 1 | K | 3408 | 61% 39% |
| 1 | L | 3408 | 61% 39% |
| 1 | M | 3408 | 61% 38% |
| 1 | N | 3408 | 61% 38% |
| 1 | O | 3408 | 61% 38% |
| 1 | P | 3408 | 61% 38% |
| 1 | Q | 3408 | 60% 39% |
| 1 | R | 3408 | 59% 41% |
| 1 | S | 3408 | 61% 38% |
| 1 | T | 3408 | 61% 39% |
| 2 | 0 | 2 | 50% 50% |
| 2 | 0A | 2 | 50% 50% |
| 2 | 2 | 2 | 100% |
| 2 | 5A | 2 | 50% 50% |
| 2 | 7 | 2 | 50% 50% |
| 2 | 8 | 2 | 100% |
| 2 | AA | 2 | 100% |
| 2 | CA | 2 | 50% 50% |
| 2 | HA | 2 | 50% 50% |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 2 | IA | 2 | 50% 50% |
| 2 | KA | 2 | 50% 50% |
| 2 | MA | 2 | 100% |
| 2 | RA | 2 | 50% 50% |
| 2 | SA | 2 | 50% 50% |
| 2 | U | 2 | 50% 50% |
| 2 | UA | 2 | 100% |
| 2 | W | 2 | 100% |
| 2 | WA | 2 | 50% 50% |
| 2 | Y | 2 | 100% |
| 2 | bA | 2 | 50% 50% |
| 2 | cA | 2 | 100% |
| 2 | d | 2 | 100% |
| 2 | e | 2 | 100% |
| 2 | eA | 2 | 100% |
| 2 | g | 2 | 100% |
| 2 | gA | 2 | 100% |
| 2 | i | 2 | 50% 50% |
| 2 | lA | 2 | 50% 50% |
| 2 | mA | 2 | 100% |
| 2 | n | 2 | 50% 50% 50% |
| 2 | o | 2 | 100% |
| 2 | oA | 2 | 50% 50% |
| 2 | q | 2 | 50% 50% |
| 2 | qA | 2 | 100% |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 2 | s | 2 | 100% |
| 2 | vA | 2 | 50% 50% |
| 2 | wA | 2 | 100% |
| 2 | x | 2 | 50% 50% |
| 2 | y | 2 | 100% |
| 2 | yA | 2 | 50% 50% |
| 3 | 1 | 3 | 33% 33% 33% |
| 3 | 1A | 3 | 100% |
| 3 | 2A | 3 | 67% 33% |
| 3 | 3 | 3 | 67% 33% |
| 3 | 3A | 3 | 100% |
| 3 | 4 | 3 | 100% |
| 3 | 4A | 3 | 33% 67% |
| 3 | 5 | 3 | 100% |
| 3 | 6 | 3 | 33% 67% |
| 3 | 9 | 3 | 67% 33% |
| 3 | BA | 3 | 33% 33% 33% |
| 3 | DA | 3 | 67% 33% |
| 3 | EA | 3 | 67% 33% |
| 3 | FA | 3 | 100% |
| 3 | GA | 3 | 33% 67% |
| 3 | JA | 3 | 67% 33% |
| 3 | LA | 3 | 33% 67% |
| 3 | NA | 3 | 67% 33% |
| 3 | OA | 3 | 100% |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 3 | PA | 3 | 100% |
| 3 | QA | 3 | 67% 33% |
| 3 | TA | 3 | 100% |
| 3 | V | 3 | 67% 33% |
| 3 | VA | 3 | 100% |
| 3 | X | 3 | 33% 33% 33% |
| 3 | XA | 3 | 67% 33% |
| 3 | YA | 3 | 67% 33% |
| 3 | Z | 3 | 33% 67% |
| 3 | ZA | 3 | 100% |
| 3 | a | 3 | 67% 33% |
| 3 | aA | 3 | 33% 67% |
| 3 | b | 3 | 67% 33% |
| 3 | c | 3 | 33% 33% 33% |
| 3 | dA | 3 | 67% 33% |
| 3 | f | 3 | 67% 33% |
| 3 | fA | 3 | 33% 67% |
| 3 | h | 3 | 67% 33% |
| 3 | hA | 3 | 33% 67% |
| 3 | iA | 3 | 100% |
| 3 | j | 3 | 100% |
| 3 | jA | 3 | 67% 33% |
| 3 | k | 3 | 100% |
| 3 | kA | 3 | 100% |
| 3 | l | 3 | 100% |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 3 | m | 3 | 33% 33% 33% |
| 3 | nA | 3 | 67% 33% |
| 3 | p | 3 | 67% 33% |
| 3 | pA | 3 | 100% |
| 3 | r | 3 | 33% 33% 33% |
| 3 | rA | 3 | 100% |
| 3 | sA | 3 | 100% |
| 3 | t | 3 | 100% |
| 3 | tA | 3 | 100% |
| 3 | u | 3 | 100% |
| 3 | uA | 3 | 33% 33% 33% |
| 3 | v | 3 | 100% |
| 3 | w | 3 | 67% 33% |
| 3 | xA | 3 | 100% |
| 3 | z | 3 | 67% 33% |
| 3 | zA | 3 | 33% 33% 33% 33% |

# 2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 549912 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Hemocyanin.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 1 | A | 3387 | Total | C | N | O | S | 0 | 0 |
| | | | 27308 | 17393 | 4686 | 5138 | 91 | | |
| 1 | B | 3388 | Total | C | N | O | S | 0 | 0 |
| | | | 27308 | 17387 | 4689 | 5141 | 91 | | |
| 1 | C | 3387 | Total | C | N | O | S | 0 | 0 |
| | | | 27308 | 17393 | 4686 | 5138 | 91 | | |
| 1 | D | 3388 | Total | C | N | O | S | 0 | 0 |
| | | | 27310 | 17389 | 4689 | 5141 | 91 | | |
| 1 | E | 3387 | Total | C | N | O | S | 0 | 0 |
| | | | 27308 | 17393 | 4686 | 5138 | 91 | | |
| 1 | F | 3388 | Total | C | N | O | S | 0 | 0 |
| | | | 27310 | 17389 | 4689 | 5141 | 91 | | |
| 1 | G | 3387 | Total | C | N | O | S | 0 | 0 |
| | | | 27307 | 17393 | 4686 | 5137 | 91 | | |
| 1 | H | 3388 | Total | C | N | O | S | 0 | 0 |
| | | | 27310 | 17389 | 4689 | 5141 | 91 | | |
| 1 | I | 3387 | Total | C | N | O | S | 0 | 0 |
| | | | 27308 | 17393 | 4686 | 5138 | 91 | | |
| 1 | J | 3388 | Total | C | N | O | S | 0 | 0 |
| | | | 27309 | 17388 | 4689 | 5141 | 91 | | |
| 1 | K | 3387 | Total | C | N | O | S | 0 | 0 |
| | | | 27308 | 17393 | 4686 | 5138 | 91 | | |
| 1 | L | 3388 | Total | C | N | O | S | 0 | 0 |
| | | | 27308 | 17387 | 4689 | 5141 | 91 | | |
| 1 | M | 3387 | Total | C | N | O | S | 0 | 0 |
| | | | 27308 | 17393 | 4686 | 5138 | 91 | | |
| 1 | N | 3388 | Total | C | N | O | S | 0 | 0 |
| | | | 27310 | 17389 | 4689 | 5141 | 91 | | |
| 1 | O | 3387 | Total | C | N | O | S | 0 | 0 |
| | | | 27308 | 17393 | 4686 | 5138 | 91 | | |
| 1 | P | 3388 | Total | C | N | O | S | 0 | 0 |
| | | | 27310 | 17389 | 4689 | 5141 | 91 | | |
| 1 | Q | 3387 | Total | C | N | O | S | 0 | 0 |
| | | | 27307 | 17393 | 4686 | 5137 | 91 | | |

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| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 1 | R | 3388 | Total | C | N | O | S | 0 | 0 |
| | | | 27310 | 17389 | 4689 | 5141 | 91 | | |
| 1 | S | 3387 | Total | C | N | O | S | 0 | 0 |
| | | | 27308 | 17393 | 4686 | 5138 | 91 | | |
| 1 | T | 3388 | Total | C | N | O | S | 0 | 0 |
| | | | 27309 | 17388 | 4689 | 5141 | 91 | | |

- Molecule 2 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.




| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| 2 | U | 2 | Total | C | N | O | 0 | 0 |
| | | | 28 | 16 | 2 | 10 | | |
| 2 | W | 2 | Total | C | N | O | 0 | 0 |
| | | | 28 | 16 | 2 | 10 | | |
| 2 | Y | 2 | Total | C | N | O | 0 | 0 |
| | | | 28 | 16 | 2 | 10 | | |
| 2 | d | 2 | Total | C | N | O | 0 | 0 |
| | | | 28 | 16 | 2 | 10 | | |
| 2 | e | 2 | Total | C | N | O | 0 | 0 |
| | | | 28 | 16 | 2 | 10 | | |
| 2 | g | 2 | Total | C | N | O | 0 | 0 |
| | | | 28 | 16 | 2 | 10 | | |
| 2 | i | 2 | Total | C | N | O | 0 | 0 |
| | | | 28 | 16 | 2 | 10 | | |
| 2 | n | 2 | Total | C | N | O | 0 | 0 |
| | | | 28 | 16 | 2 | 10 | | |
| 2 | o | 2 | Total | C | N | O | 0 | 0 |
| | | | 28 | 16 | 2 | 10 | | |
| 2 | q | 2 | Total | C | N | O | 0 | 0 |
| | | | 28 | 16 | 2 | 10 | | |
| 2 | s | 2 | Total | C | N | O | 0 | 0 |
| | | | 28 | 16 | 2 | 10 | | |
| 2 | x | 2 | Total | C | N | O | 0 | 0 |
| | | | 28 | 16 | 2 | 10 | | |
| 2 | y | 2 | Total | C | N | O | 0 | 0 |
| | | | 28 | 16 | 2 | 10 | | |
| 2 | 0 | 2 | Total | C | N | O | 0 | 0 |
| | | | 28 | 16 | 2 | 10 | | |

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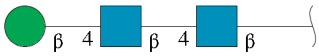
| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| 2 | 2 | 2 | Total | C | N | O | 0 | 0 |
| | | | 28 | 16 | 2 | 10 | | |
| 2 | 7 | 2 | Total | C | N | O | 0 | 0 |
| | | | 28 | 16 | 2 | 10 | | |
| 2 | 8 | 2 | Total | C | N | O | 0 | 0 |
| | | | 28 | 16 | 2 | 10 | | |
| 2 | AA | 2 | Total | C | N | O | 0 | 0 |
| | | | 28 | 16 | 2 | 10 | | |
| 2 | CA | 2 | Total | C | N | O | 0 | 0 |
| | | | 28 | 16 | 2 | 10 | | |
| 2 | HA | 2 | Total | C | N | O | 0 | 0 |
| | | | 28 | 16 | 2 | 10 | | |
| 2 | IA | 2 | Total | C | N | O | 0 | 0 |
| | | | 28 | 16 | 2 | 10 | | |
| 2 | KA | 2 | Total | C | N | O | 0 | 0 |
| | | | 28 | 16 | 2 | 10 | | |
| 2 | MA | 2 | Total | C | N | O | 0 | 0 |
| | | | 28 | 16 | 2 | 10 | | |
| 2 | RA | 2 | Total | C | N | O | 0 | 0 |
| | | | 28 | 16 | 2 | 10 | | |
| 2 | SA | 2 | Total | C | N | O | 0 | 0 |
| | | | 28 | 16 | 2 | 10 | | |
| 2 | UA | 2 | Total | C | N | O | 0 | 0 |
| | | | 28 | 16 | 2 | 10 | | |
| 2 | WA | 2 | Total | C | N | O | 0 | 0 |
| | | | 28 | 16 | 2 | 10 | | |
| 2 | bA | 2 | Total | C | N | O | 0 | 0 |
| | | | 28 | 16 | 2 | 10 | | |
| 2 | cA | 2 | Total | C | N | O | 0 | 0 |
| | | | 28 | 16 | 2 | 10 | | |
| 2 | eA | 2 | Total | C | N | O | 0 | 0 |
| | | | 28 | 16 | 2 | 10 | | |
| 2 | gA | 2 | Total | C | N | O | 0 | 0 |
| | | | 28 | 16 | 2 | 10 | | |
| 2 | lA | 2 | Total | C | N | O | 0 | 0 |
| | | | 28 | 16 | 2 | 10 | | |
| 2 | mA | 2 | Total | C | N | O | 0 | 0 |
| | | | 28 | 16 | 2 | 10 | | |
| 2 | oA | 2 | Total | C | N | O | 0 | 0 |
| | | | 28 | 16 | 2 | 10 | | |
| 2 | qA | 2 | Total | C | N | O | 0 | 0 |
| | | | 28 | 16 | 2 | 10 | | |

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| Mol | Chain | Residues | Atoms | AltConf | Trace |
|---|---|---|---|---|---|
| 2 | vA | 2 | Total C N O<br>28 16 2 10 | 0 | 0 |
| 2 | wA | 2 | Total C N O<br>28 16 2 10 | 0 | 0 |
| 2 | yA | 2 | Total C N O<br>28 16 2 10 | 0 | 0 |
| 2 | 0A | 2 | Total C N O<br>28 16 2 10 | 0 | 0 |
| 2 | 5A | 2 | Total C N O<br>28 16 2 10 | 0 | 0 |

- Molecule 3 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.




| Mol | Chain | Residues | Atoms | AltConf | Trace |
|---|---|---|---|---|---|
| 3 | V | 3 | Total C N O<br>39 22 2 15 | 0 | 0 |
| 3 | X | 3 | Total C N O<br>39 22 2 15 | 0 | 0 |
| 3 | Z | 3 | Total C N O<br>39 22 2 15 | 0 | 0 |
| 3 | a | 3 | Total C N O<br>39 22 2 15 | 0 | 0 |
| 3 | b | 3 | Total C N O<br>39 22 2 15 | 0 | 0 |
| 3 | c | 3 | Total C N O<br>39 22 2 15 | 0 | 0 |
| 3 | f | 3 | Total C N O<br>39 22 2 15 | 0 | 0 |
| 3 | h | 3 | Total C N O<br>39 22 2 15 | 0 | 0 |
| 3 | j | 3 | Total C N O<br>39 22 2 15 | 0 | 0 |
| 3 | k | 3 | Total C N O<br>39 22 2 15 | 0 | 0 |
| 3 | l | 3 | Total C N O<br>39 22 2 15 | 0 | 0 |
| 3 | m | 3 | Total C N O<br>39 22 2 15 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| 3 | p | 3 | Total | C | N | O | 0 | 0 |
| | | | 39 | 22 | 2 | 15 | | |
| 3 | r | 3 | Total | C | N | O | 0 | 0 |
| | | | 39 | 22 | 2 | 15 | | |
| 3 | t | 3 | Total | C | N | O | 0 | 0 |
| | | | 39 | 22 | 2 | 15 | | |
| 3 | u | 3 | Total | C | N | O | 0 | 0 |
| | | | 39 | 22 | 2 | 15 | | |
| 3 | v | 3 | Total | C | N | O | 0 | 0 |
| | | | 39 | 22 | 2 | 15 | | |
| 3 | w | 3 | Total | C | N | O | 0 | 0 |
| | | | 39 | 22 | 2 | 15 | | |
| 3 | z | 3 | Total | C | N | O | 0 | 0 |
| | | | 39 | 22 | 2 | 15 | | |
| 3 | 1 | 3 | Total | C | N | O | 0 | 0 |
| | | | 39 | 22 | 2 | 15 | | |
| 3 | 3 | 3 | Total | C | N | O | 0 | 0 |
| | | | 39 | 22 | 2 | 15 | | |
| 3 | 4 | 3 | Total | C | N | O | 0 | 0 |
| | | | 39 | 22 | 2 | 15 | | |
| 3 | 5 | 3 | Total | C | N | O | 0 | 0 |
| | | | 39 | 22 | 2 | 15 | | |
| 3 | 6 | 3 | Total | C | N | O | 0 | 0 |
| | | | 39 | 22 | 2 | 15 | | |
| 3 | 9 | 3 | Total | C | N | O | 0 | 0 |
| | | | 39 | 22 | 2 | 15 | | |
| 3 | BA | 3 | Total | C | N | O | 0 | 0 |
| | | | 39 | 22 | 2 | 15 | | |
| 3 | DA | 3 | Total | C | N | O | 0 | 0 |
| | | | 39 | 22 | 2 | 15 | | |
| 3 | EA | 3 | Total | C | N | O | 0 | 0 |
| | | | 39 | 22 | 2 | 15 | | |
| 3 | FA | 3 | Total | C | N | O | 0 | 0 |
| | | | 39 | 22 | 2 | 15 | | |
| 3 | GA | 3 | Total | C | N | O | 0 | 0 |
| | | | 39 | 22 | 2 | 15 | | |
| 3 | JA | 3 | Total | C | N | O | 0 | 0 |
| | | | 39 | 22 | 2 | 15 | | |
| 3 | LA | 3 | Total | C | N | O | 0 | 0 |
| | | | 39 | 22 | 2 | 15 | | |
| 3 | NA | 3 | Total | C | N | O | 0 | 0 |
| | | | 39 | 22 | 2 | 15 | | |

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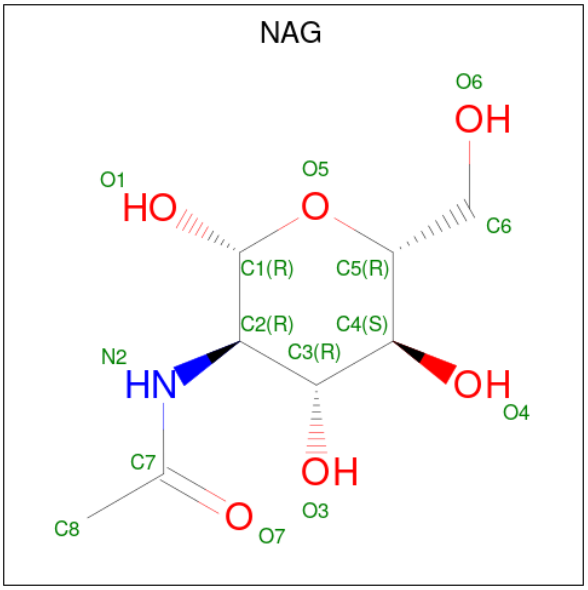
| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| 3 | OA | 3 | Total | C | N | O | 0 | 0 |
| | | | 39 | 22 | 2 | 15 | | |
| 3 | PA | 3 | Total | C | N | O | 0 | 0 |
| | | | 39 | 22 | 2 | 15 | | |
| 3 | QA | 3 | Total | C | N | O | 0 | 0 |
| | | | 39 | 22 | 2 | 15 | | |
| 3 | TA | 3 | Total | C | N | O | 0 | 0 |
| | | | 39 | 22 | 2 | 15 | | |
| 3 | VA | 3 | Total | C | N | O | 0 | 0 |
| | | | 39 | 22 | 2 | 15 | | |
| 3 | XA | 3 | Total | C | N | O | 0 | 0 |
| | | | 39 | 22 | 2 | 15 | | |
| 3 | YA | 3 | Total | C | N | O | 0 | 0 |
| | | | 39 | 22 | 2 | 15 | | |
| 3 | ZA | 3 | Total | C | N | O | 0 | 0 |
| | | | 39 | 22 | 2 | 15 | | |
| 3 | aA | 3 | Total | C | N | O | 0 | 0 |
| | | | 39 | 22 | 2 | 15 | | |
| 3 | dA | 3 | Total | C | N | O | 0 | 0 |
| | | | 39 | 22 | 2 | 15 | | |
| 3 | fA | 3 | Total | C | N | O | 0 | 0 |
| | | | 39 | 22 | 2 | 15 | | |
| 3 | hA | 3 | Total | C | N | O | 0 | 0 |
| | | | 39 | 22 | 2 | 15 | | |
| 3 | iA | 3 | Total | C | N | O | 0 | 0 |
| | | | 39 | 22 | 2 | 15 | | |
| 3 | jA | 3 | Total | C | N | O | 0 | 0 |
| | | | 39 | 22 | 2 | 15 | | |
| 3 | kA | 3 | Total | C | N | O | 0 | 0 |
| | | | 39 | 22 | 2 | 15 | | |
| 3 | nA | 3 | Total | C | N | O | 0 | 0 |
| | | | 39 | 22 | 2 | 15 | | |
| 3 | pA | 3 | Total | C | N | O | 0 | 0 |
| | | | 39 | 22 | 2 | 15 | | |
| 3 | rA | 3 | Total | C | N | O | 0 | 0 |
| | | | 39 | 22 | 2 | 15 | | |
| 3 | sA | 3 | Total | C | N | O | 0 | 0 |
| | | | 39 | 22 | 2 | 15 | | |
| 3 | tA | 3 | Total | C | N | O | 0 | 0 |
| | | | 39 | 22 | 2 | 15 | | |
| 3 | uA | 3 | Total | C | N | O | 0 | 0 |
| | | | 39 | 22 | 2 | 15 | | |

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| Mol | Chain | Residues | Atoms | AltConf | Trace |
|---|---|---|---|---|---|
| 3 | xA | 3 | Total C N O<br>39 22 2 15 | 0 | 0 |
| 3 | zA | 3 | Total C N O<br>39 22 2 15 | 0 | 0 |
| 3 | 1A | 3 | Total C N O<br>39 22 2 15 | 0 | 0 |
| 3 | 2A | 3 | Total C N O<br>39 22 2 15 | 0 | 0 |
| 3 | 3A | 3 | Total C N O<br>39 22 2 15 | 0 | 0 |
| 3 | 4A | 3 | Total C N O<br>39 22 2 15 | 0 | 0 |

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$) (labeled as "Ligand of Interest" by depositor).




| Mol | Chain | Residues | Atoms | AltConf |
|---|---|---|---|---|
| 4 | A | 1 | Total C N O<br>14 8 1 5 | 0 |
| 4 | B | 1 | Total C N O<br>14 8 1 5 | 0 |
| 4 | C | 1 | Total C N O<br>14 8 1 5 | 0 |
| 4 | D | 1 | Total C N O<br>14 8 1 5 | 0 |
| 4 | E | 1 | Total C N O<br>14 8 1 5 | 0 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Residues | Atoms | | | | AltConf |
|---|---|---|---|---|---|---|---|
| 4 | F | 1 | Total | C | N | O | 0 |
| | | | 14 | 8 | 1 | 5 | |
| 4 | G | 1 | Total | C | N | O | 0 |
| | | | 14 | 8 | 1 | 5 | |
| 4 | H | 1 | Total | C | N | O | 0 |
| | | | 14 | 8 | 1 | 5 | |
| 4 | I | 1 | Total | C | N | O | 0 |
| | | | 14 | 8 | 1 | 5 | |
| 4 | J | 1 | Total | C | N | O | 0 |
| | | | 14 | 8 | 1 | 5 | |
| 4 | K | 1 | Total | C | N | O | 0 |
| | | | 14 | 8 | 1 | 5 | |
| 4 | L | 1 | Total | C | N | O | 0 |
| | | | 14 | 8 | 1 | 5 | |
| 4 | M | 1 | Total | C | N | O | 0 |
| | | | 14 | 8 | 1 | 5 | |
| 4 | N | 1 | Total | C | N | O | 0 |
| | | | 14 | 8 | 1 | 5 | |
| 4 | O | 1 | Total | C | N | O | 0 |
| | | | 14 | 8 | 1 | 5 | |
| 4 | P | 1 | Total | C | N | O | 0 |
| | | | 14 | 8 | 1 | 5 | |
| 4 | Q | 1 | Total | C | N | O | 0 |
| | | | 14 | 8 | 1 | 5 | |
| 4 | R | 1 | Total | C | N | O | 0 |
| | | | 14 | 8 | 1 | 5 | |
| 4 | S | 1 | Total | C | N | O | 0 |
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| 4 | T | 1 | Total | C | N | O | 0 |
| | | | 14 | 8 | 1 | 5 | |

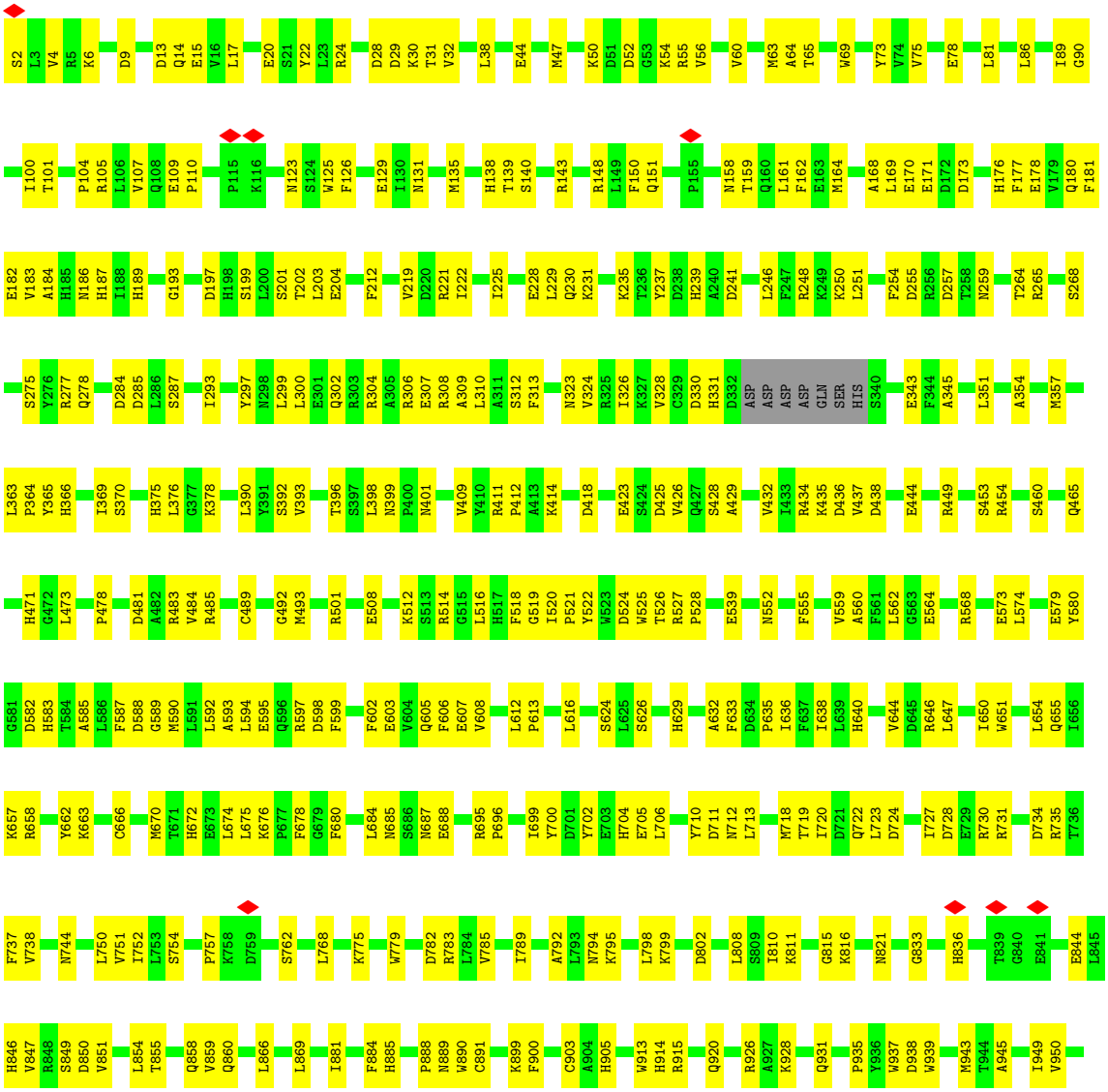
# 3 Residue-property plots (i)

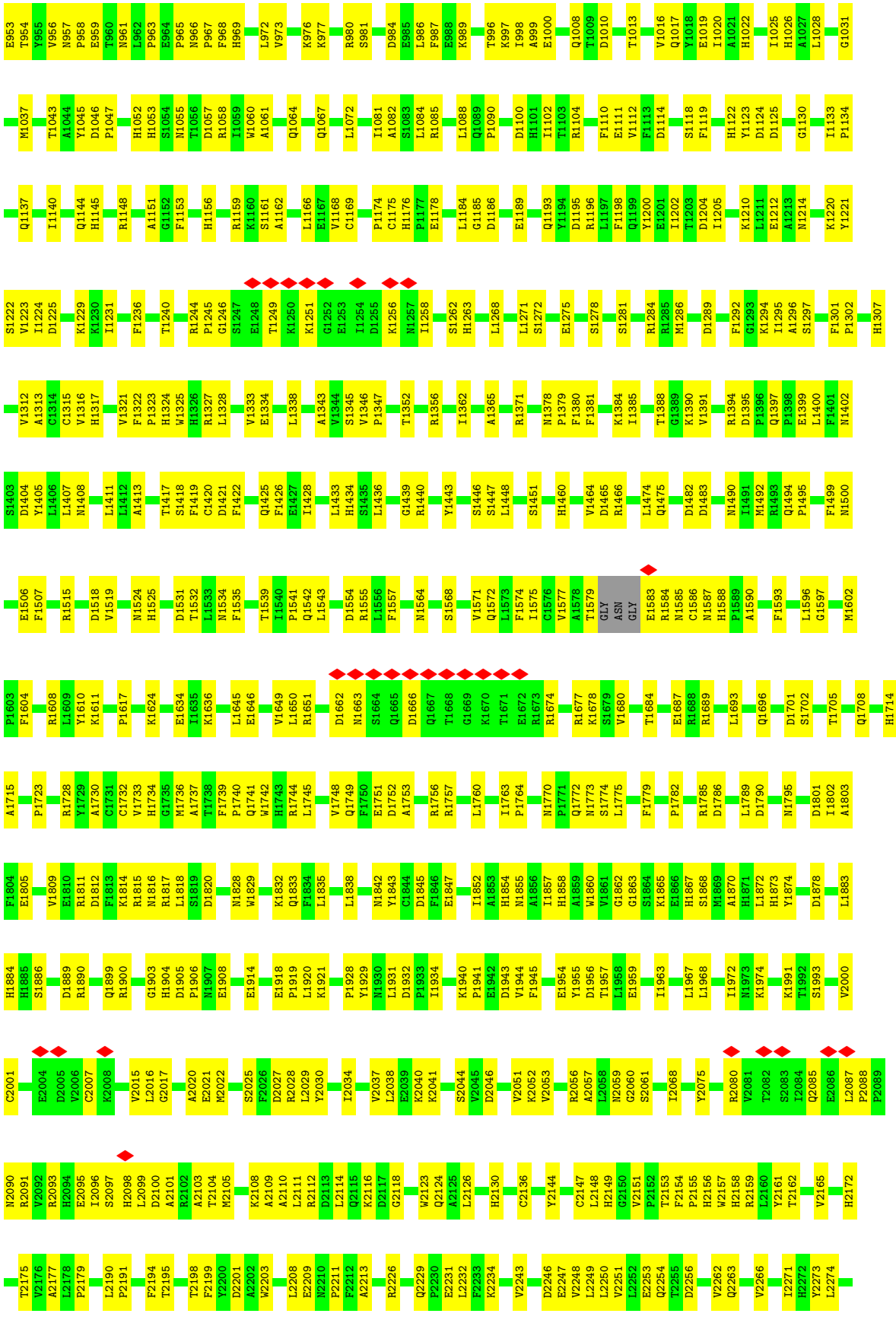
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: Hemocyanin

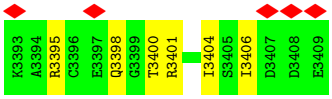
Chain A:




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M1037 T1043 A1044 Y1045 D1046 P1047 H1052 H1053 S1054 N1055 T1056 D1057 R1058 I1059 W1060 A1061 Q1064 Q1067 L1072 I1081 A1082 S1083 L1084 R1085 L1088 Q1089 P1090 D1100 H1101 I1102 T1103 R1104 F1110 E1111 V1112 F1113 D1114 S1118 F1119 H1122 Y1123 D1124 D1125 G1130 I1133 P1134
Q1137 I1140 Q1144 H1145 R1148 A1151 G1152 F1153 H1156 R1159 K1160 S1161 A1162 L1166 E1167 V1168 C1169 P1174 C1175 H1176 P1177 E1178 L1184 G1185 D1186 E1189 Q1193 Y1194 D1195 R1196 L1197 F1198 Q1199 Y1200 E1201 I1202 T1203 D1204 I1205 K1210 L1211 E1212 A1213 N1214 K1220 Y1221
S1222 V1223 I1224 D1225 K1229 K1230 I1231 F1236 T1240 R1244 P1245 G1246 S1247 E1248 T1249 K1250 K1251 G1252 E1253 I1254 D1255 K1256 N1257 I1258 S1262 H1263 L1268 L1271 S1272 E1275 S1278 S1281 R1284 R1285 M1286 D1289 F1292 G1293 K1294 I1295 A1296 S1297 F1301 P1302 H1307
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P1603 F1604 R1608 L1609 Y1610 K1611 P1617 K1624 E1634 I1635 K1636 L1645 E1646 V1649 L1650 R1651 D1662 N1663 S1664 Q1665 D1666 Q1667 T1668 G1669 K1670 T1671 E1672 R1673 R1674 R1677 K1678 S1679 V1680 T1684 E1687 R1688 R1689 L1693 Q1696 D1701 S1702 T1705 Q1708 H1714
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C2001 E2004 D2005 V2006 C2007 K2008 V2015 L2016 G2017 A2020 E2021 M2022 S2025 F2026 D2027 R2028 L2029 Y2030 I2034 V2037 L2038 E2039 K2040 K2041 S2044 V2045 D2046 V2051 K2052 V2053 R2056 A2057 L2058 N2059 G2060 S2061 I2068 Y2075 R2080 V2081 T2082 S2083 I2084 Q2085 E2086 L2087 P2088 P2089
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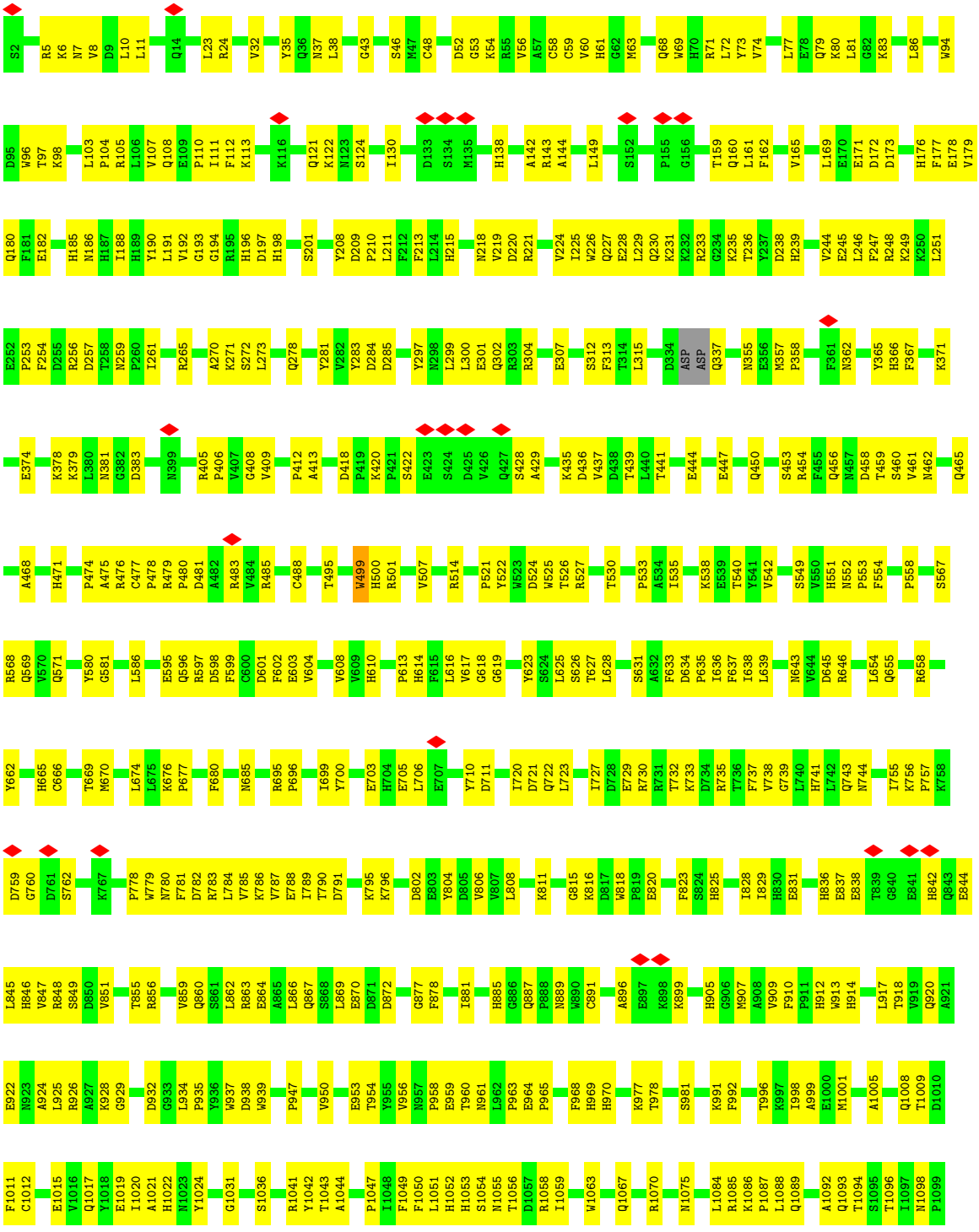
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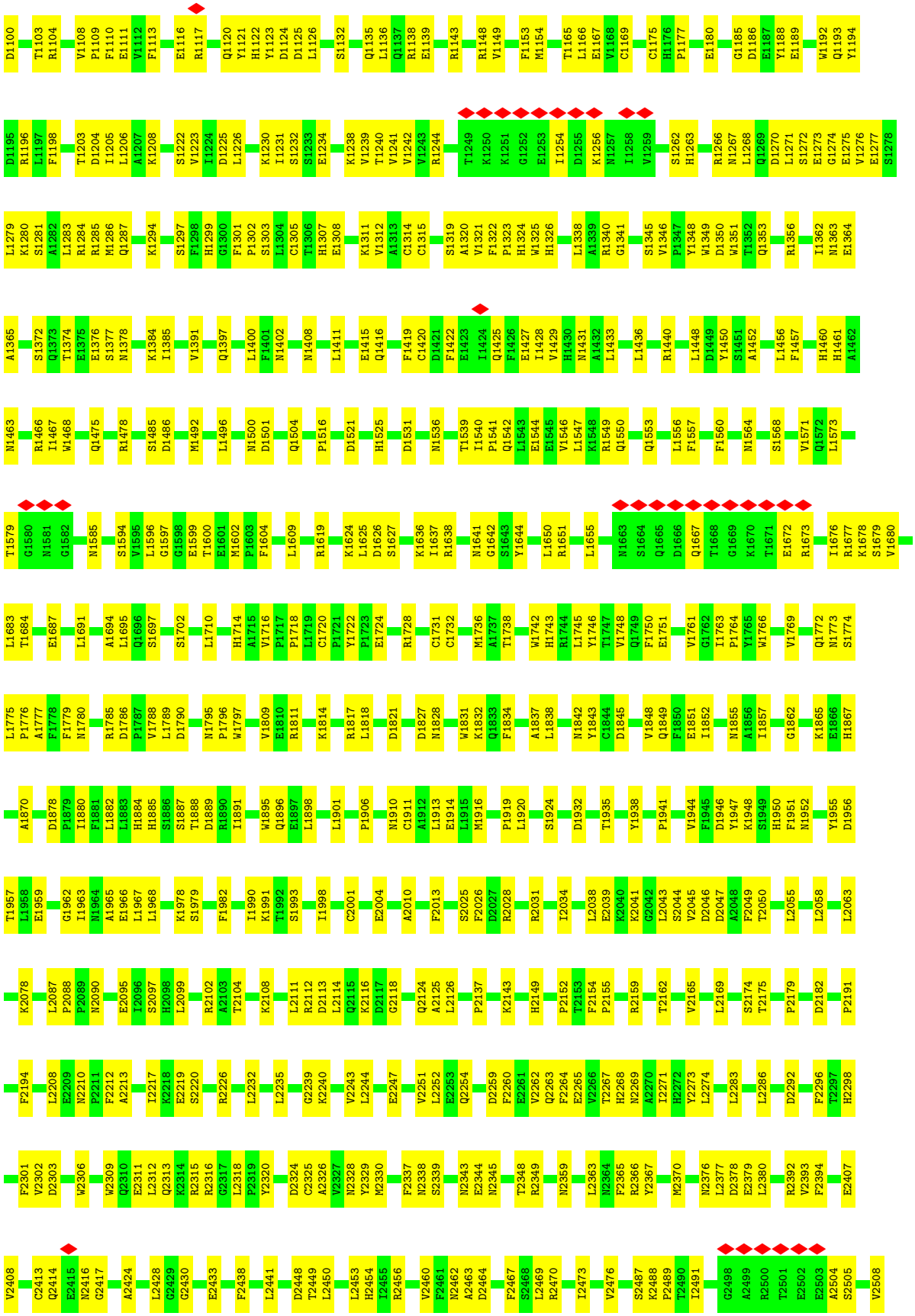


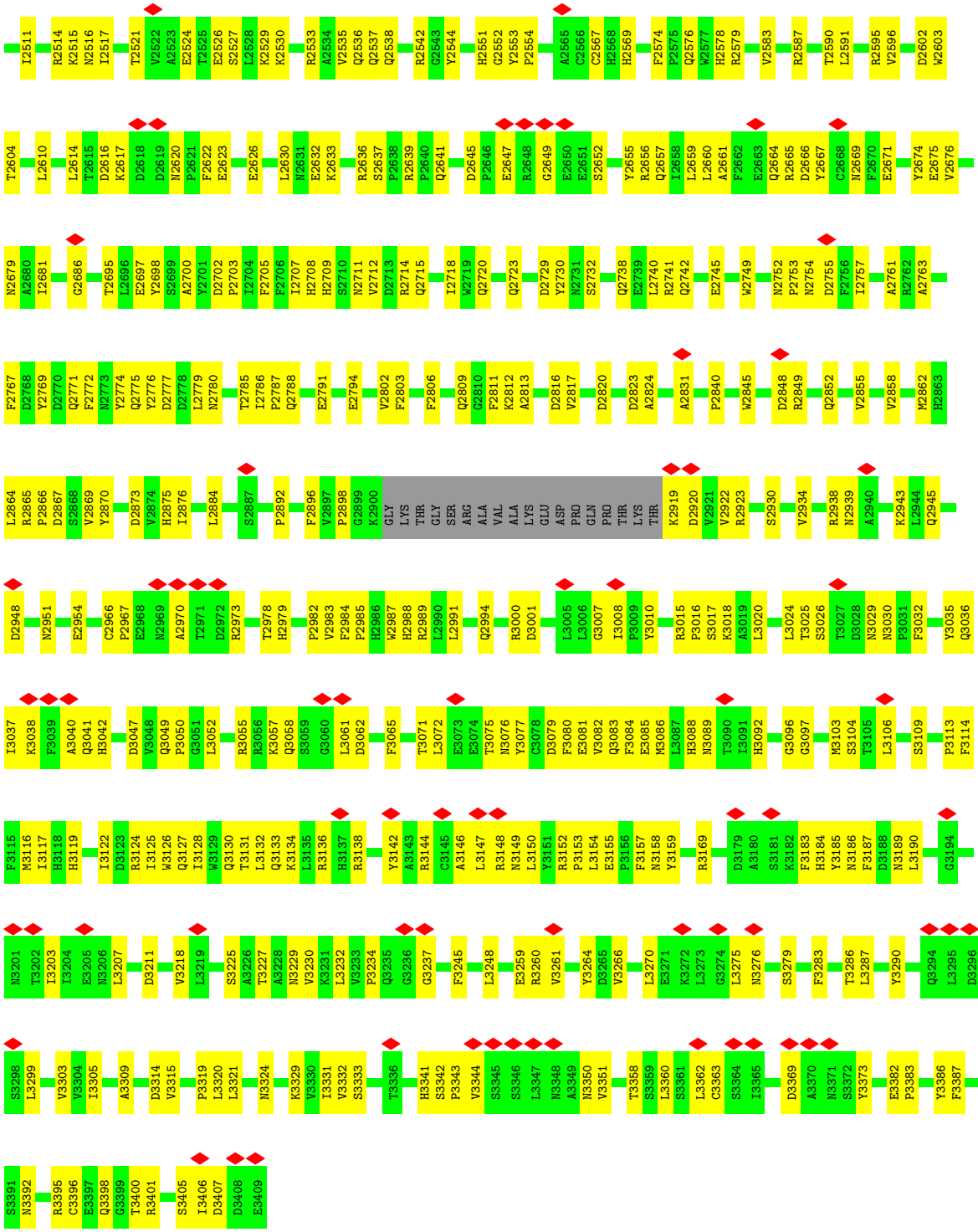

• Molecule 1: Hemocyanin

Chain B:



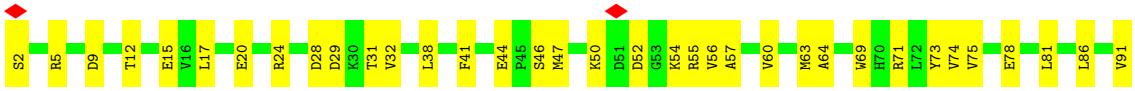

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T1957 L1958 E1959 G1962 I1963 N1964 A1965 E1966 L1967 L1968 K1978 S1979 F1982 I1990 K1991 T1992 S1993 I1998 C2001 E2004 A2010 F2013 S2025 F2026 D2027 R2028 R2031 I2034 L2038 E2039 K2040 K2041 G2042 L2043 S2044 V2045 D2046 D2047 A2048 F2049 T2050 L2055 L2058 L2063
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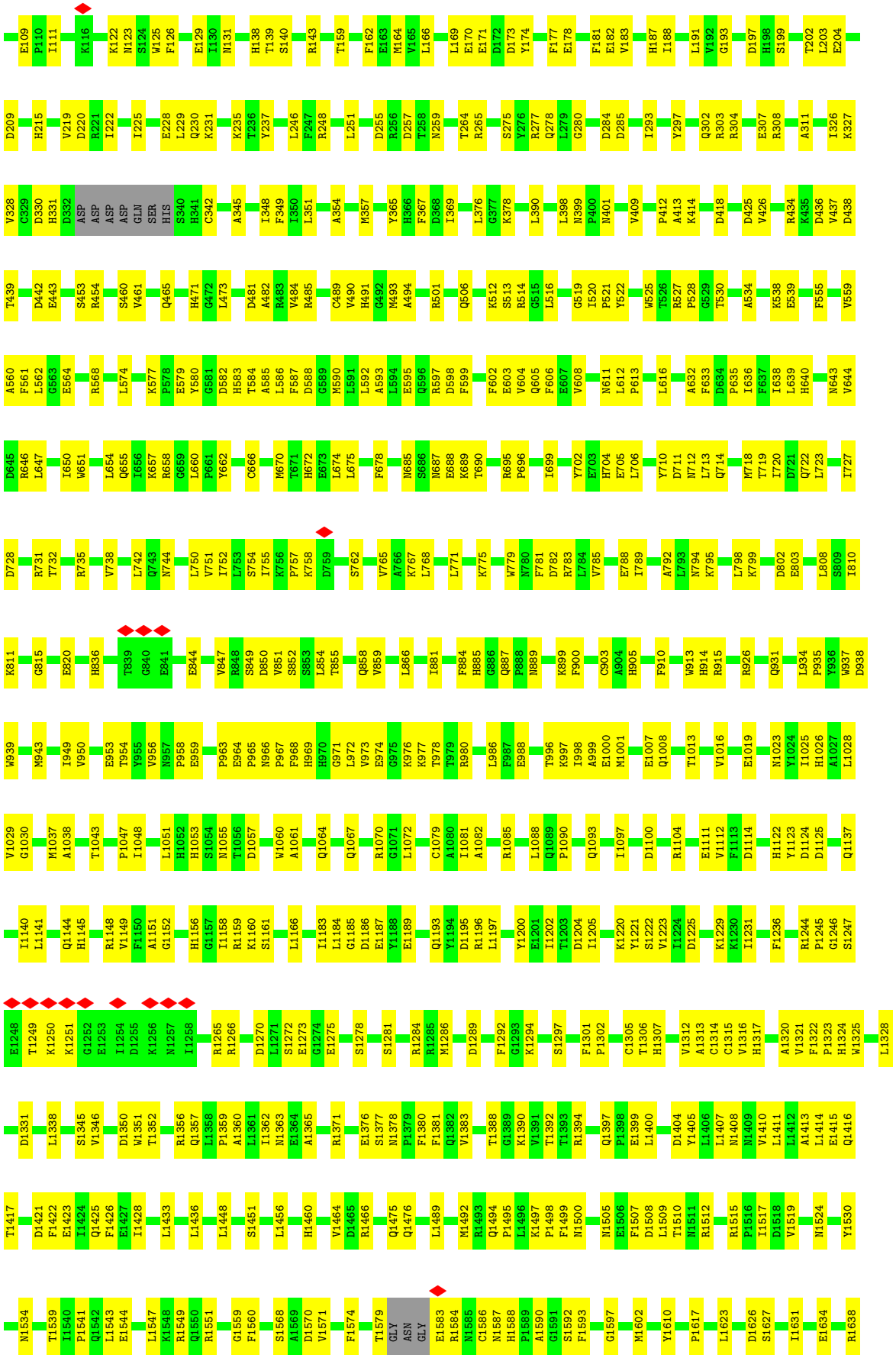


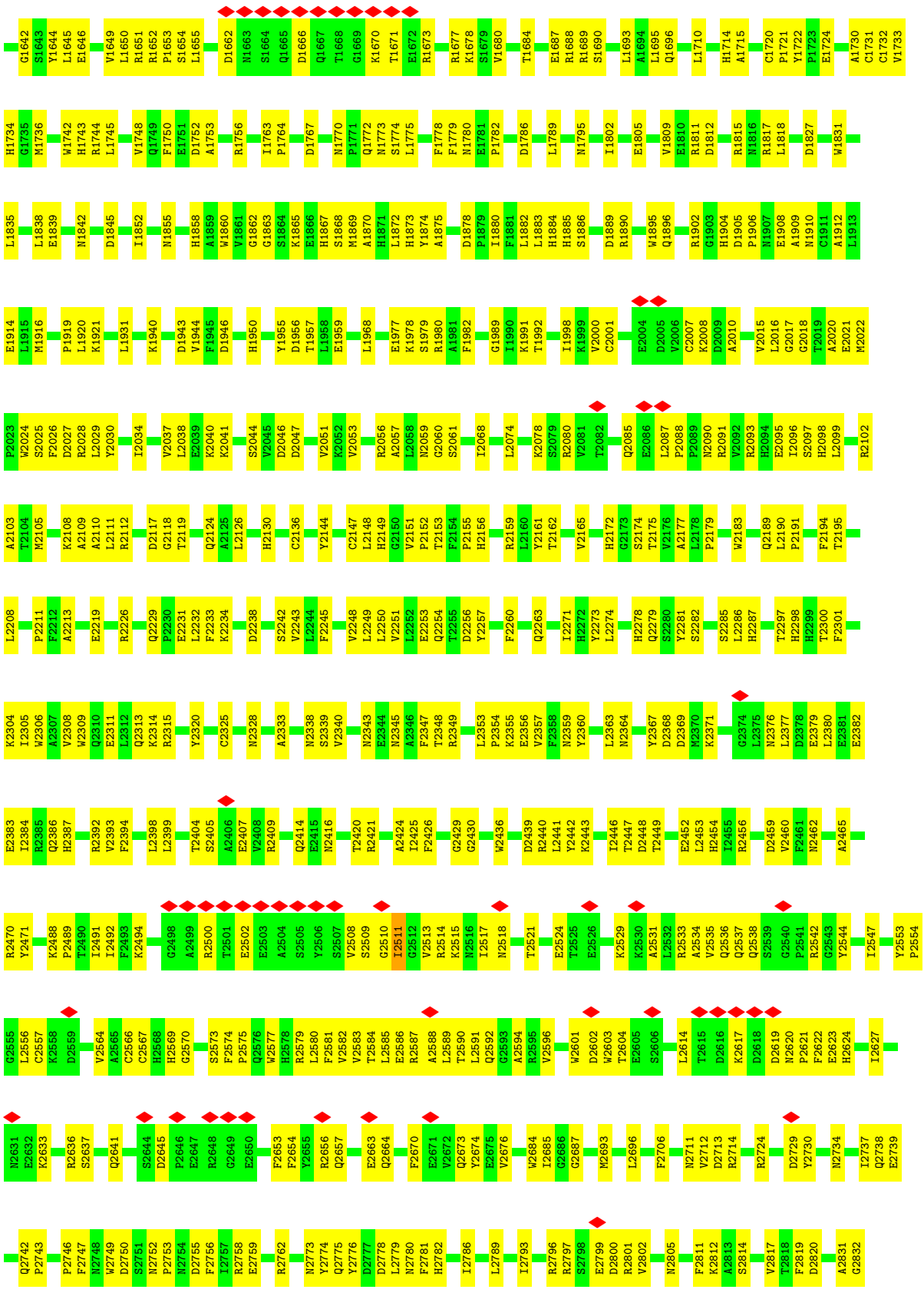
• Molecule 1: Hemocyanin

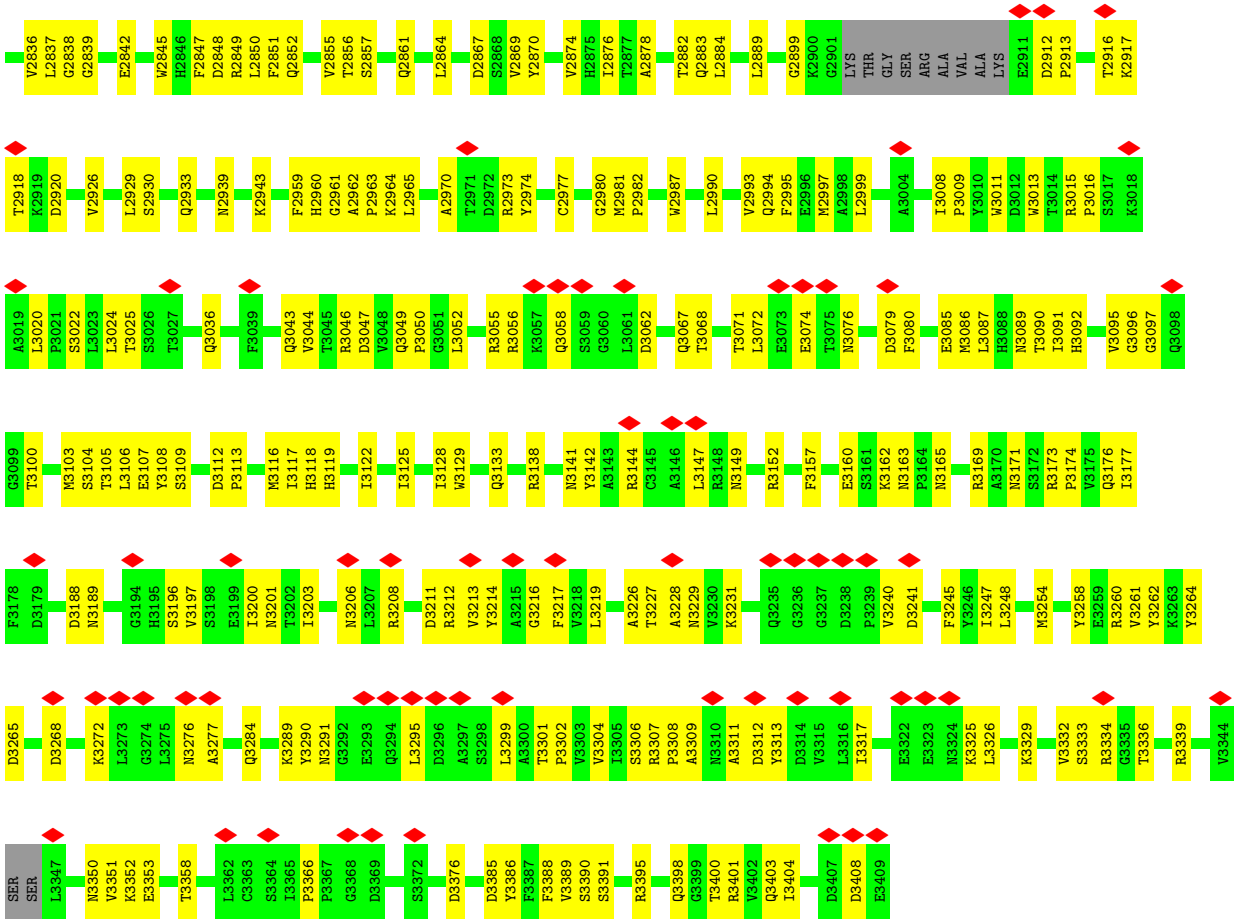
Chain C:




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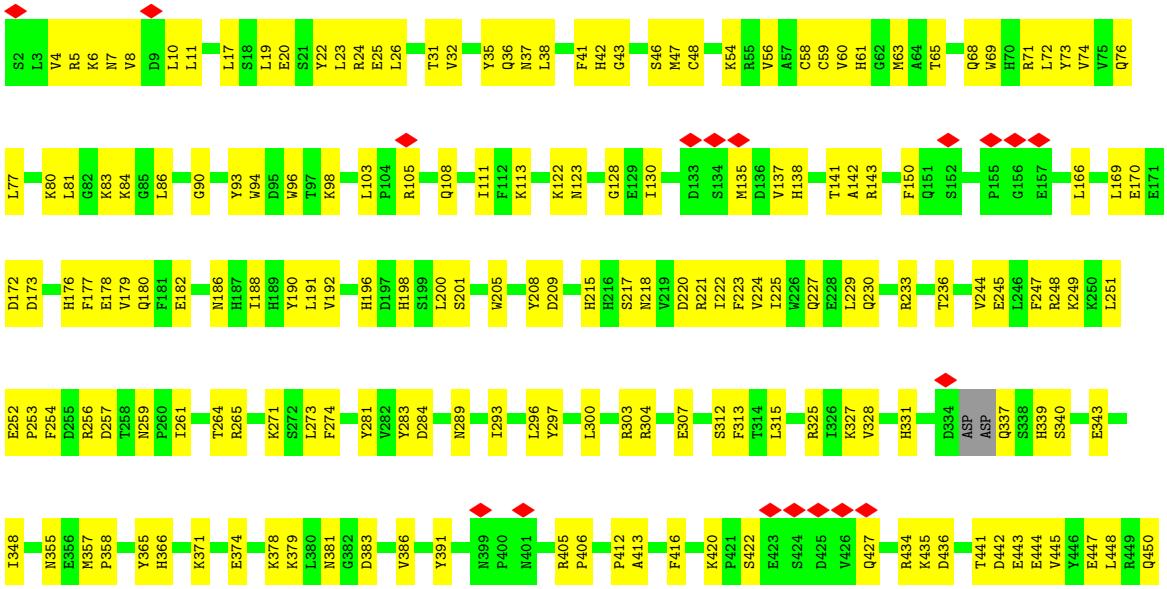


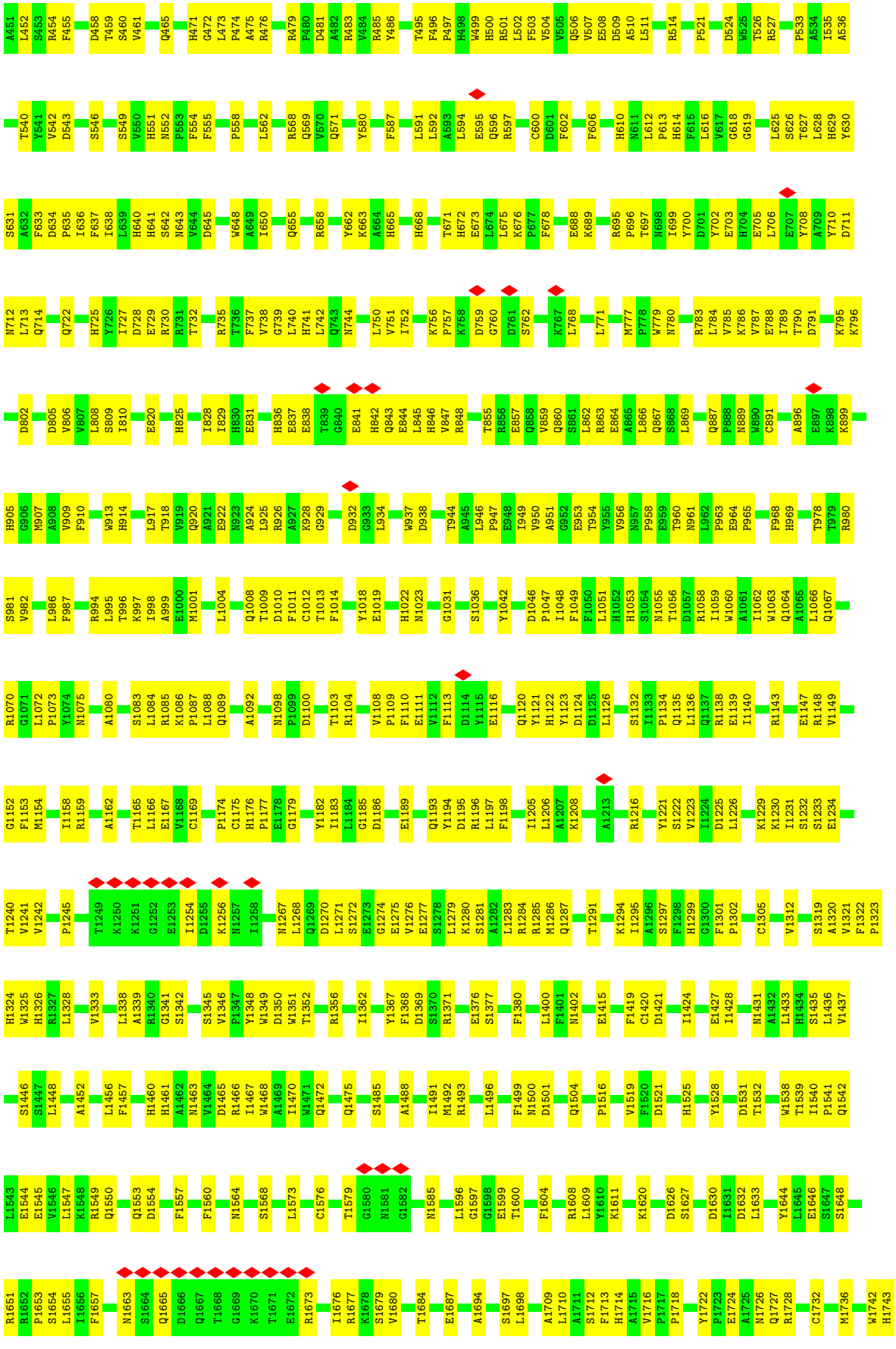


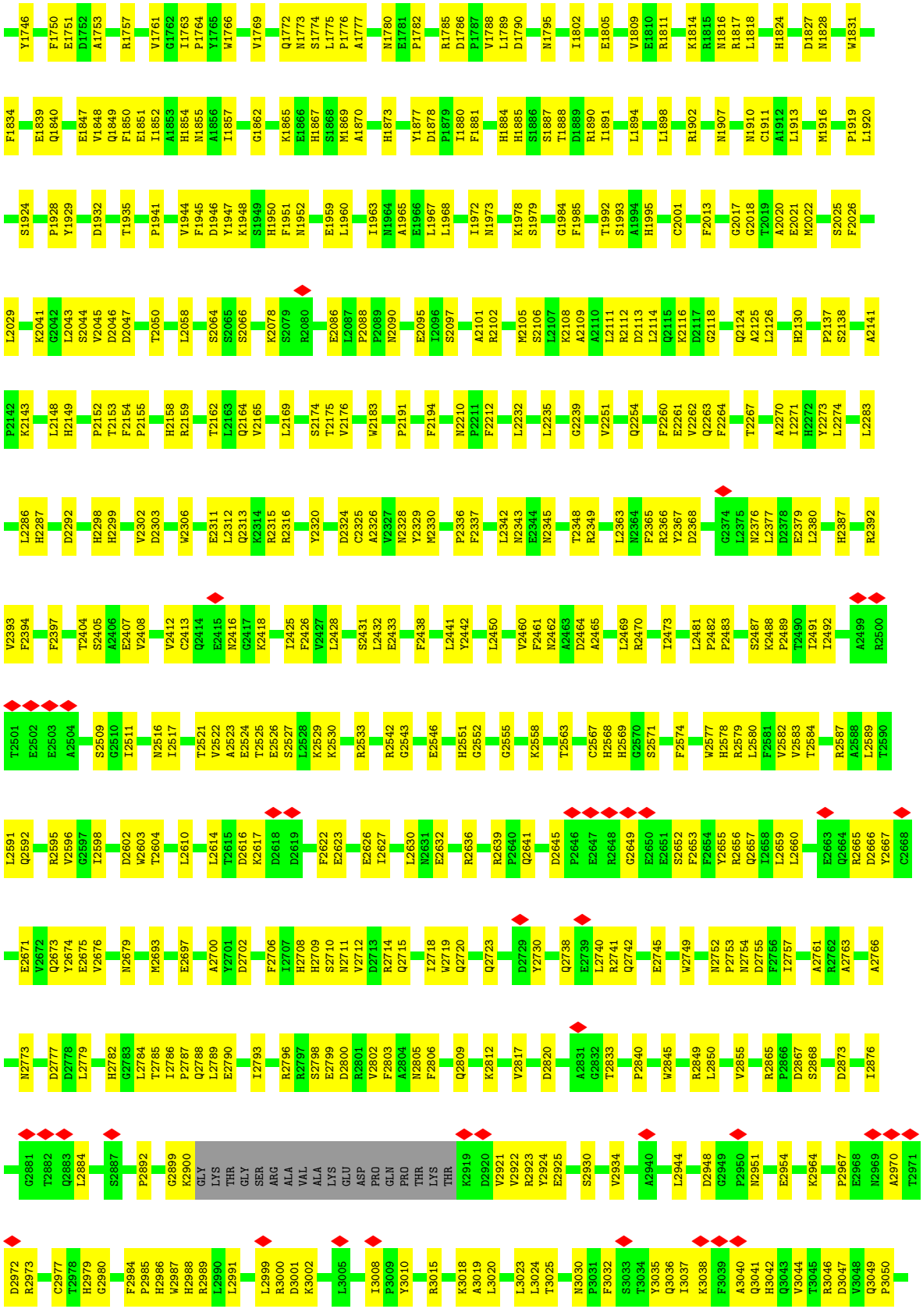
• Molecule 1: Hemocyanin

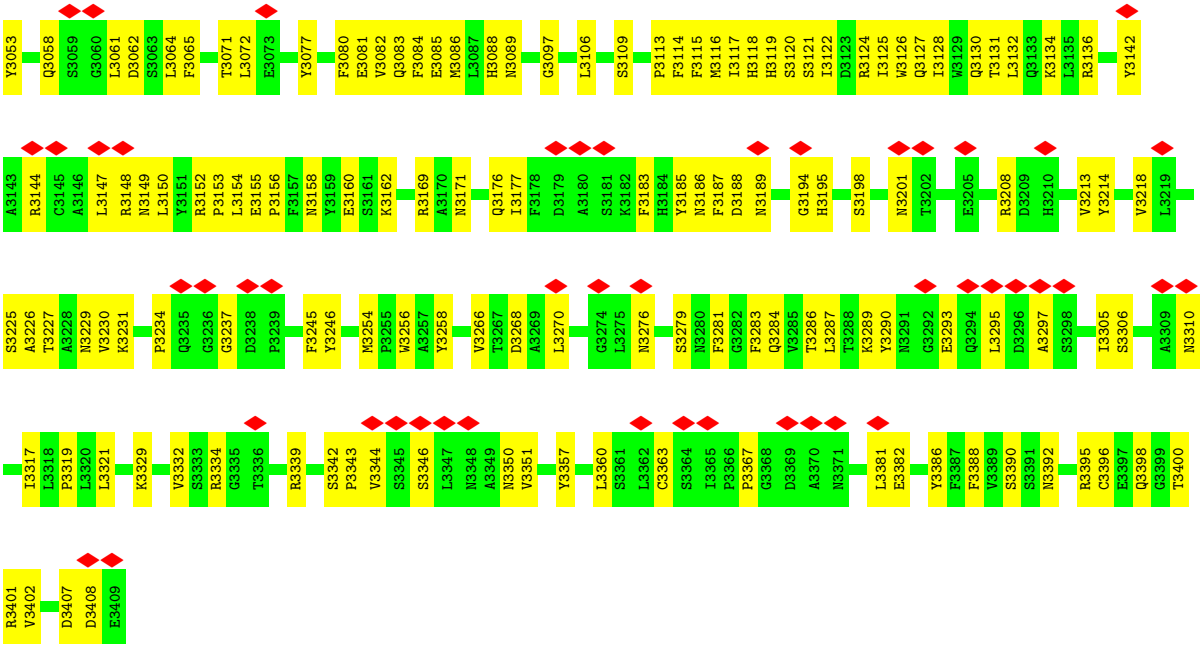
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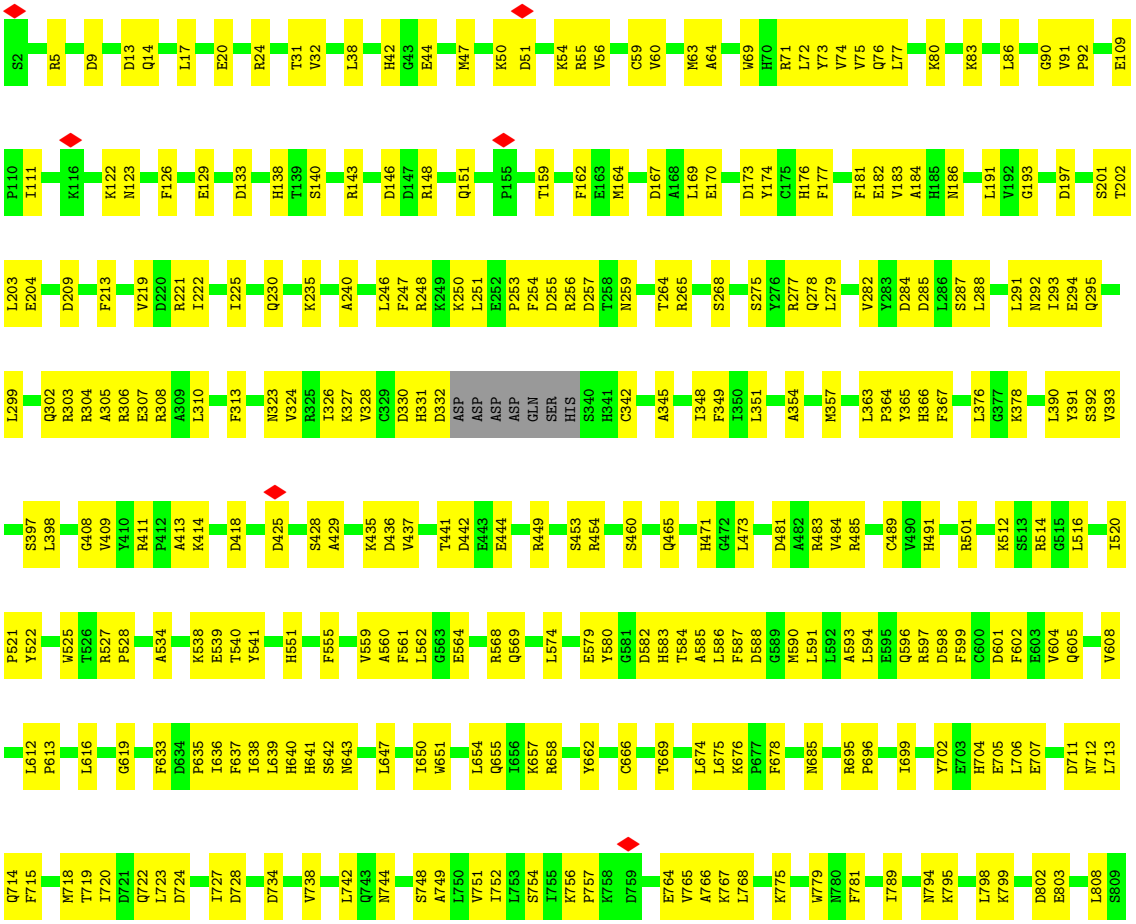

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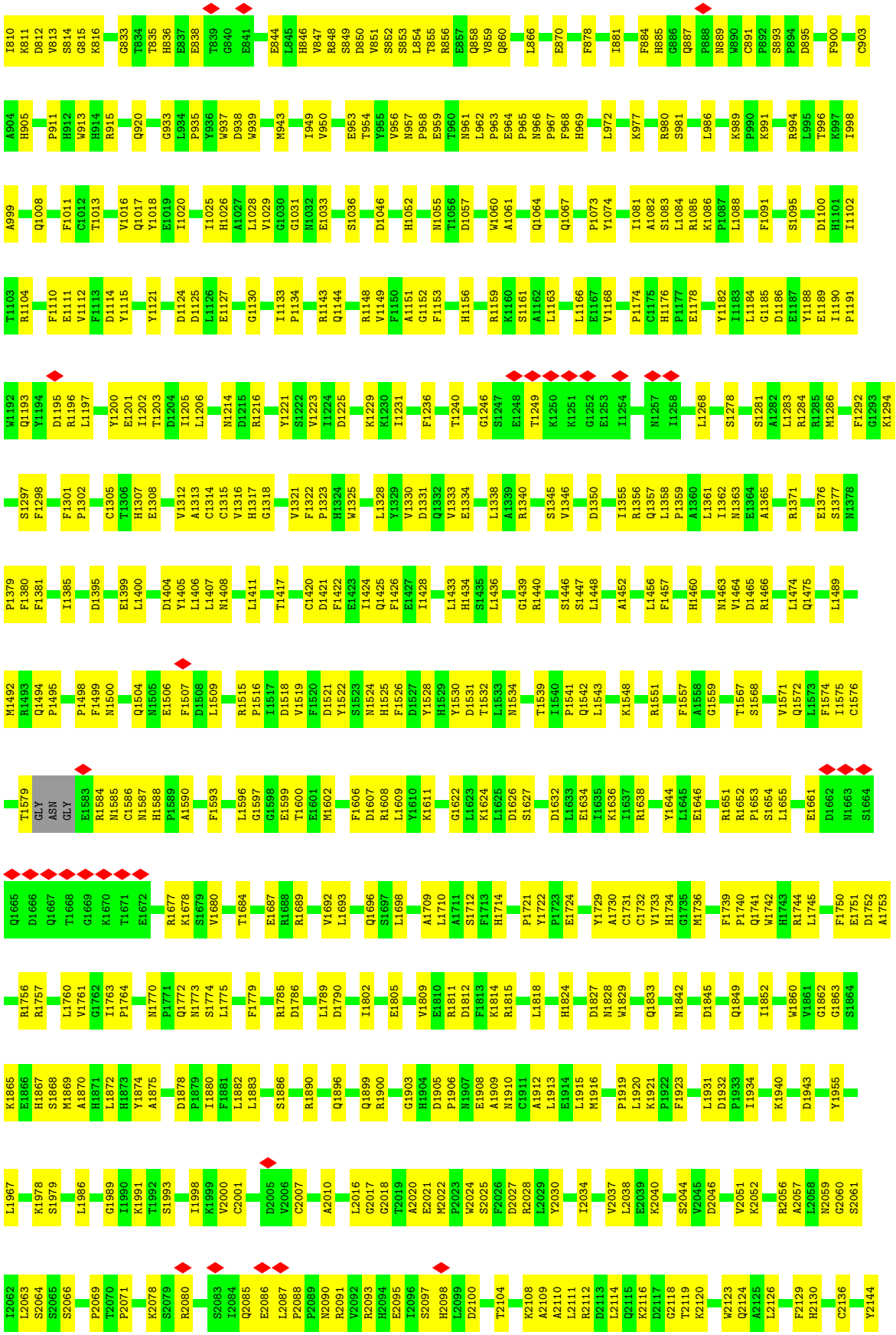


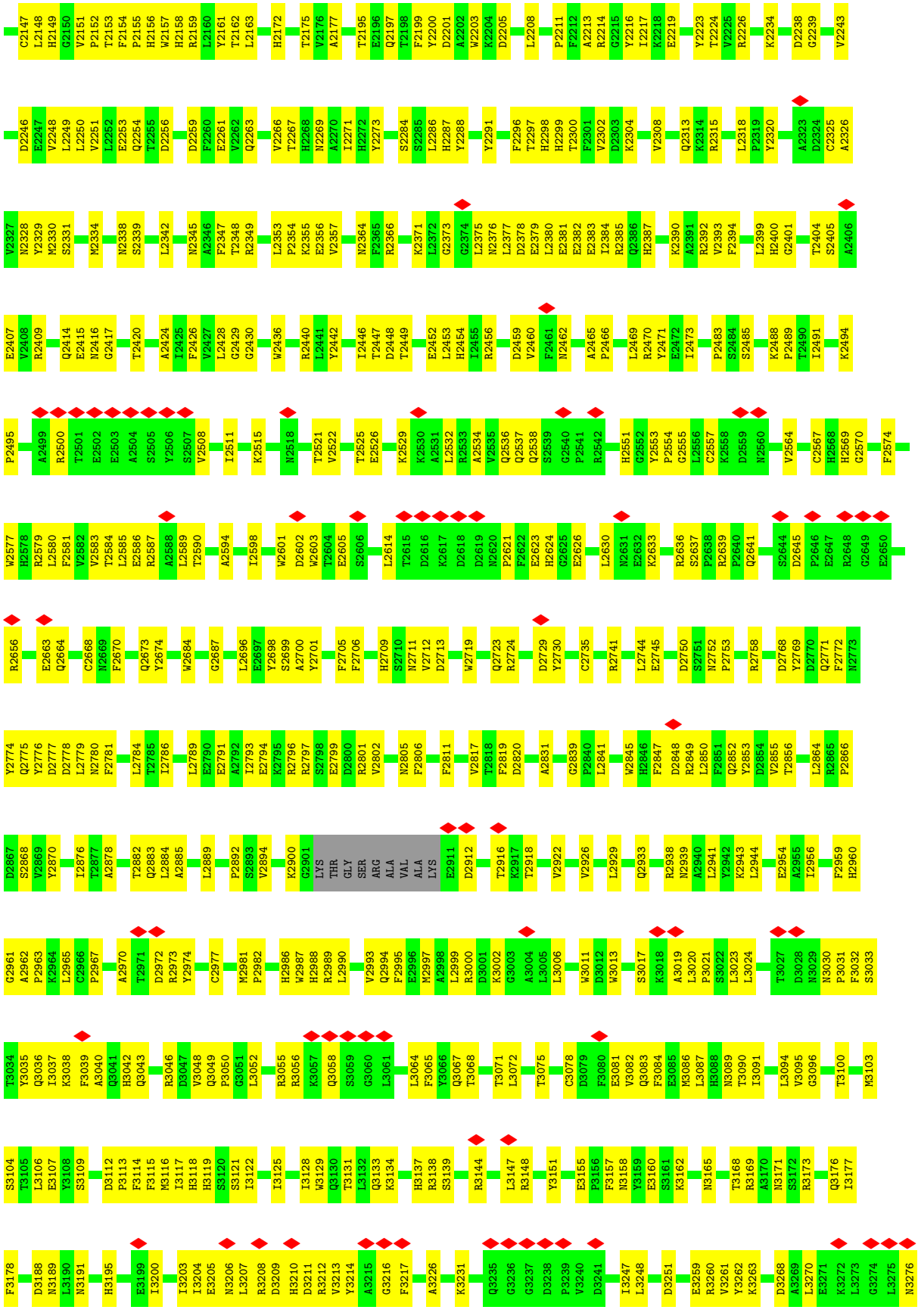
• Molecule 1: Hemocyanin

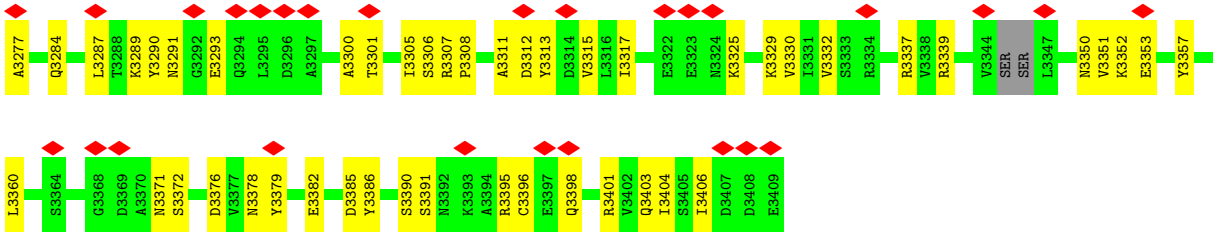
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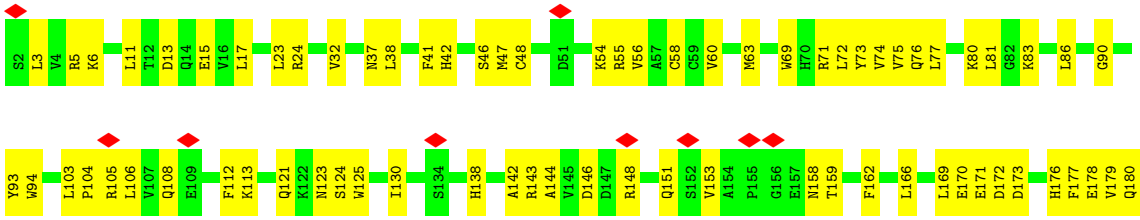

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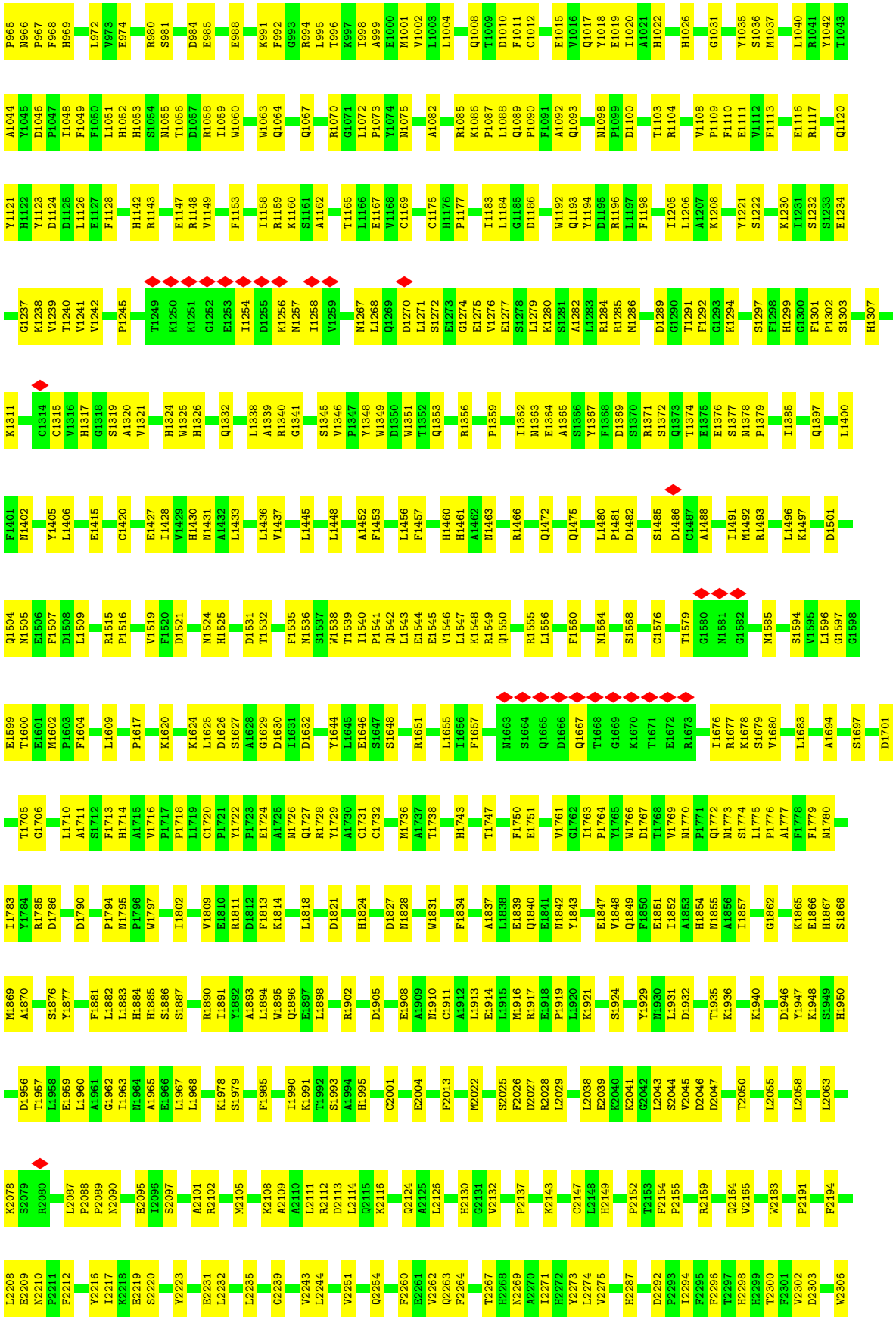


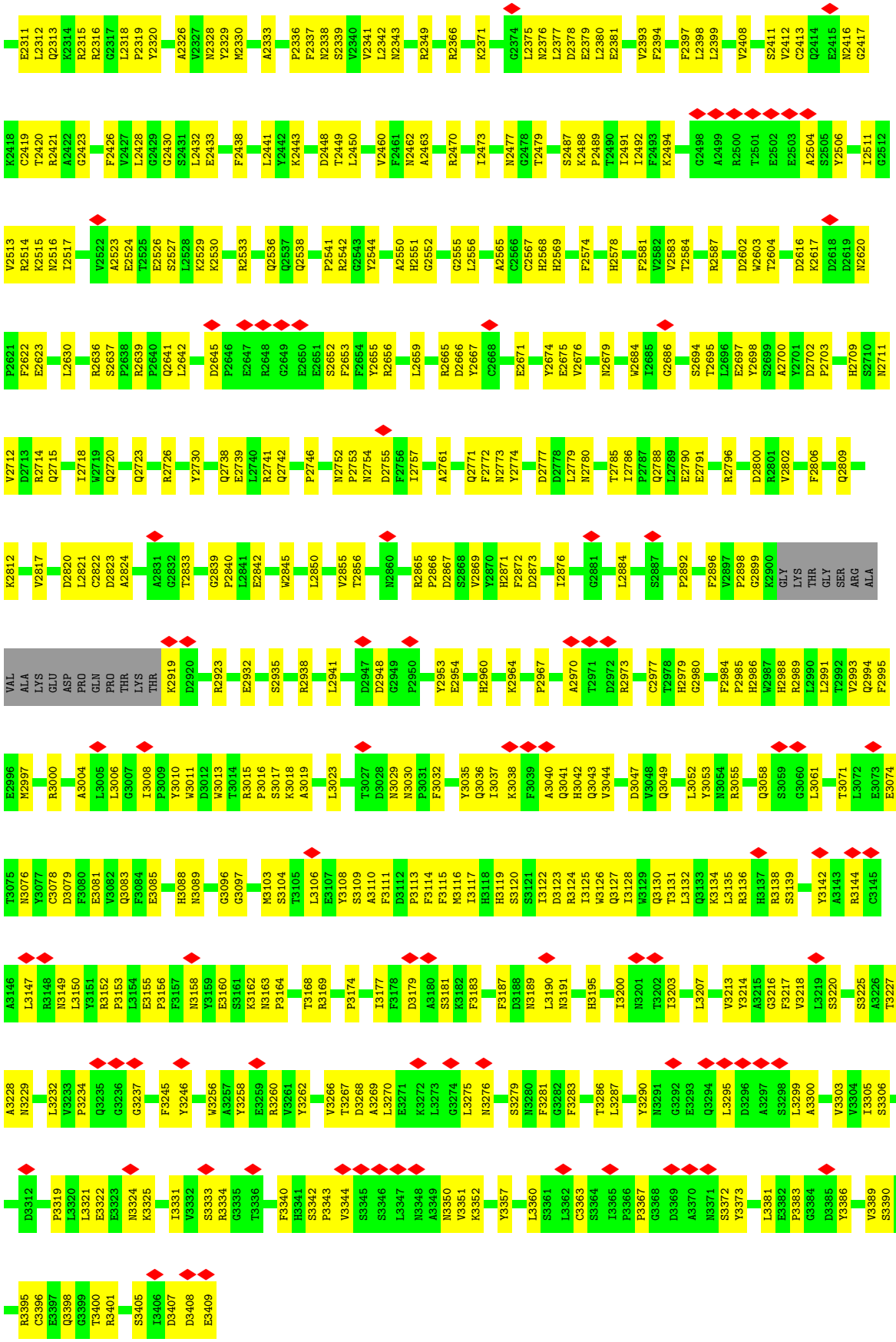

• Molecule 1: Hemocyanin

Chain F:



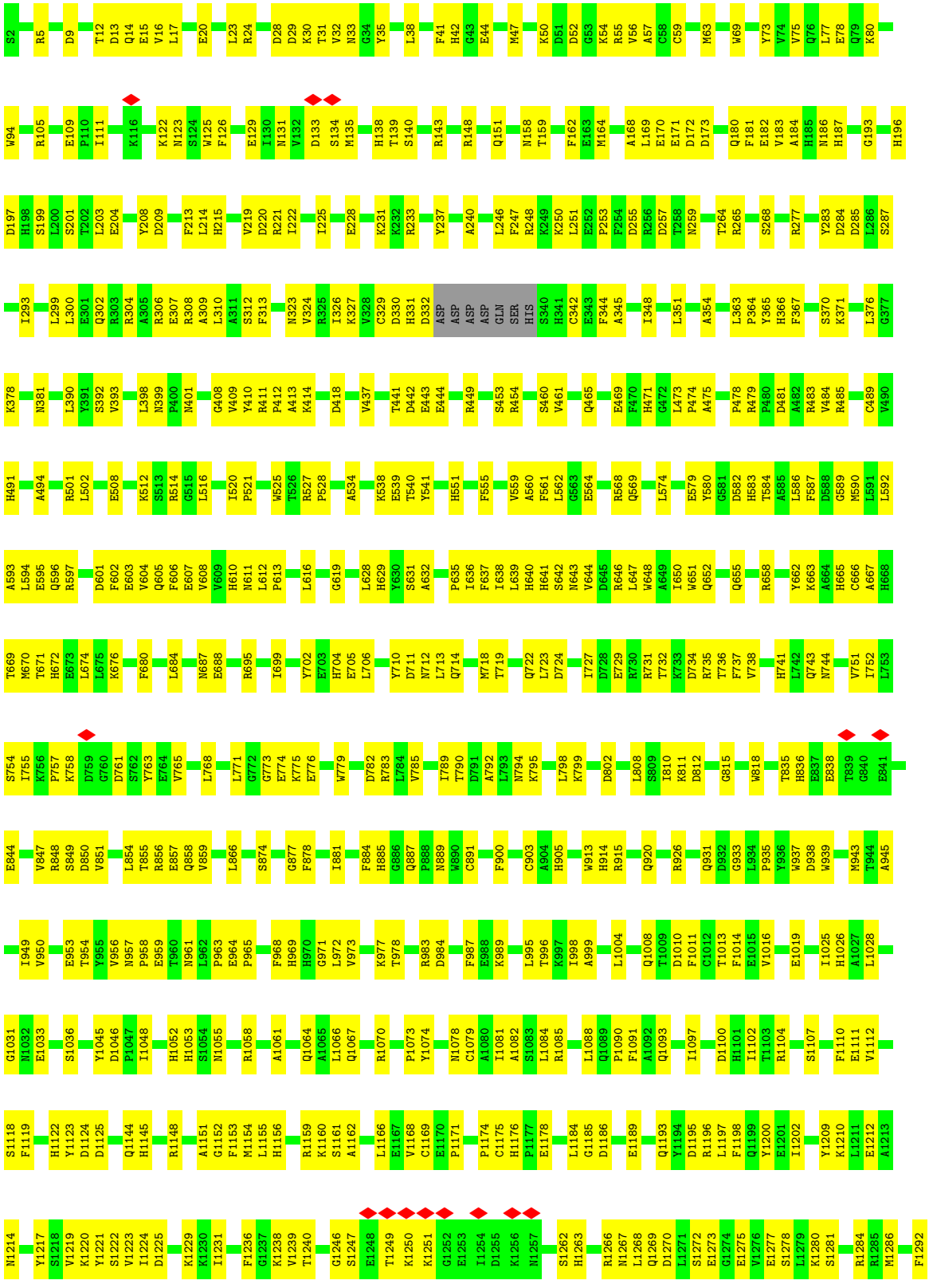

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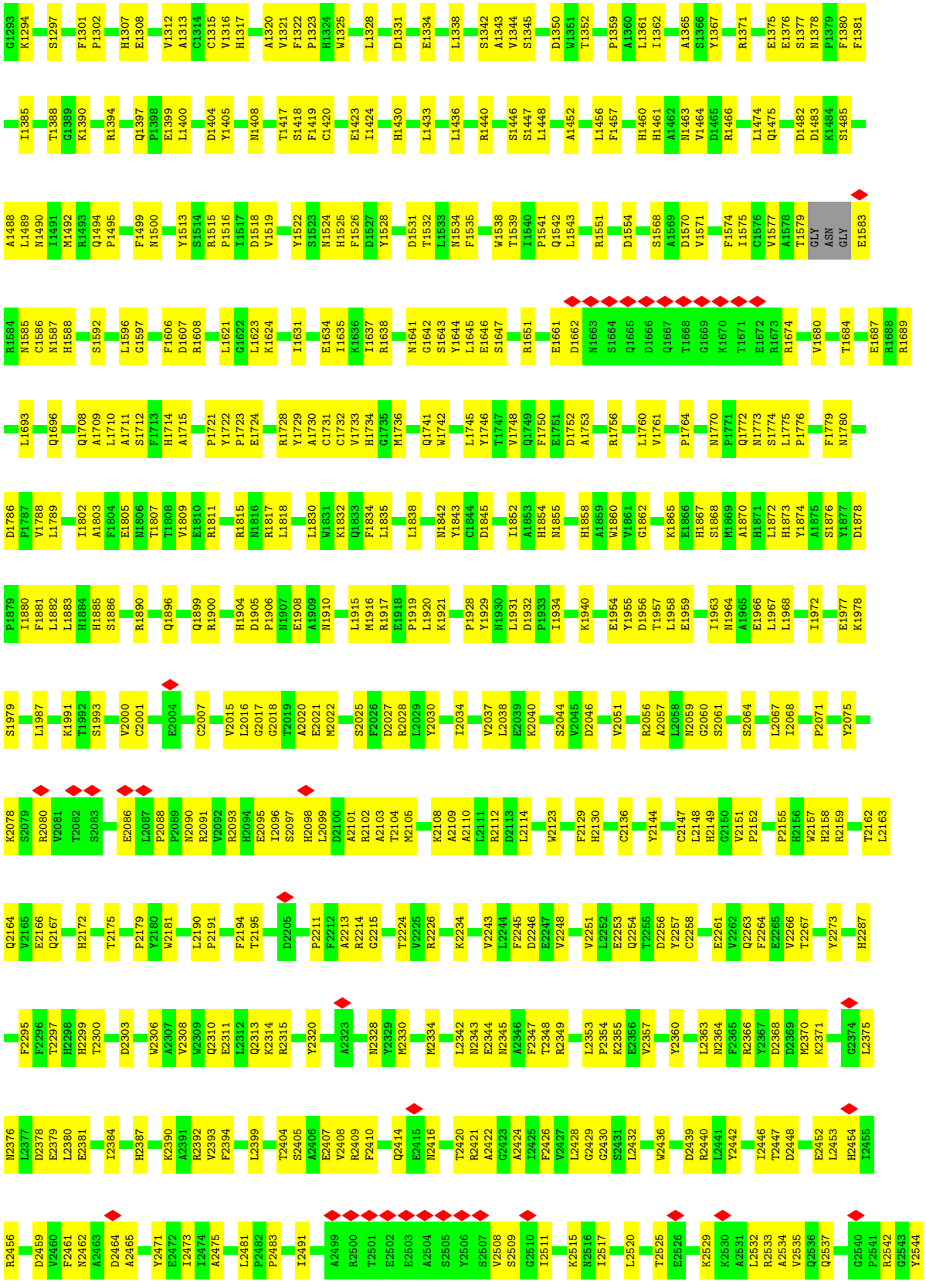

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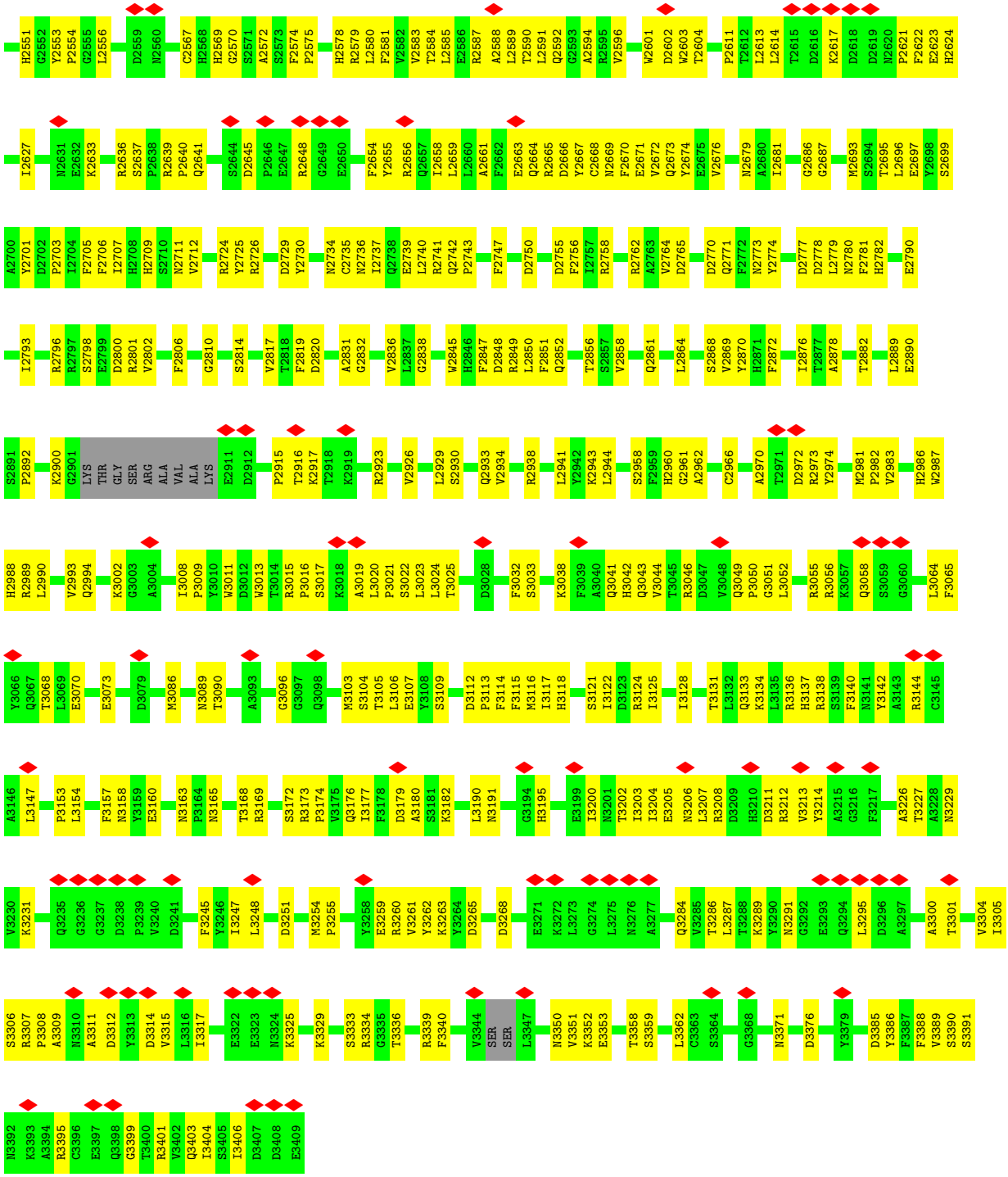
• Molecule 1: Hemocyanin

Chain G:



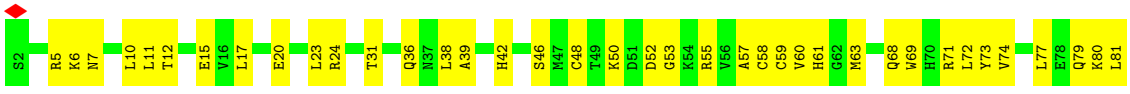


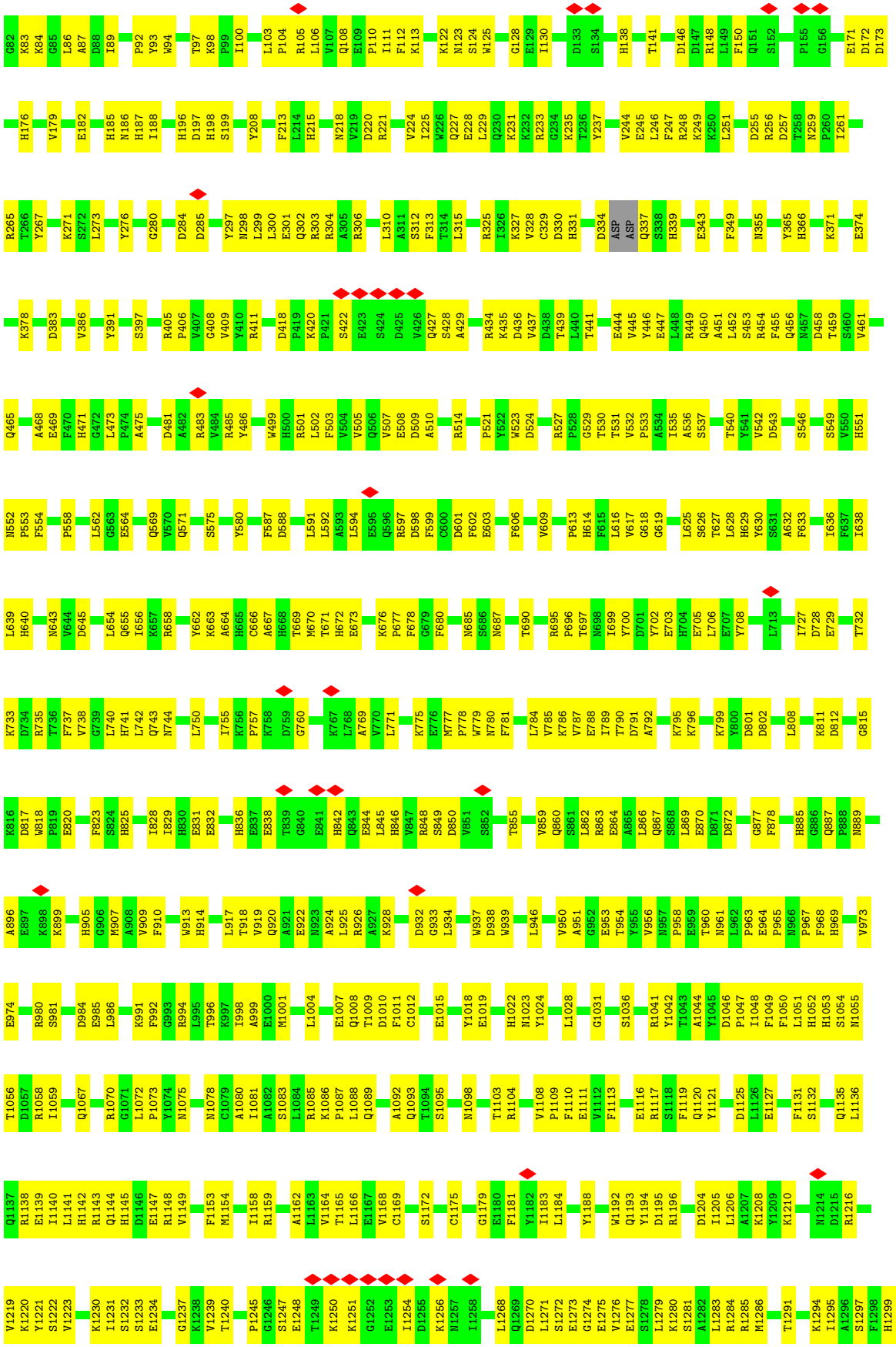


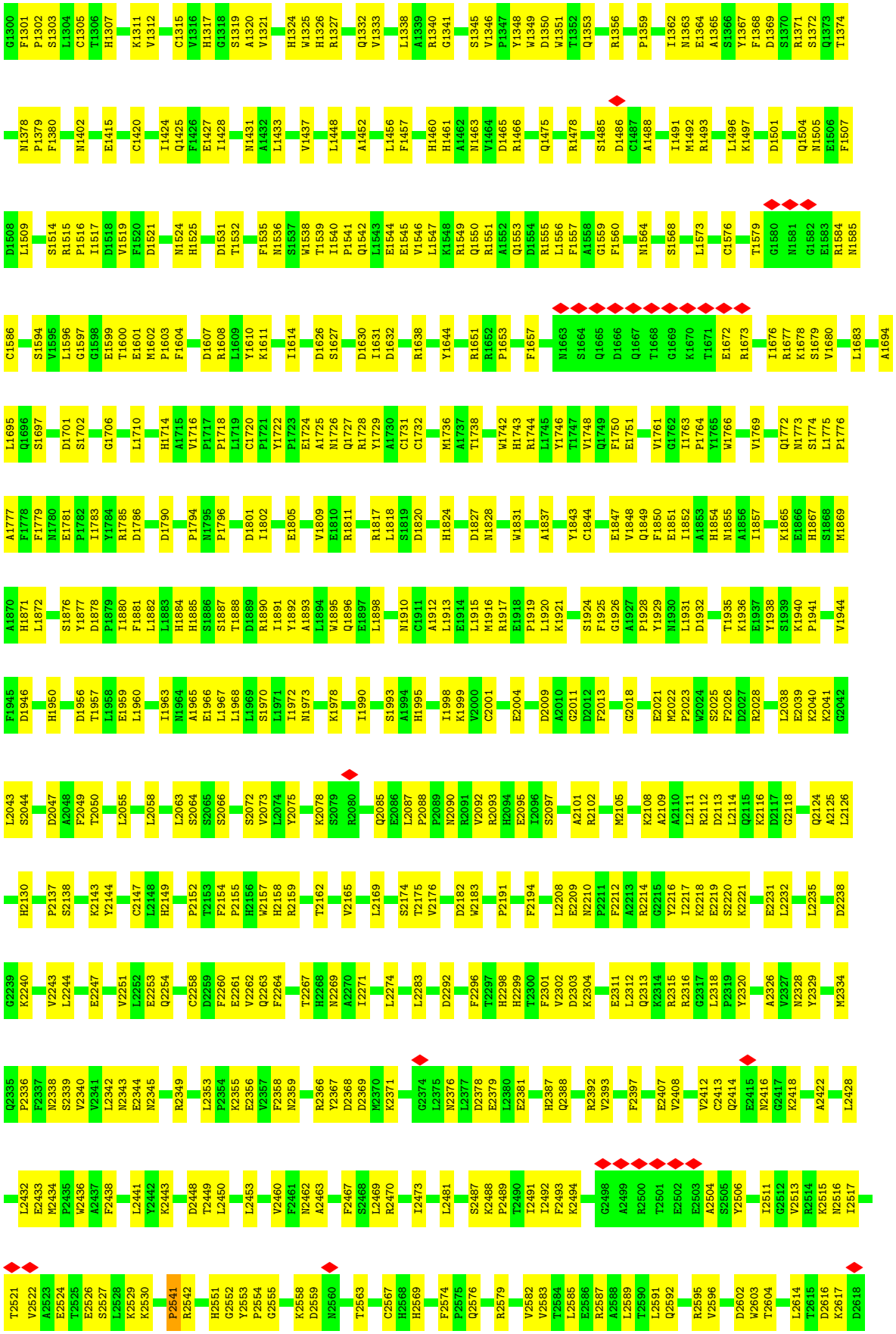
• Molecule 1: Hemocyanin

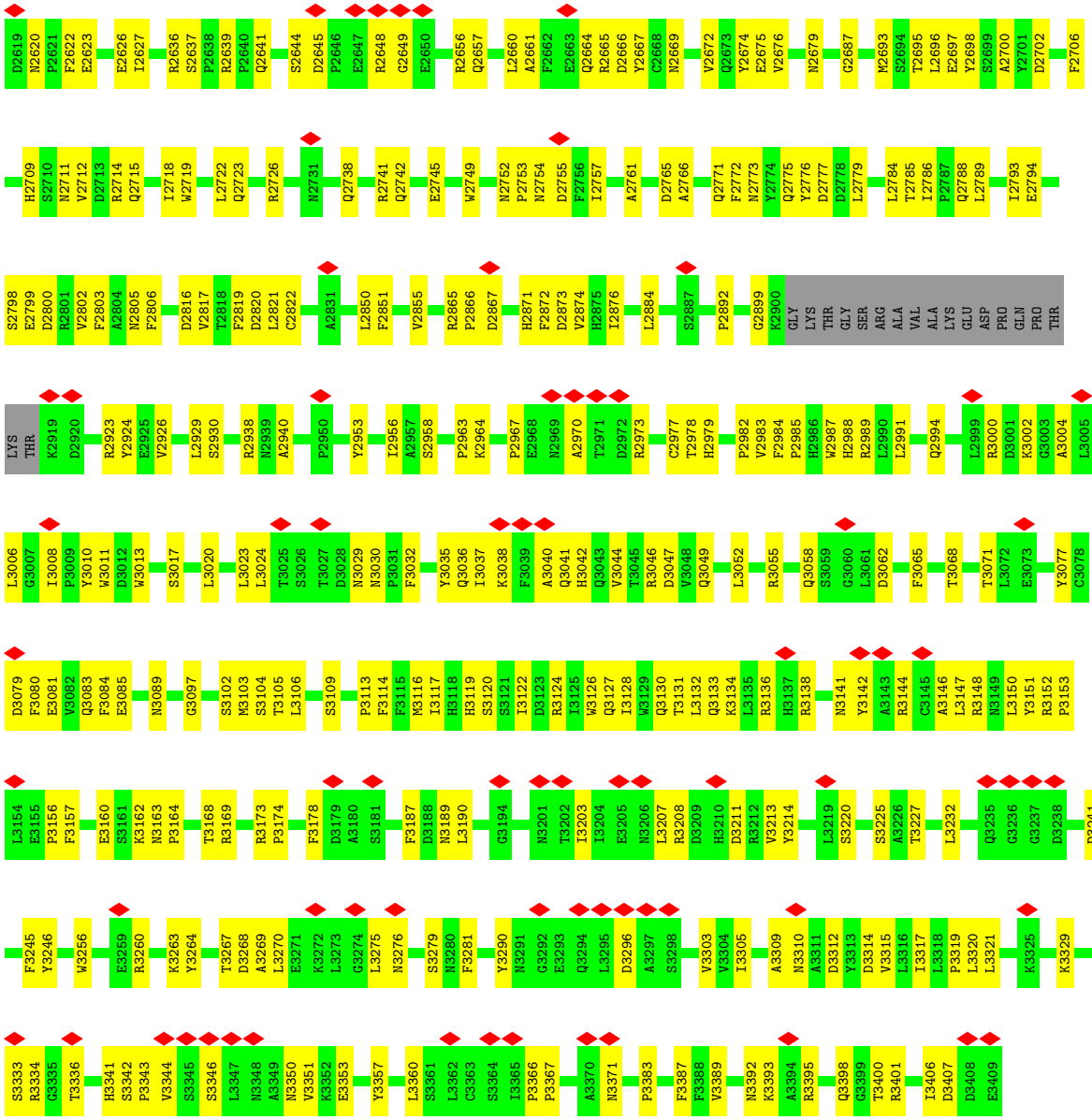
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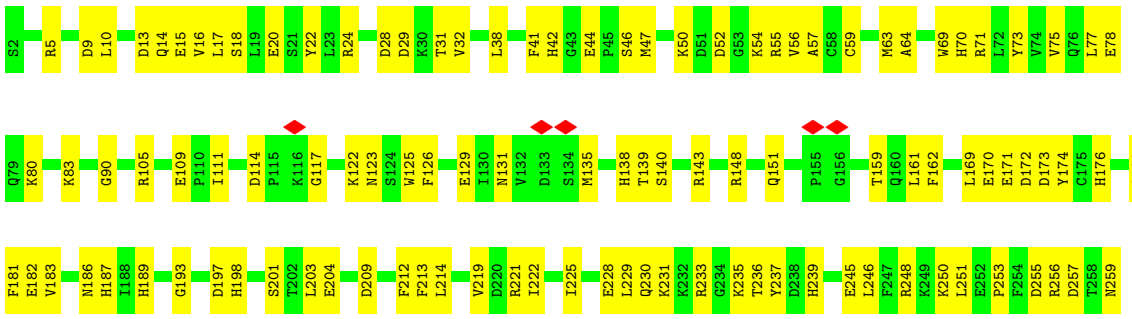

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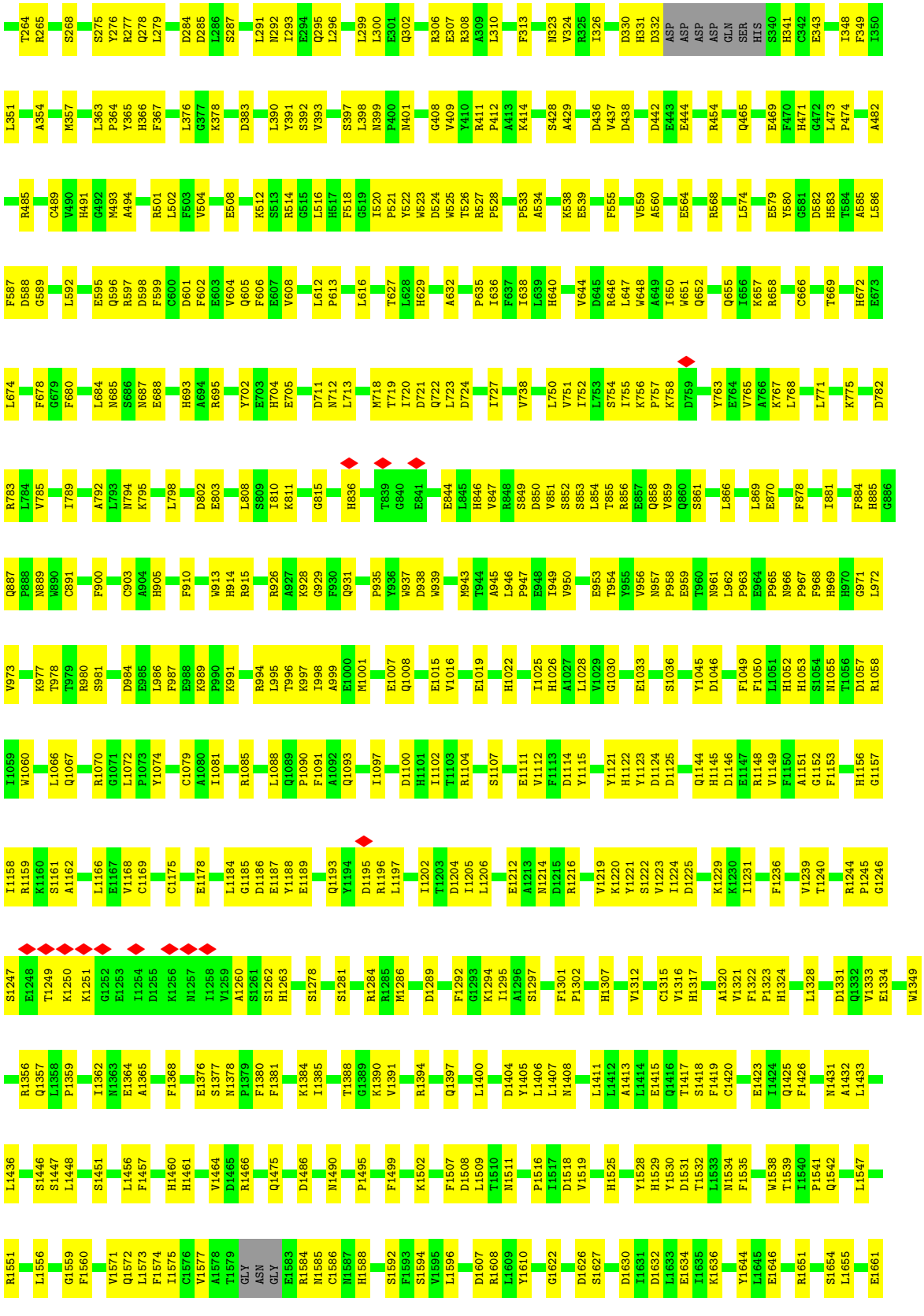


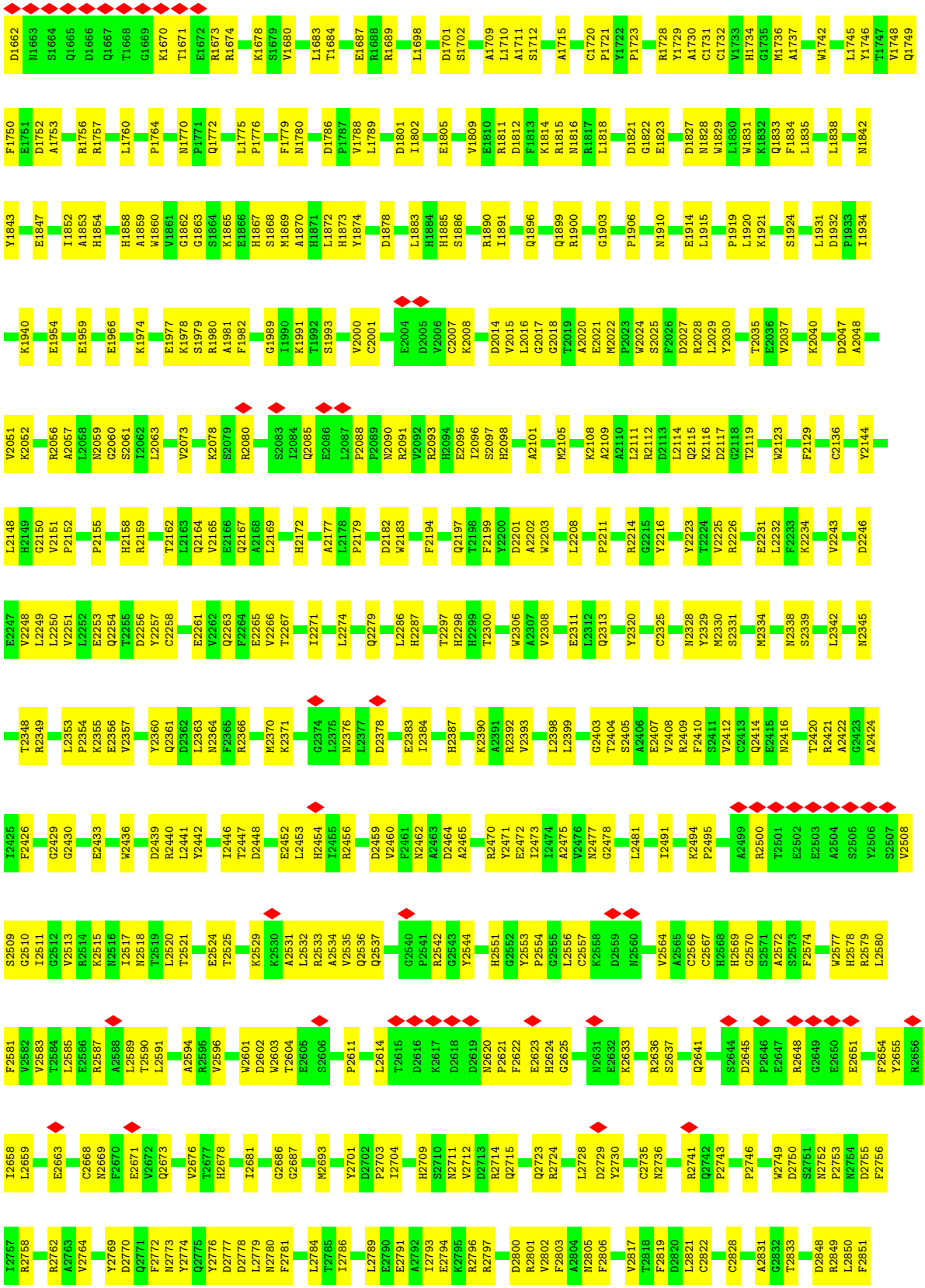
• Molecule 1: Hemocyanin

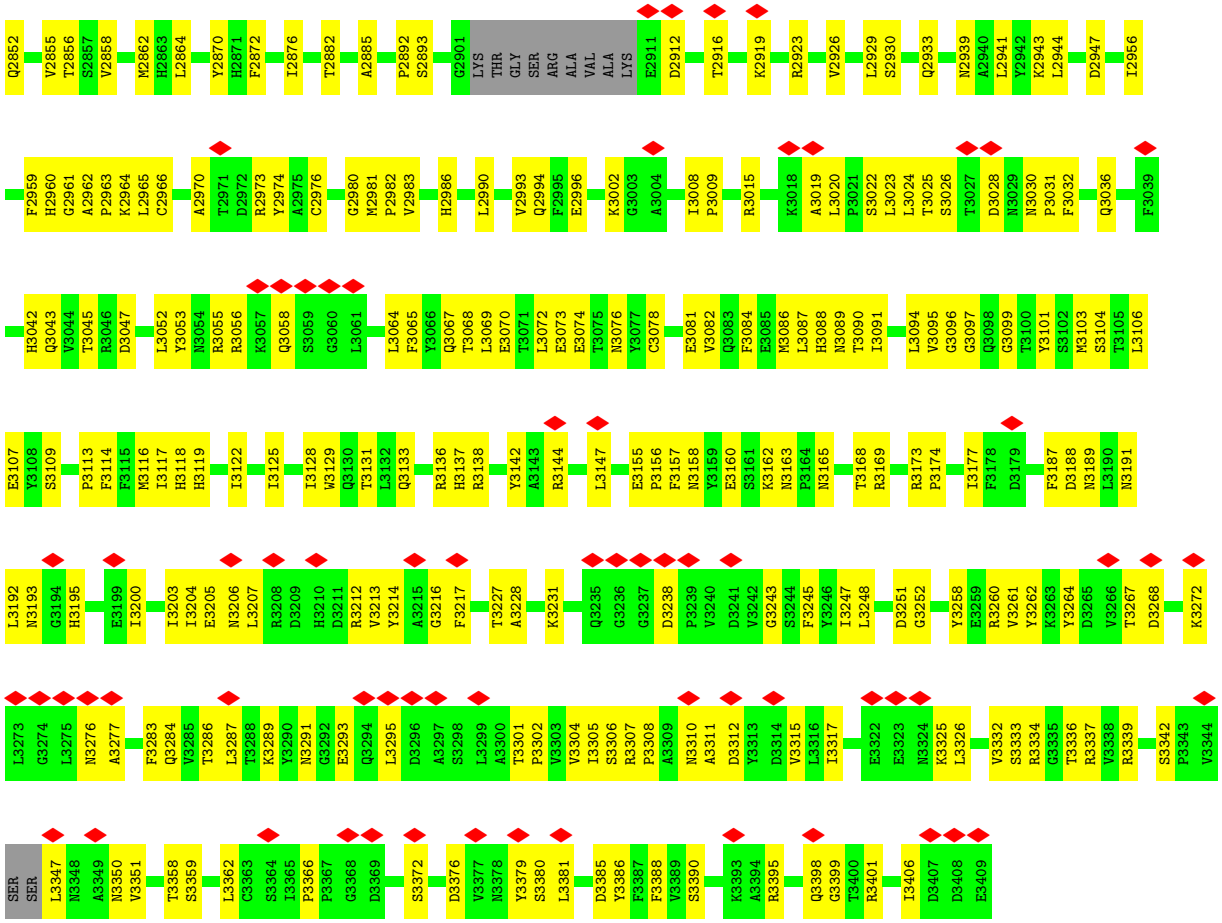
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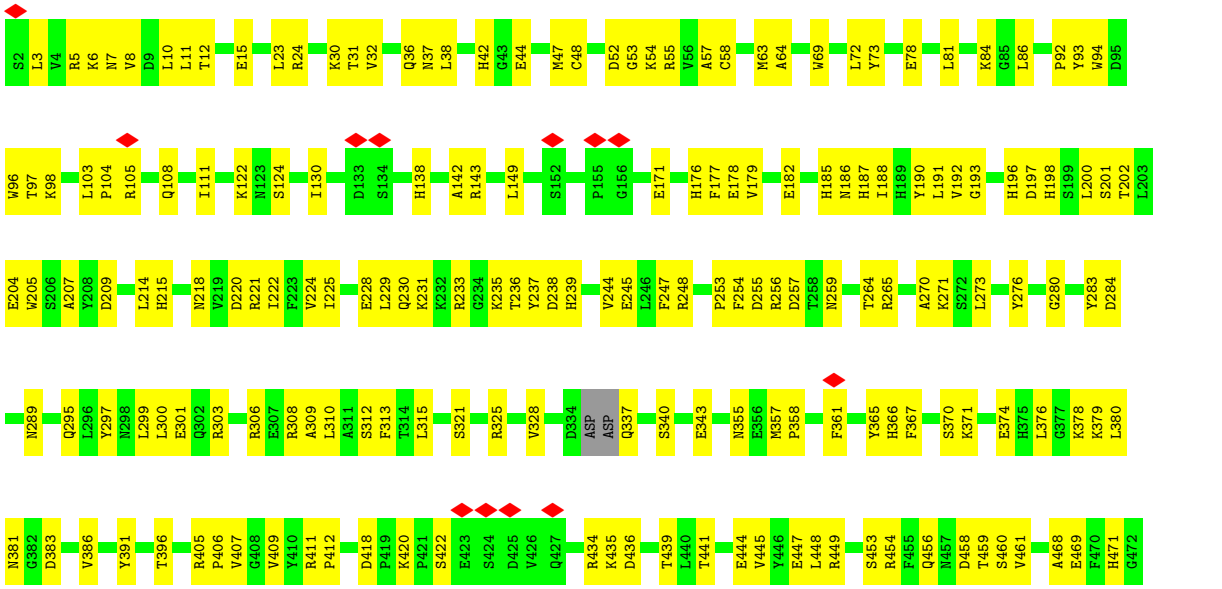

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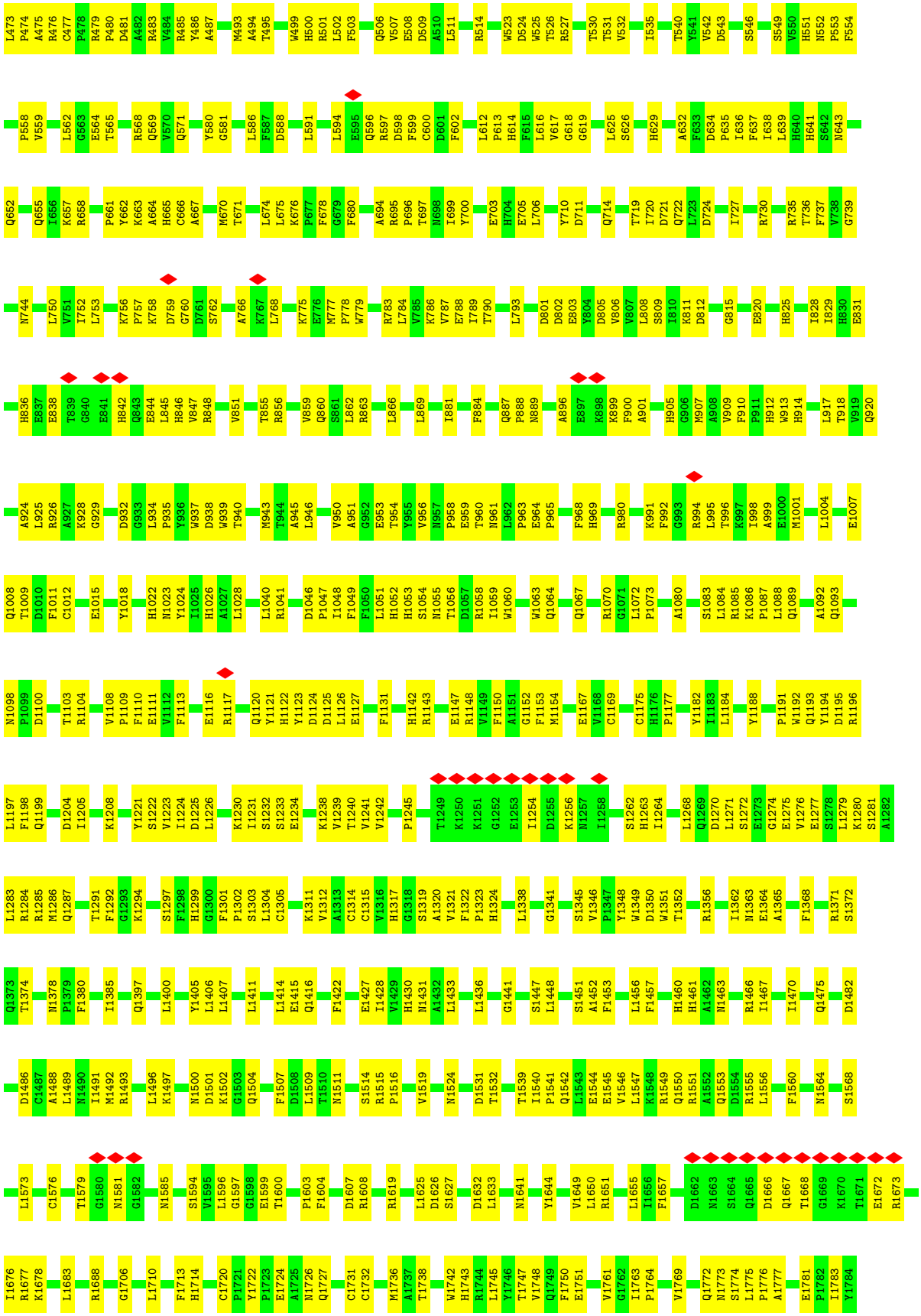


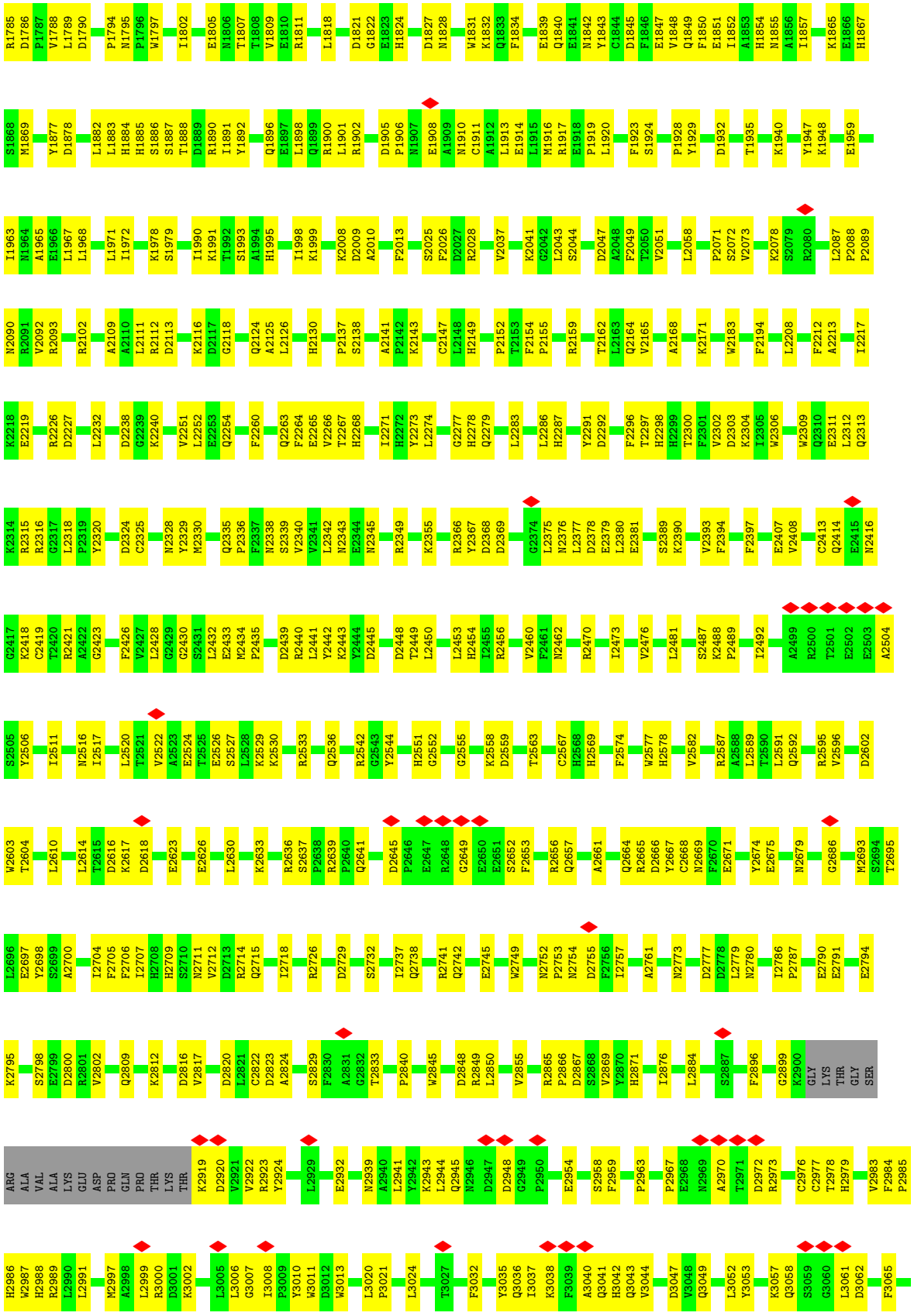
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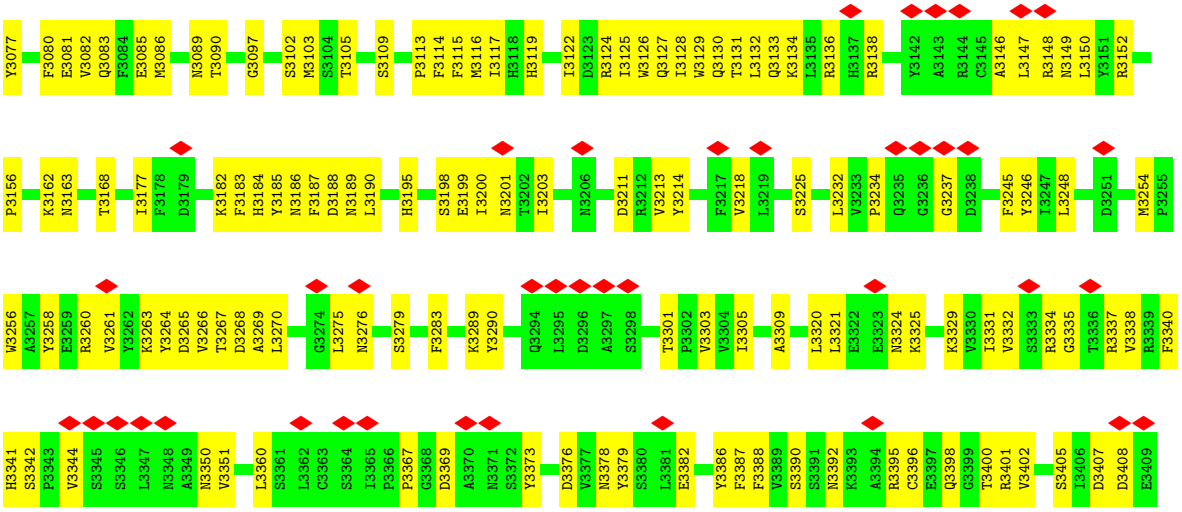
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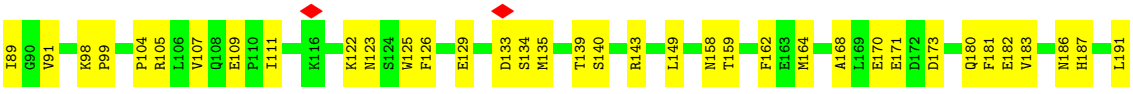


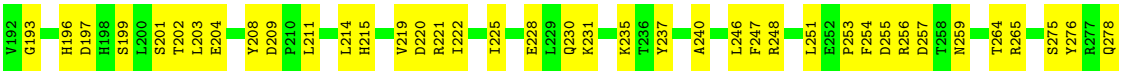
• Molecule 1: Hemocyanin

Chain K:













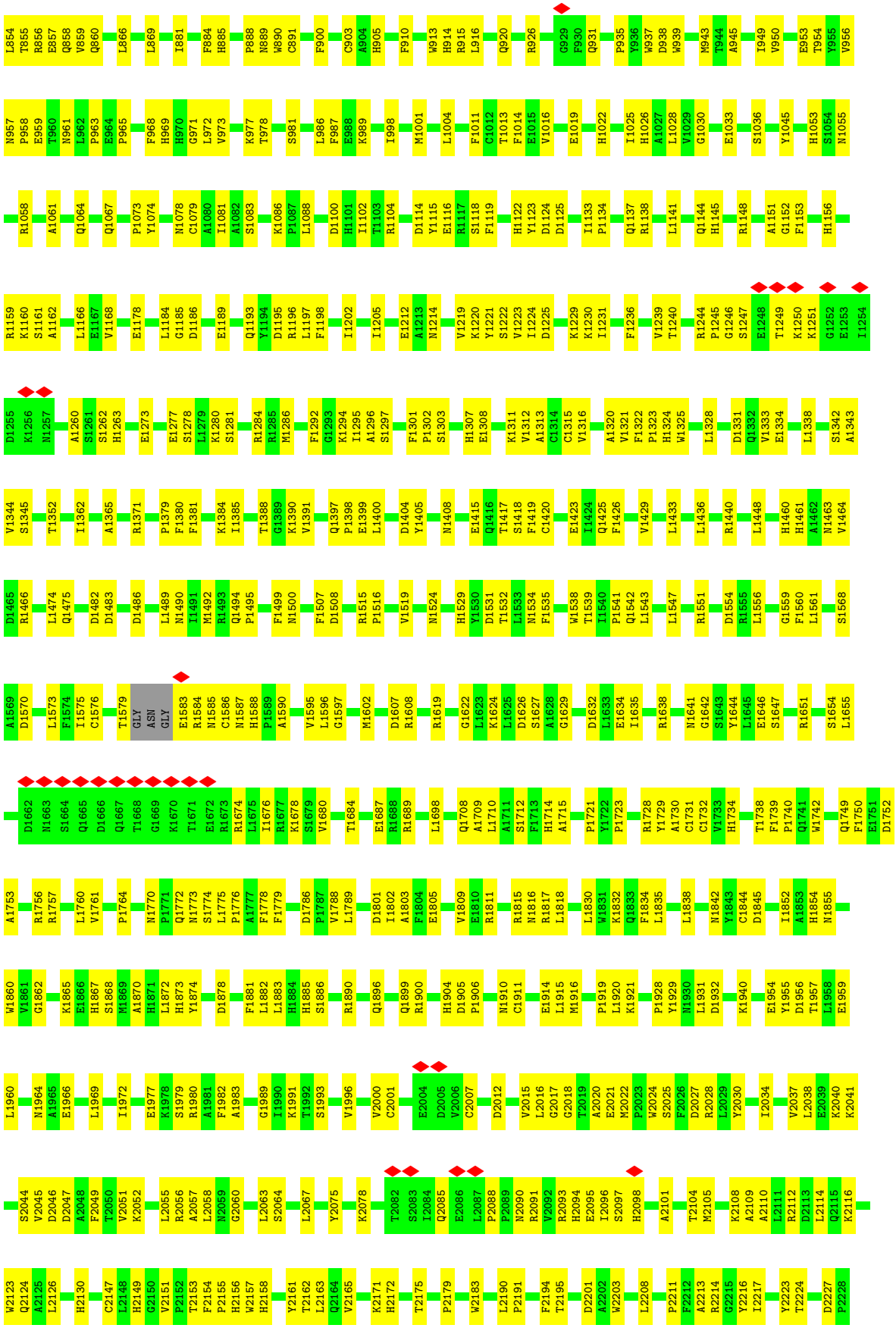


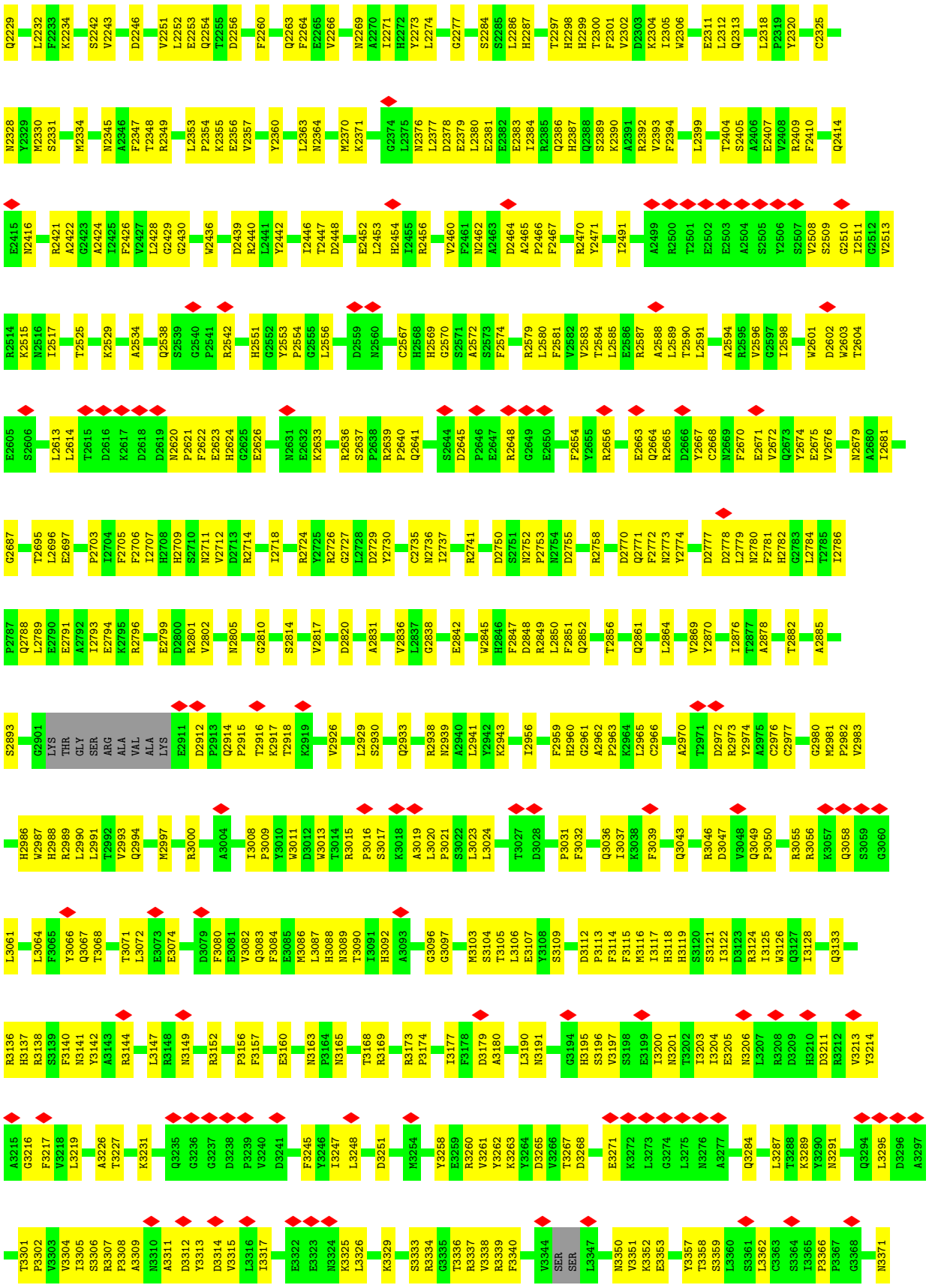


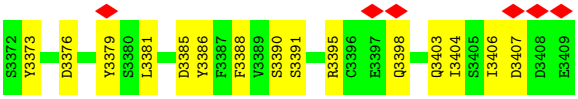







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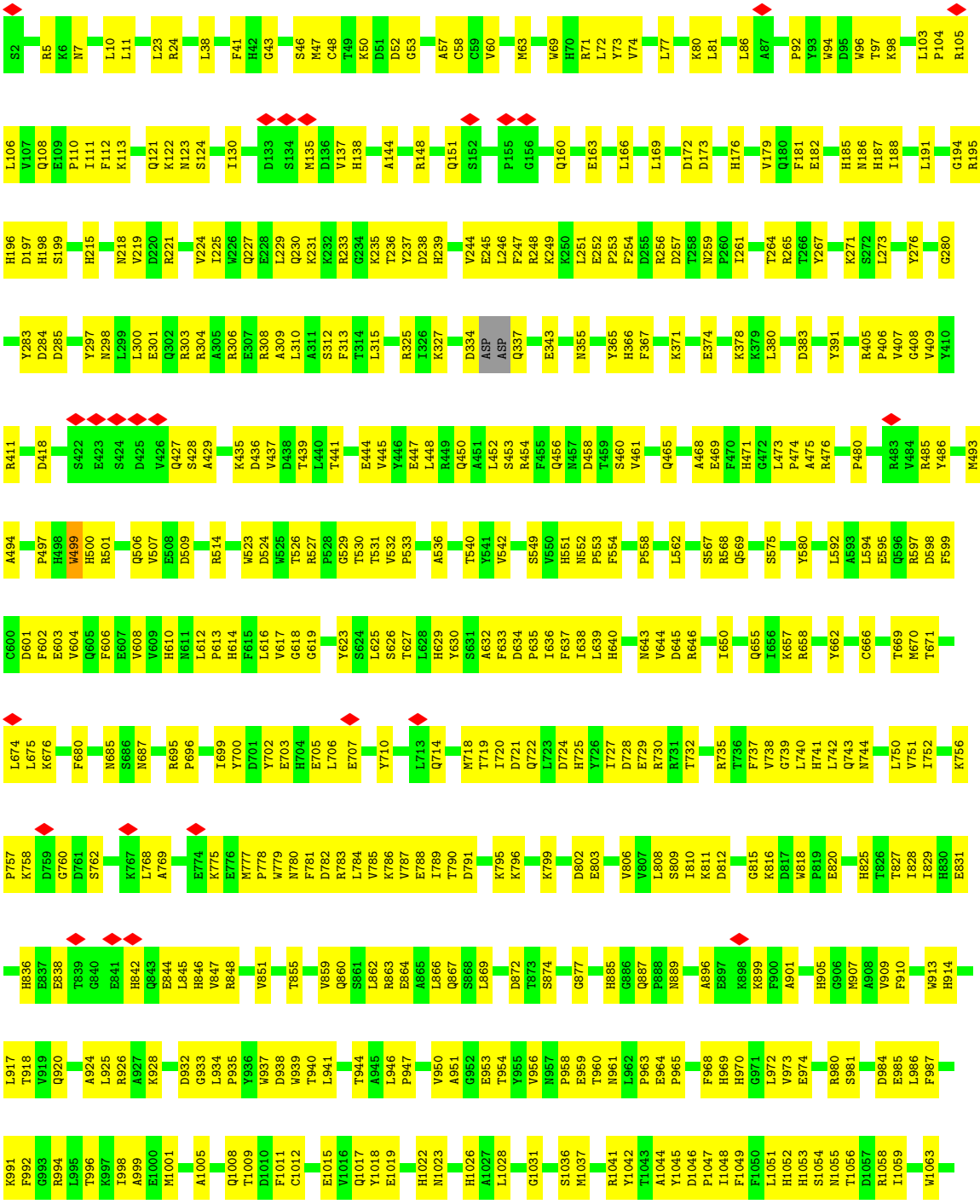


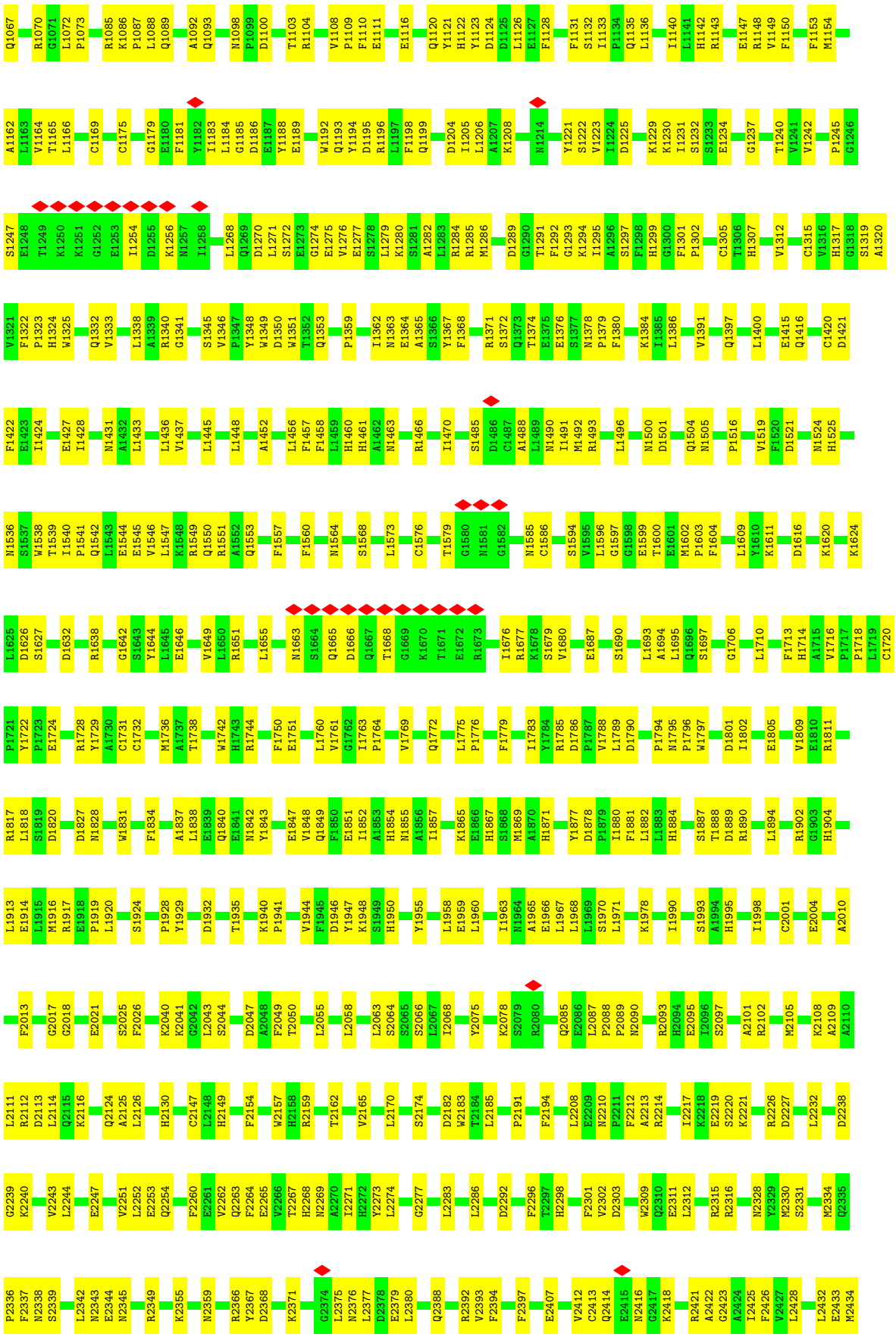


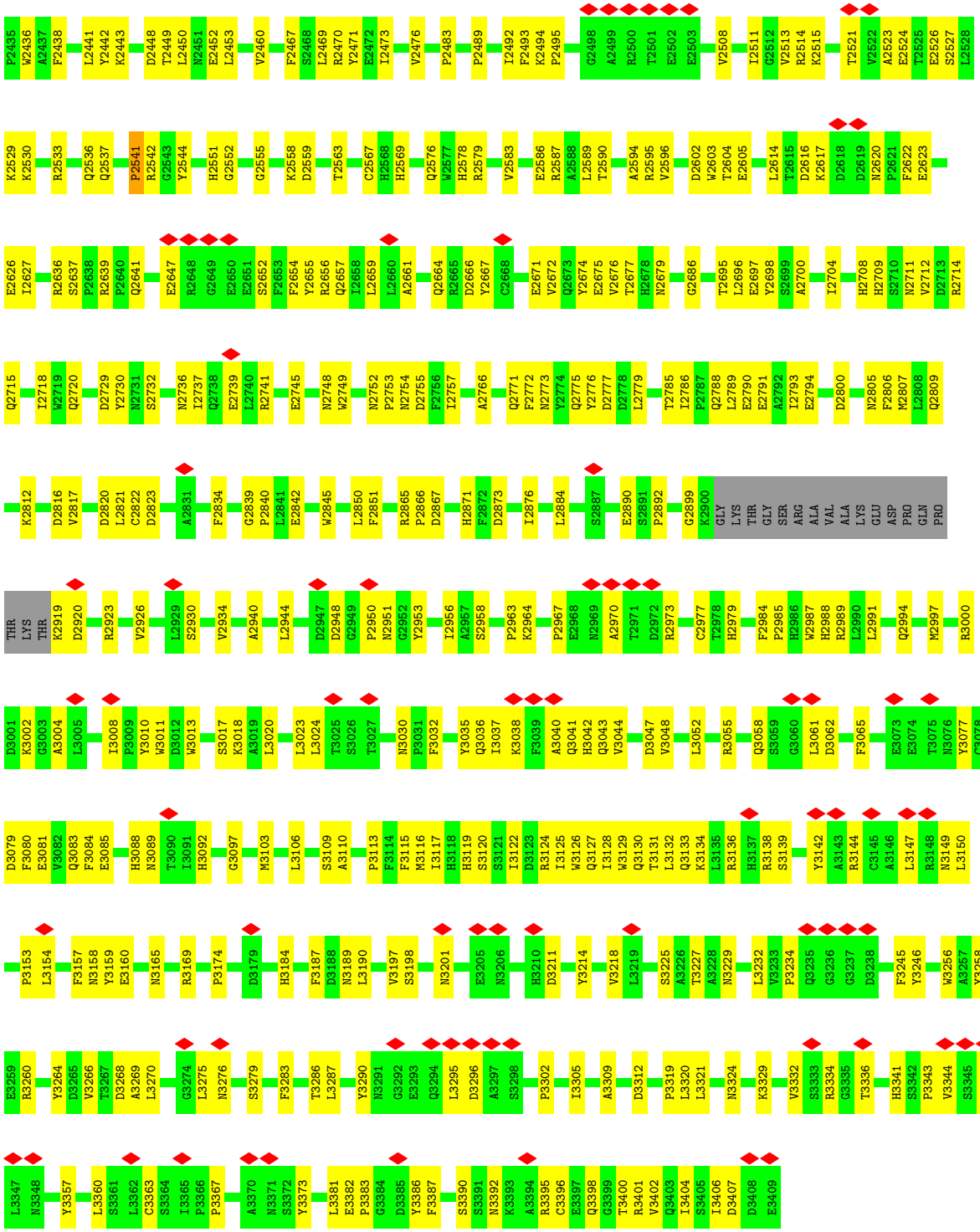
• Molecule 1: Hemocyanin

Chain L:



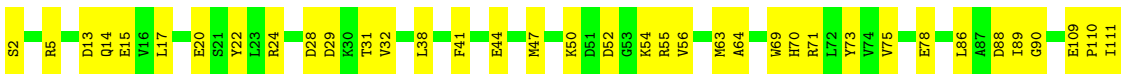


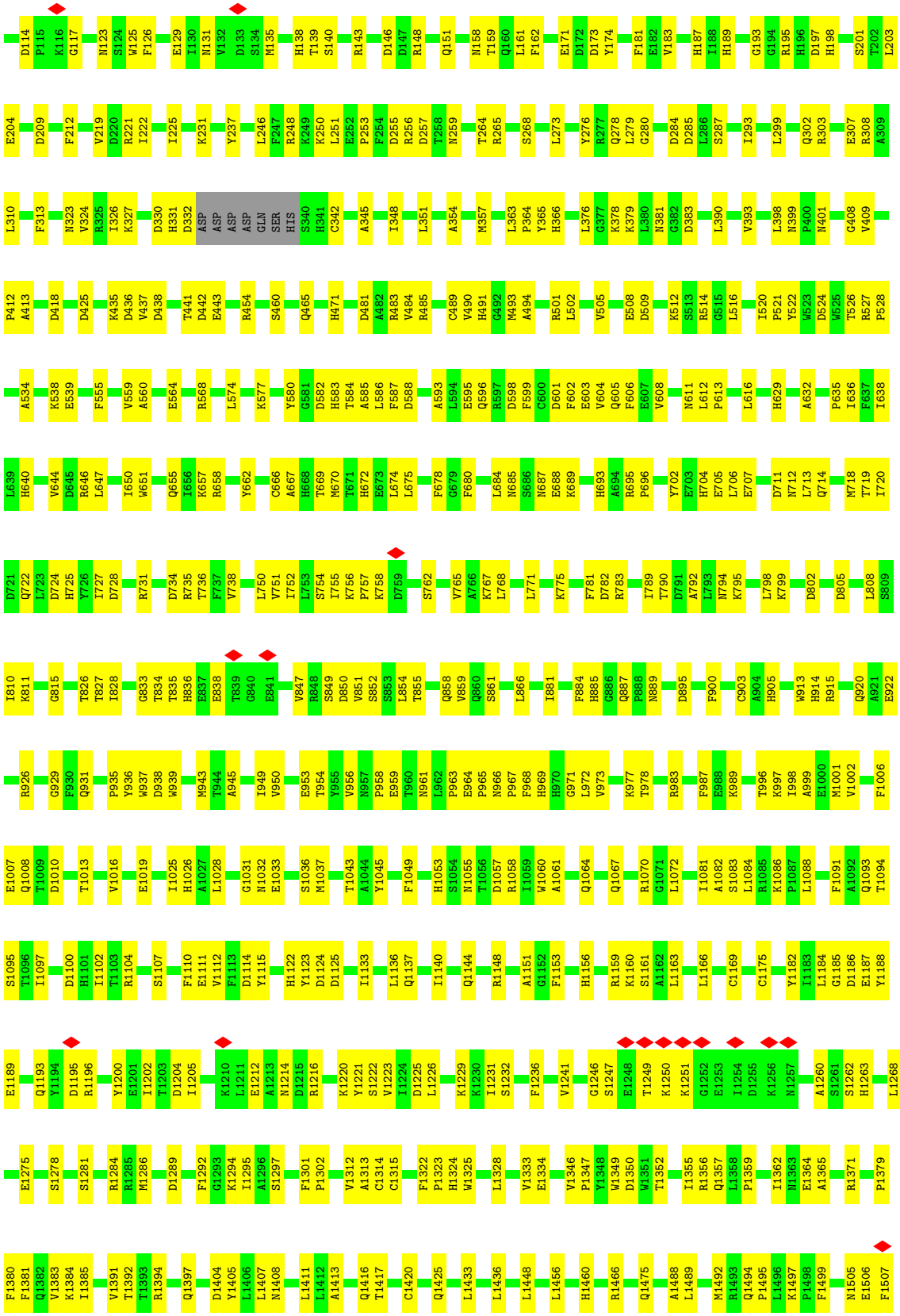


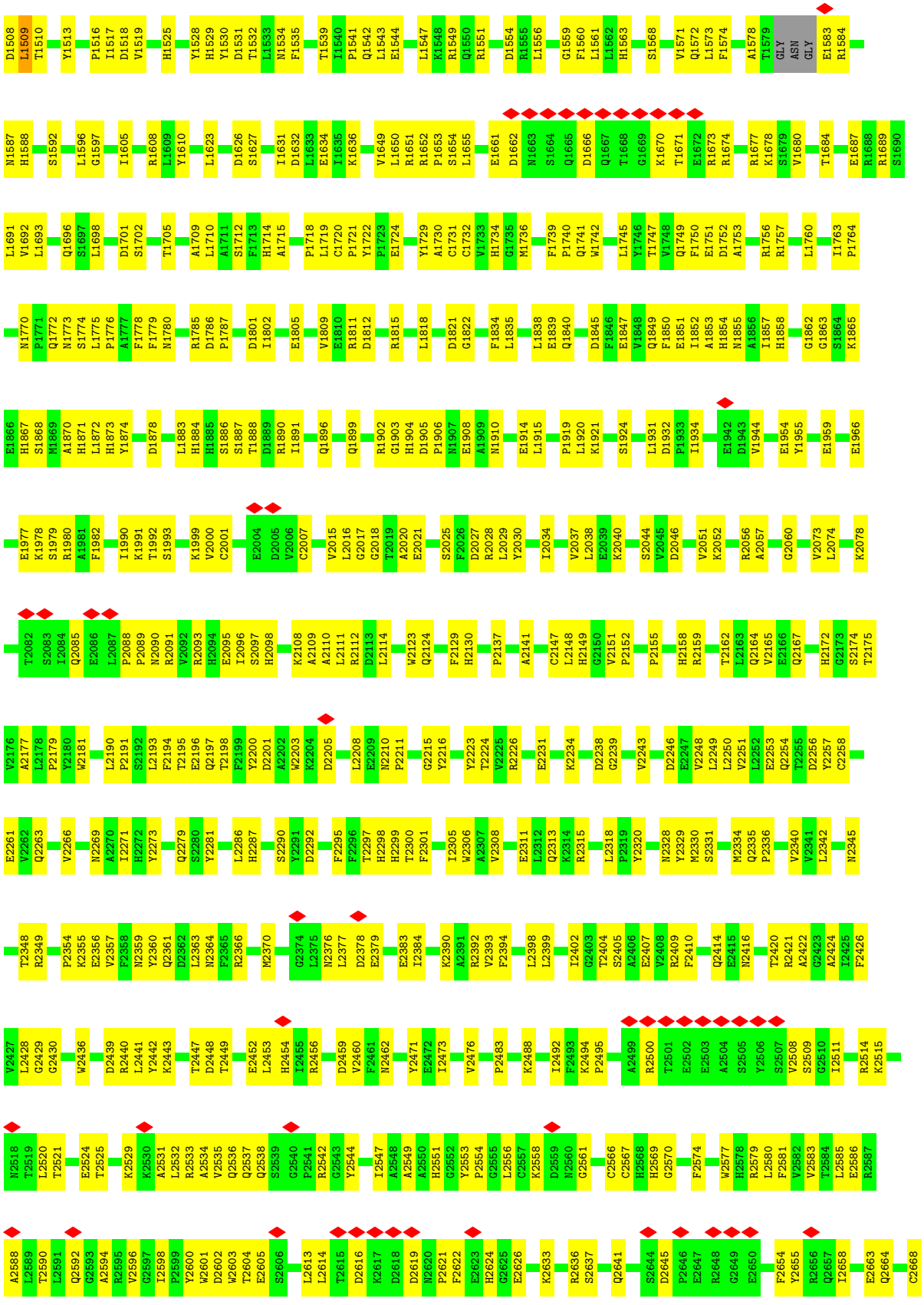
• Molecule 1: Hemocyanin

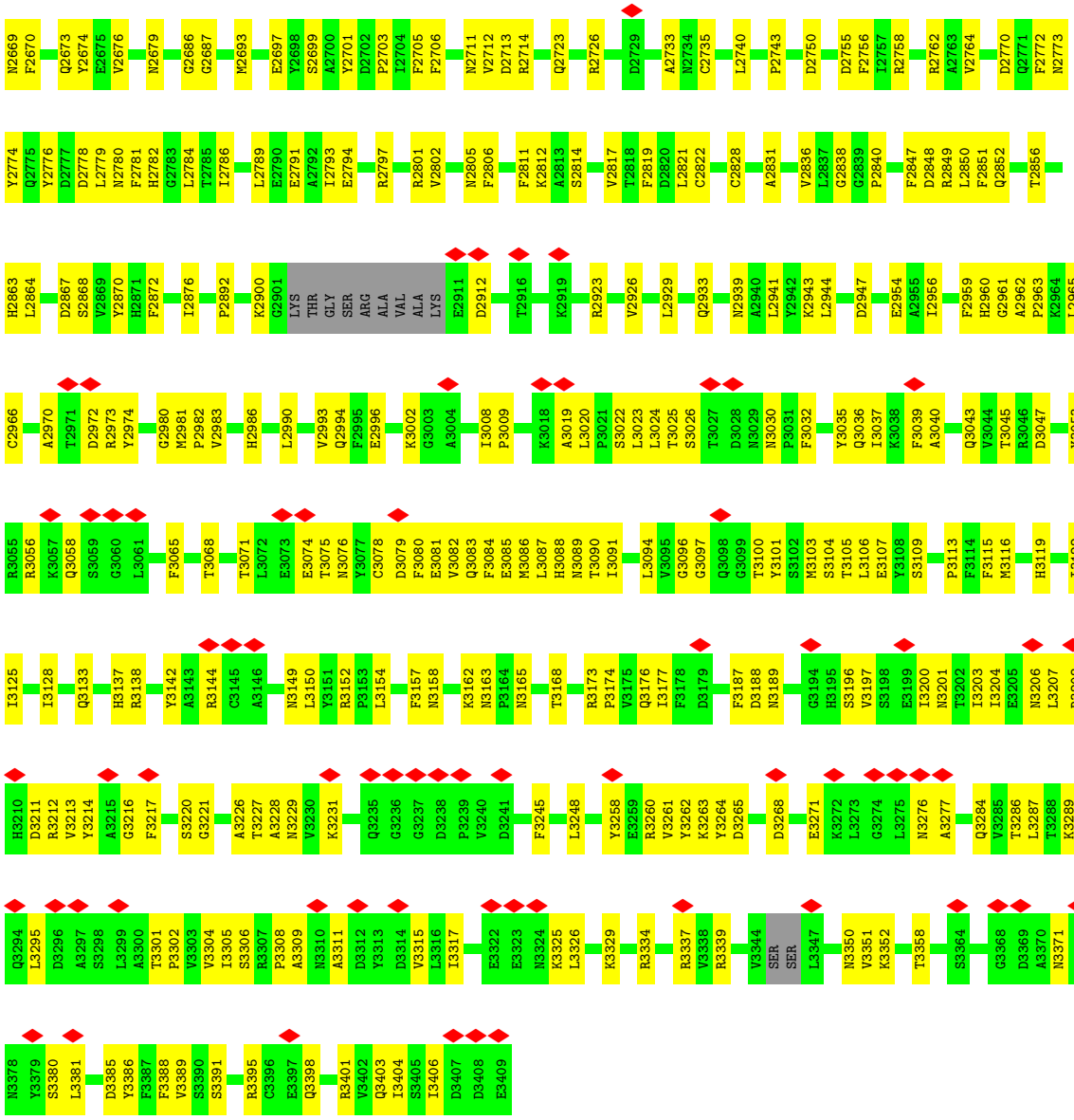
Chain M:




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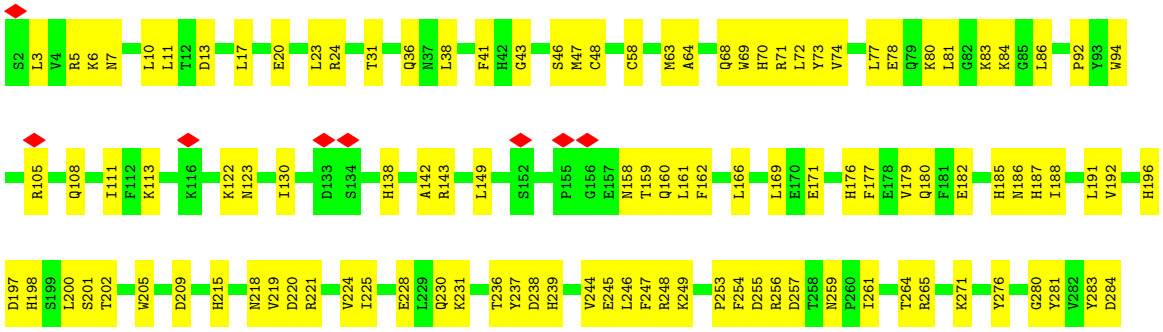

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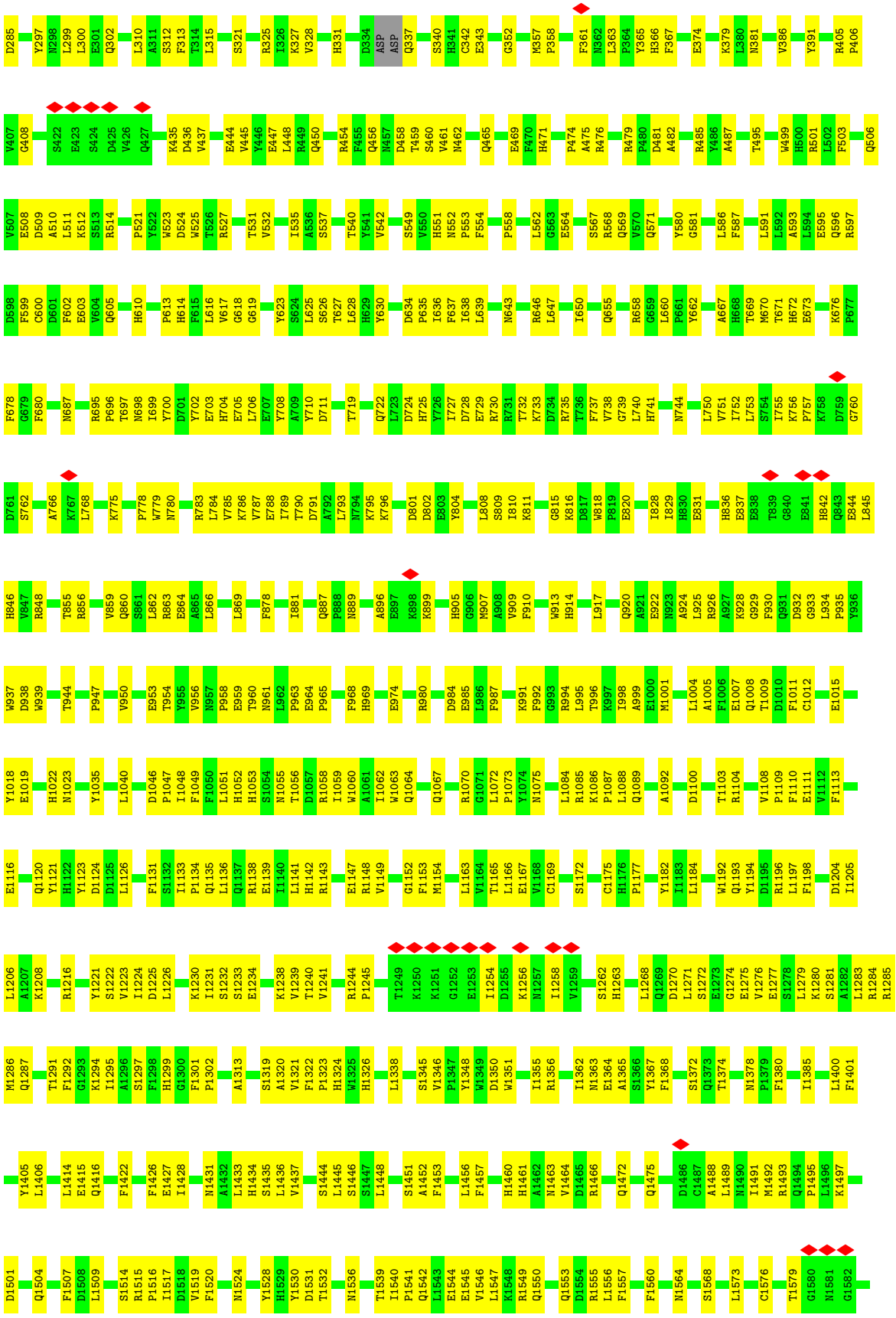


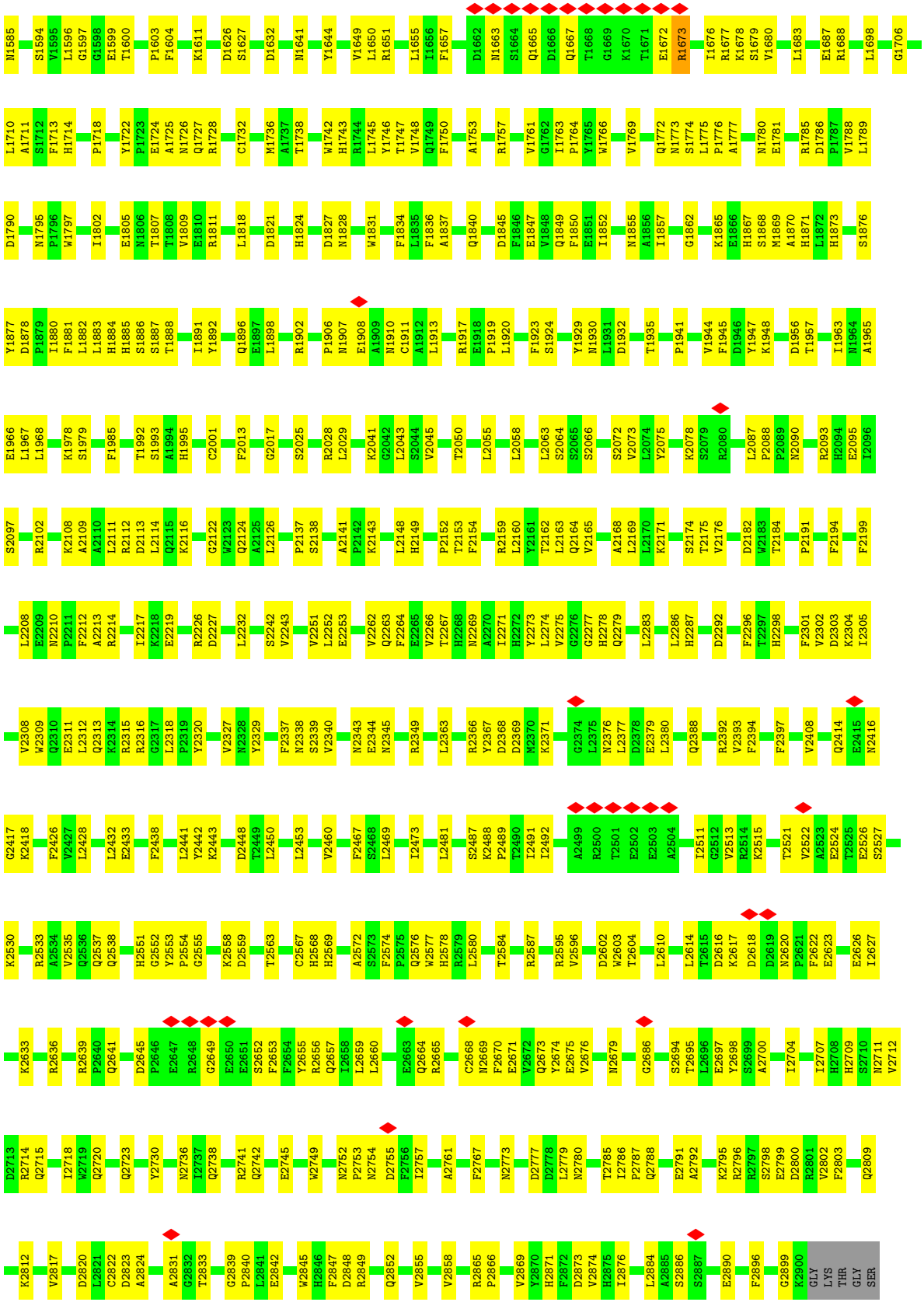
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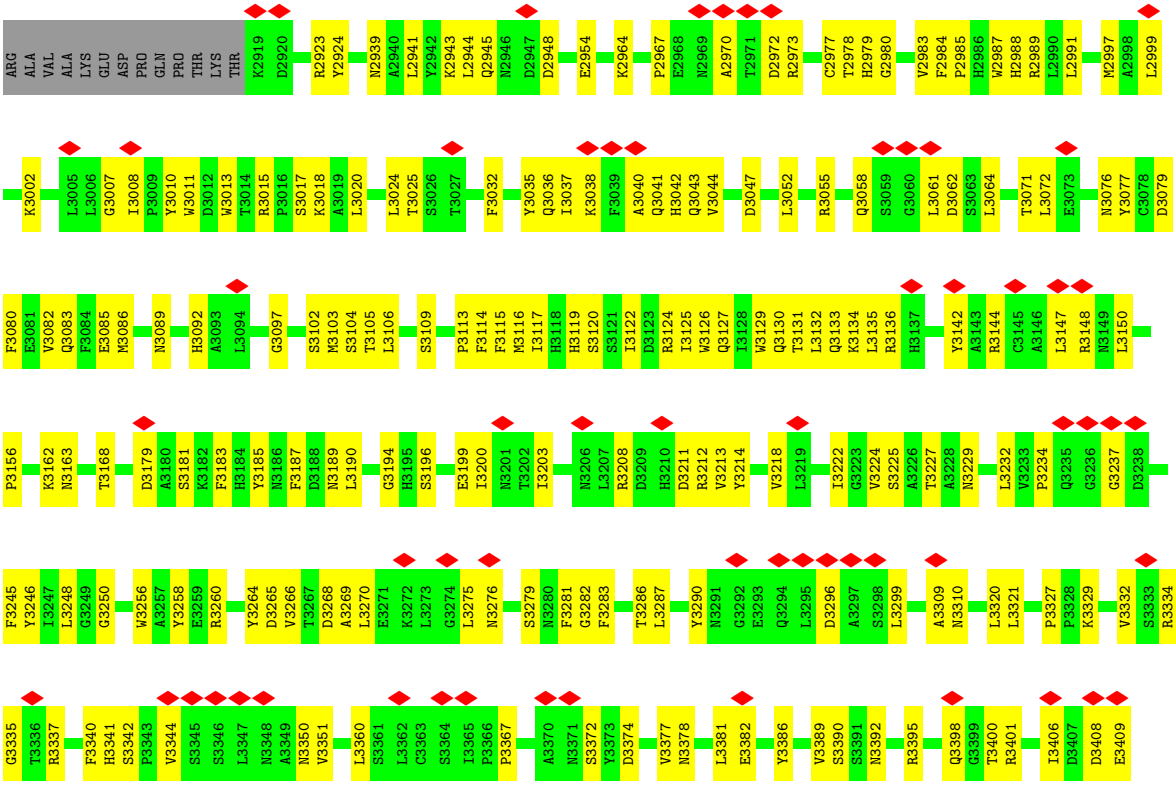
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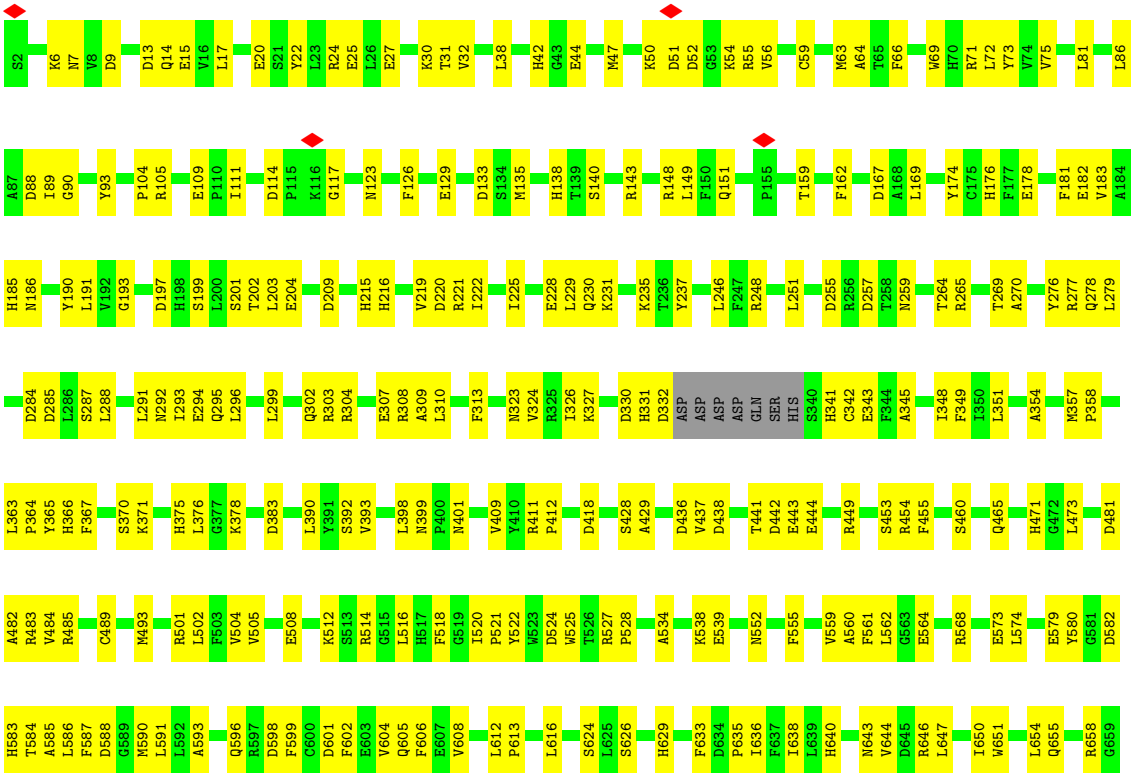

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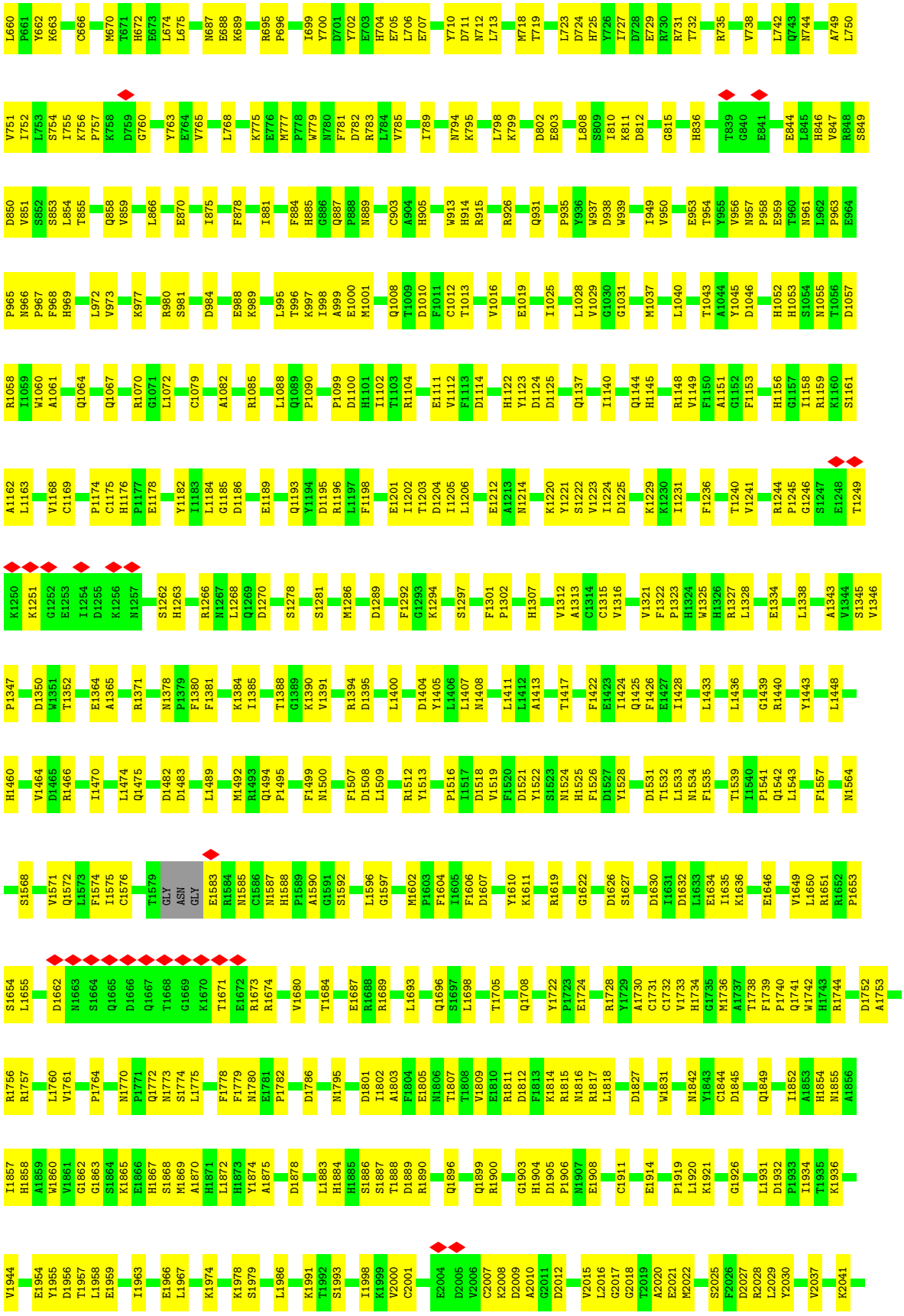


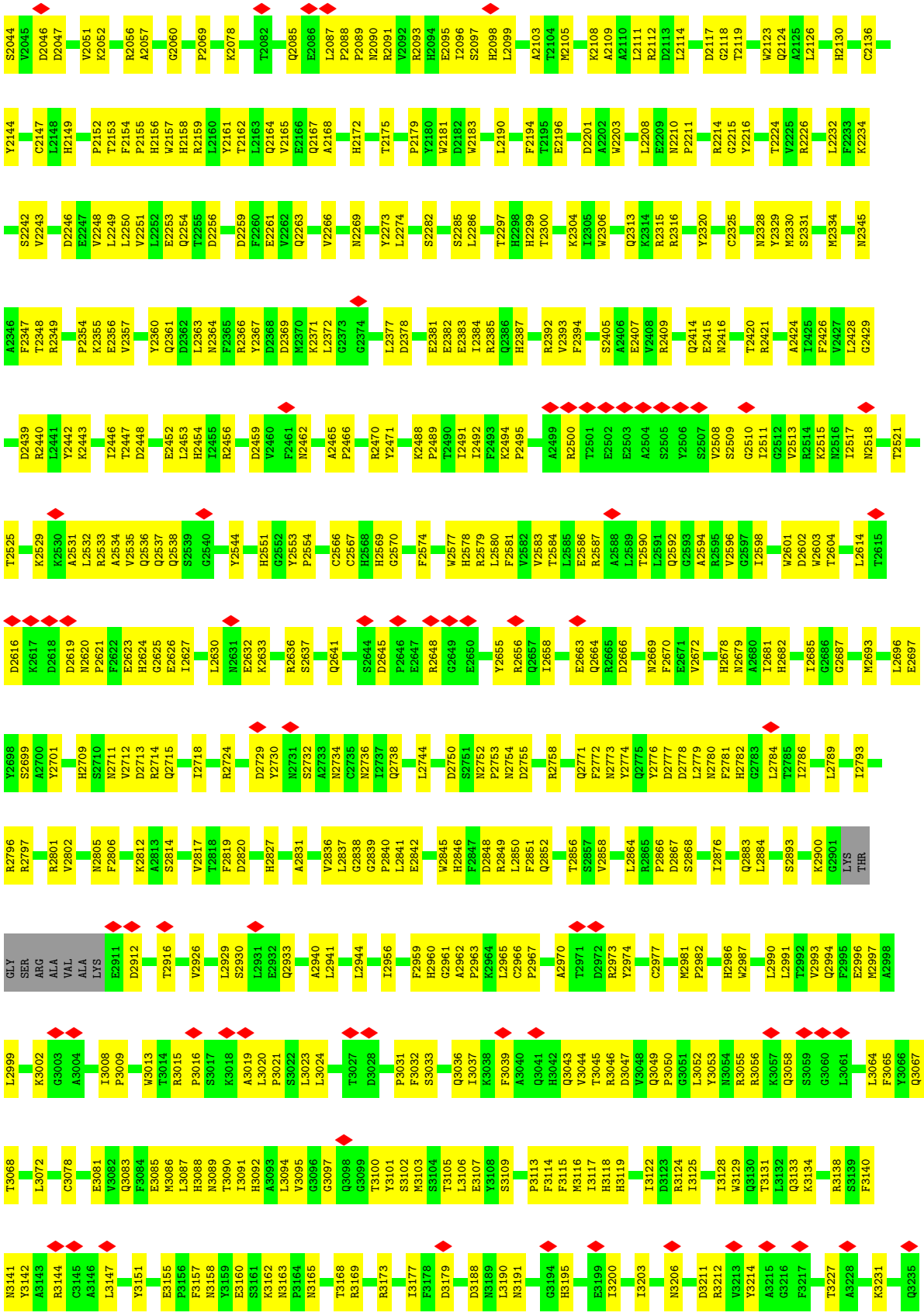
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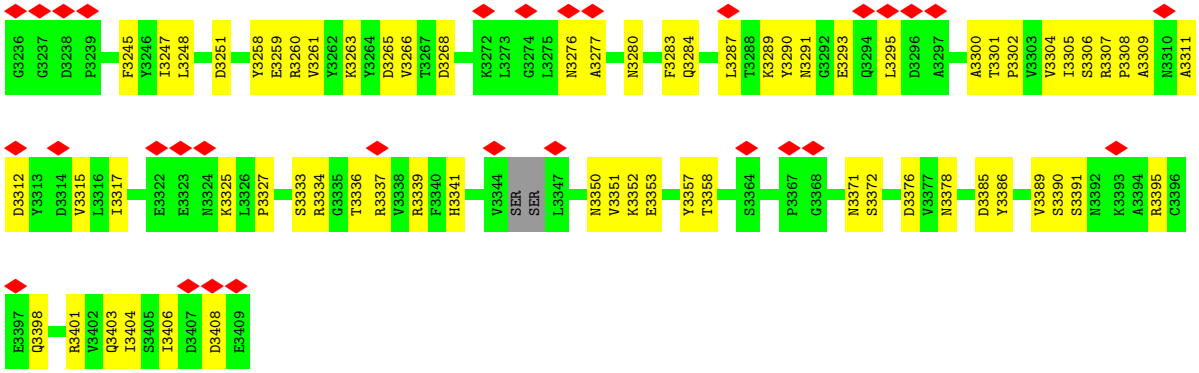
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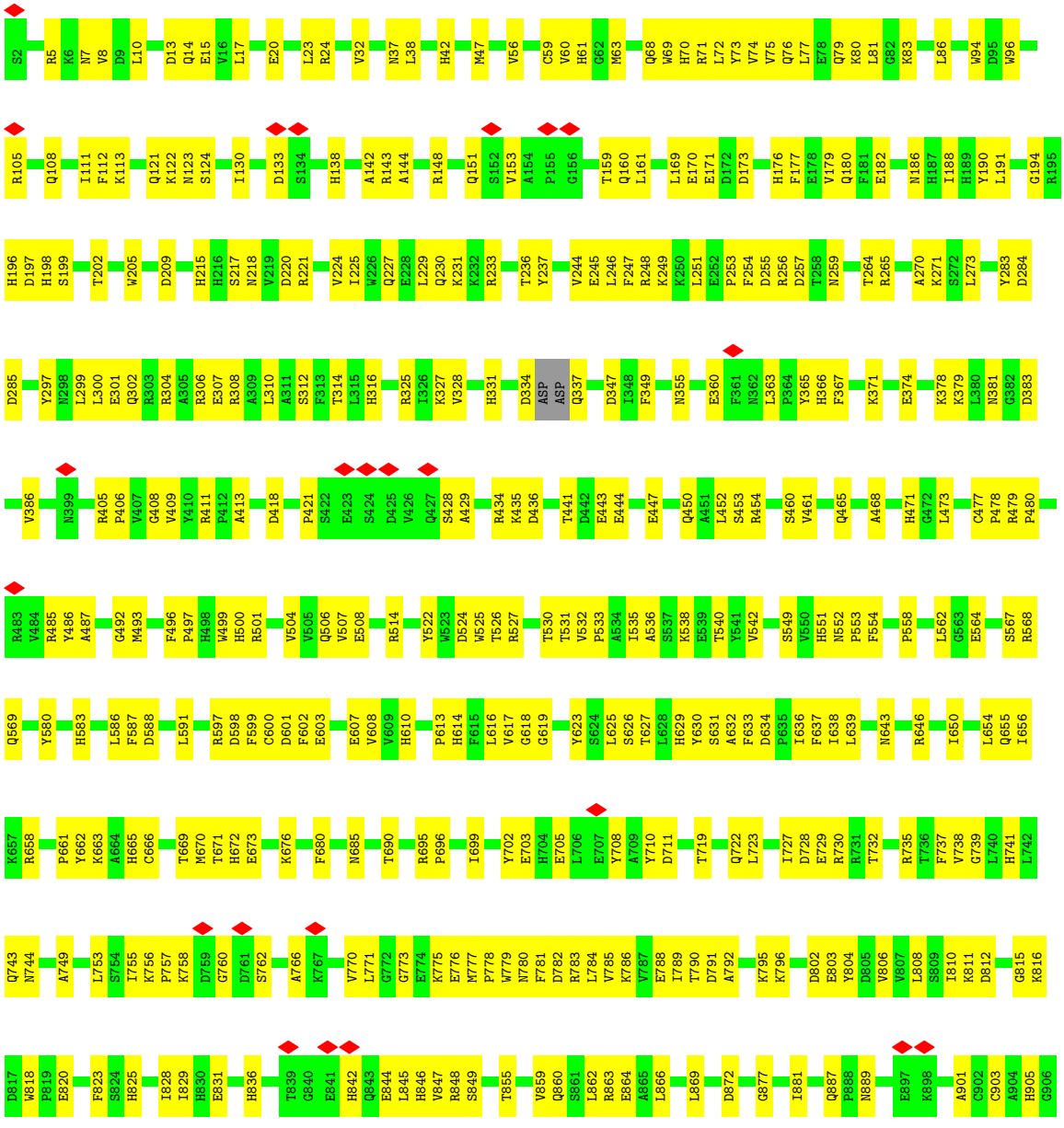


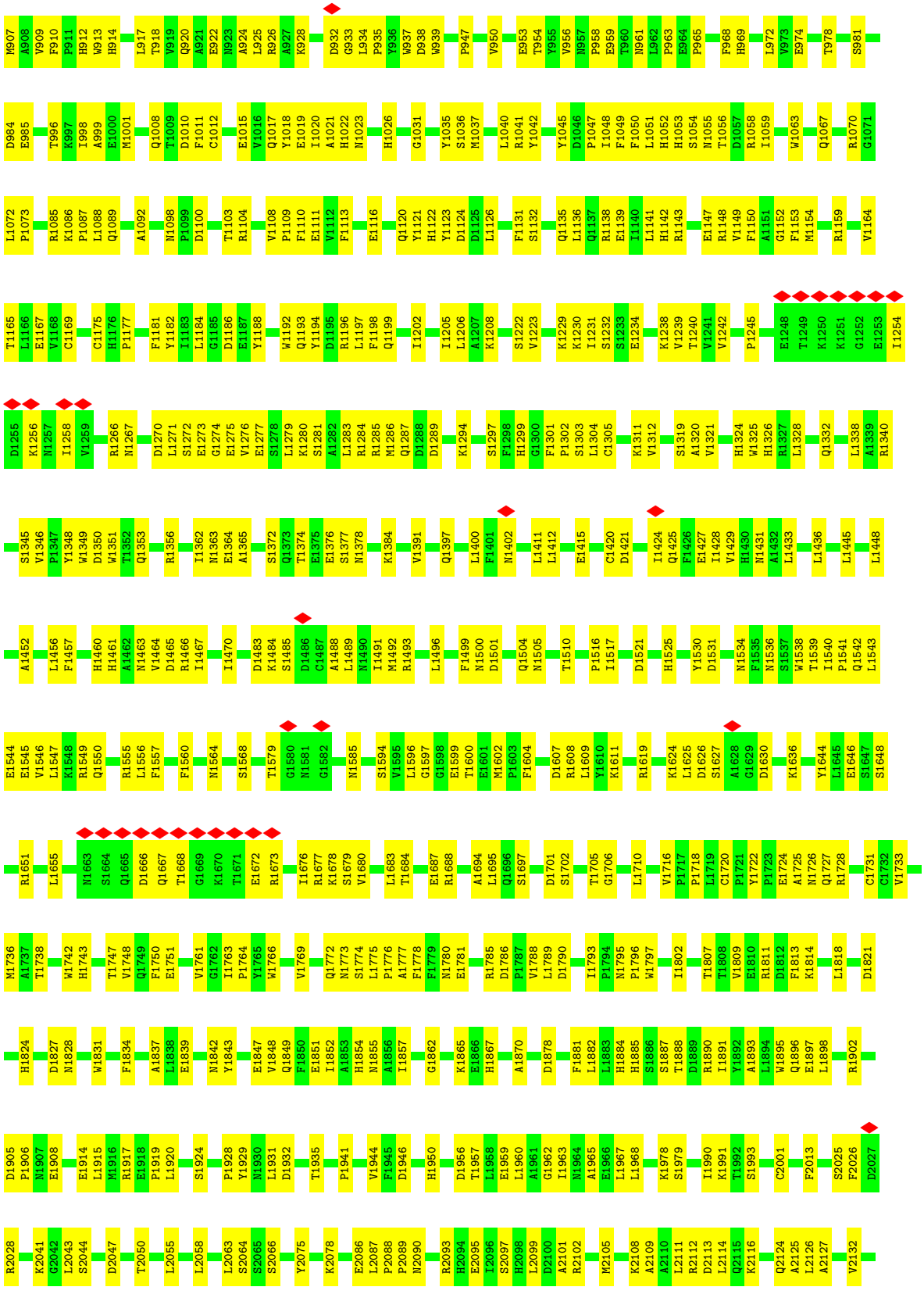


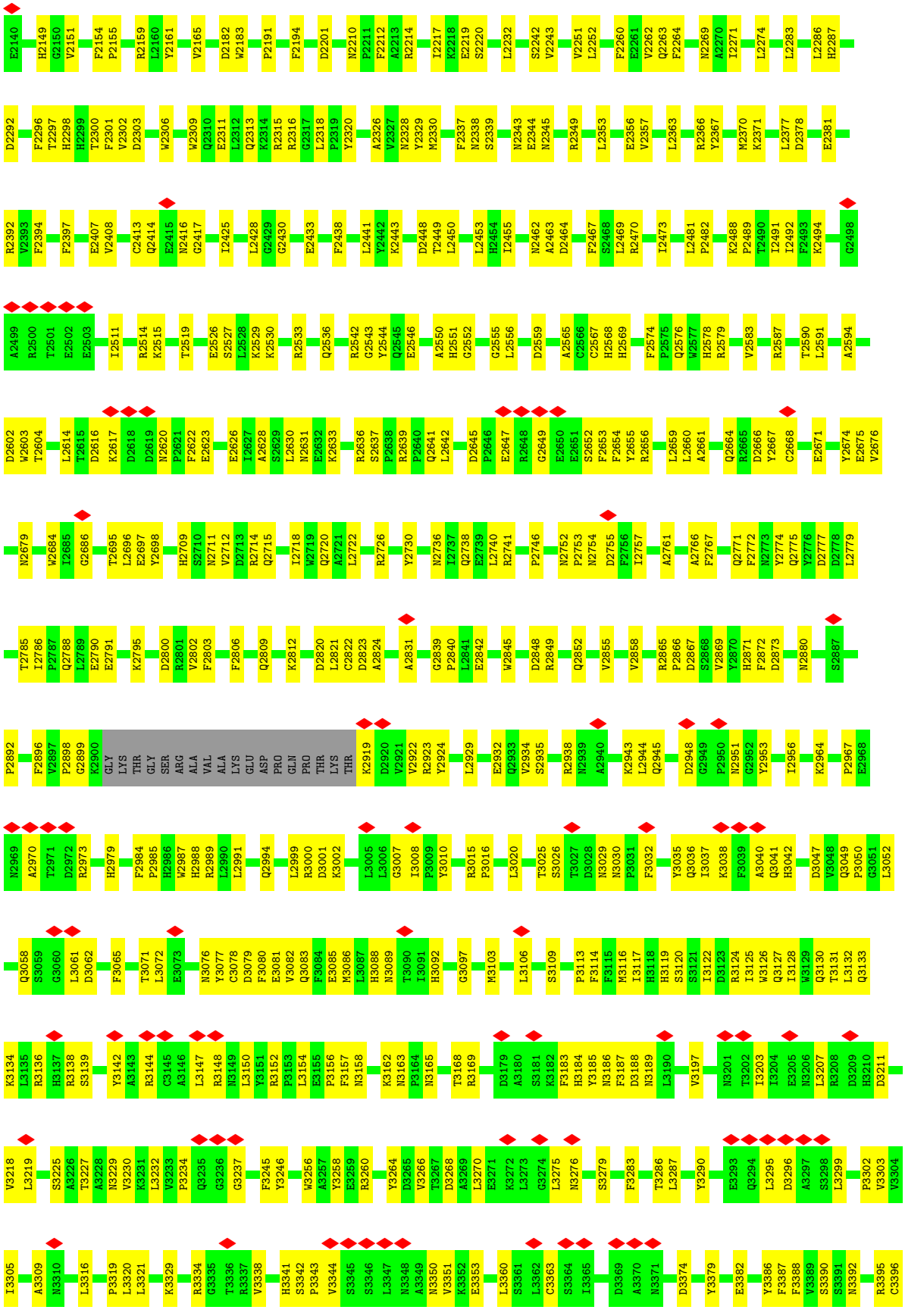

• Molecule 1: Hemocyanin

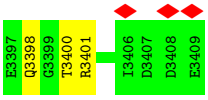
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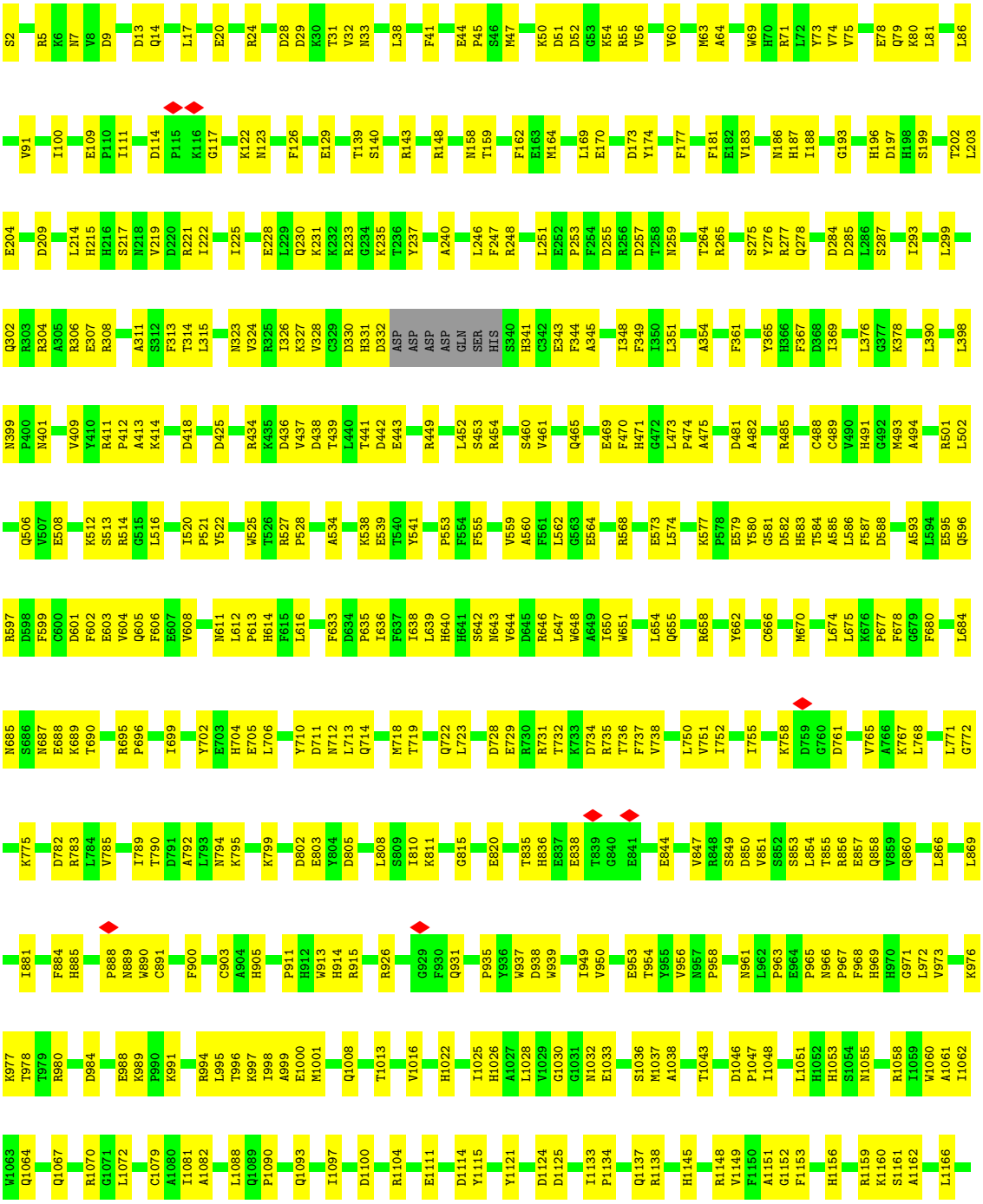


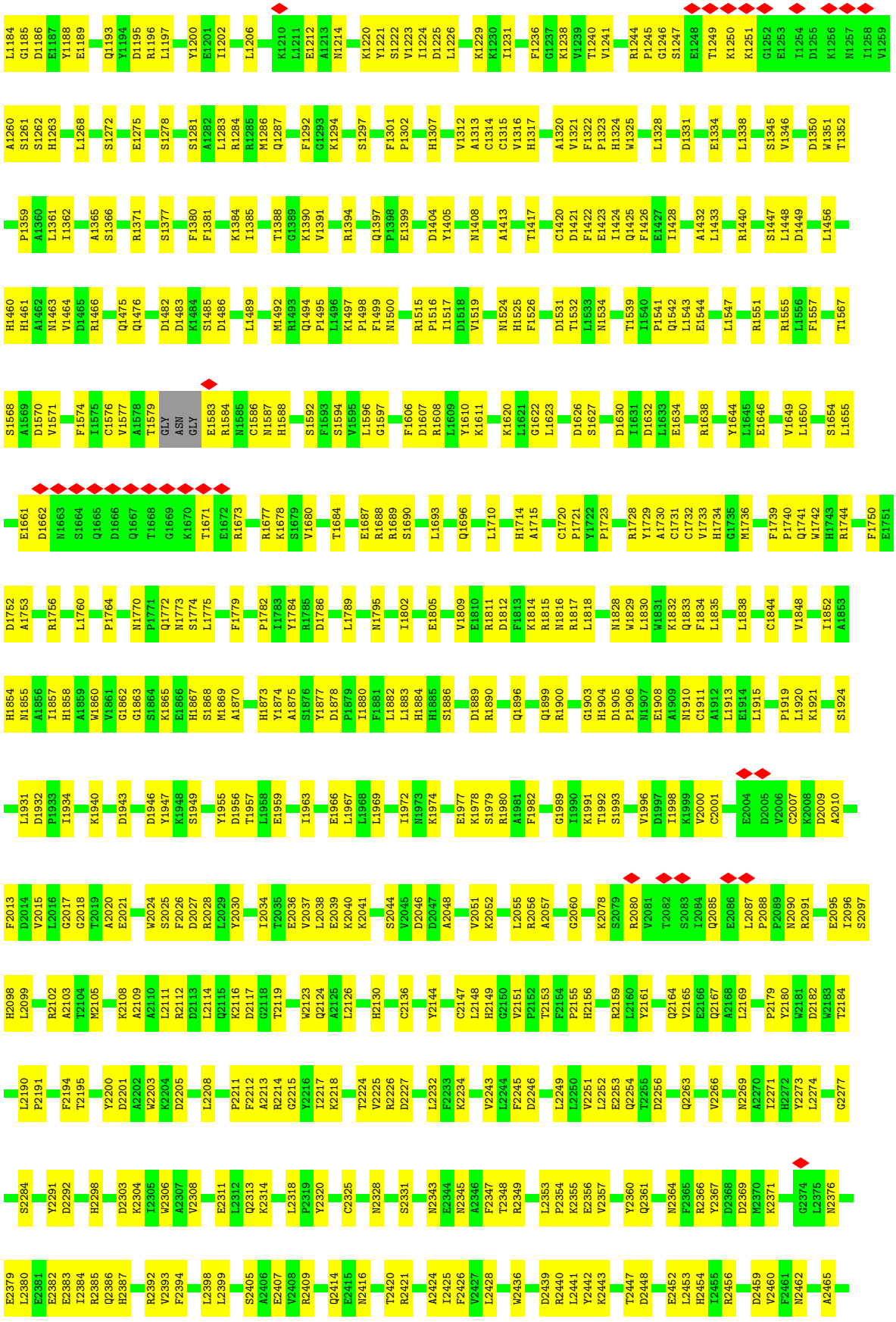


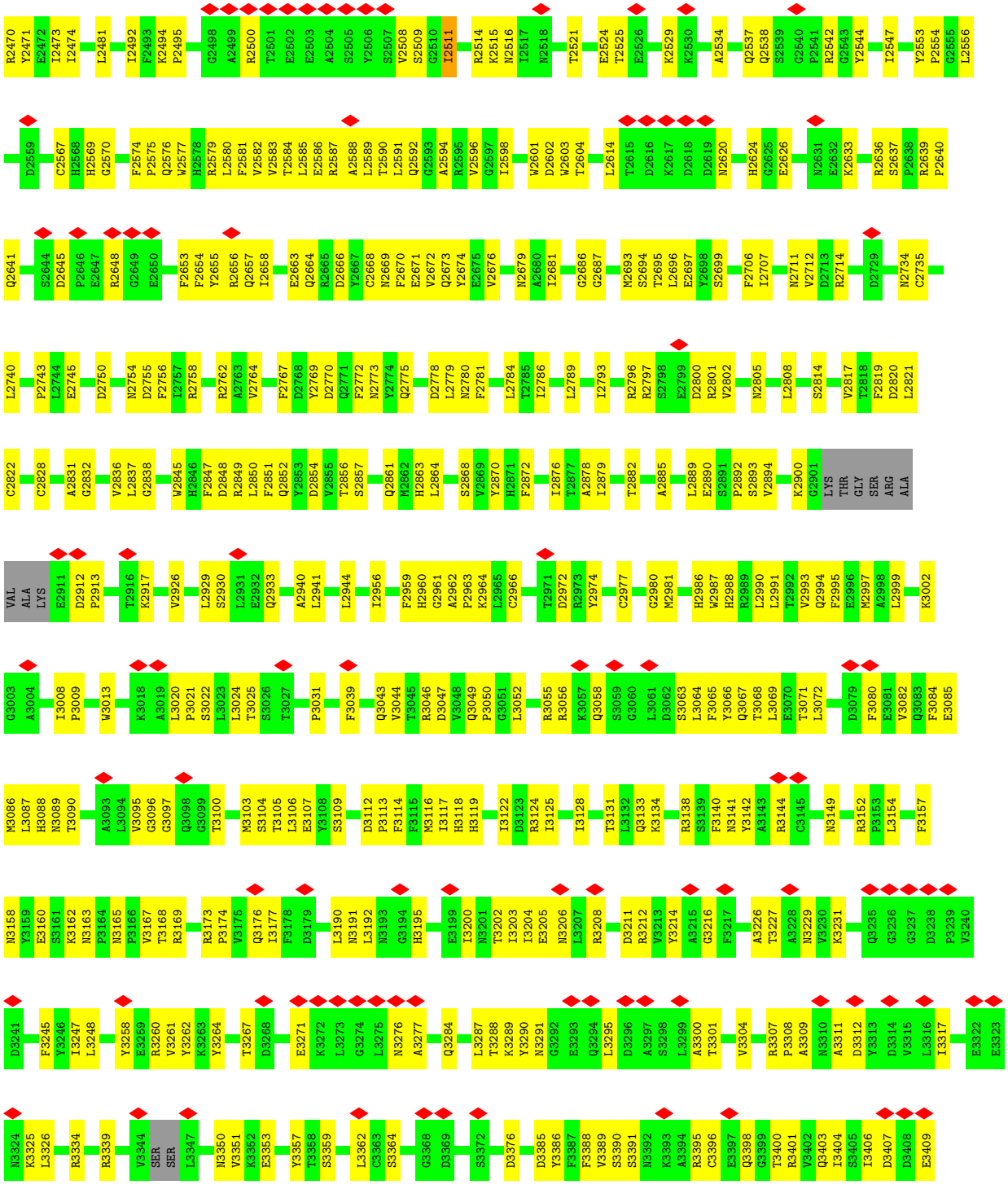

• Molecule 1: Hemocyanin

Chain Q:



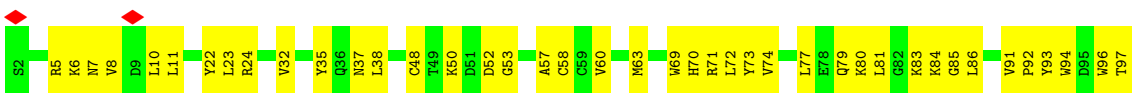

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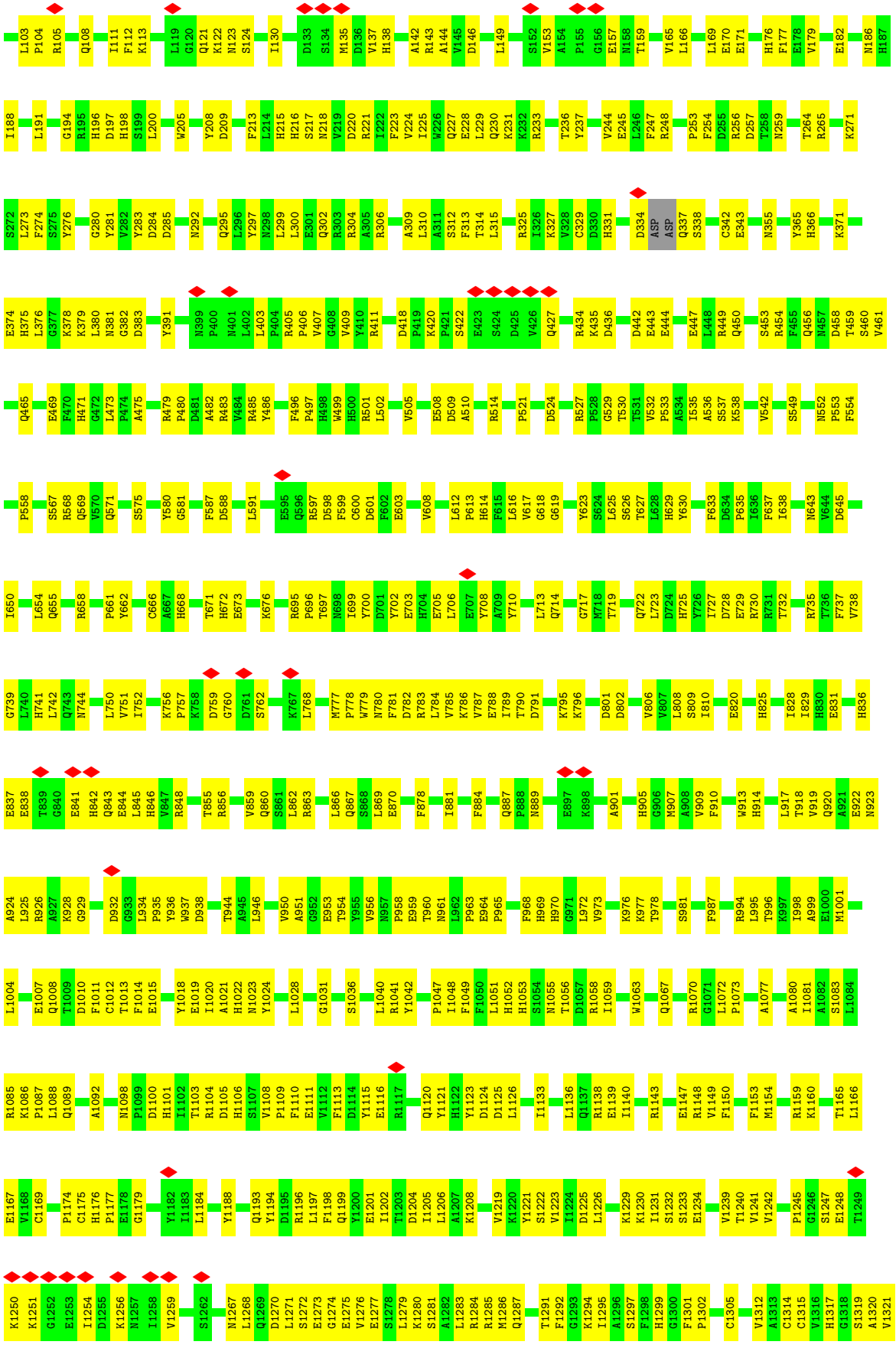


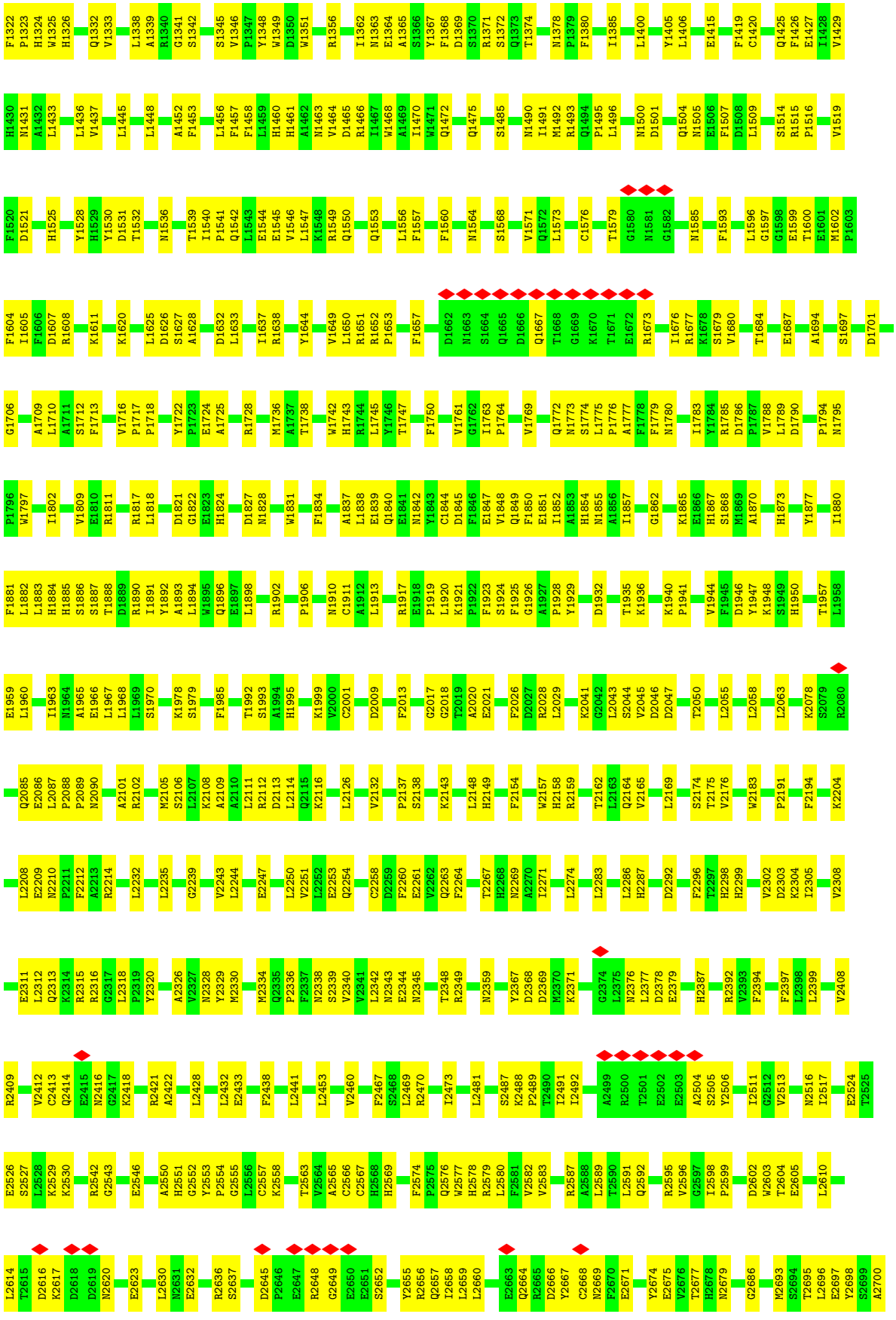
• Molecule 1: Hemocyanin

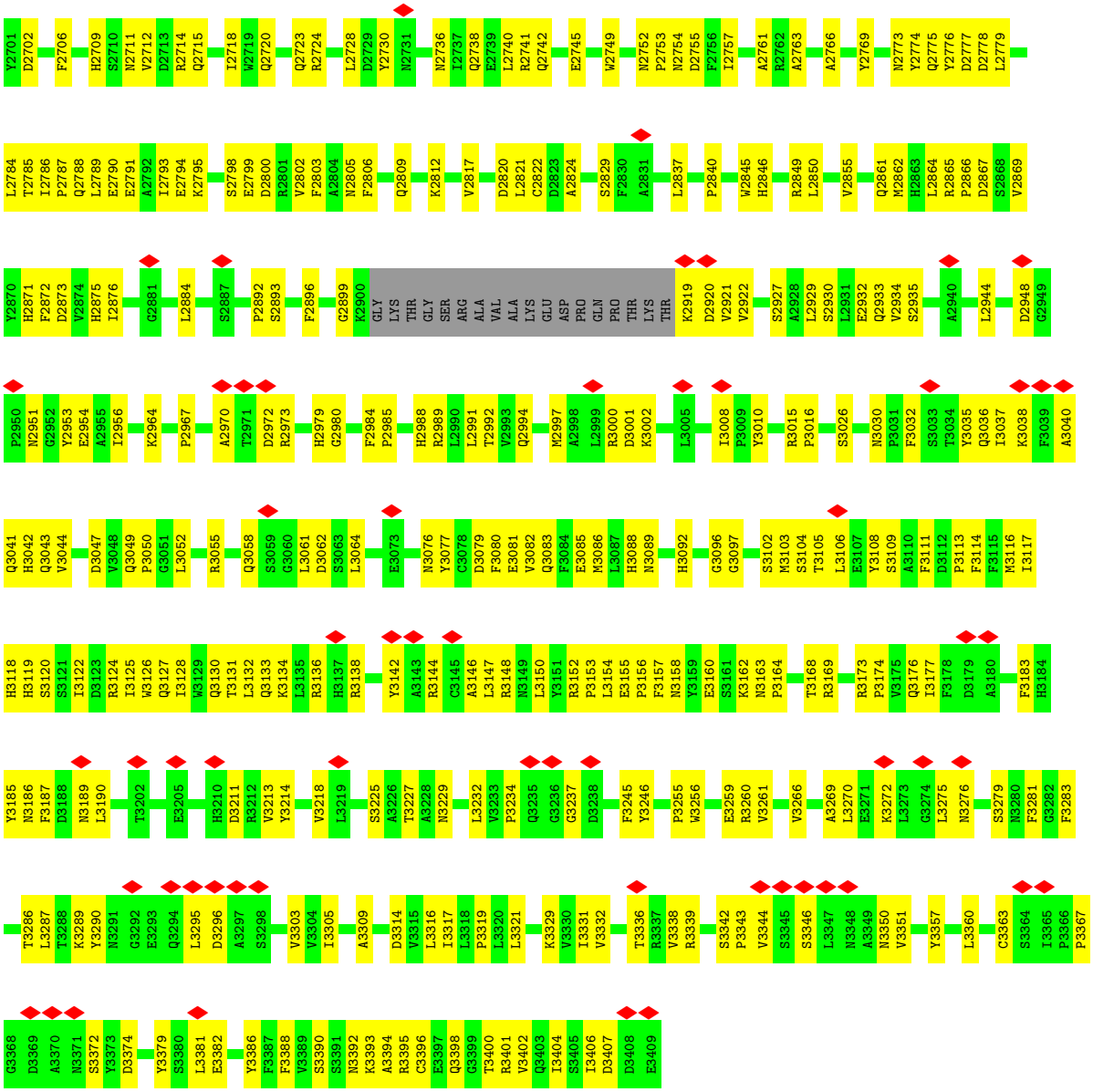
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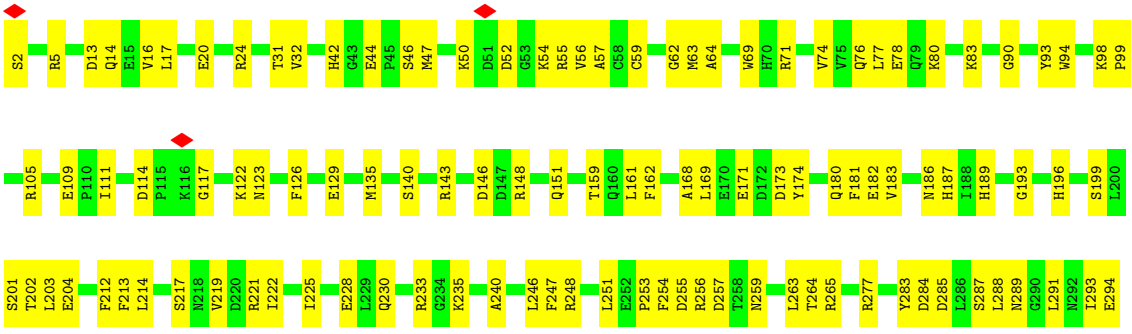

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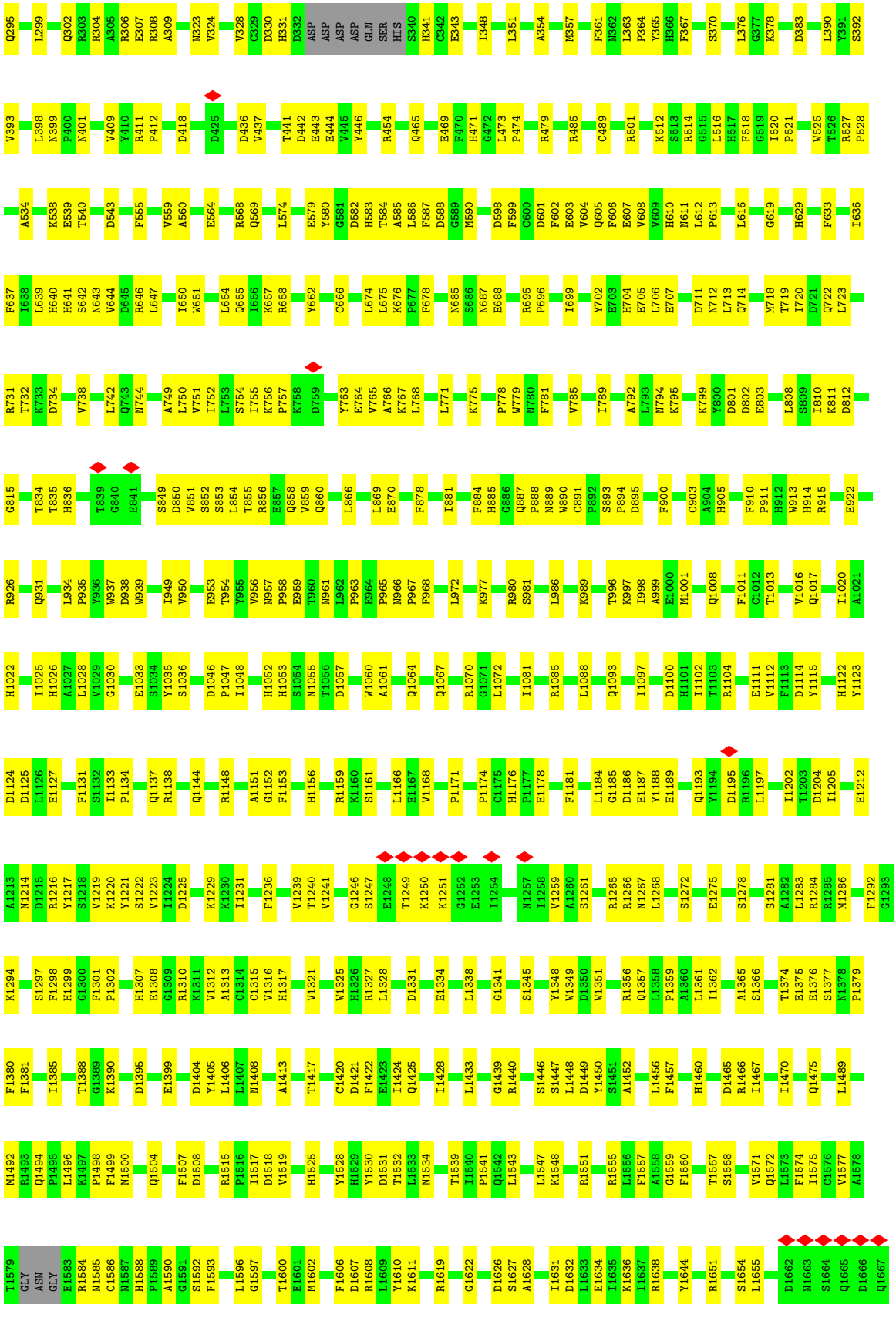


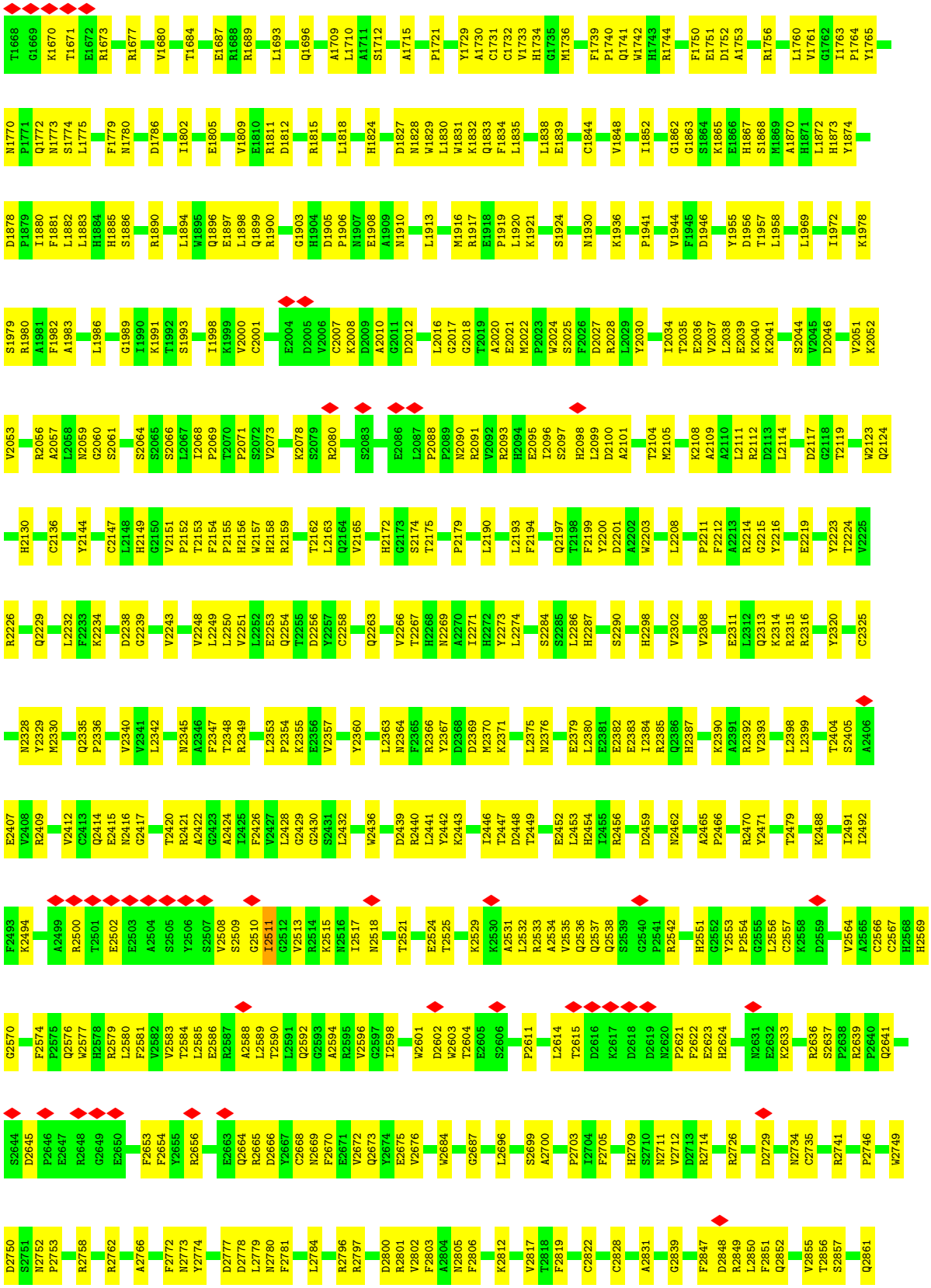
• Molecule 1: Hemocyanin

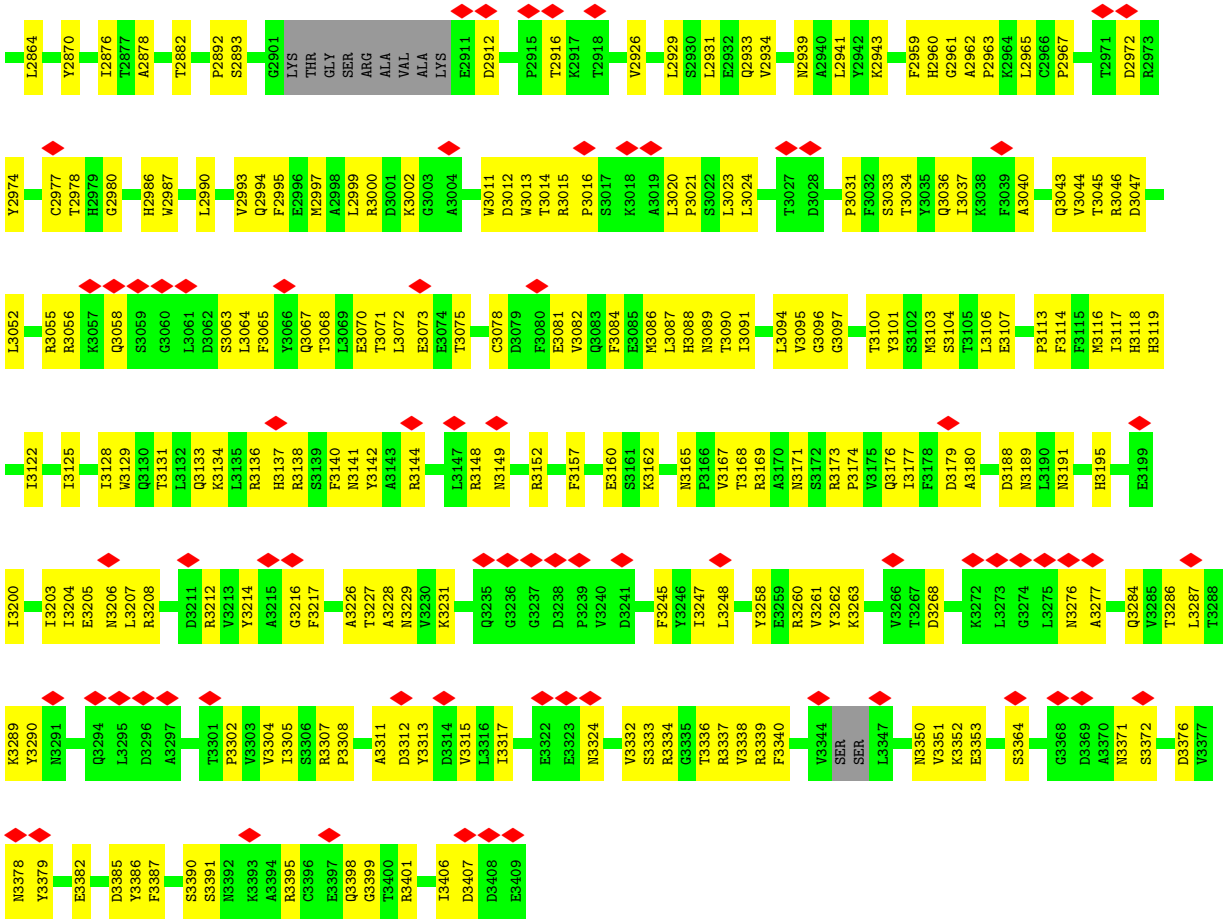
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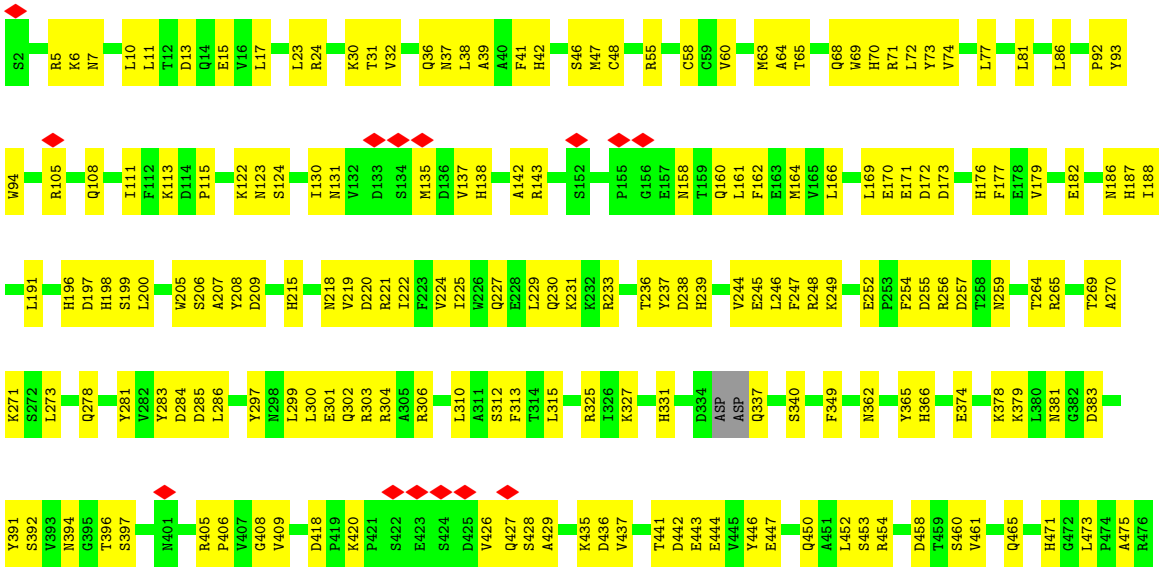

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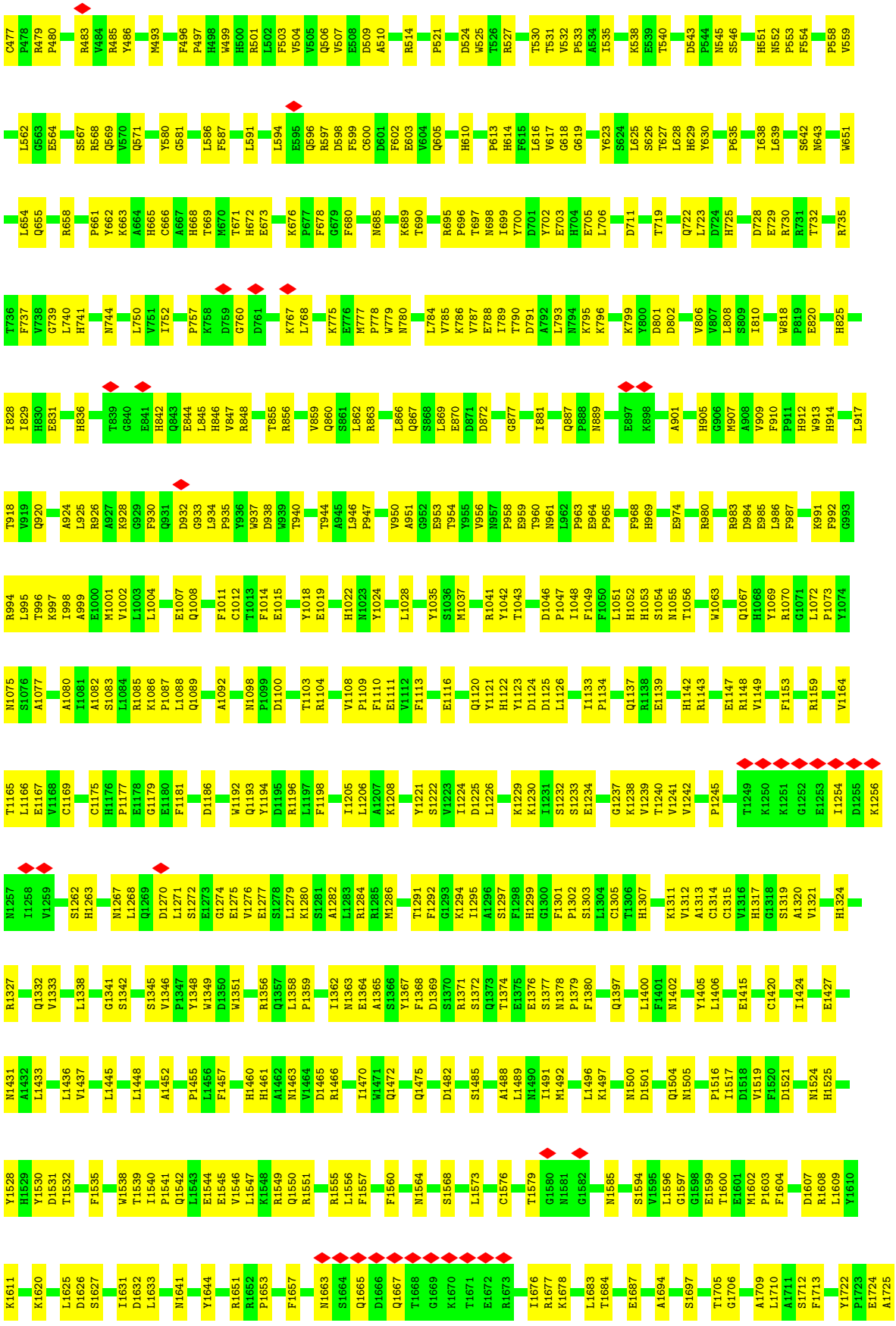


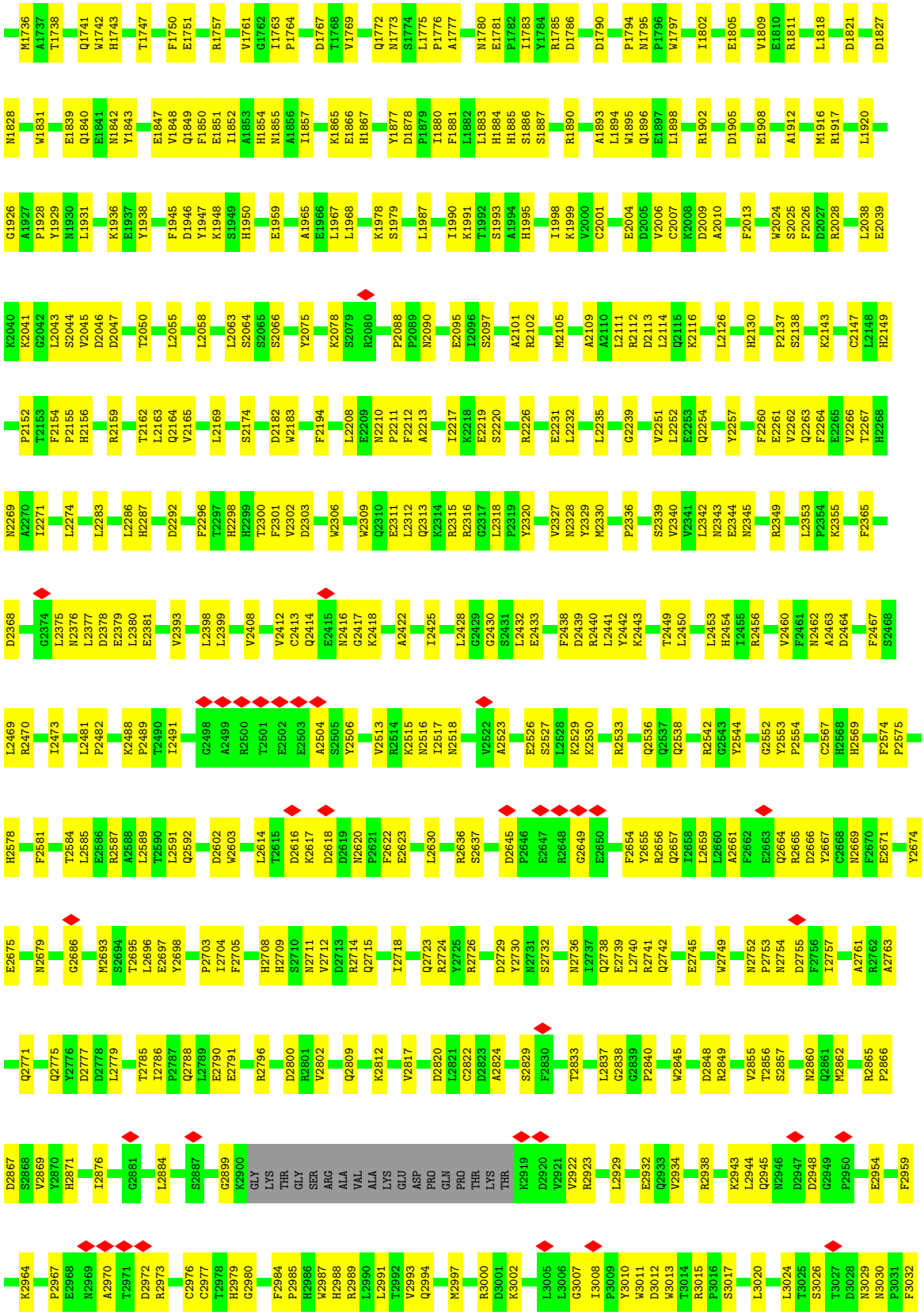
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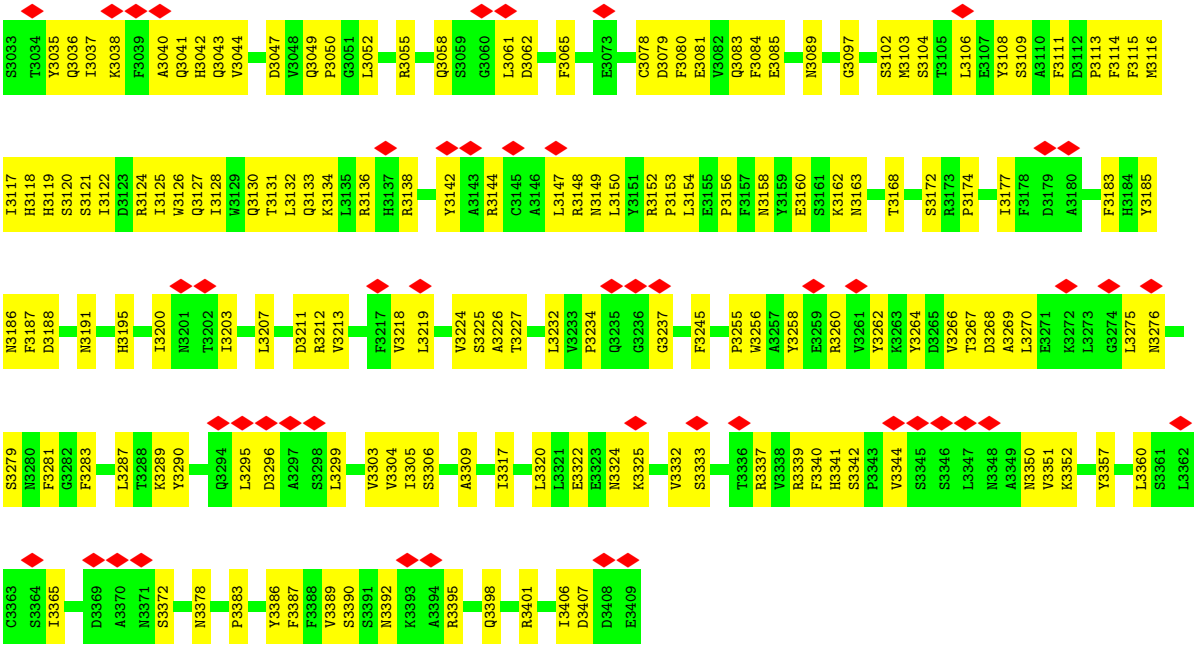
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D2867 S2868 V2869 Y2870 H2871 I2876 G2881 L2884 S2887 G2899 K2900 GLY LYS THR GLY SER ARG ALA VAL ALA LYS GLU ASP PRO GLN PRO THR LYS THR K2919 D2920 V2921 V2922 R2923 L2929 E2932 Q2933 V2934 R2938 K2943 L2944 Q2945 N2946 D2947 D2948 G2949 P2950 E2954 F2959
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• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain U:

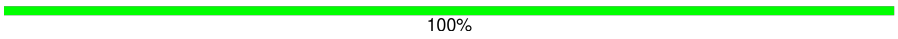






• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain W:

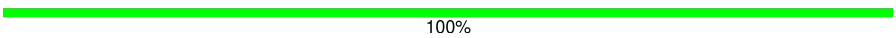






• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Y:

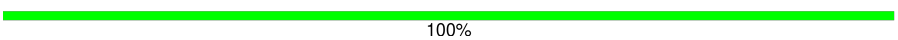






• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

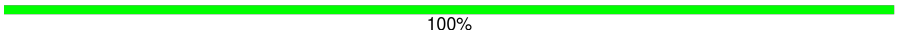
Chain d:






• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain e:

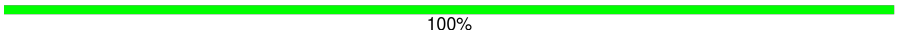






• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain g:







• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain i:







• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain n:

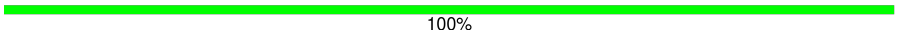






• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain o:







• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain q:







• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain s:







• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain x:

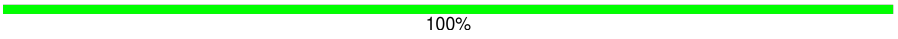






• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain y:







• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 0:

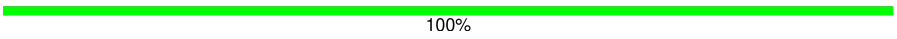






• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 2:







• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 7:

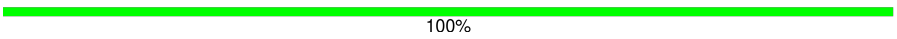






• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

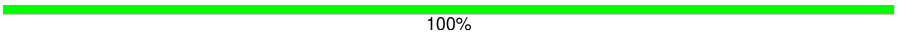
Chain 8:






• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain AA:







• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain CA:







• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain HA:







• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain IA:







• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain KA:

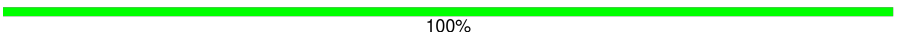






• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain MA:







• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain RA:






• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain SA:

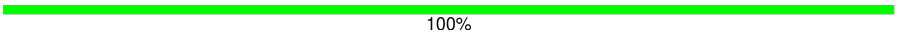






• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain UA:







• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain WA:







• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain bA:

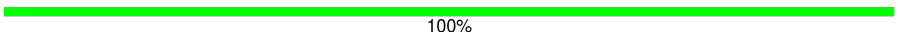






• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain cA:

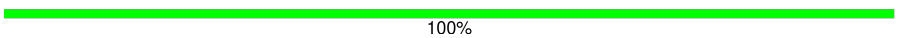






• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

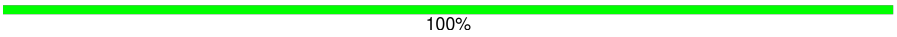
Chain eA:






• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain gA:







• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain lA:

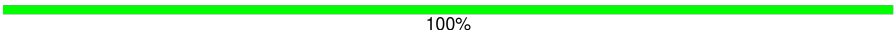






• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain mA:







• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain oA:

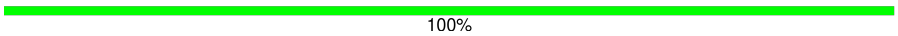






• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain qA:







• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain vA:







• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain wA:







• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain yA:







• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 0A:







• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 5A:







• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain V:

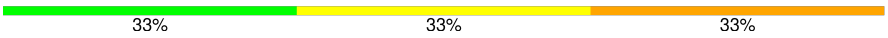






• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain X:







• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Z:






• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain a:







• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain b:

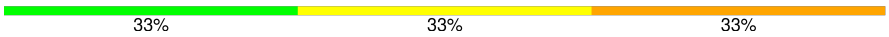






• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain c:







• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain f:







• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain h:

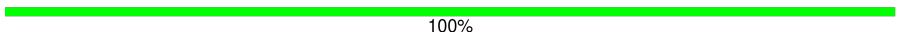






• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain j:







• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

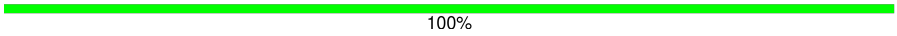
Chain k:






• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain l:

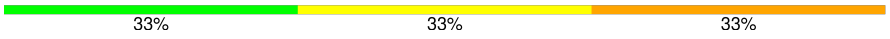






• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain m:







• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain p:

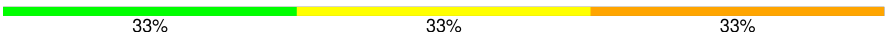






• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain r:

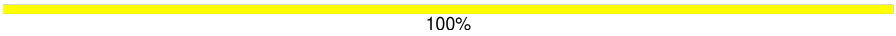






• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain t:







• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

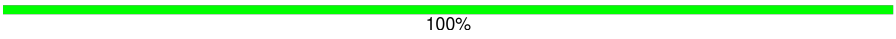
Chain u:






• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain v:







• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain w:







• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain z:

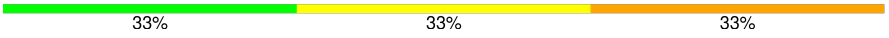






• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 1:







• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 3:

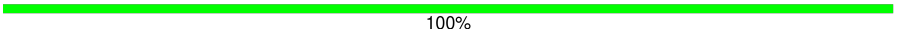






• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 4:

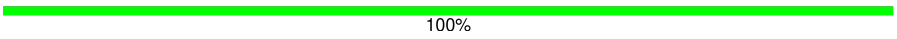






• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

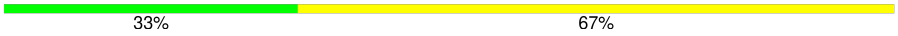
Chain 5:






• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 6:







• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 9:

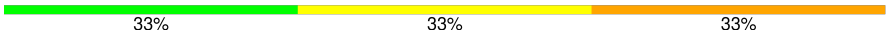






• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain BA:







• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain DA:







• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain EA:

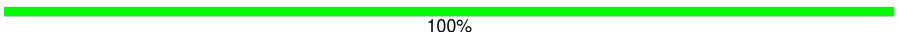






• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain FA:






• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain GA:







• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain JA:

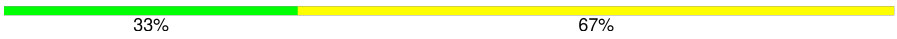






• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain LA:







• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain NA:

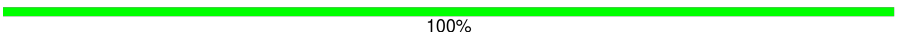






• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain OA:

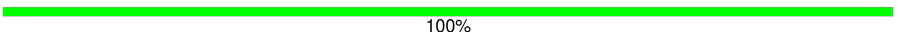






• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain PA:







• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

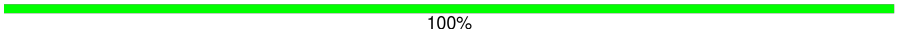
Chain QA:






• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain TA:

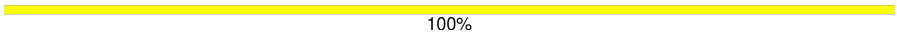






• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain VA:







• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain XA:







• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain YA:

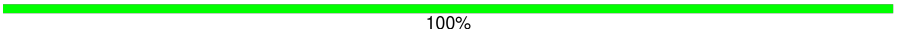






• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain ZA:

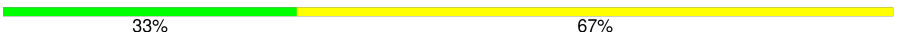






• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain aA:






• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain dA:







• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain fA:

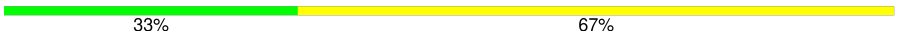






• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain hA:

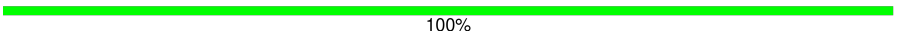






• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain iA:







• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain jA:

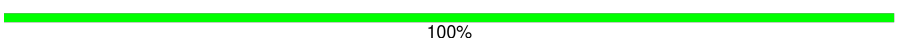






• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain kA:







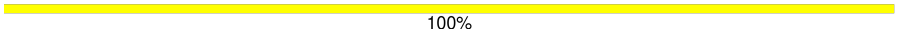
• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain nA:





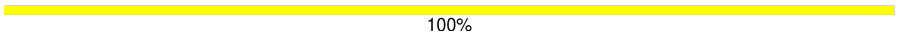

• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain pA: 





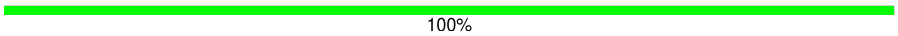
• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain rA: 





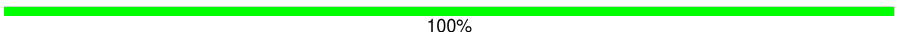
• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain sA: 





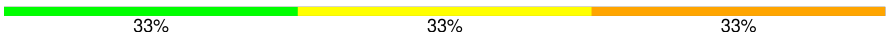
• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain tA: 





• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain uA: 





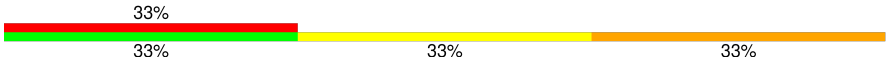
• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain xA: 




• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain zA:

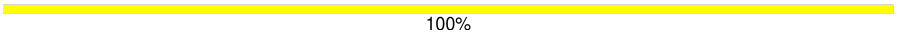






• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 1A:







• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 2A:

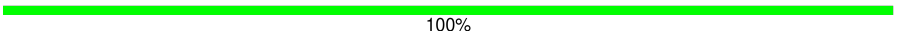






• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 3A:







• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 4A:






# 4 Experimental information (i)

| Property | Value | Source |
|---|---|---|
| EM reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, D5 | Depositor |
| Number of particles used | 29935 | Depositor |
| Resolution determination method | FSC 0.143 CUT-OFF | Depositor |
| CTF correction method | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope | FEI TITAN KRIOS | Depositor |
| Voltage (kV) | 300 | Depositor |
| Electron dose ($e^-/Å^2$) | 36.75 | Depositor |
| Minimum defocus (nm) | 1100 | Depositor |
| Maximum defocus (nm) | 1900 | Depositor |
| Magnification | 59000 | Depositor |
| Image detector | FEI FALCON III (4k x 4k) | Depositor |
| Maximum map value | 3.862 | Depositor |
| Minimum map value | -2.136 | Depositor |
| Average map value | 0.033 | Depositor |
| Map value standard deviation | 0.212 | Depositor |
| Recommended contour level | 0.637 | Depositor |
| Map size (Å) | 597.77997, 597.77997, 597.77997 | wwPDB |
| Map dimensions | 300, 300, 300 | wwPDB |
| Map angles (°) | 90.0, 90.0, 90.0 | wwPDB |
| Pixel spacing (Å) | 1.9925998, 1.9925998, 1.9925998 | Depositor |

# 5 Model quality

## 5.1 Standard geometry

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

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

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | #$\|Z\|>5$ | RMSZ | #$\|Z\|>5$ |
| 1 | A | 0.16 | 0/28074 | 0.36 | 0/38177 |
| 1 | B | 0.15 | 0/28072 | 0.34 | 0/38172 |
| 1 | C | 0.16 | 0/28074 | 0.35 | 0/38177 |
| 1 | D | 0.15 | 0/28077 | 0.35 | 1/38182 (0.0%) |
| 1 | E | 0.16 | 0/28074 | 0.35 | 0/38177 |
| 1 | F | 0.15 | 0/28077 | 0.34 | 1/38182 (0.0%) |
| 1 | G | 0.16 | 0/28073 | 0.35 | 0/38176 |
| 1 | H | 0.15 | 0/28077 | 0.36 | 2/38182 (0.0%) |
| 1 | I | 0.16 | 0/28074 | 0.35 | 0/38177 |
| 1 | J | 0.15 | 0/28074 | 0.35 | 0/38175 |
| 1 | K | 0.16 | 0/28074 | 0.35 | 0/38177 |
| 1 | L | 0.16 | 0/28072 | 0.36 | 1/38172 (0.0%) |
| 1 | M | 0.16 | 0/28074 | 0.35 | 0/38177 |
| 1 | N | 0.15 | 0/28077 | 0.35 | 1/38182 (0.0%) |
| 1 | O | 0.16 | 0/28074 | 0.35 | 0/38177 |
| 1 | P | 0.15 | 0/28077 | 0.34 | 0/38182 |
| 1 | Q | 0.16 | 0/28073 | 0.35 | 0/38176 |
| 1 | R | 0.15 | 0/28077 | 0.35 | 1/38182 (0.0%) |
| 1 | S | 0.16 | 0/28074 | 0.36 | 0/38177 |
| 1 | T | 0.15 | 0/28074 | 0.35 | 0/38175 |
| All | All | 0.16 | 0/561492 | 0.35 | 7/763554 (0.0%) |

There are no bond length outliers.

All (7) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | H | 2541 | PRO | CA-N-CD | -6.58 | 102.78 | 112.00 |
| 1 | H | 3142 | TYR | CA-CB-CG | 5.96 | 124.63 | 113.90 |
| 1 | N | 1673 | ARG | CB-CA-C | -5.33 | 110.45 | 116.63 |
| 1 | F | 745 | ILE | N-CA-C | -5.31 | 108.33 | 113.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | D | 1673 | ARG | CB-CA-C | -5.30 | 110.48 | 116.63 |
| 1 | L | 2541 | PRO | CA-N-CD | -5.25 | 104.65 | 112.00 |
| 1 | R | 1673 | ARG | CB-CA-C | -5.22 | 110.58 | 116.63 |

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 | A | 27308 | 0 | 26081 | 1005 | 0 |
| 1 | B | 27308 | 0 | 26066 | 1001 | 0 |
| 1 | C | 27308 | 0 | 26081 | 1000 | 0 |
| 1 | D | 27310 | 0 | 26071 | 1024 | 0 |
| 1 | E | 27308 | 0 | 26081 | 1001 | 0 |
| 1 | F | 27310 | 0 | 26071 | 1030 | 0 |
| 1 | G | 27307 | 0 | 26078 | 1041 | 0 |
| 1 | H | 27310 | 0 | 26071 | 1045 | 0 |
| 1 | I | 27308 | 0 | 26081 | 986 | 0 |
| 1 | J | 27309 | 0 | 26067 | 1015 | 0 |
| 1 | K | 27308 | 0 | 26081 | 995 | 0 |
| 1 | L | 27308 | 0 | 26066 | 1005 | 0 |
| 1 | M | 27308 | 0 | 26081 | 961 | 0 |
| 1 | N | 27310 | 0 | 26071 | 1001 | 0 |
| 1 | O | 27308 | 0 | 26081 | 960 | 0 |
| 1 | P | 27310 | 0 | 26071 | 1007 | 0 |
| 1 | Q | 27307 | 0 | 26078 | 1023 | 0 |
| 1 | R | 27310 | 0 | 26071 | 1075 | 0 |
| 1 | S | 27308 | 0 | 26081 | 985 | 0 |
| 1 | T | 27309 | 0 | 26068 | 1012 | 0 |
| 2 | 0 | 28 | 0 | 25 | 0 | 0 |
| 2 | 0A | 28 | 0 | 25 | 1 | 0 |
| 2 | 2 | 28 | 0 | 25 | 0 | 0 |
| 2 | 5A | 28 | 0 | 25 | 0 | 0 |
| 2 | 7 | 28 | 0 | 25 | 0 | 0 |
| 2 | 8 | 28 | 0 | 25 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 2 | AA | 28 | 0 | 25 | 0 | 0 |
| 2 | CA | 28 | 0 | 25 | 1 | 0 |
| 2 | HA | 28 | 0 | 25 | 0 | 0 |
| 2 | IA | 28 | 0 | 25 | 1 | 0 |
| 2 | KA | 28 | 0 | 25 | 1 | 0 |
| 2 | MA | 28 | 0 | 25 | 0 | 0 |
| 2 | RA | 28 | 0 | 25 | 0 | 0 |
| 2 | SA | 28 | 0 | 25 | 1 | 0 |
| 2 | U | 28 | 0 | 25 | 2 | 0 |
| 2 | UA | 28 | 0 | 25 | 0 | 0 |
| 2 | W | 28 | 0 | 25 | 0 | 0 |
| 2 | WA | 28 | 0 | 25 | 0 | 0 |
| 2 | Y | 28 | 0 | 25 | 0 | 0 |
| 2 | bA | 28 | 0 | 25 | 0 | 0 |
| 2 | cA | 28 | 0 | 25 | 0 | 0 |
| 2 | d | 28 | 0 | 25 | 0 | 0 |
| 2 | e | 28 | 0 | 25 | 0 | 0 |
| 2 | eA | 28 | 0 | 25 | 0 | 0 |
| 2 | g | 28 | 0 | 25 | 0 | 0 |
| 2 | gA | 28 | 0 | 25 | 0 | 0 |
| 2 | i | 28 | 0 | 25 | 0 | 0 |
| 2 | lA | 28 | 0 | 25 | 2 | 0 |
| 2 | mA | 28 | 0 | 25 | 0 | 0 |
| 2 | n | 28 | 0 | 25 | 0 | 0 |
| 2 | o | 28 | 0 | 25 | 0 | 0 |
| 2 | oA | 28 | 0 | 25 | 1 | 0 |
| 2 | q | 28 | 0 | 25 | 1 | 0 |
| 2 | qA | 28 | 0 | 25 | 0 | 0 |
| 2 | s | 28 | 0 | 25 | 0 | 0 |
| 2 | vA | 28 | 0 | 25 | 0 | 0 |
| 2 | wA | 28 | 0 | 25 | 0 | 0 |
| 2 | x | 28 | 0 | 25 | 0 | 0 |
| 2 | y | 28 | 0 | 25 | 0 | 0 |
| 2 | yA | 28 | 0 | 25 | 1 | 0 |
| 3 | 1 | 39 | 0 | 34 | 2 | 0 |
| 3 | 1A | 39 | 0 | 34 | 1 | 0 |
| 3 | 2A | 39 | 0 | 34 | 1 | 0 |
| 3 | 3 | 39 | 0 | 34 | 0 | 0 |
| 3 | 3A | 39 | 0 | 34 | 0 | 0 |
| 3 | 4 | 39 | 0 | 34 | 0 | 0 |
| 3 | 4A | 39 | 0 | 34 | 2 | 0 |
| 3 | 5 | 39 | 0 | 34 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 3 | 6 | 39 | 0 | 34 | 1 | 0 |
| 3 | 9 | 39 | 0 | 34 | 0 | 0 |
| 3 | BA | 39 | 0 | 34 | 2 | 0 |
| 3 | DA | 39 | 0 | 34 | 0 | 0 |
| 3 | EA | 39 | 0 | 34 | 1 | 0 |
| 3 | FA | 39 | 0 | 34 | 0 | 0 |
| 3 | GA | 39 | 0 | 34 | 1 | 0 |
| 3 | JA | 39 | 0 | 34 | 1 | 0 |
| 3 | LA | 39 | 0 | 34 | 1 | 0 |
| 3 | NA | 39 | 0 | 34 | 0 | 0 |
| 3 | OA | 39 | 0 | 34 | 0 | 0 |
| 3 | PA | 39 | 0 | 34 | 0 | 0 |
| 3 | QA | 39 | 0 | 34 | 0 | 0 |
| 3 | TA | 39 | 0 | 34 | 0 | 0 |
| 3 | V | 39 | 0 | 34 | 1 | 0 |
| 3 | VA | 39 | 0 | 34 | 2 | 0 |
| 3 | X | 39 | 0 | 34 | 1 | 0 |
| 3 | XA | 39 | 0 | 34 | 0 | 0 |
| 3 | YA | 39 | 0 | 34 | 1 | 0 |
| 3 | Z | 39 | 0 | 34 | 1 | 0 |
| 3 | ZA | 39 | 0 | 34 | 0 | 0 |
| 3 | a | 39 | 0 | 34 | 1 | 0 |
| 3 | aA | 39 | 0 | 34 | 1 | 0 |
| 3 | b | 39 | 0 | 34 | 1 | 0 |
| 3 | c | 39 | 0 | 34 | 1 | 0 |
| 3 | dA | 39 | 0 | 34 | 1 | 0 |
| 3 | f | 39 | 0 | 34 | 1 | 0 |
| 3 | fA | 39 | 0 | 34 | 2 | 0 |
| 3 | h | 39 | 0 | 34 | 0 | 0 |
| 3 | hA | 39 | 0 | 34 | 1 | 0 |
| 3 | iA | 39 | 0 | 34 | 0 | 0 |
| 3 | j | 39 | 0 | 34 | 0 | 0 |
| 3 | jA | 39 | 0 | 34 | 1 | 0 |
| 3 | k | 39 | 0 | 34 | 0 | 0 |
| 3 | kA | 39 | 0 | 34 | 0 | 0 |
| 3 | l | 39 | 0 | 34 | 0 | 0 |
| 3 | m | 39 | 0 | 34 | 2 | 0 |
| 3 | nA | 39 | 0 | 34 | 1 | 0 |
| 3 | p | 39 | 0 | 34 | 2 | 0 |
| 3 | pA | 39 | 0 | 34 | 1 | 0 |
| 3 | r | 39 | 0 | 34 | 3 | 0 |
| 3 | rA | 39 | 0 | 34 | 2 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 3 | sA | 39 | 0 | 34 | 0 | 0 |
| 3 | t | 39 | 0 | 34 | 2 | 0 |
| 3 | tA | 39 | 0 | 34 | 0 | 0 |
| 3 | u | 39 | 0 | 34 | 0 | 0 |
| 3 | uA | 39 | 0 | 34 | 2 | 0 |
| 3 | v | 39 | 0 | 34 | 0 | 0 |
| 3 | w | 39 | 0 | 34 | 1 | 0 |
| 3 | xA | 39 | 0 | 34 | 0 | 0 |
| 3 | z | 39 | 0 | 34 | 1 | 0 |
| 3 | zA | 39 | 0 | 34 | 1 | 0 |
| 4 | A | 14 | 0 | 13 | 0 | 0 |
| 4 | B | 14 | 0 | 13 | 0 | 0 |
| 4 | C | 14 | 0 | 13 | 1 | 0 |
| 4 | D | 14 | 0 | 13 | 1 | 0 |
| 4 | E | 14 | 0 | 13 | 1 | 0 |
| 4 | F | 14 | 0 | 13 | 1 | 0 |
| 4 | G | 14 | 0 | 13 | 1 | 0 |
| 4 | H | 14 | 0 | 13 | 1 | 0 |
| 4 | I | 14 | 0 | 13 | 1 | 0 |
| 4 | J | 14 | 0 | 13 | 0 | 0 |
| 4 | K | 14 | 0 | 13 | 1 | 0 |
| 4 | L | 14 | 0 | 13 | 0 | 0 |
| 4 | M | 14 | 0 | 13 | 0 | 0 |
| 4 | N | 14 | 0 | 13 | 1 | 0 |
| 4 | O | 14 | 0 | 13 | 0 | 0 |
| 4 | P | 14 | 0 | 13 | 0 | 0 |
| 4 | Q | 14 | 0 | 13 | 0 | 0 |
| 4 | R | 14 | 0 | 13 | 1 | 0 |
| 4 | S | 14 | 0 | 13 | 0 | 0 |
| 4 | T | 14 | 0 | 13 | 3 | 0 |
| All | All | 549912 | 0 | 524797 | 19650 | 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 18.

All (19650) 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:N:2720:GLN:HE22 | 1:N:2730:TYR:HB2 | 1.34 | 0.92 |
| 1:A:754:SER:HG | 1:A:762:SER:HG | 1.18 | 0.92 |
| 1:M:2533:ARG:NH2 | 1:M:2619:ASP:O | 2.04 | 0.91 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:J:597:ARG:HH21 | 1:J:658:ARG:HB2 | 1.34 | 0.91 |
| 1:L:486:TYR:HB3 | 1:L:777:MET:HE1 | 1.53 | 0.90 |
| 1:H:2738:GLN:HE22 | 1:I:2893:SER:HA | 1.36 | 0.90 |
| 1:K:754:SER:HG | 1:K:762:SER:HG | 1.21 | 0.89 |
| 1:H:597:ARG:HH21 | 1:H:658:ARG:HB2 | 1.37 | 0.89 |
| 1:K:2511:ILE:H | 1:K:2596:VAL:HG12 | 1.39 | 0.87 |
| 1:P:405:ARG:NH1 | 1:P:406:PRO:O | 2.06 | 0.87 |
| 1:A:257:ASP:HA | 1:A:265:ARG:HE | 1.40 | 0.87 |
| 1:H:486:TYR:HB3 | 1:H:777:MET:HE1 | 1.55 | 0.86 |
| 1:C:257:ASP:HA | 1:C:265:ARG:HE | 1.37 | 0.86 |
| 1:Q:257:ASP:HA | 1:Q:265:ARG:HE | 1.38 | 0.86 |
| 1:O:2664:GLN:HE21 | 1:O:2670:PHE:HA | 1.40 | 0.86 |
| 1:I:2511:ILE:H | 1:I:2596:VAL:HG12 | 1.40 | 0.86 |
| 1:E:1587:ASN:H | 1:H:337:GLN:HG3 | 1.40 | 0.86 |
| 1:K:1587:ASN:H | 1:N:337:GLN:HG3 | 1.41 | 0.86 |
| 1:I:257:ASP:HA | 1:I:265:ARG:HE | 1.38 | 0.85 |
| 1:C:277:ARG:HH21 | 1:K:836:HIS:CD2 | 1.95 | 0.85 |
| 1:L:1400:LEU:HD21 | 1:L:1436:LEU:HB3 | 1.58 | 0.85 |
| 1:S:2590:THR:HA | 1:S:2594:ALA:HB3 | 1.59 | 0.85 |
| 1:H:3213:VAL:HG21 | 1:H:3270:LEU:HD12 | 1.54 | 0.85 |
| 1:L:454:ARG:HB2 | 1:L:514:ARG:HD3 | 1.59 | 0.85 |
| 1:B:1400:LEU:HD21 | 1:B:1436:LEU:HB3 | 1.59 | 0.85 |
| 1:S:1865:LYS:HZ2 | 1:S:1867:HIS:H | 1.26 | 0.84 |
| 1:C:277:ARG:HH21 | 1:K:836:HIS:HD2 | 1.25 | 0.84 |
| 1:D:357:MET:HE3 | 1:D:358:PRO:HD2 | 1.59 | 0.84 |
| 1:K:50:LYS:HB3 | 1:K:54:LYS:H | 1.42 | 0.84 |
| 1:S:751:VAL:HG12 | 1:S:810:ILE:HG22 | 1.58 | 0.84 |
| 1:A:885:HIS:NE2 | 1:A:903:CYS:SG | 2.51 | 0.84 |
| 1:R:581:GLY:H | 1:R:856:ARG:HH22 | 1.25 | 0.84 |
| 1:Q:885:HIS:NE2 | 1:Q:903:CYS:SG | 2.50 | 0.84 |
| 1:D:1978:LYS:HA | 1:D:2078:LYS:HZ3 | 1.43 | 0.84 |
| 1:S:257:ASP:HA | 1:S:265:ARG:HE | 1.43 | 0.83 |
| 1:L:254:PHE:HD2 | 1:L:264:THR:HB | 1.44 | 0.83 |
| 1:S:1760:LEU:HD12 | 1:S:1761:VAL:HG13 | 1.60 | 0.83 |
| 1:E:1400:LEU:HD21 | 1:E:1436:LEU:HB3 | 1.59 | 0.83 |
| 1:T:405:ARG:NH1 | 1:T:406:PRO:O | 2.12 | 0.83 |
| 1:T:1539:THR:HG23 | 1:T:1541:PRO:HD2 | 1.61 | 0.83 |
| 1:O:885:HIS:NE2 | 1:O:903:CYS:SG | 2.52 | 0.82 |
| 1:O:1587:ASN:H | 1:R:337:GLN:HG3 | 1.42 | 0.82 |
| 1:J:1579:THR:HG21 | 1:J:1585:ASN:HB3 | 1.61 | 0.82 |
| 1:H:2775:GLN:NE2 | 1:H:2776:TYR:O | 2.12 | 0.82 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:G:885:HIS:NE2 | 1:G:903:CYS:SG | 2.53 | 0.82 |
| 1:R:994:ARG:HE | 1:R:995:LEU:H | 1.25 | 0.82 |
| 1:G:50:LYS:HB3 | 1:G:54:LYS:H | 1.44 | 0.82 |
| 1:H:735:ARG:HB3 | 1:H:831:GLU:HB3 | 1.60 | 0.82 |
| 1:P:454:ARG:HH22 | 1:P:1338:LEU:HG | 1.44 | 0.82 |
| 1:C:885:HIS:NE2 | 1:C:903:CYS:SG | 2.53 | 0.82 |
| 1:H:454:ARG:HH22 | 1:H:1338:LEU:HG | 1.44 | 0.82 |
| 1:M:1151:ALA:HB2 | 1:M:1202:ILE:HD11 | 1.62 | 0.82 |
| 1:O:2253:GLU:HG3 | 1:O:2384:ILE:HG12 | 1.61 | 0.82 |
| 1:S:885:HIS:NE2 | 1:S:903:CYS:SG | 2.53 | 0.82 |
| 1:G:257:ASP:HA | 1:G:265:ARG:HE | 1.44 | 0.81 |
| 1:O:887:GLN:HE21 | 1:O:889:ASN:HD21 | 1.28 | 0.81 |
| 1:P:2587:ARG:HH22 | 1:P:2753:PRO:HG2 | 1.45 | 0.81 |
| 1:Q:50:LYS:HB3 | 1:Q:54:LYS:H | 1.46 | 0.81 |
| 1:K:885:HIS:NE2 | 1:K:903:CYS:SG | 2.53 | 0.81 |
| 1:L:3113:PRO:HA | 1:L:3116:MET:HE2 | 1.62 | 0.81 |
| 1:Q:2251:VAL:HG22 | 1:Q:2263:GLN:HB3 | 1.62 | 0.81 |
| 1:B:454:ARG:HB2 | 1:B:514:ARG:HD3 | 1.62 | 0.81 |
| 1:B:454:ARG:HH22 | 1:B:1338:LEU:HG | 1.44 | 0.81 |
| 1:M:1914:GLU:OE2 | 1:N:1655:LEU:N | 2.13 | 0.81 |
| 1:C:751:VAL:HG12 | 1:C:810:ILE:HG22 | 1.62 | 0.81 |
| 1:S:3317:ILE:HG12 | 1:S:3339:ARG:HB3 | 1.62 | 0.81 |
| 1:I:50:LYS:HB3 | 1:I:54:LYS:H | 1.45 | 0.81 |
| 1:R:3128:ILE:HD11 | 1:R:3190:LEU:HD22 | 1.62 | 0.81 |
| 1:I:69:TRP:HD1 | 1:I:251:LEU:HD12 | 1.46 | 0.81 |
| 1:I:3078:CYS:HA | 1:I:3081:GLU:HG2 | 1.61 | 0.81 |
| 1:E:885:HIS:NE2 | 1:E:903:CYS:SG | 2.54 | 0.80 |
| 1:L:1978:LYS:HA | 1:L:2078:LYS:HZ3 | 1.46 | 0.80 |
| 1:R:1978:LYS:HA | 1:R:2078:LYS:HZ3 | 1.46 | 0.80 |
| 1:T:486:TYR:HB3 | 1:T:777:MET:HE1 | 1.61 | 0.80 |
| 1:Q:2590:THR:HA | 1:Q:2594:ALA:HB3 | 1.63 | 0.80 |
| 1:S:50:LYS:HB3 | 1:S:54:LYS:H | 1.45 | 0.80 |
| 1:I:3334:ARG:HH21 | 1:I:3406:ILE:HG23 | 1.46 | 0.80 |
| 1:N:454:ARG:HH22 | 1:N:1338:LEU:HG | 1.45 | 0.80 |
| 1:E:50:LYS:HB3 | 1:E:54:LYS:H | 1.44 | 0.80 |
| 1:N:2738:GLN:HE22 | 1:O:2893:SER:HA | 1.47 | 0.80 |
| 1:E:866:LEU:HD23 | 1:E:967:PRO:HB2 | 1.62 | 0.80 |
| 1:P:1072:LEU:HD12 | 1:P:1073:PRO:HD2 | 1.61 | 0.80 |
| 1:A:2511:ILE:H | 1:A:2596:VAL:HG12 | 1.46 | 0.80 |
| 1:M:1736:MET:HB3 | 1:M:1915:LEU:HD13 | 1.63 | 0.80 |
| 1:J:1400:LEU:HD21 | 1:J:1436:LEU:HB3 | 1.62 | 0.80 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:O:2392:ARG:HB2 | 1:O:2494:LYS:HB3 | 1.64 | 0.80 |
| 1:Q:2226:ARG:O | 1:T:113:LYS:NZ | 2.12 | 0.80 |
| 1:T:617:VAL:HB | 1:T:625:LEU:HD23 | 1.64 | 0.80 |
| 1:T:1147:GLU:HG3 | 1:T:1245:PRO:HA | 1.62 | 0.80 |
| 1:A:2392:ARG:HB2 | 1:A:2494:LYS:HB3 | 1.63 | 0.80 |
| 1:H:617:VAL:HB | 1:H:625:LEU:HD23 | 1.62 | 0.80 |
| 1:M:915:ARG:HD3 | 1:M:1112:VAL:HG22 | 1.64 | 0.80 |
| 1:P:937:TRP:HB3 | 1:P:1051:LEU:HD13 | 1.64 | 0.80 |
| 1:E:1284:ARG:HE | 1:E:1379:PRO:HG3 | 1.46 | 0.79 |
| 1:K:731:ARG:NH1 | 1:K:834:THR:O | 2.13 | 0.79 |
| 1:L:2720:GLN:NE2 | 1:L:2730:TYR:O | 2.14 | 0.79 |
| 1:M:50:LYS:HB3 | 1:M:54:LYS:H | 1.47 | 0.79 |
| 1:N:1153:PHE:HB2 | 1:N:1198:PHE:HD2 | 1.46 | 0.79 |
| 1:R:2806:PHE:HE1 | 1:R:2892:PRO:HB3 | 1.46 | 0.79 |
| 1:L:1019:GLU:HA | 1:L:1022:HIS:CE1 | 2.17 | 0.79 |
| 1:B:1539:THR:HG23 | 1:B:1541:PRO:HD2 | 1.63 | 0.79 |
| 1:M:731:ARG:HG2 | 1:M:735:ARG:HH22 | 1.46 | 0.79 |
| 1:B:2775:GLN:NE2 | 1:B:2776:TYR:O | 2.15 | 0.79 |
| 1:R:313:PHE:HE2 | 1:R:406:PRO:HB3 | 1.47 | 0.79 |
| 1:N:1492:MET:HA | 1:N:1516:PRO:HG2 | 1.65 | 0.79 |
| 1:I:1914:GLU:OE1 | 1:J:1655:LEU:N | 2.16 | 0.79 |
| 1:Q:2224:THR:HB | 1:Q:2226:ARG:HH12 | 1.47 | 0.79 |
| 1:E:2108:LYS:HG3 | 1:E:2112:ARG:HH12 | 1.47 | 0.79 |
| 1:I:2590:THR:HA | 1:I:2594:ALA:HB3 | 1.65 | 0.79 |
| 1:L:937:TRP:HB3 | 1:L:1051:LEU:HD13 | 1.64 | 0.79 |
| 1:T:581:GLY:H | 1:T:856:ARG:HH22 | 1.28 | 0.79 |
| 1:B:1539:THR:HG22 | 1:B:1542:GLN:HE22 | 1.48 | 0.79 |
| 1:G:1680:VAL:HG12 | 1:G:1764:PRO:HB2 | 1.65 | 0.79 |
| 1:N:735:ARG:HB3 | 1:N:831:GLU:HB3 | 1.63 | 0.79 |
| 1:Q:751:VAL:HG12 | 1:Q:810:ILE:HG22 | 1.65 | 0.79 |
| 1:A:50:LYS:HB3 | 1:A:54:LYS:H | 1.46 | 0.78 |
| 1:B:937:TRP:HB3 | 1:B:1051:LEU:HD13 | 1.65 | 0.78 |
| 1:C:1081:ILE:HD13 | 1:D:2460:VAL:HG12 | 1.65 | 0.78 |
| 1:F:1539:THR:HG23 | 1:F:1541:PRO:HD2 | 1.64 | 0.78 |
| 1:T:3115:PHE:O | 1:T:3119:HIS:ND1 | 2.17 | 0.78 |
| 1:B:2865:ARG:HD3 | 1:B:2867:ASP:H | 1.48 | 0.78 |
| 1:D:1400:LEU:HD21 | 1:D:1436:LEU:HB3 | 1.66 | 0.78 |
| 1:F:937:TRP:HB3 | 1:F:1051:LEU:HD13 | 1.66 | 0.78 |
| 1:O:751:VAL:HG12 | 1:O:810:ILE:HG22 | 1.65 | 0.78 |
| 1:P:1539:THR:HG23 | 1:P:1541:PRO:HD2 | 1.65 | 0.78 |
| 1:R:3036:GLN:NE2 | 1:R:3043:GLN:OE1 | 2.16 | 0.78 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:2614:LEU:HD11 | 1:B:2636:ARG:HH12 | 1.48 | 0.78 |
| 1:J:2434:MET:HE3 | 1:J:2435:PRO:HD2 | 1.65 | 0.78 |
| 1:Q:1622:GLY:HA2 | 1:R:2779:LEU:HD21 | 1.66 | 0.78 |
| 1:F:538:LYS:HZ2 | 1:F:552:ASN:HB2 | 1.47 | 0.78 |
| 1:G:1151:ALA:HB2 | 1:G:1202:ILE:HD11 | 1.64 | 0.78 |
| 1:Q:1286:MET:HG3 | 1:Q:1292:PHE:HB2 | 1.66 | 0.78 |
| 1:D:1072:LEU:HD12 | 1:D:1073:PRO:HD2 | 1.66 | 0.78 |
| 1:F:1400:LEU:HD21 | 1:F:1436:LEU:HB3 | 1.65 | 0.78 |
| 1:O:3337:ARG:HD2 | 1:O:3378:ASN:HB2 | 1.65 | 0.78 |
| 1:F:454:ARG:HH22 | 1:F:1338:LEU:HG | 1.48 | 0.78 |
| 1:H:103:LEU:HD12 | 1:H:104:PRO:HD2 | 1.66 | 0.78 |
| 1:A:2939:ASN:ND2 | 1:J:2932:GLU:OE1 | 2.16 | 0.78 |
| 1:I:1286:MET:HG3 | 1:I:1292:PHE:HB2 | 1.66 | 0.78 |
| 1:K:2253:GLU:HG3 | 1:K:2384:ILE:HG12 | 1.66 | 0.78 |
| 1:L:103:LEU:HD12 | 1:L:104:PRO:HD2 | 1.66 | 0.78 |
| 1:L:2775:GLN:NE2 | 1:L:2776:TYR:O | 2.17 | 0.78 |
| 1:M:203:LEU:HD21 | 1:M:351:LEU:HB3 | 1.66 | 0.78 |
| 1:N:937:TRP:HB3 | 1:N:1051:LEU:HD13 | 1.64 | 0.78 |
| 1:S:1151:ALA:HB2 | 1:S:1202:ILE:HD11 | 1.66 | 0.78 |
| 1:S:3212:ARG:HG3 | 1:S:3214:TYR:HE1 | 1.47 | 0.78 |
| 1:E:3078:CYS:HA | 1:E:3081:GLU:HG2 | 1.65 | 0.78 |
| 1:I:751:VAL:HG12 | 1:I:810:ILE:HG22 | 1.66 | 0.77 |
| 1:P:597:ARG:HE | 1:P:658:ARG:HG3 | 1.48 | 0.77 |
| 1:D:405:ARG:NH1 | 1:D:406:PRO:O | 2.18 | 0.77 |
| 1:M:1680:VAL:HG12 | 1:M:1764:PRO:HB2 | 1.64 | 0.77 |
| 1:C:1862:GLY:HA3 | 1:C:1870:ALA:HB2 | 1.65 | 0.77 |
| 1:L:1539:THR:HG23 | 1:L:1541:PRO:HD2 | 1.63 | 0.77 |
| 1:Q:926:ARG:NH1 | 1:Q:931:GLN:O | 2.17 | 0.77 |
| 1:Q:2392:ARG:HB2 | 1:Q:2494:LYS:HB3 | 1.67 | 0.77 |
| 1:D:111:ILE:HG23 | 1:D:122:LYS:HB2 | 1.67 | 0.77 |
| 1:N:1579:THR:HG21 | 1:N:1585:ASN:HB3 | 1.67 | 0.77 |
| 1:P:3144:ARG:HE | 1:P:3147:LEU:HD21 | 1.48 | 0.77 |
| 1:Q:2637:SER:HB2 | 1:Q:2687:GLY:HA3 | 1.65 | 0.77 |
| 1:S:915:ARG:HD3 | 1:S:1112:VAL:HG22 | 1.67 | 0.77 |
| 1:P:846:HIS:HB3 | 1:P:1121:TYR:HA | 1.66 | 0.77 |
| 1:R:2964:LYS:HG2 | 1:R:2973:ARG:HB2 | 1.66 | 0.77 |
| 1:C:248:ARG:NH2 | 1:C:802:ASP:O | 2.17 | 0.77 |
| 1:I:885:HIS:NE2 | 1:I:903:CYS:SG | 2.57 | 0.77 |
| 1:I:1151:ALA:HB2 | 1:I:1202:ILE:HD11 | 1.66 | 0.77 |
| 1:K:2603:TRP:CD1 | 1:K:2711:ASN:HD22 | 2.03 | 0.77 |
| 1:Q:574:LEU:HB3 | 1:Q:616:LEU:HD21 | 1.65 | 0.77 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:D:1049:PHE:O | 1:D:1053:HIS:ND1 | 2.17 | 0.77 |
| 1:O:148:ARG:HA | 1:O:151:GLN:HE22 | 1.50 | 0.77 |
| 1:T:1400:LEU:HD21 | 1:T:1436:LEU:HB3 | 1.67 | 0.77 |
| 1:A:751:VAL:HG12 | 1:A:810:ILE:HG22 | 1.66 | 0.77 |
| 1:G:2253:GLU:HG3 | 1:G:2384:ILE:HG12 | 1.65 | 0.77 |
| 1:J:3115:PHE:O | 1:J:3119:HIS:ND1 | 2.18 | 0.77 |
| 1:N:1400:LEU:HD21 | 1:N:1436:LEU:HB3 | 1.64 | 0.77 |
| 1:D:3115:PHE:O | 1:D:3119:HIS:ND1 | 2.17 | 0.77 |
| 1:F:594:LEU:HA | 1:F:602:PHE:HE2 | 1.48 | 0.77 |
| 1:L:1072:LEU:HD12 | 1:L:1073:PRO:HD2 | 1.67 | 0.77 |
| 1:N:1072:LEU:HD12 | 1:N:1073:PRO:HD2 | 1.67 | 0.77 |
| 1:C:1400:LEU:HD21 | 1:C:1436:LEU:HB3 | 1.66 | 0.76 |
| 1:C:1680:VAL:HG12 | 1:C:1764:PRO:HB2 | 1.65 | 0.76 |
| 1:S:2392:ARG:HB2 | 1:S:2494:LYS:HB3 | 1.67 | 0.76 |
| 1:D:1873:HIS:HE2 | 1:D:2020:ALA:HB3 | 1.48 | 0.76 |
| 1:R:111:ILE:HG23 | 1:R:122:LYS:HB2 | 1.67 | 0.76 |
| 1:E:2392:ARG:HB2 | 1:E:2494:LYS:HB3 | 1.67 | 0.76 |
| 1:G:2603:TRP:CD1 | 1:G:2711:ASN:HD22 | 2.03 | 0.76 |
| 1:H:937:TRP:HB3 | 1:H:1051:LEU:HD13 | 1.67 | 0.76 |
| 1:S:2251:VAL:HG22 | 1:S:2263:GLN:HB3 | 1.66 | 0.76 |
| 1:E:2251:VAL:HG22 | 1:E:2263:GLN:HB3 | 1.66 | 0.76 |
| 1:J:454:ARG:NH2 | 1:J:1338:LEU:O | 2.18 | 0.76 |
| 1:R:1072:LEU:HD12 | 1:R:1073:PRO:HD2 | 1.67 | 0.76 |
| 1:H:1539:THR:HG23 | 1:H:1541:PRO:HD2 | 1.65 | 0.76 |
| 1:N:848:ARG:HE | 1:N:934:LEU:H | 1.32 | 0.76 |
| 1:Q:1587:ASN:OD1 | 1:T:337:GLN:NE2 | 2.18 | 0.76 |
| 1:R:1539:THR:HG23 | 1:R:1541:PRO:HD2 | 1.66 | 0.76 |
| 1:E:1151:ALA:HB2 | 1:E:1202:ILE:HD11 | 1.66 | 0.76 |
| 1:J:480:PRO:HA | 1:J:485:ARG:HH22 | 1.49 | 0.76 |
| 1:M:1862:GLY:HA3 | 1:M:1870:ALA:HB2 | 1.66 | 0.76 |
| 1:R:617:VAL:HB | 1:R:625:LEU:HD23 | 1.67 | 0.76 |
| 1:C:1842:ASN:HB3 | 1:C:1845:ASP:HB2 | 1.68 | 0.76 |
| 1:E:915:ARG:NH1 | 1:E:1057:ASP:OD2 | 2.19 | 0.76 |
| 1:J:1116:GLU:HA | 1:J:1120:GLN:HA | 1.68 | 0.76 |
| 1:G:2256:ASP:OD2 | 1:G:2440:ARG:NH2 | 2.18 | 0.76 |
| 1:G:2664:GLN:HE21 | 1:G:2670:PHE:HA | 1.51 | 0.76 |
| 1:G:2773:ASN:HD21 | 1:G:3142:TYR:HB2 | 1.51 | 0.76 |
| 1:O:1433:LEU:HD11 | 1:O:1460:HIS:CD2 | 2.21 | 0.76 |
| 1:R:2985:PRO:HB2 | 1:R:2989:ARG:HH21 | 1.49 | 0.76 |
| 1:A:731:ARG:HA | 1:A:735:ARG:HH12 | 1.49 | 0.76 |
| 1:A:1328:LEU:HB3 | 1:A:1499:PHE:HE2 | 1.50 | 0.76 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:G:594:LEU:O | 1:G:597:ARG:NH2 | 2.18 | 0.76 |
| 1:Q:2817:VAL:HG22 | 1:Q:2876:ILE:HG22 | 1.67 | 0.76 |
| 1:C:2000:VAL:HG12 | 1:C:2051:VAL:HG22 | 1.67 | 0.76 |
| 1:A:2590:THR:HA | 1:A:2594:ALA:HB3 | 1.68 | 0.75 |
| 1:J:1072:LEU:HD12 | 1:J:1073:PRO:HD2 | 1.69 | 0.75 |
| 1:A:1587:ASN:H | 1:D:337:GLN:HG3 | 1.48 | 0.75 |
| 1:E:2614:LEU:HB3 | 1:E:2636:ARG:HH12 | 1.52 | 0.75 |
| 1:E:257:ASP:HA | 1:E:265:ARG:HE | 1.51 | 0.75 |
| 1:E:437:VAL:HG12 | 1:E:521:PRO:HB2 | 1.68 | 0.75 |
| 1:H:405:ARG:NH1 | 1:H:406:PRO:O | 2.18 | 0.75 |
| 1:I:915:ARG:HD3 | 1:I:1112:VAL:HG22 | 1.68 | 0.75 |
| 1:L:808:LEU:HB2 | 1:L:820:GLU:HG3 | 1.68 | 0.75 |
| 1:A:3142:TYR:OH | 1:A:3144:ARG:NH1 | 2.19 | 0.75 |
| 1:B:1116:GLU:HA | 1:B:1120:GLN:HA | 1.68 | 0.75 |
| 1:F:1965:ALA:HA | 1:F:1968:LEU:HB2 | 1.67 | 0.75 |
| 1:F:2251:VAL:HG22 | 1:F:2263:GLN:HG3 | 1.68 | 0.75 |
| 1:H:2541:PRO:HD2 | 1:H:2542:ARG:H | 1.51 | 0.75 |
| 1:S:2108:LYS:HG3 | 1:S:2112:ARG:HH12 | 1.51 | 0.75 |
| 1:A:654:LEU:HD21 | 1:A:658:ARG:HH21 | 1.52 | 0.75 |
| 1:A:2253:GLU:HG3 | 1:A:2384:ILE:HG12 | 1.68 | 0.75 |
| 1:A:2796:ARG:O | 1:A:2801:ARG:NH2 | 2.20 | 0.75 |
| 1:J:405:ARG:NH1 | 1:J:406:PRO:O | 2.19 | 0.75 |
| 1:K:191:LEU:HG | 1:K:349:PHE:HE2 | 1.51 | 0.75 |
| 1:K:2251:VAL:HG22 | 1:K:2263:GLN:HB3 | 1.68 | 0.75 |
| 1:M:50:LYS:HE2 | 1:M:357:MET:HG2 | 1.68 | 0.75 |
| 1:R:2595:ARG:HG3 | 1:R:2596:VAL:HG13 | 1.68 | 0.75 |
| 1:T:907:MET:HG2 | 1:T:909:VAL:H | 1.51 | 0.75 |
| 1:E:2637:SER:HB2 | 1:E:2687:GLY:HA3 | 1.68 | 0.75 |
| 1:F:3398:GLN:NE2 | 1:F:3400:THR:OG1 | 2.19 | 0.75 |
| 1:M:1286:MET:HG3 | 1:M:1292:PHE:HB2 | 1.67 | 0.75 |
| 1:O:3078:CYS:HA | 1:O:3081:GLU:HG2 | 1.69 | 0.75 |
| 1:E:465:GLN:HG2 | 1:E:560:ALA:HB2 | 1.69 | 0.75 |
| 1:F:486:TYR:HB3 | 1:F:777:MET:HE1 | 1.67 | 0.75 |
| 1:S:465:GLN:HG2 | 1:S:560:ALA:HB2 | 1.68 | 0.75 |
| 1:C:1151:ALA:HB2 | 1:C:1202:ILE:HD11 | 1.69 | 0.75 |
| 1:C:2637:SER:HB2 | 1:C:2687:GLY:HA3 | 1.68 | 0.75 |
| 1:C:2664:GLN:HE21 | 1:C:2670:PHE:HA | 1.52 | 0.75 |
| 1:D:2595:ARG:HG3 | 1:D:2596:VAL:HG13 | 1.69 | 0.75 |
| 1:E:605:GLN:HA | 1:E:608:VAL:HG12 | 1.69 | 0.75 |
| 1:E:3386:TYR:HB2 | 1:E:3404:ILE:HG22 | 1.69 | 0.75 |
| 1:F:3047:ASP:HB2 | 1:F:3097:GLY:HA3 | 1.69 | 0.75 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:2470:ARG:NH1 | 1:A:2471:TYR:O | 2.20 | 0.75 |
| 1:E:2253:GLU:HG3 | 1:E:2384:ILE:HG12 | 1.68 | 0.75 |
| 1:E:2796:ARG:HH12 | 1:E:2801:ARG:HE | 1.35 | 0.75 |
| 1:H:1098:ASN:O | 1:H:1104:ARG:NH1 | 2.19 | 0.75 |
| 1:L:617:VAL:HB | 1:L:625:LEU:HD23 | 1.69 | 0.75 |
| 1:Q:1862:GLY:HA3 | 1:Q:1870:ALA:HB2 | 1.69 | 0.75 |
| 1:D:594:LEU:HA | 1:D:602:PHE:HE2 | 1.52 | 0.74 |
| 1:E:751:VAL:HG12 | 1:E:810:ILE:HG22 | 1.67 | 0.74 |
| 1:F:2919:LYS:HZ1 | 1:F:2997:MET:HE1 | 1.51 | 0.74 |
| 1:Q:2325:CYS:HA | 1:R:1242:VAL:HG13 | 1.68 | 0.74 |
| 1:S:69:TRP:HD1 | 1:S:251:LEU:HD12 | 1.51 | 0.74 |
| 1:S:2511:ILE:H | 1:S:2596:VAL:HG12 | 1.52 | 0.74 |
| 1:C:50:LYS:HB3 | 1:C:54:LYS:H | 1.52 | 0.74 |
| 1:F:94:TRP:O | 1:F:218:ASN:ND2 | 2.19 | 0.74 |
| 1:F:1959:GLU:OE2 | 1:F:1963:ILE:N | 2.20 | 0.74 |
| 1:M:2534:ALA:O | 1:M:2538:GLN:NE2 | 2.17 | 0.74 |
| 1:P:907:MET:HG2 | 1:P:909:VAL:H | 1.52 | 0.74 |
| 1:S:2470:ARG:NH1 | 1:S:2471:TYR:O | 2.19 | 0.74 |
| 1:S:3337:ARG:NH2 | 1:S:3379:TYR:O | 2.19 | 0.74 |
| 1:F:2313:GLN:HG2 | 1:F:2320:TYR:HB3 | 1.69 | 0.74 |
| 1:J:617:VAL:HB | 1:J:625:LEU:HD23 | 1.69 | 0.74 |
| 1:K:259:ASN:O | 1:K:265:ARG:NH2 | 2.21 | 0.74 |
| 1:M:611:ASN:HD22 | 1:M:771:LEU:H | 1.33 | 0.74 |
| 1:S:1127:GLU:OE2 | 1:S:1131:PHE:N | 2.20 | 0.74 |
| 1:T:1072:LEU:HD12 | 1:T:1073:PRO:HD2 | 1.69 | 0.74 |
| 1:J:1965:ALA:HA | 1:J:1968:LEU:HD13 | 1.67 | 0.74 |
| 1:J:2286:LEU:HB3 | 1:J:2428:LEU:HD21 | 1.67 | 0.74 |
| 1:M:2590:THR:HA | 1:M:2594:ALA:HB3 | 1.70 | 0.74 |
| 1:P:3398:GLN:NE2 | 1:P:3400:THR:OG1 | 2.20 | 0.74 |
| 1:S:1284:ARG:NH2 | 1:S:1376:GLU:OE2 | 2.20 | 0.74 |
| 1:S:1539:THR:HG23 | 1:S:1541:PRO:HD2 | 1.69 | 0.74 |
| 1:B:846:HIS:HB3 | 1:B:1121:TYR:HA | 1.69 | 0.74 |
| 1:D:3156:PRO:HB2 | 1:D:3162:LYS:HG3 | 1.70 | 0.74 |
| 1:G:1359:PRO:HD2 | 1:G:1362:ILE:HD11 | 1.70 | 0.74 |
| 1:M:2390:LYS:HB2 | 1:M:2392:ARG:HH22 | 1.53 | 0.74 |
| 1:A:3074:GLU:HB3 | 1:A:3080:PHE:HE1 | 1.51 | 0.74 |
| 1:M:2614:LEU:HD12 | 1:M:2636:ARG:HH22 | 1.52 | 0.74 |
| 1:S:866:LEU:HD23 | 1:S:967:PRO:HB2 | 1.70 | 0.74 |
| 1:A:2420:THR:HG21 | 1:A:2453:LEU:HD21 | 1.70 | 0.74 |
| 1:C:914:HIS:CE1 | 1:C:1053:HIS:HE1 | 2.05 | 0.74 |
| 1:F:739:GLY:HA3 | 1:F:784:LEU:HB3 | 1.70 | 0.74 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:J:254:PHE:HD2 | 1:J:264:THR:HB | 1.53 | 0.74 |
| 1:M:885:HIS:NE2 | 1:M:903:CYS:SG | 2.60 | 0.74 |
| 1:P:597:ARG:HH22 | 1:P:655:GLN:HA | 1.53 | 0.74 |
| 1:R:454:ARG:NH2 | 1:R:1338:LEU:O | 2.20 | 0.74 |
| 1:S:2253:GLU:HG3 | 1:S:2384:ILE:HG12 | 1.70 | 0.74 |
| 1:B:2587:ARG:HH22 | 1:B:2753:PRO:HG2 | 1.53 | 0.74 |
| 1:C:2511:ILE:H | 1:C:2596:VAL:HG12 | 1.51 | 0.74 |
| 1:F:1072:LEU:HD12 | 1:F:1073:PRO:HD2 | 1.70 | 0.74 |
| 1:A:1286:MET:HG3 | 1:A:1292:PHE:HB2 | 1.69 | 0.74 |
| 1:C:2392:ARG:HB2 | 1:C:2494:LYS:HB3 | 1.69 | 0.74 |
| 1:E:1127:GLU:OE2 | 1:E:1130:GLY:N | 2.19 | 0.74 |
| 1:J:2865:ARG:NH1 | 1:J:2867:ASP:OD2 | 2.20 | 0.74 |
| 1:L:2587:ARG:HH22 | 1:L:2753:PRO:HG2 | 1.53 | 0.74 |
| 1:T:2251:VAL:HG22 | 1:T:2263:GLN:HG3 | 1.70 | 0.74 |
| 1:A:2637:SER:HB2 | 1:A:2687:GLY:HA3 | 1.68 | 0.74 |
| 1:B:1143:ARG:O | 1:B:1148:ARG:NH1 | 2.20 | 0.74 |
| 1:L:3000:ARG:NH2 | 1:L:3004:ALA:O | 2.21 | 0.74 |
| 1:P:3360:LEU:HD12 | 1:P:3387:PHE:HB3 | 1.68 | 0.74 |
| 1:Q:3357:TYR:HB3 | 1:R:3329:LYS:HD3 | 1.70 | 0.74 |
| 1:R:3047:ASP:HB2 | 1:R:3097:GLY:HA3 | 1.70 | 0.74 |
| 1:T:937:TRP:HB3 | 1:T:1051:LEU:HD13 | 1.69 | 0.74 |
| 1:B:2665:ARG:O | 1:B:2723:GLN:NE2 | 2.21 | 0.73 |
| 1:G:731:ARG:HA | 1:G:735:ARG:HH12 | 1.52 | 0.73 |
| 1:G:937:TRP:O | 1:G:1055:ASN:ND2 | 2.21 | 0.73 |
| 1:G:2148:LEU:HB3 | 1:G:2151:VAL:HG11 | 1.70 | 0.73 |
| 1:K:2817:VAL:HG22 | 1:K:2876:ILE:HG22 | 1.70 | 0.73 |
| 1:O:756:LYS:NZ | 1:O:757:PRO:O | 2.21 | 0.73 |
| 1:O:2056:ARG:HH22 | 1:O:2060:GLY:HA2 | 1.50 | 0.73 |
| 1:O:2420:THR:HG21 | 1:O:2453:LEU:HD21 | 1.69 | 0.73 |
| 3:fA:1:NAG:H62 | 3:fA:2:NAG:HN2 | 1.52 | 0.73 |
| 1:A:1756:ARG:HH12 | 1:B:2175:THR:HB | 1.52 | 0.73 |
| 1:F:1677:ARG:NH1 | 1:F:1751:GLU:OE2 | 2.21 | 0.73 |
| 1:G:855:THR:H | 1:G:858:GLN:NE2 | 1.86 | 0.73 |
| 1:K:1286:MET:HG3 | 1:K:1292:PHE:HB2 | 1.71 | 0.73 |
| 1:N:3213:VAL:HG21 | 1:N:3270:LEU:HD12 | 1.69 | 0.73 |
| 1:O:1862:GLY:HA3 | 1:O:1870:ALA:HB2 | 1.69 | 0.73 |
| 1:O:2108:LYS:HG3 | 1:O:2112:ARG:HH12 | 1.53 | 0.73 |
| 1:R:1865:LYS:HE3 | 1:R:1867:HIS:H | 1.51 | 0.73 |
| 1:O:1963:ILE:HG23 | 1:O:1967:LEU:HD23 | 1.70 | 0.73 |
| 1:R:735:ARG:HB3 | 1:R:831:GLU:HB3 | 1.70 | 0.73 |
| 1:D:475:ALA:HB3 | 1:D:485:ARG:HB3 | 1.70 | 0.73 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:G:63:MET:HB3 | 1:G:246:LEU:HD21 | 1.71 | 0.73 |
| 1:G:1156:HIS:HB3 | 1:G:1193:GLN:HE22 | 1.53 | 0.73 |
| 1:H:1072:LEU:HD12 | 1:H:1073:PRO:HD2 | 1.70 | 0.73 |
| 1:L:7:ASN:HB3 | 1:L:10:LEU:HD13 | 1.69 | 0.73 |
| 1:M:756:LYS:NZ | 1:M:757:PRO:O | 2.21 | 0.73 |
| 1:T:698:ASN:ND2 | 1:T:705:GLU:OE2 | 2.21 | 0.73 |
| 1:A:605:GLN:HA | 1:A:608:VAL:HG12 | 1.69 | 0.73 |
| 1:E:915:ARG:HD3 | 1:E:1112:VAL:HG22 | 1.68 | 0.73 |
| 1:F:1837:ALA:HA | 1:F:1849:GLN:HE21 | 1.53 | 0.73 |
| 1:G:751:VAL:HG12 | 1:G:810:ILE:HG22 | 1.71 | 0.73 |
| 1:I:756:LYS:NZ | 1:I:757:PRO:O | 2.21 | 0.73 |
| 1:J:514:ARG:HH12 | 1:J:1341:GLY:HA2 | 1.53 | 0.73 |
| 1:K:1081:ILE:HD13 | 1:L:2460:VAL:HG12 | 1.68 | 0.73 |
| 1:P:1143:ARG:O | 1:P:1148:ARG:NH1 | 2.21 | 0.73 |
| 1:T:94:TRP:O | 1:T:218:ASN:ND2 | 2.21 | 0.73 |
| 1:F:2616:ASP:OD1 | 1:F:2617:LYS:N | 2.22 | 0.73 |
| 1:G:866:LEU:HD13 | 1:G:968:PHE:HE1 | 1.54 | 0.73 |
| 1:L:454:ARG:NH2 | 1:L:1338:LEU:O | 2.22 | 0.73 |
| 1:P:454:ARG:HB2 | 1:P:514:ARG:HD3 | 1.69 | 0.73 |
| 1:C:1286:MET:HG3 | 1:C:1292:PHE:HB2 | 1.68 | 0.73 |
| 1:E:3171:ASN:HA | 1:E:3176:GLN:HE22 | 1.54 | 0.73 |
| 1:H:673:GLU:O | 1:H:695:ARG:NH2 | 2.22 | 0.73 |
| 1:H:1677:ARG:NH2 | 1:H:1751:GLU:OE1 | 2.22 | 0.73 |
| 1:O:1195:ASP:HB2 | 1:P:2441:LEU:HD21 | 1.71 | 0.73 |
| 1:O:1286:MET:HG3 | 1:O:1292:PHE:HB2 | 1.70 | 0.73 |
| 1:E:756:LYS:NZ | 1:E:757:PRO:O | 2.22 | 0.73 |
| 1:F:2311:GLU:O | 1:F:2315:ARG:NH1 | 2.22 | 0.73 |
| 1:H:229:LEU:HB3 | 1:H:233:ARG:HH21 | 1.52 | 0.73 |
| 1:H:2667:TYR:HA | 1:H:2719:TRP:HH2 | 1.54 | 0.73 |
| 1:J:1750:PHE:HD2 | 1:J:1882:LEU:HD11 | 1.52 | 0.73 |
| 1:K:1862:GLY:HA3 | 1:K:1870:ALA:HB2 | 1.71 | 0.73 |
| 1:O:534:ALA:O | 1:O:538:LYS:NZ | 2.22 | 0.73 |
| 1:O:1328:LEU:HB3 | 1:O:1499:PHE:HE2 | 1.52 | 0.73 |
| 1:O:2470:ARG:NH1 | 1:O:2471:TYR:O | 2.21 | 0.73 |
| 1:O:2817:VAL:HG22 | 1:O:2876:ILE:HG22 | 1.69 | 0.73 |
| 1:S:1680:VAL:HG12 | 1:S:1764:PRO:HB2 | 1.71 | 0.73 |
| 1:B:1638:ARG:HH22 | 1:B:1642:GLY:HA2 | 1.54 | 0.73 |
| 1:C:2673:GLN:HE22 | 1:C:2852:GLN:H | 1.33 | 0.73 |
| 1:G:1466:ARG:NH2 | 1:G:1534:ASN:O | 2.20 | 0.73 |
| 1:G:2405:SER:HB3 | 1:G:2426:PHE:HE1 | 1.54 | 0.73 |
| 1:K:2252:LEU:HD11 | 1:K:2312:LEU:HD21 | 1.69 | 0.73 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:R:907:MET:HG2 | 1:R:909:VAL:H | 1.54 | 0.73 |
| 1:C:2253:GLU:HG3 | 1:C:2384:ILE:HG12 | 1.71 | 0.72 |
| 1:G:1286:MET:HG3 | 1:G:1292:PHE:HB2 | 1.71 | 0.72 |
| 1:L:1089:GLN:HE22 | 1:L:1092:ALA:HB3 | 1.54 | 0.72 |
| 1:M:1328:LEU:HB3 | 1:M:1499:PHE:HE2 | 1.54 | 0.72 |
| 1:N:1965:ALA:HA | 1:N:1968:LEU:HB2 | 1.69 | 0.72 |
| 1:O:1674:ARG:HD2 | 1:O:1954:GLU:HG2 | 1.71 | 0.72 |
| 1:P:2111:LEU:HD13 | 1:P:2212:PHE:HE1 | 1.53 | 0.72 |
| 1:D:2741:ARG:NH1 | 1:E:2868:SER:O | 2.21 | 0.72 |
| 1:O:1151:ALA:HB2 | 1:O:1202:ILE:HD11 | 1.70 | 0.72 |
| 1:R:2251:VAL:HG22 | 1:R:2263:GLN:HG3 | 1.71 | 0.72 |
| 1:T:594:LEU:HA | 1:T:602:PHE:HE1 | 1.53 | 0.72 |
| 1:F:696:PRO:HA | 1:F:699:ILE:HD13 | 1.72 | 0.72 |
| 1:I:866:LEU:HD23 | 1:I:967:PRO:HB2 | 1.71 | 0.72 |
| 1:I:1680:VAL:HG12 | 1:I:1764:PRO:HB2 | 1.70 | 0.72 |
| 1:R:2785:THR:OG1 | 1:R:2788:GLN:OE1 | 2.07 | 0.72 |
| 1:A:1862:GLY:HA3 | 1:A:1870:ALA:HB2 | 1.70 | 0.72 |
| 1:E:2420:THR:HG21 | 1:E:2453:LEU:HD21 | 1.71 | 0.72 |
| 1:G:1587:ASN:H | 1:J:337:GLN:HG3 | 1.53 | 0.72 |
| 1:J:907:MET:HG2 | 1:J:909:VAL:H | 1.55 | 0.72 |
| 1:M:1815:ARG:HD2 | 1:M:1818:LEU:HD21 | 1.71 | 0.72 |
| 1:P:1965:ALA:HA | 1:P:1968:LEU:HB2 | 1.70 | 0.72 |
| 1:S:756:LYS:NZ | 1:S:757:PRO:O | 2.23 | 0.72 |
| 1:T:7:ASN:HB3 | 1:T:10:LEU:HD13 | 1.72 | 0.72 |
| 1:A:1905:ASP:HB3 | 1:A:1908:GLU:HB2 | 1.72 | 0.72 |
| 1:E:2817:VAL:HG22 | 1:E:2876:ILE:HG22 | 1.71 | 0.72 |
| 1:F:617:VAL:HB | 1:F:625:LEU:HD23 | 1.70 | 0.72 |
| 1:G:3013:TRP:HZ3 | 1:G:3064:LEU:HB3 | 1.55 | 0.72 |
| 1:N:1837:ALA:HA | 1:N:1849:GLN:HE21 | 1.54 | 0.72 |
| 1:O:2534:ALA:O | 1:O:2538:GLN:NE2 | 2.18 | 0.72 |
| 1:R:1993:SER:HB2 | 1:R:2058:LEU:HD11 | 1.70 | 0.72 |
| 1:S:437:VAL:HG12 | 1:S:521:PRO:HB2 | 1.70 | 0.72 |
| 1:T:446:TYR:OH | 1:T:543:ASP:OD1 | 2.03 | 0.72 |
| 1:T:1492:MET:HA | 1:T:1516:PRO:HG2 | 1.72 | 0.72 |
| 1:T:2311:GLU:O | 1:T:2315:ARG:NH1 | 2.22 | 0.72 |
| 1:C:1466:ARG:NH2 | 1:C:1534:ASN:O | 2.22 | 0.72 |
| 1:M:1574:PHE:HB2 | 1:M:1634:GLU:HB3 | 1.70 | 0.72 |
| 1:Q:1359:PRO:HD2 | 1:Q:1362:ILE:HD11 | 1.70 | 0.72 |
| 1:R:2414:GLN:HE22 | 1:R:2453:LEU:HD22 | 1.54 | 0.72 |
| 1:S:3340:PHE:HE2 | 1:S:3351:VAL:HG11 | 1.55 | 0.72 |
| 1:C:738:VAL:HG23 | 1:C:789:ILE:HD13 | 1.72 | 0.72 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:E:1286:MET:HG3 | 1:E:1292:PHE:HB2 | 1.71 | 0.72 |
| 1:F:454:ARG:HB2 | 1:F:514:ARG:HD3 | 1.71 | 0.72 |
| 1:F:1677:ARG:NE | 1:F:1763:ILE:O | 2.22 | 0.72 |
| 1:I:465:GLN:HG2 | 1:I:560:ALA:HB2 | 1.71 | 0.72 |
| 1:I:534:ALA:O | 1:I:538:LYS:NZ | 2.22 | 0.72 |
| 1:T:1475:GLN:HG2 | 1:T:1482:ASP:HB3 | 1.70 | 0.72 |
| 1:B:2709:HIS:HA | 1:B:2712:VAL:HG22 | 1.72 | 0.72 |
| 1:D:2785:THR:OG1 | 1:D:2788:GLN:OE1 | 2.06 | 0.72 |
| 1:G:1420:CYS:HB2 | 1:G:1608:ARG:HH21 | 1.55 | 0.72 |
| 1:G:3020:LEU:HB3 | 1:G:3024:LEU:HD11 | 1.71 | 0.72 |
| 1:N:2414:GLN:HE22 | 1:N:2453:LEU:HD22 | 1.54 | 0.72 |
| 1:Q:493:MET:HE1 | 1:Q:670:MET:HE3 | 1.72 | 0.72 |
| 1:R:3360:LEU:HG | 1:R:3401:ARG:HD3 | 1.70 | 0.72 |
| 1:S:2286:LEU:HD12 | 1:S:2429:GLY:HA2 | 1.72 | 0.72 |
| 1:A:1842:ASN:HB3 | 1:A:1845:ASP:HB2 | 1.72 | 0.72 |
| 1:E:2673:GLN:HE22 | 1:E:2852:GLN:H | 1.36 | 0.72 |
| 1:F:379:LYS:HD3 | 1:F:381:ASN:H | 1.53 | 0.72 |
| 1:F:925:LEU:HD13 | 1:F:928:LYS:HE2 | 1.69 | 0.72 |
| 1:H:2414:GLN:HE22 | 1:H:2453:LEU:HD22 | 1.55 | 0.72 |
| 1:I:2256:ASP:OD2 | 1:I:2440:ARG:NH2 | 2.23 | 0.72 |
| 1:K:3142:TYR:OH | 1:K:3144:ARG:NH1 | 2.23 | 0.72 |
| 1:L:1919:PRO:HB2 | 1:L:1924:SER:HB2 | 1.72 | 0.72 |
| 1:M:248:ARG:NH2 | 1:M:802:ASP:O | 2.23 | 0.72 |
| 1:O:2511:ILE:H | 1:O:2596:VAL:HG12 | 1.53 | 0.72 |
| 1:P:617:VAL:HB | 1:P:625:LEU:HD23 | 1.70 | 0.72 |
| 1:P:655:GLN:HG2 | 1:P:662:TYR:HB3 | 1.69 | 0.72 |
| 1:S:2817:VAL:HG22 | 1:S:2876:ILE:HG22 | 1.70 | 0.72 |
| 3:pA:1:NAG:H62 | 3:pA:2:NAG:HN2 | 1.54 | 0.72 |
| 1:C:926:ARG:NH1 | 1:C:931:GLN:O | 2.23 | 0.72 |
| 1:D:1743:HIS:HD2 | 1:D:1885:HIS:HD2 | 1.37 | 0.72 |
| 1:E:248:ARG:NH2 | 1:E:802:ASP:O | 2.23 | 0.72 |
| 1:H:1089:GLN:HE22 | 1:H:1092:ALA:HB3 | 1.54 | 0.72 |
| 1:I:2420:THR:HG21 | 1:I:2453:LEU:HD21 | 1.71 | 0.72 |
| 1:J:3360:LEU:HD12 | 1:J:3387:PHE:HB3 | 1.72 | 0.72 |
| 1:K:20:GLU:O | 1:K:24:ARG:HD3 | 1.90 | 0.72 |
| 1:Q:2602:ASP:HA | 1:Q:2711:ASN:HD21 | 1.55 | 0.72 |
| 1:A:1067:GLN:HE21 | 1:A:1072:LEU:HB2 | 1.54 | 0.71 |
| 1:D:244:VAL:HG22 | 1:D:828:ILE:HG21 | 1.71 | 0.71 |
| 1:K:2709:HIS:HA | 1:K:2712:VAL:HG12 | 1.72 | 0.71 |
| 1:L:1742:TRP:HD1 | 1:L:1920:LEU:HD12 | 1.54 | 0.71 |
| 1:L:2622:PHE:O | 1:L:2636:ARG:NH2 | 2.23 | 0.71 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:M:2273:TYR:HB2 | 1:M:2428:LEU:HD21 | 1.70 | 0.71 |
| 1:M:2664:GLN:HE21 | 1:M:2670:PHE:HA | 1.54 | 0.71 |
| 1:P:1149:VAL:HG11 | 1:P:1206:LEU:HD13 | 1.71 | 0.71 |
| 1:P:1321:VAL:HA | 1:P:1324:HIS:HD2 | 1.52 | 0.71 |
| 1:R:3142:TYR:O | 1:R:3144:ARG:NH1 | 2.23 | 0.71 |
| 1:S:2364:ASN:OD1 | 1:S:2366:ARG:NH1 | 2.22 | 0.71 |
| 1:T:441:THR:OG1 | 1:T:444:GLU:OE1 | 2.08 | 0.71 |
| 1:E:126:PHE:O | 1:E:143:ARG:NH2 | 2.24 | 0.71 |
| 1:F:1865:LYS:HE3 | 1:F:1867:HIS:H | 1.55 | 0.71 |
| 1:G:471:HIS:NE2 | 1:G:489:CYS:SG | 2.63 | 0.71 |
| 1:K:2570:GLY:HA3 | 1:K:2845:TRP:HB2 | 1.72 | 0.71 |
| 1:M:534:ALA:O | 1:M:538:LYS:NZ | 2.22 | 0.71 |
| 1:Q:1899:GLN:HE21 | 1:Q:1904:HIS:HB2 | 1.54 | 0.71 |
| 1:R:80:LYS:HA | 1:R:83:LYS:HZ3 | 1.55 | 0.71 |
| 1:R:1098:ASN:O | 1:R:1104:ARG:NH1 | 2.23 | 0.71 |
| 1:A:2096:ILE:HD13 | 1:A:2179:PRO:HG2 | 1.73 | 0.71 |
| 1:F:1978:LYS:HA | 1:F:2078:LYS:HZ3 | 1.54 | 0.71 |
| 1:I:3088:HIS:HD2 | 1:I:3122:ILE:HG13 | 1.55 | 0.71 |
| 1:K:1914:GLU:OE2 | 1:L:1655:LEU:N | 2.16 | 0.71 |
| 1:M:465:GLN:HG2 | 1:M:560:ALA:HB2 | 1.70 | 0.71 |
| 1:M:750:LEU:HD11 | 1:M:767:LYS:HE3 | 1.72 | 0.71 |
| 1:O:2637:SER:HB2 | 1:O:2687:GLY:HA3 | 1.70 | 0.71 |
| 1:R:1116:GLU:HA | 1:R:1120:GLN:HA | 1.72 | 0.71 |
| 1:S:2978:THR:H | 1:S:2987:TRP:HZ3 | 1.38 | 0.71 |
| 1:G:437:VAL:HG12 | 1:G:521:PRO:HB2 | 1.72 | 0.71 |
| 1:H:3000:ARG:NH2 | 1:H:3004:ALA:O | 2.21 | 0.71 |
| 1:K:1320:ALA:HA | 1:K:1423:GLU:HG3 | 1.71 | 0.71 |
| 1:O:654:LEU:HD21 | 1:O:658:ARG:HH21 | 1.56 | 0.71 |
| 1:P:247:PHE:O | 1:P:271:LYS:NZ | 2.23 | 0.71 |
| 1:Q:534:ALA:O | 1:Q:538:LYS:NZ | 2.24 | 0.71 |
| 1:R:105:ARG:HA | 1:R:108:GLN:HE22 | 1.54 | 0.71 |
| 1:T:3392:ASN:HB3 | 1:T:3395:ARG:HG2 | 1.72 | 0.71 |
| 1:I:1862:GLY:HA3 | 1:I:1870:ALA:HB2 | 1.71 | 0.71 |
| 1:D:1993:SER:HB2 | 1:D:2058:LEU:HD11 | 1.71 | 0.71 |
| 1:E:2534:ALA:O | 1:E:2538:GLN:NE2 | 2.20 | 0.71 |
| 1:H:808:LEU:HB2 | 1:H:820:GLU:HG3 | 1.71 | 0.71 |
| 1:K:937:TRP:O | 1:K:1055:ASN:ND2 | 2.24 | 0.71 |
| 1:K:1156:HIS:HB3 | 1:K:1193:GLN:HE22 | 1.53 | 0.71 |
| 1:L:1284:ARG:HH22 | 1:L:1379:PRO:HB3 | 1.55 | 0.71 |
| 1:O:555:PHE:HA | 1:O:568:ARG:HH22 | 1.56 | 0.71 |
| 1:S:2420:THR:HG21 | 1:S:2453:LEU:HD21 | 1.73 | 0.71 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:808:LEU:HB2 | 1:B:820:GLU:HG3 | 1.72 | 0.71 |
| 1:G:2579:ARG:NH1 | 1:G:2774:TYR:OH | 2.23 | 0.71 |
| 1:J:441:THR:OG1 | 1:J:444:GLU:OE1 | 2.08 | 0.71 |
| 1:L:454:ARG:HH22 | 1:L:1338:LEU:HG | 1.56 | 0.71 |
| 1:M:3334:ARG:HH21 | 1:M:3406:ILE:HG23 | 1.55 | 0.71 |
| 1:P:1400:LEU:HD21 | 1:P:1436:LEU:HB3 | 1.72 | 0.71 |
| 1:R:486:TYR:HB3 | 1:R:777:MET:HE1 | 1.73 | 0.71 |
| 1:S:1575:ILE:HD11 | 1:S:1590:ALA:HB2 | 1.72 | 0.71 |
| 1:T:735:ARG:HB3 | 1:T:831:GLU:HB3 | 1.73 | 0.71 |
| 1:A:2664:GLN:NE2 | 1:A:2669:ASN:OD1 | 2.24 | 0.71 |
| 1:G:2078:LYS:HB3 | 1:G:2080:ARG:HH22 | 1.56 | 0.71 |
| 1:I:2614:LEU:HD12 | 1:I:2636:ARG:HH22 | 1.55 | 0.71 |
| 1:I:2803:PHE:HB3 | 1:I:2852:GLN:OE1 | 1.91 | 0.71 |
| 1:K:866:LEU:HD13 | 1:K:968:PHE:HE1 | 1.56 | 0.71 |
| 1:K:2572:ALA:HB3 | 1:K:2736:ASN:HD21 | 1.56 | 0.71 |
| 1:K:2579:ARG:NH1 | 1:K:2774:TYR:OH | 2.23 | 0.71 |
| 1:L:735:ARG:HH22 | 1:L:790:THR:H | 1.39 | 0.71 |
| 1:L:2087:LEU:HD13 | 1:L:2366:ARG:HD3 | 1.73 | 0.71 |
| 1:M:2511:ILE:H | 1:M:2596:VAL:HG12 | 1.56 | 0.71 |
| 1:N:2741:ARG:NH2 | 1:O:2866:PRO:O | 2.24 | 0.71 |
| 1:Q:1899:GLN:NE2 | 1:Q:1905:ASP:O | 2.24 | 0.71 |
| 1:R:454:ARG:HH22 | 1:R:1338:LEU:HG | 1.56 | 0.71 |
| 1:S:1284:ARG:HD3 | 1:S:1379:PRO:HG3 | 1.70 | 0.71 |
| 1:D:2251:VAL:HG22 | 1:D:2263:GLN:HG3 | 1.73 | 0.71 |
| 1:F:3360:LEU:HG | 1:F:3401:ARG:HD3 | 1.72 | 0.71 |
| 1:T:1019:GLU:HA | 1:T:1022:HIS:CE1 | 2.25 | 0.71 |
| 1:C:2044:SER:OG | 1:C:2046:ASP:OD1 | 2.08 | 0.71 |
| 1:D:2964:LYS:HG2 | 1:D:2973:ARG:HB2 | 1.72 | 0.71 |
| 1:K:1815:ARG:HD3 | 1:K:1818:LEU:HD21 | 1.72 | 0.71 |
| 1:M:20:GLU:O | 1:M:24:ARG:HD3 | 1.91 | 0.71 |
| 1:M:1785:ARG:NH1 | 1:M:1786:ASP:O | 2.24 | 0.71 |
| 1:M:2392:ARG:HB2 | 1:M:2494:LYS:HB3 | 1.72 | 0.71 |
| 1:N:405:ARG:NH1 | 1:N:406:PRO:O | 2.23 | 0.71 |
| 1:Q:2227:ASP:HB3 | 1:Q:2277:GLY:HA3 | 1.73 | 0.71 |
| 1:Q:3142:TYR:OH | 1:Q:3144:ARG:NH1 | 2.24 | 0.71 |
| 1:S:605:GLN:HA | 1:S:608:VAL:HG12 | 1.73 | 0.71 |
| 1:A:20:GLU:O | 1:A:24:ARG:HD3 | 1.91 | 0.70 |
| 1:A:2803:PHE:HB3 | 1:A:2852:GLN:OE1 | 1.89 | 0.70 |
| 1:K:63:MET:HB3 | 1:K:246:LEU:HD21 | 1.72 | 0.70 |
| 1:O:1067:GLN:HE21 | 1:O:1072:LEU:HB2 | 1.56 | 0.70 |
| 1:O:1914:GLU:OE1 | 1:P:1655:LEU:N | 2.17 | 0.70 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:S:629:HIS:HA | 1:S:775:LYS:HZ1 | 1.56 | 0.70 |
| 1:S:915:ARG:NH1 | 1:S:1057:ASP:OD2 | 2.23 | 0.70 |
| 1:T:614:HIS:HA | 1:T:625:LEU:HG | 1.73 | 0.70 |
| 1:C:1811:ARG:NH2 | 1:C:1878:ASP:OD1 | 2.24 | 0.70 |
| 1:F:465:GLN:NE2 | 1:F:558:PRO:O | 2.24 | 0.70 |
| 1:H:94:TRP:O | 1:H:218:ASN:ND2 | 2.24 | 0.70 |
| 1:J:2587:ARG:HH22 | 1:J:2753:PRO:HG2 | 1.56 | 0.70 |
| 1:L:499:TRP:CH2 | 1:L:499:TRP:CE2 | 2.78 | 0.70 |
| 1:L:1677:ARG:NH1 | 1:L:1763:ILE:O | 2.24 | 0.70 |
| 1:N:1448:LEU:HD21 | 1:N:1596:LEU:HG | 1.73 | 0.70 |
| 1:N:2665:ARG:O | 1:N:2723:GLN:NE2 | 2.25 | 0.70 |
| 1:S:2805:ASN:HB3 | 1:S:2850:LEU:HD21 | 1.72 | 0.70 |
| 1:T:3047:ASP:HB2 | 1:T:3097:GLY:HA3 | 1.71 | 0.70 |
| 1:B:1089:GLN:HE22 | 1:B:1092:ALA:HB3 | 1.56 | 0.70 |
| 1:D:1147:GLU:HG3 | 1:D:1245:PRO:HA | 1.72 | 0.70 |
| 1:F:1492:MET:HA | 1:F:1516:PRO:HG2 | 1.74 | 0.70 |
| 1:G:20:GLU:O | 1:G:24:ARG:HD3 | 1.91 | 0.70 |
| 1:L:1286:MET:HE1 | 1:L:1292:PHE:HB2 | 1.72 | 0.70 |
| 1:M:956:VAL:HA | 1:M:963:PRO:HA | 1.73 | 0.70 |
| 1:P:8:VAL:O | 1:P:105:ARG:NH1 | 2.24 | 0.70 |
| 1:Q:2981:MET:HE3 | 1:Q:3149:ASN:HD22 | 1.54 | 0.70 |
| 1:R:1677:ARG:NH1 | 1:R:1763:ILE:O | 2.24 | 0.70 |
| 1:S:3052:LEU:O | 1:S:3055:ARG:NH2 | 2.25 | 0.70 |
| 1:T:229:LEU:HB3 | 1:T:233:ARG:HH21 | 1.55 | 0.70 |
| 1:T:3232:LEU:HD13 | 1:T:3269:ALA:HB3 | 1.72 | 0.70 |
| 1:B:244:VAL:HG22 | 1:B:828:ILE:HG21 | 1.73 | 0.70 |
| 1:C:2148:LEU:HB3 | 1:C:2151:VAL:HG11 | 1.73 | 0.70 |
| 1:G:309:ALA:H | 1:G:370:SER:HG | 1.37 | 0.70 |
| 1:G:1899:GLN:HE21 | 1:G:1904:HIS:HB2 | 1.56 | 0.70 |
| 1:H:2587:ARG:HH22 | 1:H:2753:PRO:HG2 | 1.56 | 0.70 |
| 1:I:1081:ILE:HD13 | 1:J:2460:VAL:HG12 | 1.73 | 0.70 |
| 1:K:512:LYS:HA | 1:K:516:LEU:HB2 | 1.72 | 0.70 |
| 1:K:1811:ARG:NH2 | 1:K:1878:ASP:OD1 | 2.23 | 0.70 |
| 1:K:2405:SER:HB3 | 1:K:2426:PHE:HE1 | 1.55 | 0.70 |
| 1:A:69:TRP:HD1 | 1:A:251:LEU:HD12 | 1.55 | 0.70 |
| 1:B:617:VAL:HB | 1:B:625:LEU:HD23 | 1.71 | 0.70 |
| 1:I:63:MET:HB3 | 1:I:246:LEU:HD21 | 1.72 | 0.70 |
| 1:K:534:ALA:O | 1:K:538:LYS:NZ | 2.24 | 0.70 |
| 1:O:1732:CYS:O | 1:O:1734:HIS:ND1 | 2.23 | 0.70 |
| 1:P:144:ALA:HB3 | 1:P:194:GLY:HA3 | 1.73 | 0.70 |
| 1:Q:1815:ARG:HD3 | 1:Q:1818:LEU:HD21 | 1.73 | 0.70 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:256:ARG:O | 1:B:265:ARG:NH1 | 2.25 | 0.70 |
| 1:I:2462:ASN:O | 1:J:1085:ARG:NH1 | 2.25 | 0.70 |
| 1:L:991:LYS:NZ | 1:L:992:PHE:O | 2.25 | 0.70 |
| 1:N:2264:PHE:HZ | 1:N:2302:VAL:HG13 | 1.56 | 0.70 |
| 1:O:69:TRP:HD1 | 1:O:251:LEU:HD12 | 1.56 | 0.70 |
| 1:Q:2253:GLU:HG3 | 1:Q:2384:ILE:HG12 | 1.71 | 0.70 |
| 1:S:534:ALA:O | 1:S:538:LYS:NZ | 2.25 | 0.70 |
| 1:S:3332:VAL:O | 1:S:3334:ARG:NH2 | 2.24 | 0.70 |
| 1:T:991:LYS:NZ | 1:T:992:PHE:O | 2.25 | 0.70 |
| 1:C:574:LEU:HB3 | 1:C:616:LEU:HD21 | 1.72 | 0.70 |
| 1:C:915:ARG:HD3 | 1:C:1112:VAL:HG22 | 1.74 | 0.70 |
| 1:D:2985:PRO:HB2 | 1:D:2989:ARG:HH21 | 1.55 | 0.70 |
| 1:H:1837:ALA:HA | 1:H:1849:GLN:HE21 | 1.55 | 0.70 |
| 1:J:1775:LEU:HD12 | 1:J:1776:PRO:HD2 | 1.74 | 0.70 |
| 1:J:2809:GLN:NE2 | 1:J:2845:TRP:O | 2.25 | 0.70 |
| 1:L:735:ARG:HB3 | 1:L:831:GLU:HB3 | 1.74 | 0.70 |
| 1:N:94:TRP:O | 1:N:218:ASN:ND2 | 2.25 | 0.70 |
| 1:Q:1680:VAL:HG12 | 1:Q:1764:PRO:HB2 | 1.71 | 0.70 |
| 1:R:2148:LEU:HD13 | 1:R:2334:MET:HE1 | 1.72 | 0.70 |
| 1:R:2149:HIS:HA | 1:R:2154:PHE:HD2 | 1.56 | 0.70 |
| 1:S:2637:SER:HB2 | 1:S:2687:GLY:HA3 | 1.72 | 0.70 |
| 3:VA:1:NAG:H62 | 3:VA:2:NAG:HN2 | 1.55 | 0.70 |
| 1:D:907:MET:HG2 | 1:D:909:VAL:H | 1.56 | 0.70 |
| 1:E:148:ARG:HA | 1:E:151:GLN:HE22 | 1.54 | 0.70 |
| 1:H:501:ARG:HH22 | 1:H:702:TYR:HB3 | 1.57 | 0.70 |
| 1:I:915:ARG:NH1 | 1:I:1057:ASP:OD2 | 2.25 | 0.70 |
| 1:I:1815:ARG:HD2 | 1:I:1818:LEU:HD21 | 1.74 | 0.70 |
| 1:L:925:LEU:HD13 | 1:L:928:LYS:HE2 | 1.74 | 0.70 |
| 1:Q:20:GLU:O | 1:Q:24:ARG:HD3 | 1.92 | 0.70 |
| 1:R:420:LYS:NZ | 1:R:422:SER:O | 2.22 | 0.70 |
| 1:S:63:MET:HB3 | 1:S:246:LEU:HD21 | 1.72 | 0.70 |
| 1:S:1862:GLY:HA3 | 1:S:1870:ALA:HB2 | 1.74 | 0.70 |
| 1:S:1917:ARG:NH2 | 1:T:1631:ILE:O | 2.24 | 0.70 |
| 1:A:3089:ASN:HD21 | 1:A:3248:LEU:H | 1.40 | 0.70 |
| 1:B:499:TRP:CH2 | 1:B:499:TRP:CE2 | 2.78 | 0.70 |
| 1:E:20:GLU:O | 1:E:24:ARG:HD3 | 1.91 | 0.70 |
| 1:G:2572:ALA:HB3 | 1:G:2736:ASN:HD21 | 1.57 | 0.70 |
| 1:G:2590:THR:HA | 1:G:2594:ALA:HB3 | 1.74 | 0.70 |
| 1:I:1539:THR:HG23 | 1:I:1541:PRO:HD2 | 1.74 | 0.70 |
| 1:J:420:LYS:NZ | 1:J:422:SER:O | 2.23 | 0.70 |
| 1:K:1067:GLN:HG2 | 1:K:1074:TYR:HB3 | 1.74 | 0.70 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:L:1147:GLU:HG3 | 1:L:1245:PRO:HA | 1.71 | 0.70 |
| 1:M:3385:ASP:O | 1:N:3148:ARG:NH2 | 2.25 | 0.70 |
| 1:O:1811:ARG:NH2 | 1:O:1878:ASP:OD1 | 2.24 | 0.70 |
| 1:T:465:GLN:NE2 | 1:T:558:PRO:O | 2.23 | 0.70 |
| 1:A:738:VAL:HG23 | 1:A:789:ILE:HD13 | 1.74 | 0.70 |
| 1:A:3386:TYR:HB2 | 1:A:3404:ILE:HG22 | 1.73 | 0.70 |
| 1:C:20:GLU:O | 1:C:24:ARG:HD3 | 1.92 | 0.70 |
| 1:C:493:MET:HE3 | 1:C:670:MET:HE2 | 1.72 | 0.70 |
| 1:C:3231:LYS:HB2 | 1:C:3284:GLN:HE21 | 1.56 | 0.70 |
| 1:D:937:TRP:HB3 | 1:D:1051:LEU:HD13 | 1.74 | 0.70 |
| 1:G:1811:ARG:NH2 | 1:G:1878:ASP:OD1 | 2.24 | 0.70 |
| 1:H:247:PHE:HB3 | 1:H:271:LYS:HD2 | 1.72 | 0.70 |
| 1:H:2964:LYS:HG2 | 1:H:2973:ARG:HB2 | 1.73 | 0.70 |
| 1:I:20:GLU:O | 1:I:24:ARG:HD3 | 1.91 | 0.70 |
| 1:K:751:VAL:HG12 | 1:K:810:ILE:HG22 | 1.73 | 0.70 |
| 1:K:2939:ASN:ND2 | 1:T:2932:GLU:OE1 | 2.25 | 0.70 |
| 1:L:907:MET:HG2 | 1:L:909:VAL:H | 1.56 | 0.70 |
| 1:N:1089:GLN:HE22 | 1:N:1092:ALA:HB3 | 1.57 | 0.70 |
| 1:P:3032:PHE:HA | 1:P:3113:PRO:HG2 | 1.74 | 0.70 |
| 1:R:673:GLU:O | 1:R:695:ARG:NH2 | 2.22 | 0.70 |
| 1:A:1770:ASN:OD1 | 1:A:1772:GLN:NE2 | 2.25 | 0.69 |
| 1:B:2232:LEU:HD12 | 1:B:2274:LEU:HB3 | 1.74 | 0.69 |
| 1:C:1714:HIS:NE2 | 1:C:1732:CYS:SG | 2.64 | 0.69 |
| 1:F:1116:GLU:HA | 1:F:1120:GLN:HA | 1.74 | 0.69 |
| 1:F:1284:ARG:NH2 | 1:F:1377:SER:O | 2.25 | 0.69 |
| 1:H:907:MET:HG2 | 1:H:909:VAL:H | 1.55 | 0.69 |
| 1:H:991:LYS:NZ | 1:H:992:PHE:O | 2.25 | 0.69 |
| 1:H:1919:PRO:HB2 | 1:H:1924:SER:HB2 | 1.73 | 0.69 |
| 1:J:1448:LEU:HD21 | 1:J:1596:LEU:HG | 1.73 | 0.69 |
| 1:J:2112:ARG:HE | 1:J:2116:LYS:HE2 | 1.56 | 0.69 |
| 1:K:1417:THR:O | 1:K:1475:GLN:NE2 | 2.25 | 0.69 |
| 1:K:1680:VAL:HG12 | 1:K:1764:PRO:HB2 | 1.73 | 0.69 |
| 1:L:1710:LEU:HD22 | 1:L:1750:PHE:HE1 | 1.57 | 0.69 |
| 1:L:2414:GLN:HE22 | 1:L:2453:LEU:HD22 | 1.57 | 0.69 |
| 1:N:2149:HIS:HA | 1:N:2154:PHE:HD2 | 1.57 | 0.69 |
| 1:O:2656:ARG:HD2 | 1:O:2656:ARG:H | 1.57 | 0.69 |
| 1:R:3037:ILE:HG22 | 1:R:3042:HIS:H | 1.57 | 0.69 |
| 1:A:1575:ILE:HD11 | 1:A:1590:ALA:HB2 | 1.73 | 0.69 |
| 1:G:514:ARG:HH12 | 1:G:1343:ALA:HA | 1.56 | 0.69 |
| 1:H:1677:ARG:NH1 | 1:H:1763:ILE:O | 2.25 | 0.69 |
| 1:H:1742:TRP:HD1 | 1:H:1920:LEU:HD12 | 1.56 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:K:1714:HIS:NE2 | 1:K:1732:CYS:SG | 2.65 | 0.69 |
| 1:N:597:ARG:HH22 | 1:N:655:GLN:HA | 1.57 | 0.69 |
| 1:T:2809:GLN:NE2 | 1:T:2845:TRP:O | 2.25 | 0.69 |
| 1:A:1732:CYS:O | 1:A:1734:HIS:ND1 | 2.25 | 0.69 |
| 1:B:1098:ASN:O | 1:B:1104:ARG:NH1 | 2.26 | 0.69 |
| 1:C:1732:CYS:O | 1:C:1734:HIS:ND1 | 2.22 | 0.69 |
| 1:D:2126:LEU:HD21 | 1:D:2165:VAL:HG12 | 1.74 | 0.69 |
| 1:E:534:ALA:O | 1:E:538:LYS:NZ | 2.25 | 0.69 |
| 1:F:1993:SER:HB2 | 1:F:2058:LEU:HD11 | 1.75 | 0.69 |
| 1:G:1714:HIS:NE2 | 1:G:1732:CYS:SG | 2.65 | 0.69 |
| 1:H:1284:ARG:HH22 | 1:H:1379:PRO:HB3 | 1.58 | 0.69 |
| 1:L:1098:ASN:O | 1:L:1104:ARG:NH1 | 2.26 | 0.69 |
| 1:P:887:GLN:HE22 | 1:P:889:ASN:HB2 | 1.56 | 0.69 |
| 1:P:2414:GLN:HE22 | 1:P:2453:LEU:HD22 | 1.56 | 0.69 |
| 1:P:2709:HIS:HA | 1:P:2712:VAL:HG22 | 1.74 | 0.69 |
| 1:A:1742:TRP:HD1 | 1:A:1920:LEU:HD12 | 1.58 | 0.69 |
| 1:E:50:LYS:NZ | 1:E:357:MET:SD | 2.64 | 0.69 |
| 1:H:2232:LEU:HD12 | 1:H:2274:LEU:HB3 | 1.74 | 0.69 |
| 1:H:3047:ASP:HB2 | 1:H:3097:GLY:HA3 | 1.74 | 0.69 |
| 1:I:2108:LYS:HG3 | 1:I:2112:ARG:HH12 | 1.56 | 0.69 |
| 1:J:1993:SER:HB2 | 1:J:2058:LEU:HD11 | 1.74 | 0.69 |
| 1:L:3154:LEU:O | 1:L:3158:ASN:N | 2.24 | 0.69 |
| 1:M:69:TRP:HD1 | 1:M:251:LEU:HD12 | 1.58 | 0.69 |
| 1:P:673:GLU:O | 1:P:695:ARG:NH2 | 2.24 | 0.69 |
| 1:R:2159:ARG:NE | 1:R:2303:ASP:OD1 | 2.26 | 0.69 |
| 1:S:937:TRP:O | 1:S:1055:ASN:ND2 | 2.26 | 0.69 |
| 1:A:1674:ARG:HD2 | 1:A:1954:GLU:HG2 | 1.74 | 0.69 |
| 1:B:1677:ARG:NH2 | 1:B:1751:GLU:OE1 | 2.25 | 0.69 |
| 1:C:2883:GLN:NE2 | 1:C:2884:LEU:O | 2.26 | 0.69 |
| 1:F:144:ALA:HB3 | 1:F:194:GLY:HA3 | 1.75 | 0.69 |
| 1:H:2087:LEU:HD13 | 1:H:2366:ARG:HD3 | 1.73 | 0.69 |
| 1:I:1770:ASN:OD1 | 1:I:1772:GLN:NE2 | 2.26 | 0.69 |
| 1:J:1546:VAL:HA | 1:J:1549:ARG:HG2 | 1.75 | 0.69 |
| 1:L:2243:VAL:HG23 | 1:L:2244:LEU:HD12 | 1.73 | 0.69 |
| 1:N:1539:THR:HG23 | 1:N:1541:PRO:HD2 | 1.75 | 0.69 |
| 1:P:2232:LEU:HD12 | 1:P:2274:LEU:HB3 | 1.74 | 0.69 |
| 1:R:2191:PRO:HG2 | 1:R:2194:PHE:HD2 | 1.58 | 0.69 |
| 1:T:1089:GLN:HE22 | 1:T:1092:ALA:HB3 | 1.56 | 0.69 |
| 1:C:203:LEU:HD21 | 1:C:351:LEU:HB3 | 1.74 | 0.69 |
| 1:C:2056:ARG:NH1 | 1:C:2057:ALA:O | 2.25 | 0.69 |
| 1:D:1349:TRP:O | 1:D:1463:ASN:ND2 | 2.25 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:D:1865:LYS:HE3 | 1:D:1867:HIS:H | 1.56 | 0.69 |
| 1:E:846:HIS:HB2 | 1:E:1121:TYR:HB2 | 1.74 | 0.69 |
| 1:L:2311:GLU:O | 1:L:2315:ARG:NH1 | 2.25 | 0.69 |
| 1:M:751:VAL:HG12 | 1:M:810:ILE:HG22 | 1.75 | 0.69 |
| 1:M:2256:ASP:OD2 | 1:M:2440:ARG:NH2 | 2.25 | 0.69 |
| 1:P:94:TRP:O | 1:P:218:ASN:ND2 | 2.26 | 0.69 |
| 1:P:3049:GLN:H | 1:P:3052:LEU:HD12 | 1.56 | 0.69 |
| 1:R:1837:ALA:HA | 1:R:1849:GLN:HE21 | 1.57 | 0.69 |
| 1:T:1677:ARG:NH1 | 1:T:1763:ILE:O | 2.25 | 0.69 |
| 1:E:3052:LEU:O | 1:E:3055:ARG:NH2 | 2.25 | 0.69 |
| 1:E:3385:ASP:OD2 | 1:E:3403:GLN:NE2 | 2.26 | 0.69 |
| 1:G:512:LYS:HA | 1:G:516:LEU:HB2 | 1.74 | 0.69 |
| 1:I:2253:GLU:HG3 | 1:I:2384:ILE:HG12 | 1.74 | 0.69 |
| 1:I:3047:ASP:HB2 | 1:I:3097:GLY:HA3 | 1.74 | 0.69 |
| 1:M:2533:ARG:NH2 | 1:M:2621:PRO:HD3 | 2.07 | 0.69 |
| 1:T:913:TRP:HD1 | 1:T:1088:LEU:HD12 | 1.57 | 0.69 |
| 1:A:63:MET:HB3 | 1:A:246:LEU:HD21 | 1.73 | 0.69 |
| 1:A:915:ARG:HD3 | 1:A:1112:VAL:HG22 | 1.73 | 0.69 |
| 1:A:956:VAL:HA | 1:A:963:PRO:HA | 1.73 | 0.69 |
| 1:C:1359:PRO:HD2 | 1:C:1362:ILE:HD11 | 1.74 | 0.69 |
| 1:D:727:ILE:HG22 | 1:D:730:ARG:HH21 | 1.57 | 0.69 |
| 1:E:608:VAL:HG22 | 1:E:768:LEU:HD11 | 1.73 | 0.69 |
| 1:E:1896:GLN:OE1 | 1:E:1899:GLN:NE2 | 2.26 | 0.69 |
| 1:F:1098:ASN:O | 1:F:1104:ARG:NH1 | 2.26 | 0.69 |
| 1:G:1067:GLN:HG2 | 1:G:1074:TYR:HB3 | 1.74 | 0.69 |
| 1:G:2755:ASP:OD2 | 1:G:2756:PHE:N | 2.25 | 0.69 |
| 1:H:939:TRP:HZ3 | 1:H:1052:HIS:HA | 1.56 | 0.69 |
| 1:I:956:VAL:HA | 1:I:963:PRO:HA | 1.73 | 0.69 |
| 1:I:1828:ASN:HB3 | 1:I:1831:TRP:HB3 | 1.75 | 0.69 |
| 1:J:846:HIS:HB3 | 1:J:1121:TYR:HA | 1.74 | 0.69 |
| 1:J:994:ARG:HE | 1:J:995:LEU:H | 1.41 | 0.69 |
| 1:K:2570:GLY:HA2 | 1:K:2847:PHE:HE1 | 1.58 | 0.69 |
| 1:K:2590:THR:HA | 1:K:2594:ALA:HB3 | 1.73 | 0.69 |
| 1:M:1811:ARG:NH2 | 1:M:1878:ASP:OD1 | 2.26 | 0.69 |
| 1:O:257:ASP:HA | 1:O:265:ARG:HE | 1.58 | 0.69 |
| 1:O:1070:ARG:HH12 | 1:O:1137:GLN:HE22 | 1.41 | 0.69 |
| 1:O:2926:VAL:HB | 1:O:3023:LEU:HD21 | 1.73 | 0.69 |
| 1:O:3334:ARG:HH21 | 1:O:3406:ILE:HG23 | 1.58 | 0.69 |
| 1:P:331:HIS:NE2 | 1:P:672:HIS:O | 2.26 | 0.69 |
| 1:R:1560:PHE:HZ | 1:R:1573:LEU:HD11 | 1.58 | 0.69 |
| 1:S:3337:ARG:CZ | 1:S:3378:ASN:HB2 | 2.22 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:956:VAL:HA | 1:C:963:PRO:HA | 1.73 | 0.69 |
| 1:C:2802:VAL:H | 1:C:2856:THR:HG22 | 1.58 | 0.69 |
| 1:D:6:LYS:NZ | 1:D:10:LEU:O | 2.26 | 0.69 |
| 1:D:1560:PHE:HZ | 1:D:1573:LEU:HD11 | 1.58 | 0.69 |
| 1:F:3321:LEU:O | 1:F:3395:ARG:NH2 | 2.26 | 0.69 |
| 1:H:1232:SER:OG | 1:H:1234:GLU:OE1 | 2.11 | 0.69 |
| 1:I:1574:PHE:HB2 | 1:I:1634:GLU:HB3 | 1.73 | 0.69 |
| 1:K:465:GLN:HG2 | 1:K:560:ALA:HB2 | 1.74 | 0.69 |
| 1:M:555:PHE:HA | 1:M:568:ARG:HH22 | 1.58 | 0.69 |
| 1:M:3036:GLN:OE1 | 1:M:3043:GLN:NE2 | 2.26 | 0.69 |
| 1:Q:473:LEU:HD23 | 1:Q:775:LYS:HZ1 | 1.57 | 0.69 |
| 1:R:1349:TRP:O | 1:R:1463:ASN:ND2 | 2.26 | 0.69 |
| 1:S:1328:LEU:HB3 | 1:S:1499:PHE:HE2 | 1.58 | 0.69 |
| 1:S:1574:PHE:HB2 | 1:S:1634:GLU:HB3 | 1.74 | 0.69 |
| 1:S:2025:SER:O | 1:T:1651:ARG:NH2 | 2.26 | 0.69 |
| 1:E:1574:PHE:HB2 | 1:E:1634:GLU:HB3 | 1.75 | 0.69 |
| 1:E:1815:ARG:HD2 | 1:E:1818:LEU:HD21 | 1.75 | 0.69 |
| 1:G:534:ALA:O | 1:G:538:LYS:NZ | 2.25 | 0.69 |
| 1:G:1862:GLY:HA3 | 1:G:1870:ALA:HB2 | 1.73 | 0.69 |
| 1:H:1012:CYS:SG | 1:H:1196:ARG:NH1 | 2.66 | 0.69 |
| 1:H:1488:ALA:HB1 | 1:H:1491:ILE:HD13 | 1.73 | 0.69 |
| 1:K:2256:ASP:OD2 | 1:K:2440:ARG:NH2 | 2.25 | 0.69 |
| 1:L:3080:PHE:HA | 1:L:3083:GLN:HE22 | 1.58 | 0.69 |
| 1:N:617:VAL:HB | 1:N:625:LEU:HD23 | 1.75 | 0.69 |
| 1:N:1993:SER:HB2 | 1:N:2058:LEU:HD11 | 1.74 | 0.69 |
| 1:O:1156:HIS:HB3 | 1:O:1193:GLN:HE22 | 1.57 | 0.69 |
| 1:P:808:LEU:HB2 | 1:P:820:GLU:HG3 | 1.75 | 0.69 |
| 1:P:1153:PHE:HB2 | 1:P:1198:PHE:HD2 | 1.56 | 0.69 |
| 1:Q:248:ARG:NH2 | 1:Q:802:ASP:O | 2.26 | 0.69 |
| 1:Q:1466:ARG:NH2 | 1:Q:1534:ASN:O | 2.26 | 0.69 |
| 1:Q:1741:GLN:N | 1:Q:1741:GLN:OE1 | 2.26 | 0.69 |
| 1:Q:2001:CYS:HA | 1:Q:2007:CYS:HB3 | 1.75 | 0.69 |
| 1:A:1156:HIS:HB3 | 1:A:1193:GLN:HE22 | 1.57 | 0.68 |
| 1:A:1195:ASP:HB2 | 1:B:2441:LEU:HD21 | 1.74 | 0.68 |
| 1:A:1811:ARG:NH2 | 1:A:1878:ASP:OD1 | 2.25 | 0.68 |
| 1:B:2159:ARG:NE | 1:B:2303:ASP:OD1 | 2.24 | 0.68 |
| 1:C:534:ALA:O | 1:C:538:LYS:NZ | 2.24 | 0.68 |
| 1:E:1842:ASN:HB3 | 1:E:1845:ASP:HB2 | 1.75 | 0.68 |
| 1:E:2805:ASN:HB3 | 1:E:2850:LEU:HD21 | 1.73 | 0.68 |
| 1:G:956:VAL:HA | 1:G:963:PRO:HA | 1.74 | 0.68 |
| 1:H:2866:PRO:O | 1:I:2741:ARG:NH1 | 2.27 | 0.68 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:K:2094:HIS:HD2 | 1:K:2098:HIS:HB3 | 1.57 | 0.68 |
| 1:K:2664:GLN:HE21 | 1:K:2670:PHE:HA | 1.58 | 0.68 |
| 1:L:738:VAL:HG23 | 1:L:789:ILE:HG13 | 1.73 | 0.68 |
| 1:L:3360:LEU:HG | 1:L:3401:ARG:HD3 | 1.74 | 0.68 |
| 1:M:1839:GLU:HA | 1:M:1902:ARG:HH22 | 1.58 | 0.68 |
| 1:M:2251:VAL:HG22 | 1:M:2263:GLN:HB3 | 1.74 | 0.68 |
| 1:P:735:ARG:HB3 | 1:P:831:GLU:HB3 | 1.73 | 0.68 |
| 1:P:1993:SER:HB2 | 1:P:2058:LEU:HD11 | 1.74 | 0.68 |
| 1:P:2622:PHE:O | 1:P:2636:ARG:NH2 | 2.25 | 0.68 |
| 1:Q:3395:ARG:HH21 | 1:Q:3398:GLN:HE22 | 1.41 | 0.68 |
| 1:T:46:SER:O | 1:T:55:ARG:NH1 | 2.26 | 0.68 |
| 1:T:1098:ASN:O | 1:T:1104:ARG:NH1 | 2.26 | 0.68 |
| 1:A:2962:ALA:HB2 | 1:A:3107:GLU:HG2 | 1.75 | 0.68 |
| 1:C:2796:ARG:NH1 | 1:C:2799:GLU:OE2 | 2.26 | 0.68 |
| 1:G:1328:LEU:HB3 | 1:G:1499:PHE:HE2 | 1.57 | 0.68 |
| 1:H:2785:THR:OG1 | 1:H:2788:GLN:OE1 | 2.11 | 0.68 |
| 1:I:2579:ARG:NE | 1:I:2774:TYR:OH | 2.24 | 0.68 |
| 1:J:991:LYS:NZ | 1:J:992:PHE:O | 2.26 | 0.68 |
| 1:M:1689:ARG:NE | 1:M:1786:ASP:OD1 | 2.27 | 0.68 |
| 1:M:1714:HIS:NE2 | 1:M:1732:CYS:SG | 2.66 | 0.68 |
| 1:O:109:GLU:O | 1:O:123:ASN:ND2 | 2.26 | 0.68 |
| 1:O:454:ARG:HH21 | 1:O:514:ARG:HB3 | 1.59 | 0.68 |
| 1:O:915:ARG:HD3 | 1:O:1112:VAL:HG22 | 1.74 | 0.68 |
| 1:O:956:VAL:HA | 1:O:963:PRO:HA | 1.75 | 0.68 |
| 1:Q:1587:ASN:OD1 | 1:Q:1588:HIS:ND1 | 2.26 | 0.68 |
| 1:S:903:CYS:O | 1:S:905:HIS:ND1 | 2.26 | 0.68 |
| 1:S:1770:ASN:OD1 | 1:S:1772:GLN:NE2 | 2.26 | 0.68 |
| 1:T:454:ARG:HH22 | 1:T:1338:LEU:HG | 1.57 | 0.68 |
| 1:T:1579:THR:HG21 | 1:T:1585:ASN:HB3 | 1.75 | 0.68 |
| 1:T:2665:ARG:O | 1:T:2723:GLN:NE2 | 2.27 | 0.68 |
| 1:B:2414:GLN:HE22 | 1:B:2453:LEU:HD22 | 1.59 | 0.68 |
| 1:E:1494:GLN:NE2 | 1:E:1500:ASN:OD1 | 2.25 | 0.68 |
| 1:G:2817:VAL:HG22 | 1:G:2876:ILE:HG22 | 1.74 | 0.68 |
| 1:I:3395:ARG:HH21 | 1:I:3398:GLN:HE22 | 1.42 | 0.68 |
| 1:L:244:VAL:HG22 | 1:L:828:ILE:HG21 | 1.75 | 0.68 |
| 1:L:1012:CYS:SG | 1:L:1196:ARG:NH1 | 2.66 | 0.68 |
| 1:L:2232:LEU:HD12 | 1:L:2274:LEU:HB3 | 1.73 | 0.68 |
| 1:M:1384:LYS:NZ | 1:M:1385:ILE:O | 2.25 | 0.68 |
| 1:O:38:LEU:O | 1:O:73:TYR:OH | 2.11 | 0.68 |
| 1:S:3305:ILE:HA | 1:S:3315:VAL:O | 1.93 | 0.68 |
| 1:A:2980:GLY:HA2 | 1:A:3258:TYR:HE1 | 1.59 | 0.68 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:2191:PRO:HG2 | 1:B:2194:PHE:HD2 | 1.57 | 0.68 |
| 1:E:2256:ASP:OD2 | 1:E:2440:ARG:NH2 | 2.23 | 0.68 |
| 1:F:991:LYS:NZ | 1:F:992:PHE:O | 2.26 | 0.68 |
| 1:G:611:ASN:HD22 | 1:G:771:LEU:H | 1.41 | 0.68 |
| 1:G:1417:THR:O | 1:G:1475:GLN:NE2 | 2.27 | 0.68 |
| 1:H:671:THR:O | 1:H:695:ARG:NH2 | 2.26 | 0.68 |
| 1:H:2311:GLU:O | 1:H:2315:ARG:NH1 | 2.26 | 0.68 |
| 1:L:2785:THR:OG1 | 1:L:2788:GLN:OE1 | 2.10 | 0.68 |
| 1:M:1890:ARG:NH2 | 1:M:1959:GLU:O | 2.26 | 0.68 |
| 1:M:2533:ARG:HH22 | 1:M:2619:ASP:C | 2.01 | 0.68 |
| 1:Q:78:GLU:OE2 | 1:Q:79:GLN:NE2 | 2.25 | 0.68 |
| 1:Q:555:PHE:HA | 1:Q:568:ARG:HH22 | 1.57 | 0.68 |
| 1:Q:2256:ASP:OD2 | 1:Q:2440:ARG:NH2 | 2.26 | 0.68 |
| 1:R:244:VAL:HG22 | 1:R:828:ILE:HG21 | 1.75 | 0.68 |
| 1:R:1089:GLN:HE22 | 1:R:1092:ALA:HB3 | 1.58 | 0.68 |
| 1:B:420:LYS:NZ | 1:B:422:SER:OG | 2.26 | 0.68 |
| 1:E:1067:GLN:NE2 | 1:E:1073:PRO:O | 2.26 | 0.68 |
| 1:E:1862:GLY:HA3 | 1:E:1870:ALA:HB2 | 1.73 | 0.68 |
| 1:G:2570:GLY:HA3 | 1:G:2845:TRP:HB2 | 1.74 | 0.68 |
| 1:G:2637:SER:HB2 | 1:G:2687:GLY:HA3 | 1.76 | 0.68 |
| 1:I:3212:ARG:HG2 | 1:I:3267:THR:HG21 | 1.76 | 0.68 |
| 1:K:109:GLU:O | 1:K:123:ASN:ND2 | 2.25 | 0.68 |
| 1:M:1710:LEU:HB3 | 1:M:1750:PHE:HE1 | 1.57 | 0.68 |
| 1:N:3115:PHE:O | 1:N:3119:HIS:ND1 | 2.18 | 0.68 |
| 1:P:905:HIS:HA | 1:P:910:PHE:HD2 | 1.58 | 0.68 |
| 1:Q:2018:GLY:N | 1:Q:2021:GLU:OE2 | 2.22 | 0.68 |
| 1:T:220:ASP:OD1 | 1:T:283:TYR:OH | 2.11 | 0.68 |
| 1:B:907:MET:HG2 | 1:B:909:VAL:H | 1.57 | 0.68 |
| 1:B:912:HIS:HE2 | 1:B:1113:PHE:HE1 | 1.41 | 0.68 |
| 1:C:3386:TYR:HB2 | 1:C:3404:ILE:HG22 | 1.76 | 0.68 |
| 1:D:1763:ILE:HD12 | 1:D:1764:PRO:HD2 | 1.75 | 0.68 |
| 1:F:1546:VAL:HA | 1:F:1549:ARG:HG2 | 1.76 | 0.68 |
| 1:F:2622:PHE:O | 1:F:2636:ARG:NH2 | 2.25 | 0.68 |
| 1:G:465:GLN:HG2 | 1:G:560:ALA:HB2 | 1.76 | 0.68 |
| 1:K:2462:ASN:O | 1:L:1085:ARG:NH1 | 2.26 | 0.68 |
| 1:L:2552:GLY:HA3 | 1:L:2697:GLU:HA | 1.75 | 0.68 |
| 1:M:1506:GLU:HG3 | 1:M:1507:PHE:H | 1.58 | 0.68 |
| 1:M:2025:SER:O | 1:N:1651:ARG:NH2 | 2.25 | 0.68 |
| 1:O:191:LEU:HG | 1:O:349:PHE:HE2 | 1.58 | 0.68 |
| 1:O:1575:ILE:HD11 | 1:O:1590:ALA:HB2 | 1.75 | 0.68 |
| 1:Q:2000:VAL:HG12 | 1:Q:2051:VAL:HG22 | 1.76 | 0.68 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:R:2243:VAL:HG23 | 1:R:2244:LEU:HD12 | 1.74 | 0.68 |
| 1:S:1917:ARG:NH1 | 1:T:1632:ASP:OD2 | 2.27 | 0.68 |
| 1:S:2534:ALA:O | 1:S:2538:GLN:NE2 | 2.23 | 0.68 |
| 1:A:38:LEU:O | 1:A:73:TYR:OH | 2.11 | 0.68 |
| 1:A:555:PHE:HA | 1:A:568:ARG:HH22 | 1.57 | 0.68 |
| 1:A:1151:ALA:HB2 | 1:A:1202:ILE:HD11 | 1.74 | 0.68 |
| 1:B:1677:ARG:NH1 | 1:B:1763:ILE:O | 2.27 | 0.68 |
| 1:C:277:ARG:HH22 | 1:K:731:ARG:HH12 | 1.42 | 0.68 |
| 1:C:434:ARG:HD2 | 1:C:710:TYR:HE1 | 1.58 | 0.68 |
| 1:C:593:ALA:HA | 1:C:605:GLN:HG3 | 1.74 | 0.68 |
| 1:E:555:PHE:HA | 1:E:568:ARG:HH22 | 1.57 | 0.68 |
| 1:E:2224:THR:HB | 1:E:2226:ARG:HH12 | 1.59 | 0.68 |
| 1:F:185:HIS:CE1 | 1:F:219:VAL:HG21 | 2.28 | 0.68 |
| 1:I:2025:SER:O | 1:J:1651:ARG:NH2 | 2.27 | 0.68 |
| 1:M:937:TRP:O | 1:M:1055:ASN:ND2 | 2.27 | 0.68 |
| 1:N:1489:LEU:HA | 1:N:1492:MET:HE1 | 1.76 | 0.68 |
| 1:P:1098:ASN:O | 1:P:1104:ARG:NH1 | 2.26 | 0.68 |
| 1:T:1349:TRP:O | 1:T:1463:ASN:ND2 | 2.22 | 0.68 |
| 1:B:2286:LEU:HB3 | 1:B:2428:LEU:HD21 | 1.76 | 0.68 |
| 1:C:3149:ASN:OD1 | 1:C:3152:ARG:NH1 | 2.25 | 0.68 |
| 1:D:954:THR:HG22 | 1:D:965:PRO:HA | 1.76 | 0.68 |
| 1:D:1539:THR:HG23 | 1:D:1541:PRO:HD2 | 1.75 | 0.68 |
| 1:E:1067:GLN:HG2 | 1:E:1074:TYR:HB3 | 1.76 | 0.68 |
| 1:E:1359:PRO:HD2 | 1:E:1362:ILE:HD11 | 1.76 | 0.68 |
| 1:F:907:MET:HG2 | 1:F:909:VAL:H | 1.58 | 0.68 |
| 1:G:1802:ILE:HD12 | 1:G:1805:GLU:HB2 | 1.73 | 0.68 |
| 1:H:2113:ASP:OD1 | 1:H:2114:LEU:N | 2.26 | 0.68 |
| 1:I:307:GLU:O | 1:I:308:ARG:NE | 2.26 | 0.68 |
| 1:J:937:TRP:HB3 | 1:J:1051:LEU:HD13 | 1.74 | 0.68 |
| 1:K:1723:PRO:HA | 1:K:1728:ARG:HH22 | 1.59 | 0.68 |
| 1:M:2253:GLU:HG3 | 1:M:2384:ILE:HG12 | 1.75 | 0.68 |
| 1:O:3056:ARG:NH1 | 1:O:3058:GLN:OE1 | 2.26 | 0.68 |
| 1:P:256:ARG:O | 1:P:265:ARG:NH1 | 2.26 | 0.68 |
| 1:P:1677:ARG:NH2 | 1:P:1751:GLU:OE1 | 2.27 | 0.68 |
| 1:R:1272:SER:N | 1:R:1275:GLU:OE2 | 2.26 | 0.68 |
| 1:S:1067:GLN:HE21 | 1:S:1072:LEU:HB2 | 1.58 | 0.68 |
| 1:B:3049:GLN:H | 1:B:3052:LEU:HD12 | 1.59 | 0.68 |
| 1:D:3047:ASP:HB2 | 1:D:3097:GLY:HA3 | 1.75 | 0.68 |
| 1:F:143:ARG:NH2 | 1:F:209:ASP:OD2 | 2.27 | 0.68 |
| 1:L:1448:LEU:HD21 | 1:L:1596:LEU:HG | 1.76 | 0.68 |
| 1:M:731:ARG:HA | 1:M:735:ARG:HH12 | 1.58 | 0.68 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:M:1539:THR:HG23 | 1:M:1541:PRO:HD2 | 1.76 | 0.68 |
| 1:Q:1714:HIS:NE2 | 1:Q:1732:CYS:SG | 2.67 | 0.68 |
| 1:Q:2108:LYS:HG3 | 1:Q:2112:ARG:HH12 | 1.59 | 0.68 |
| 1:R:247:PHE:HB3 | 1:R:271:LYS:HD2 | 1.76 | 0.68 |
| 1:R:581:GLY:H | 1:R:856:ARG:NH2 | 1.92 | 0.68 |
| 1:R:1400:LEU:HD21 | 1:R:1436:LEU:HB3 | 1.74 | 0.68 |
| 1:R:2809:GLN:NE2 | 1:R:2845:TRP:O | 2.26 | 0.68 |
| 1:T:846:HIS:HB3 | 1:T:1121:TYR:HA | 1.76 | 0.68 |
| 1:A:44:GLU:HG3 | 1:A:135:MET:HE1 | 1.76 | 0.68 |
| 1:A:1723:PRO:HA | 1:A:1728:ARG:HH22 | 1.59 | 0.68 |
| 1:B:405:ARG:NH1 | 1:B:406:PRO:O | 2.26 | 0.68 |
| 1:C:654:LEU:HD21 | 1:C:658:ARG:HH21 | 1.58 | 0.68 |
| 1:C:937:TRP:O | 1:C:1055:ASN:ND2 | 2.27 | 0.68 |
| 1:C:1388:THR:OG1 | 1:C:1390:LYS:NZ | 2.27 | 0.68 |
| 1:E:675:LEU:HD11 | 1:E:696:PRO:HG3 | 1.76 | 0.68 |
| 1:E:3231:LYS:HB2 | 1:E:3284:GLN:HE21 | 1.59 | 0.68 |
| 1:G:1732:CYS:O | 1:G:1734:HIS:ND1 | 2.25 | 0.68 |
| 1:G:2861:GLN:OE1 | 1:H:1538:TRP:NE1 | 2.26 | 0.68 |
| 1:N:1005:ALA:HA | 1:N:1008:GLN:HE22 | 1.59 | 0.68 |
| 1:P:74:VAL:HA | 1:P:77:LEU:HD23 | 1.76 | 0.68 |
| 1:P:247:PHE:HB3 | 1:P:271:LYS:HD2 | 1.76 | 0.68 |
| 1:Q:1811:ARG:NH2 | 1:Q:1878:ASP:OD1 | 2.27 | 0.68 |
| 1:R:1105:ASP:OD1 | 1:R:1106:HIS:ND1 | 2.27 | 0.68 |
| 1:R:3321:LEU:O | 1:R:3395:ARG:NH2 | 2.27 | 0.68 |
| 1:S:555:PHE:HA | 1:S:568:ARG:HH22 | 1.59 | 0.68 |
| 1:A:2509:SER:O | 1:A:3138:ARG:NH1 | 2.27 | 0.67 |
| 1:B:1041:ARG:NH2 | 1:B:1188:TYR:OH | 2.27 | 0.67 |
| 1:B:1743:HIS:HD2 | 1:B:1885:HIS:HD2 | 1.40 | 0.67 |
| 1:D:1272:SER:N | 1:D:1275:GLU:OE2 | 2.28 | 0.67 |
| 1:D:2666:ASP:OD2 | 1:D:2849:ARG:NH2 | 2.28 | 0.67 |
| 1:E:1448:LEU:HB3 | 1:E:1596:LEU:HD11 | 1.76 | 0.67 |
| 1:E:1575:ILE:HD11 | 1:E:1590:ALA:HB2 | 1.76 | 0.67 |
| 1:F:3037:ILE:HG22 | 1:F:3042:HIS:H | 1.58 | 0.67 |
| 1:F:3049:GLN:H | 1:F:3052:LEU:HD12 | 1.59 | 0.67 |
| 1:J:735:ARG:HB3 | 1:J:831:GLU:HB3 | 1.76 | 0.67 |
| 1:K:1328:LEU:HB3 | 1:K:1499:PHE:HE2 | 1.56 | 0.67 |
| 1:M:63:MET:HB3 | 1:M:246:LEU:HD21 | 1.75 | 0.67 |
| 1:R:1147:GLU:HG3 | 1:R:1245:PRO:HA | 1.76 | 0.67 |
| 1:B:1448:LEU:HD21 | 1:B:1596:LEU:HG | 1.76 | 0.67 |
| 1:B:3008:ILE:HG21 | 1:B:3116:MET:HB3 | 1.76 | 0.67 |
| 1:E:937:TRP:O | 1:E:1055:ASN:ND2 | 2.27 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:F:3074:GLU:OE2 | 1:F:3083:GLN:NE2 | 2.27 | 0.67 |
| 1:F:3103:MET:HA | 1:F:3109:SER:HA | 1.75 | 0.67 |
| 1:G:1723:PRO:HA | 1:G:1728:ARG:HH22 | 1.58 | 0.67 |
| 1:G:2604:THR:HA | 1:G:2654:PHE:HE2 | 1.59 | 0.67 |
| 1:I:2194:PHE:HZ | 1:I:2226:ARG:HH22 | 1.43 | 0.67 |
| 1:K:248:ARG:NH1 | 1:K:802:ASP:O | 2.28 | 0.67 |
| 1:K:949:ILE:HG23 | 1:K:950:VAL:HG13 | 1.76 | 0.67 |
| 1:K:2637:SER:HB2 | 1:K:2687:GLY:HA3 | 1.75 | 0.67 |
| 1:L:2113:ASP:OD1 | 1:L:2114:LEU:N | 2.26 | 0.67 |
| 1:M:2673:GLN:HE22 | 1:M:2852:GLN:H | 1.40 | 0.67 |
| 1:N:160:GLN:HE22 | 1:N:161:LEU:HG | 1.60 | 0.67 |
| 1:O:2325:CYS:HA | 1:P:1242:VAL:HG13 | 1.76 | 0.67 |
| 1:P:2626:GLU:HB2 | 1:P:2633:LYS:HD3 | 1.76 | 0.67 |
| 1:C:1651:ARG:NH2 | 1:D:2025:SER:O | 2.26 | 0.67 |
| 1:D:94:TRP:O | 1:D:218:ASN:ND2 | 2.27 | 0.67 |
| 1:D:2311:GLU:O | 1:D:2315:ARG:NH1 | 2.28 | 0.67 |
| 1:E:1026:HIS:HD2 | 1:E:1184:LEU:HD11 | 1.58 | 0.67 |
| 1:G:2056:ARG:NH1 | 1:G:2057:ALA:O | 2.27 | 0.67 |
| 1:G:3089:ASN:HD21 | 1:G:3248:LEU:H | 1.41 | 0.67 |
| 1:J:1475:GLN:HG2 | 1:J:1482:ASP:HB3 | 1.75 | 0.67 |
| 1:K:2882:THR:OG1 | 4:K:3501:NAG:N2 | 2.27 | 0.67 |
| 1:L:1638:ARG:HH22 | 1:L:1642:GLY:HA2 | 1.59 | 0.67 |
| 1:L:1993:SER:HB2 | 1:L:2058:LEU:HD11 | 1.75 | 0.67 |
| 1:M:257:ASP:O | 1:M:265:ARG:NH2 | 2.26 | 0.67 |
| 1:S:2000:VAL:HG12 | 1:S:2051:VAL:HG22 | 1.76 | 0.67 |
| 1:T:3360:LEU:HD12 | 1:T:3387:PHE:HB3 | 1.76 | 0.67 |
| 1:E:69:TRP:HD1 | 1:E:251:LEU:HD12 | 1.59 | 0.67 |
| 1:E:1770:ASN:OD1 | 1:E:1772:GLN:NE2 | 2.27 | 0.67 |
| 1:E:2025:SER:O | 1:F:1651:ARG:NH2 | 2.27 | 0.67 |
| 1:E:2579:ARG:NH1 | 1:E:2774:TYR:OH | 2.26 | 0.67 |
| 1:G:1741:GLN:NE2 | 1:G:1843:TYR:OH | 2.27 | 0.67 |
| 1:I:1710:LEU:HB3 | 1:I:1750:PHE:HE1 | 1.57 | 0.67 |
| 1:K:2056:ARG:HH22 | 1:K:2060:GLY:HA2 | 1.60 | 0.67 |
| 1:L:247:PHE:HB3 | 1:L:271:LYS:HD2 | 1.75 | 0.67 |
| 1:L:1917:ARG:O | 1:L:1940:LYS:NZ | 2.27 | 0.67 |
| 1:O:3072:LEU:HD23 | 1:O:3129:TRP:HD1 | 1.60 | 0.67 |
| 1:B:3154:LEU:O | 1:B:3158:ASN:N | 2.27 | 0.67 |
| 1:C:595:GLU:O | 1:C:597:ARG:NH1 | 2.28 | 0.67 |
| 1:C:2056:ARG:NH1 | 1:C:2061:SER:O | 2.28 | 0.67 |
| 1:C:2756:PHE:HA | 1:C:2759:GLU:HG2 | 1.75 | 0.67 |
| 1:F:597:ARG:HH22 | 1:F:655:GLN:HA | 1.57 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:G:605:GLN:HA | 1:G:608:VAL:HG12 | 1.77 | 0.67 |
| 1:G:1623:LEU:HD13 | 1:G:1631:ILE:HG12 | 1.76 | 0.67 |
| 1:I:555:PHE:HA | 1:I:568:ARG:HH22 | 1.57 | 0.67 |
| 1:J:913:TRP:HD1 | 1:J:1088:LEU:HD12 | 1.59 | 0.67 |
| 1:M:915:ARG:NH1 | 1:M:1057:ASP:OD1 | 2.28 | 0.67 |
| 1:N:1012:CYS:O | 1:N:1196:ARG:NH1 | 2.27 | 0.67 |
| 1:N:1348:TYR:OH | 1:N:1466:ARG:NH1 | 2.28 | 0.67 |
| 1:N:2113:ASP:OD1 | 1:N:2114:LEU:N | 2.27 | 0.67 |
| 1:O:2130:HIS:NE2 | 1:O:2147:CYS:SG | 2.68 | 0.67 |
| 1:P:2149:HIS:HA | 1:P:2154:PHE:HD2 | 1.60 | 0.67 |
| 1:Q:31:THR:OG1 | 1:Q:32:VAL:N | 2.26 | 0.67 |
| 1:Q:1494:GLN:NE2 | 1:Q:1500:ASN:OD1 | 2.28 | 0.67 |
| 1:S:1710:LEU:HB3 | 1:S:1750:PHE:HE1 | 1.57 | 0.67 |
| 1:T:3037:ILE:HG22 | 1:T:3042:HIS:H | 1.60 | 0.67 |
| 1:A:1026:HIS:HD2 | 1:A:1184:LEU:HD11 | 1.59 | 0.67 |
| 1:B:3080:PHE:HA | 1:B:3083:GLN:HE22 | 1.60 | 0.67 |
| 1:C:3052:LEU:O | 1:C:3055:ARG:NH2 | 2.28 | 0.67 |
| 1:D:1116:GLU:HA | 1:D:1120:GLN:HA | 1.76 | 0.67 |
| 1:F:474:PRO:HB2 | 1:F:476:ARG:HH12 | 1.60 | 0.67 |
| 1:G:1583:GLU:HB2 | 1:J:340:SER:HB3 | 1.77 | 0.67 |
| 1:J:94:TRP:O | 1:J:218:ASN:ND2 | 2.27 | 0.67 |
| 1:J:1467:ILE:HA | 1:J:1470:ILE:HD12 | 1.76 | 0.67 |
| 1:K:1495:PRO:HG3 | 1:K:1515:ARG:HD3 | 1.77 | 0.67 |
| 1:K:3089:ASN:HD21 | 1:K:3248:LEU:H | 1.40 | 0.67 |
| 1:K:3214:TYR:HD1 | 1:K:3265:ASP:HA | 1.60 | 0.67 |
| 1:K:3217:PHE:HE1 | 1:K:3302:PRO:HB3 | 1.59 | 0.67 |
| 1:M:231:LYS:HD3 | 1:M:237:TYR:HE1 | 1.59 | 0.67 |
| 1:M:1380:PHE:O | 1:M:1394:ARG:NH2 | 2.28 | 0.67 |
| 1:N:2191:PRO:HG2 | 1:N:2194:PHE:HD2 | 1.60 | 0.67 |
| 1:Q:2213:ALA:O | 1:Q:2226:ARG:NH2 | 2.27 | 0.67 |
| 1:Q:3089:ASN:HD21 | 1:Q:3248:LEU:H | 1.42 | 0.67 |
| 1:R:3114:PHE:HA | 1:R:3117:ILE:HG12 | 1.77 | 0.67 |
| 1:S:1328:LEU:HB3 | 1:S:1499:PHE:CE2 | 2.30 | 0.67 |
| 1:S:1815:ARG:HD2 | 1:S:1818:LEU:HD21 | 1.76 | 0.67 |
| 1:B:3047:ASP:HB2 | 1:B:3097:GLY:HA3 | 1.77 | 0.67 |
| 1:D:54:LYS:HZ3 | 1:D:56:VAL:HA | 1.60 | 0.67 |
| 1:D:2988:HIS:HA | 1:D:2991:LEU:HD12 | 1.77 | 0.67 |
| 1:E:1811:ARG:NH2 | 1:E:1878:ASP:OD1 | 2.27 | 0.67 |
| 1:G:629:HIS:HE1 | 1:G:774:GLU:H | 1.43 | 0.67 |
| 1:G:2096:ILE:HD13 | 1:G:2179:PRO:HG2 | 1.77 | 0.67 |
| 1:G:2970:ALA:O | 1:G:2973:ARG:NH1 | 2.27 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:I:1100:ASP:O | 1:I:1104:ARG:NH1 | 2.28 | 0.67 |
| 1:K:1770:ASN:OD1 | 1:K:1772:GLN:NE2 | 2.28 | 0.67 |
| 1:K:1899:GLN:HE21 | 1:K:1904:HIS:HB2 | 1.59 | 0.67 |
| 1:N:1222:SER:HB3 | 1:N:1230:LYS:HZ1 | 1.58 | 0.67 |
| 1:N:2809:GLN:NE2 | 1:N:2845:TRP:O | 2.28 | 0.67 |
| 1:Q:3307:ARG:NH1 | 1:Q:3312:ASP:O | 2.27 | 0.67 |
| 1:T:514:ARG:HH12 | 1:T:1341:GLY:HA2 | 1.60 | 0.67 |
| 1:T:1489:LEU:HA | 1:T:1492:MET:HE1 | 1.76 | 0.67 |
| 1:A:1744:ARG:NH1 | 1:A:1944:VAL:O | 2.28 | 0.67 |
| 1:B:1865:LYS:HE3 | 1:B:1867:HIS:H | 1.60 | 0.67 |
| 1:C:454:ARG:NH2 | 1:C:514:ARG:O | 2.27 | 0.67 |
| 1:C:1161:SER:OG | 1:C:1185:GLY:N | 2.28 | 0.67 |
| 1:C:2590:THR:HA | 1:C:2594:ALA:HB3 | 1.77 | 0.67 |
| 1:D:2408:VAL:HG22 | 1:D:2473:ILE:HG22 | 1.74 | 0.67 |
| 1:E:2000:VAL:HG12 | 1:E:2051:VAL:HG22 | 1.77 | 0.67 |
| 1:G:2882:THR:OG1 | 4:G:3501:NAG:N2 | 2.26 | 0.67 |
| 1:H:451:ALA:O | 1:H:514:ARG:NH1 | 2.27 | 0.67 |
| 1:K:471:HIS:NE2 | 1:K:489:CYS:SG | 2.67 | 0.67 |
| 1:K:836:HIS:HE1 | 1:K:838:GLU:HB3 | 1.58 | 0.67 |
| 1:L:1049:PHE:O | 1:L:1053:HIS:ND1 | 2.27 | 0.67 |
| 1:N:846:HIS:HB3 | 1:N:1121:TYR:HA | 1.75 | 0.67 |
| 1:N:1763:ILE:HD12 | 1:N:1764:PRO:HD2 | 1.77 | 0.67 |
| 1:O:1085:ARG:NH2 | 1:P:2463:ALA:O | 2.28 | 0.67 |
| 1:Q:3128:ILE:HG22 | 1:Q:3190:LEU:HD12 | 1.75 | 0.67 |
| 1:R:1433:LEU:HD11 | 1:R:1460:HIS:CD2 | 2.30 | 0.67 |
| 1:R:2408:VAL:HG22 | 1:R:2473:ILE:HG22 | 1.76 | 0.67 |
| 1:S:1811:ARG:NH2 | 1:S:1878:ASP:OD1 | 2.28 | 0.67 |
| 1:A:881:ILE:HA | 1:A:884:PHE:HD2 | 1.57 | 0.67 |
| 1:A:1161:SER:OG | 1:A:1185:GLY:N | 2.26 | 0.67 |
| 1:B:2741:ARG:HH12 | 1:C:2870:TYR:H | 1.42 | 0.67 |
| 1:C:1744:ARG:NH1 | 1:C:1944:VAL:O | 2.27 | 0.67 |
| 1:C:3307:ARG:NH1 | 1:C:3312:ASP:O | 2.28 | 0.67 |
| 1:G:248:ARG:NH1 | 1:G:802:ASP:O | 2.27 | 0.67 |
| 1:G:2348:THR:OG1 | 1:G:2349:ARG:NH1 | 2.28 | 0.67 |
| 1:K:1144:GLN:OE1 | 1:K:1148:ARG:NH1 | 2.27 | 0.67 |
| 1:L:247:PHE:O | 1:L:271:LYS:NZ | 2.28 | 0.67 |
| 1:M:1161:SER:OG | 1:M:1185:GLY:N | 2.28 | 0.67 |
| 1:O:159:THR:HG23 | 1:O:162:PHE:H | 1.59 | 0.67 |
| 1:O:3301:THR:HB | 1:O:3325:LYS:HB3 | 1.75 | 0.67 |
| 1:Q:1770:ASN:OD1 | 1:Q:1772:GLN:NE2 | 2.28 | 0.67 |
| 1:Q:1910:ASN:ND2 | 1:R:1657:PHE:O | 2.28 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:R:937:TRP:HB3 | 1:R:1051:LEU:HD13 | 1.76 | 0.67 |
| 1:T:2985:PRO:HB2 | 1:T:2989:ARG:HH21 | 1.59 | 0.67 |
| 1:A:2108:LYS:HG3 | 1:A:2112:ARG:HH12 | 1.60 | 0.67 |
| 1:A:2130:HIS:NE2 | 1:A:2147:CYS:SG | 2.68 | 0.67 |
| 1:D:925:LEU:HD22 | 1:D:928:LYS:HZ3 | 1.58 | 0.67 |
| 1:E:1178:GLU:HG3 | 1:E:1205:ILE:HG12 | 1.75 | 0.67 |
| 1:E:3213:VAL:HG11 | 1:E:3270:LEU:HD13 | 1.76 | 0.67 |
| 1:G:738:VAL:HG23 | 1:G:789:ILE:HD13 | 1.75 | 0.67 |
| 1:G:2025:SER:O | 1:H:1651:ARG:NH2 | 2.27 | 0.67 |
| 1:H:1116:GLU:HA | 1:H:1120:GLN:HA | 1.77 | 0.67 |
| 1:H:2757:ILE:O | 1:H:2761:ALA:HB2 | 1.95 | 0.67 |
| 1:I:2508:VAL:O | 1:I:2515:LYS:NZ | 2.28 | 0.67 |
| 1:K:3337:ARG:NH1 | 1:K:3379:TYR:O | 2.27 | 0.67 |
| 1:M:1732:CYS:O | 1:M:1734:HIS:ND1 | 2.24 | 0.67 |
| 1:N:1919:PRO:HB2 | 1:N:1924:SER:HB2 | 1.75 | 0.67 |
| 1:O:1845:ASP:OD1 | 1:O:2028:ARG:NH1 | 2.27 | 0.67 |
| 1:O:2614:LEU:HD12 | 1:O:2636:ARG:HH12 | 1.60 | 0.67 |
| 1:Q:2027:ASP:HA | 1:R:1651:ARG:HH12 | 1.60 | 0.67 |
| 1:S:1144:GLN:HA | 1:S:1148:ARG:HH22 | 1.59 | 0.67 |
| 1:S:1896:GLN:OE1 | 1:S:1899:GLN:NE2 | 2.27 | 0.67 |
| 1:S:2018:GLY:N | 1:S:2021:GLU:OE2 | 2.25 | 0.67 |
| 1:T:925:LEU:HD13 | 1:T:928:LYS:HE2 | 1.77 | 0.67 |
| 1:T:1272:SER:N | 1:T:1275:GLU:OE2 | 2.28 | 0.67 |
| 1:A:390:LEU:HD22 | 1:A:398:LEU:HB3 | 1.76 | 0.66 |
| 1:C:55:ARG:NH2 | 1:C:56:VAL:O | 2.28 | 0.66 |
| 1:C:1195:ASP:HB2 | 1:D:2441:LEU:HD21 | 1.76 | 0.66 |
| 1:C:2108:LYS:HG3 | 1:C:2112:ARG:HH12 | 1.58 | 0.66 |
| 1:D:3360:LEU:HG | 1:D:3401:ARG:HD3 | 1.76 | 0.66 |
| 1:E:31:THR:OG1 | 1:E:32:VAL:N | 2.28 | 0.66 |
| 1:H:499:TRP:NE1 | 1:H:676:LYS:O | 2.27 | 0.66 |
| 1:I:1225:ASP:OD1 | 1:I:1229:LYS:N | 2.28 | 0.66 |
| 1:J:459:THR:OG1 | 1:J:1285:ARG:NH1 | 2.29 | 0.66 |
| 1:K:143:ARG:NH1 | 1:K:209:ASP:OD2 | 2.28 | 0.66 |
| 1:K:2587:ARG:HH12 | 1:K:2753:PRO:HG2 | 1.60 | 0.66 |
| 1:N:74:VAL:HA | 1:N:77:LEU:HD23 | 1.76 | 0.66 |
| 1:N:593:ALA:O | 1:N:596:GLN:NE2 | 2.27 | 0.66 |
| 1:N:1865:LYS:HE3 | 1:N:1867:HIS:H | 1.60 | 0.66 |
| 1:N:2741:ARG:NH1 | 1:O:2868:SER:O | 2.28 | 0.66 |
| 1:P:3132:LEU:HG | 1:P:3136:ARG:HH12 | 1.60 | 0.66 |
| 1:T:2988:HIS:HA | 1:T:2991:LEU:HD12 | 1.77 | 0.66 |
| 1:B:1993:SER:HB2 | 1:B:2058:LEU:HD11 | 1.76 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:2018:GLY:N | 1:C:2021:GLU:OE2 | 2.25 | 0.66 |
| 1:E:1710:LEU:HB3 | 1:E:1750:PHE:HE1 | 1.59 | 0.66 |
| 1:E:2590:THR:HA | 1:E:2594:ALA:HB3 | 1.76 | 0.66 |
| 1:E:2724:ARG:NH1 | 1:E:2730:TYR:OH | 2.28 | 0.66 |
| 1:E:2777:ASP:O | 1:E:3137:HIS:NE2 | 2.28 | 0.66 |
| 1:F:2112:ARG:O | 1:F:2116:LYS:NZ | 2.28 | 0.66 |
| 1:G:1144:GLN:OE1 | 1:G:1148:ARG:NH1 | 2.28 | 0.66 |
| 1:G:1815:ARG:HD3 | 1:G:1818:LEU:HD21 | 1.76 | 0.66 |
| 1:G:3128:ILE:HG22 | 1:G:3190:LEU:HD22 | 1.75 | 0.66 |
| 1:H:3037:ILE:HG22 | 1:H:3042:HIS:H | 1.60 | 0.66 |
| 1:K:3020:LEU:HB3 | 1:K:3024:LEU:HD11 | 1.77 | 0.66 |
| 1:K:3219:LEU:HD21 | 1:K:3247:ILE:HD13 | 1.77 | 0.66 |
| 1:M:3386:TYR:HB2 | 1:M:3404:ILE:HG22 | 1.76 | 0.66 |
| 1:O:2579:ARG:NH1 | 1:O:2774:TYR:OH | 2.28 | 0.66 |
| 1:Q:465:GLN:HG2 | 1:Q:560:ALA:HB2 | 1.78 | 0.66 |
| 1:Q:714:GLN:OE1 | 1:Q:718:MET:N | 2.28 | 0.66 |
| 1:R:954:THR:HG22 | 1:R:965:PRO:HA | 1.76 | 0.66 |
| 1:R:2232:LEU:HD12 | 1:R:2274:LEU:HB3 | 1.78 | 0.66 |
| 1:T:143:ARG:NH2 | 1:T:209:ASP:OD2 | 2.28 | 0.66 |
| 1:A:3056:ARG:NH1 | 1:A:3058:GLN:OE1 | 2.28 | 0.66 |
| 1:B:674:LEU:HA | 1:B:695:ARG:HH12 | 1.60 | 0.66 |
| 1:D:524:ASP:OD2 | 1:D:527:ARG:NH1 | 2.28 | 0.66 |
| 1:D:1775:LEU:HD12 | 1:D:1776:PRO:HD2 | 1.77 | 0.66 |
| 1:E:1328:LEU:HB3 | 1:E:1499:PHE:HE2 | 1.61 | 0.66 |
| 1:G:926:ARG:NH1 | 1:G:931:GLN:O | 2.29 | 0.66 |
| 1:I:2392:ARG:HB2 | 1:I:2494:LYS:HB3 | 1.77 | 0.66 |
| 1:K:2096:ILE:HD13 | 1:K:2179:PRO:HG2 | 1.77 | 0.66 |
| 1:L:221:ARG:NH1 | 1:L:285:ASP:O | 2.28 | 0.66 |
| 1:L:986:LEU:HD11 | 1:L:1028:LEU:HB3 | 1.77 | 0.66 |
| 1:M:738:VAL:HG23 | 1:M:789:ILE:HG21 | 1.77 | 0.66 |
| 1:M:1225:ASP:OD1 | 1:M:1229:LYS:N | 2.28 | 0.66 |
| 1:M:1745:LEU:HD21 | 1:M:1944:VAL:HG21 | 1.77 | 0.66 |
| 1:N:2217:ILE:HG22 | 1:N:2219:GLU:H | 1.60 | 0.66 |
| 1:N:2311:GLU:O | 1:N:2315:ARG:NH1 | 2.28 | 0.66 |
| 1:N:2709:HIS:HA | 1:N:2712:VAL:HG12 | 1.78 | 0.66 |
| 1:O:574:LEU:HD23 | 1:O:616:LEU:HG | 1.76 | 0.66 |
| 1:O:1583:GLU:OE2 | 1:R:327:LYS:NZ | 2.25 | 0.66 |
| 1:Q:956:VAL:HA | 1:Q:963:PRO:HA | 1.75 | 0.66 |
| 1:T:1993:SER:HB2 | 1:T:2058:LEU:HD11 | 1.77 | 0.66 |
| 1:T:3049:GLN:H | 1:T:3052:LEU:HD12 | 1.60 | 0.66 |
| 1:A:1786:ASP:OD2 | 1:A:1789:LEU:N | 2.26 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:D:1222:SER:HB3 | 1:D:1230:LYS:HZ1 | 1.60 | 0.66 |
| 1:D:1576:CYS:N | 1:D:1632:ASP:O | 2.26 | 0.66 |
| 1:E:2153:THR:HA | 1:E:2156:HIS:HD1 | 1.61 | 0.66 |
| 1:F:269:THR:HB | 1:F:271:LYS:HZ3 | 1.60 | 0.66 |
| 1:F:1349:TRP:O | 1:F:1463:ASN:ND2 | 2.26 | 0.66 |
| 1:G:1845:ASP:OD1 | 1:G:2028:ARG:NH1 | 2.29 | 0.66 |
| 1:G:3011:TRP:CZ3 | 1:G:3013:TRP:HB3 | 2.30 | 0.66 |
| 1:H:735:ARG:HH22 | 1:H:790:THR:H | 1.41 | 0.66 |
| 1:H:3080:PHE:HA | 1:H:3083:GLN:HE22 | 1.61 | 0.66 |
| 1:M:1802:ILE:HD12 | 1:M:1805:GLU:HB2 | 1.76 | 0.66 |
| 1:M:2114:LEU:HG | 1:M:2123:TRP:HB2 | 1.77 | 0.66 |
| 1:O:1689:ARG:NE | 1:O:1786:ASP:OD1 | 2.28 | 0.66 |
| 1:P:2551:HIS:NE2 | 1:P:2567:CYS:SG | 2.68 | 0.66 |
| 1:R:671:THR:O | 1:R:695:ARG:NH2 | 2.28 | 0.66 |
| 1:S:1122:HIS:ND1 | 1:S:1123:TYR:O | 2.25 | 0.66 |
| 1:T:2113:ASP:OD1 | 1:T:2114:LEU:N | 2.28 | 0.66 |
| 1:T:2665:ARG:HE | 1:T:2726:ARG:HH21 | 1.44 | 0.66 |
| 1:A:1037:MET:HA | 1:A:1043:THR:HA | 1.78 | 0.66 |
| 1:A:2970:ALA:O | 1:A:2973:ARG:NH1 | 2.29 | 0.66 |
| 1:C:2:SER:N | 1:C:280:GLY:O | 2.27 | 0.66 |
| 1:C:376:LEU:HB3 | 1:C:378:LYS:HZ3 | 1.61 | 0.66 |
| 1:C:646:ARG:NH2 | 1:C:714:GLN:O | 2.28 | 0.66 |
| 1:D:3037:ILE:HG22 | 1:D:3042:HIS:H | 1.59 | 0.66 |
| 1:E:1680:VAL:HG12 | 1:E:1764:PRO:HB2 | 1.77 | 0.66 |
| 1:E:2325:CYS:HA | 1:F:1242:VAL:HG13 | 1.76 | 0.66 |
| 1:F:23:LEU:HD21 | 1:F:124:SER:HB2 | 1.77 | 0.66 |
| 1:F:1284:ARG:HH21 | 1:F:1376:GLU:HG3 | 1.61 | 0.66 |
| 1:J:848:ARG:HD3 | 1:J:934:LEU:HB3 | 1.78 | 0.66 |
| 1:J:3049:GLN:H | 1:J:3052:LEU:HD12 | 1.61 | 0.66 |
| 1:K:3056:ARG:NH1 | 1:K:3058:GLN:OE1 | 2.29 | 0.66 |
| 1:M:2579:ARG:NH1 | 1:M:2774:TYR:OH | 2.29 | 0.66 |
| 1:N:2876:ILE:HB | 1:N:2884:LEU:HB2 | 1.78 | 0.66 |
| 1:O:31:THR:OG1 | 1:O:32:VAL:N | 2.28 | 0.66 |
| 1:O:1905:ASP:HB3 | 1:O:1908:GLU:HB2 | 1.76 | 0.66 |
| 1:Q:2585:LEU:HD13 | 1:Q:2706:PHE:CE2 | 2.29 | 0.66 |
| 1:R:94:TRP:O | 1:R:218:ASN:ND2 | 2.29 | 0.66 |
| 1:S:1338:LEU:HD21 | 1:S:1345:SER:HA | 1.76 | 0.66 |
| 1:S:2741:ARG:HA | 1:S:2762:ARG:HH21 | 1.60 | 0.66 |
| 1:T:1926:GLY:HA2 | 1:T:1936:LYS:HE2 | 1.77 | 0.66 |
| 1:B:597:ARG:HH22 | 1:B:655:GLN:HA | 1.59 | 0.66 |
| 1:B:2126:LEU:HD11 | 1:B:2165:VAL:HG12 | 1.78 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:E:3289:LYS:HD2 | 1:E:3291:ASN:HD22 | 1.61 | 0.66 |
| 1:F:913:TRP:HD1 | 1:F:1088:LEU:HD12 | 1.58 | 0.66 |
| 1:I:1811:ARG:NH2 | 1:I:1878:ASP:OD1 | 2.29 | 0.66 |
| 1:I:2114:LEU:HG | 1:I:2123:TRP:HB2 | 1.75 | 0.66 |
| 1:K:2796:ARG:NH1 | 1:K:2799:GLU:OE2 | 2.29 | 0.66 |
| 1:K:3047:ASP:HB3 | 1:K:3097:GLY:HA3 | 1.78 | 0.66 |
| 1:L:2809:GLN:NE2 | 1:L:2845:TRP:O | 2.28 | 0.66 |
| 1:M:1756:ARG:HH22 | 1:N:2175:THR:HB | 1.60 | 0.66 |
| 1:O:2663:GLU:OE2 | 1:O:2801:ARG:NH2 | 2.28 | 0.66 |
| 1:P:671:THR:O | 1:P:695:ARG:NH2 | 2.28 | 0.66 |
| 1:Q:55:ARG:NH2 | 1:Q:56:VAL:O | 2.29 | 0.66 |
| 1:S:2059:ASN:OD1 | 1:S:2060:GLY:N | 2.28 | 0.66 |
| 1:A:1426:PHE:HE1 | 1:A:1464:VAL:HG13 | 1.60 | 0.66 |
| 1:A:1689:ARG:NE | 1:A:1786:ASP:OD1 | 2.26 | 0.66 |
| 1:C:527:ARG:NH1 | 1:C:528:PRO:O | 2.28 | 0.66 |
| 1:C:939:TRP:HE1 | 1:C:998:ILE:HG21 | 1.59 | 0.66 |
| 1:C:1156:HIS:HB3 | 1:C:1193:GLN:HE22 | 1.61 | 0.66 |
| 1:C:1539:THR:HG23 | 1:C:1541:PRO:HD2 | 1.77 | 0.66 |
| 1:C:1919:PRO:O | 1:C:1921:LYS:NZ | 2.27 | 0.66 |
| 1:D:2159:ARG:NE | 1:D:2303:ASP:OD1 | 2.24 | 0.66 |
| 1:D:2741:ARG:NH2 | 1:E:2866:PRO:O | 2.28 | 0.66 |
| 1:E:1714:HIS:NE2 | 1:E:1732:CYS:SG | 2.66 | 0.66 |
| 1:G:2251:VAL:HG22 | 1:G:2263:GLN:HB3 | 1.78 | 0.66 |
| 1:H:1501:ASP:HB3 | 1:H:1504:GLN:HB2 | 1.78 | 0.66 |
| 1:J:105:ARG:HA | 1:J:108:GLN:HE22 | 1.60 | 0.66 |
| 1:J:1539:THR:HG23 | 1:J:1541:PRO:HD2 | 1.78 | 0.66 |
| 1:K:2085:GLN:HE22 | 1:K:2088:PRO:HD2 | 1.61 | 0.66 |
| 1:M:1156:HIS:HB3 | 1:M:1193:GLN:HE22 | 1.60 | 0.66 |
| 1:M:1413:ALA:HB1 | 1:M:1425:GLN:HG3 | 1.76 | 0.66 |
| 1:M:2393:VAL:H | 1:M:2447:THR:HG22 | 1.61 | 0.66 |
| 1:N:1049:PHE:O | 1:N:1053:HIS:ND1 | 2.28 | 0.66 |
| 1:O:738:VAL:HG23 | 1:O:789:ILE:HD13 | 1.78 | 0.66 |
| 1:O:2970:ALA:O | 1:O:2973:ARG:NH1 | 2.29 | 0.66 |
| 1:P:925:LEU:HD22 | 1:P:928:LYS:HZ1 | 1.59 | 0.66 |
| 1:Q:915:ARG:NH2 | 1:Q:1121:TYR:OH | 2.28 | 0.66 |
| 1:Q:1026:HIS:HD2 | 1:Q:1184:LEU:HD11 | 1.59 | 0.66 |
| 1:Q:3056:ARG:NH1 | 1:Q:3058:GLN:OE1 | 2.27 | 0.66 |
| 1:R:1873:HIS:HE2 | 1:R:2020:ALA:HB3 | 1.61 | 0.66 |
| 1:R:2865:ARG:HD3 | 1:R:2866:PRO:HD2 | 1.77 | 0.66 |
| 1:T:454:ARG:NH2 | 1:T:1338:LEU:O | 2.28 | 0.66 |
| 1:T:2788:GLN:HA | 1:T:2791:GLU:OE2 | 1.96 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:3020:LEU:HB3 | 1:A:3024:LEU:HD11 | 1.77 | 0.66 |
| 1:B:722:GLN:NE2 | 1:B:932:ASP:OD1 | 2.28 | 0.66 |
| 1:B:2194:PHE:CD1 | 1:B:2212:PHE:HB3 | 2.31 | 0.66 |
| 1:B:3157:PHE:O | 1:B:3169:ARG:NH1 | 2.28 | 0.66 |
| 1:D:38:LEU:O | 1:D:73:TYR:OH | 2.14 | 0.66 |
| 1:D:3008:ILE:HD13 | 1:D:3116:MET:HB3 | 1.78 | 0.66 |
| 1:F:636:ILE:O | 1:F:640:HIS:ND1 | 2.27 | 0.66 |
| 1:G:3056:ARG:NH1 | 1:G:3058:GLN:OE1 | 2.28 | 0.66 |
| 1:H:925:LEU:HD13 | 1:H:928:LYS:HE2 | 1.78 | 0.66 |
| 1:J:248:ARG:NH1 | 1:J:802:ASP:O | 2.29 | 0.66 |
| 1:K:1732:CYS:O | 1:K:1734:HIS:ND1 | 2.29 | 0.66 |
| 1:K:2741:ARG:NH2 | 1:T:2867:ASP:OD1 | 2.29 | 0.66 |
| 1:L:2541:PRO:HD2 | 1:L:2542:ARG:H | 1.59 | 0.66 |
| 1:L:2639:ARG:HD3 | 1:L:2641:GLN:HE22 | 1.58 | 0.66 |
| 1:L:2964:LYS:HG2 | 1:L:2973:ARG:HB2 | 1.76 | 0.66 |
| 1:M:1100:ASP:O | 1:M:1104:ARG:NH1 | 2.27 | 0.66 |
| 1:N:925:LEU:HD22 | 1:N:928:LYS:HZ1 | 1.59 | 0.66 |
| 1:O:527:ARG:NH1 | 1:O:528:PRO:O | 2.29 | 0.66 |
| 1:P:3037:ILE:HG22 | 1:P:3042:HIS:H | 1.61 | 0.66 |
| 1:T:2666:ASP:OD2 | 1:T:2849:ARG:NH2 | 2.29 | 0.66 |
| 1:A:1931:LEU:HD13 | 1:B:2102:ARG:HB2 | 1.75 | 0.66 |
| 1:B:230:GLN:NE2 | 1:B:236:THR:O | 2.26 | 0.66 |
| 1:C:3100:THR:HA | 1:C:3290:TYR:HE2 | 1.61 | 0.66 |
| 1:E:454:ARG:HH21 | 1:E:514:ARG:HB3 | 1.59 | 0.66 |
| 1:E:1539:THR:HG23 | 1:E:1541:PRO:HD2 | 1.78 | 0.66 |
| 1:E:1651:ARG:NH2 | 1:F:2025:SER:O | 2.29 | 0.66 |
| 1:G:2462:ASN:O | 1:H:1085:ARG:NH1 | 2.29 | 0.66 |
| 1:I:750:LEU:HD11 | 1:I:767:LYS:HE3 | 1.78 | 0.66 |
| 1:K:2534:ALA:O | 1:K:2538:GLN:NE2 | 2.27 | 0.66 |
| 1:K:2997:MET:SD | 1:K:3000:ARG:NH2 | 2.69 | 0.66 |
| 1:L:540:THR:HG22 | 1:L:551:HIS:HA | 1.78 | 0.66 |
| 1:L:2469:LEU:HD11 | 1:L:2489:PRO:HG2 | 1.78 | 0.66 |
| 1:L:3142:TYR:CZ | 1:L:3144:ARG:HD3 | 2.29 | 0.66 |
| 1:M:1855:ASN:HD21 | 1:M:2015:VAL:HA | 1.59 | 0.66 |
| 1:M:2462:ASN:O | 1:N:1085:ARG:NH1 | 2.28 | 0.66 |
| 1:P:913:TRP:HD1 | 1:P:1088:LEU:HD12 | 1.61 | 0.66 |
| 1:P:1089:GLN:HE22 | 1:P:1092:ALA:HB3 | 1.59 | 0.66 |
| 1:P:1865:LYS:HE3 | 1:P:1867:HIS:H | 1.60 | 0.66 |
| 1:Q:2226:ARG:NH1 | 1:Q:2292:ASP:OD2 | 2.27 | 0.66 |
| 1:R:1143:ARG:O | 1:R:1148:ARG:NH1 | 2.25 | 0.66 |
| 1:T:2286:LEU:HB3 | 1:T:2428:LEU:HD21 | 1.78 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:454:ARG:HH21 | 1:A:514:ARG:HB3 | 1.58 | 0.66 |
| 1:A:2118:GLY:HA2 | 1:A:2124:GLN:HE22 | 1.61 | 0.66 |
| 1:B:379:LYS:HD3 | 1:B:381:ASN:H | 1.61 | 0.66 |
| 1:C:259:ASN:O | 1:C:265:ARG:NH2 | 2.29 | 0.66 |
| 1:C:3160:GLU:HG2 | 1:C:3169:ARG:HH22 | 1.61 | 0.66 |
| 1:D:473:LEU:H | 1:D:629:HIS:HB3 | 1.60 | 0.66 |
| 1:E:454:ARG:NH2 | 1:E:514:ARG:O | 2.28 | 0.66 |
| 1:H:1865:LYS:HE3 | 1:H:1867:HIS:H | 1.61 | 0.66 |
| 1:I:3317:ILE:HG12 | 1:I:3339:ARG:HB3 | 1.78 | 0.66 |
| 1:J:920:GLN:HB3 | 1:J:1103:THR:HG21 | 1.77 | 0.66 |
| 1:J:1743:HIS:HD2 | 1:J:1885:HIS:CD2 | 2.14 | 0.66 |
| 1:L:2286:LEU:HB3 | 1:L:2428:LEU:HD21 | 1.77 | 0.66 |
| 1:N:111:ILE:HG23 | 1:N:122:LYS:HB2 | 1.78 | 0.66 |
| 1:N:938:ASP:OD1 | 1:N:1055:ASN:ND2 | 2.28 | 0.66 |
| 1:N:2576:GLN:HE21 | 1:N:2767:PHE:HE1 | 1.43 | 0.66 |
| 1:O:2986:HIS:HB3 | 1:O:3177:ILE:HD13 | 1.78 | 0.66 |
| 1:S:3020:LEU:HB3 | 1:S:3024:LEU:HD11 | 1.78 | 0.66 |
| 1:B:113:LYS:NZ | 1:I:2226:ARG:O | 2.28 | 0.65 |
| 1:B:662:TYR:HE2 | 1:B:700:TYR:HB3 | 1.61 | 0.65 |
| 1:B:696:PRO:HA | 1:B:699:ILE:HD13 | 1.78 | 0.65 |
| 1:C:1756:ARG:HH22 | 1:D:2175:THR:HB | 1.61 | 0.65 |
| 1:D:2671:GLU:N | 1:D:2671:GLU:OE1 | 2.30 | 0.65 |
| 1:D:2984:PHE:O | 1:D:2988:HIS:ND1 | 2.28 | 0.65 |
| 1:D:3321:LEU:O | 1:D:3395:ARG:NH2 | 2.28 | 0.65 |
| 1:E:2152:PRO:HA | 1:E:2261:GLU:HG3 | 1.77 | 0.65 |
| 1:E:3160:GLU:HG2 | 1:E:3169:ARG:HH22 | 1.58 | 0.65 |
| 1:H:1785:ARG:NH1 | 1:H:1786:ASP:O | 2.30 | 0.65 |
| 1:H:3360:LEU:HG | 1:H:3401:ARG:HD3 | 1.78 | 0.65 |
| 1:I:596:GLN:O | 1:I:658:ARG:NH2 | 2.28 | 0.65 |
| 1:M:2345:ASN:HD22 | 1:M:2348:THR:HG23 | 1.61 | 0.65 |
| 1:N:1415:GLU:OE2 | 1:N:1555:ARG:NH2 | 2.28 | 0.65 |
| 1:N:3058:GLN:NE2 | 1:N:3268:ASP:OD2 | 2.29 | 0.65 |
| 1:O:1328:LEU:HB3 | 1:O:1499:PHE:CE2 | 2.31 | 0.65 |
| 1:O:1815:ARG:HD2 | 1:O:1818:LEU:HD21 | 1.77 | 0.65 |
| 1:P:434:ARG:NH2 | 1:P:508:GLU:OE2 | 2.29 | 0.65 |
| 1:Q:1251:LYS:HD2 | 1:Q:1476:GLN:HE22 | 1.60 | 0.65 |
| 1:R:1222:SER:HB3 | 1:R:1230:LYS:HZ1 | 1.60 | 0.65 |
| 1:R:1763:ILE:HD12 | 1:R:1764:PRO:HD2 | 1.78 | 0.65 |
| 1:T:1100:ASP:O | 1:T:1104:ARG:NH1 | 2.29 | 0.65 |
| 1:T:1116:GLU:HA | 1:T:1120:GLN:HA | 1.78 | 0.65 |
| 1:T:2979:HIS:HA | 1:T:2984:PHE:HD2 | 1.61 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:T:3103:MET:HA | 1:T:3109:SER:HA | 1.79 | 0.65 |
| 1:A:277:ARG:NH2 | 1:M:835:THR:OG1 | 2.29 | 0.65 |
| 1:B:913:TRP:HD1 | 1:B:1088:LEU:HD12 | 1.62 | 0.65 |
| 1:C:1225:ASP:OD1 | 1:C:1229:LYS:N | 2.29 | 0.65 |
| 1:C:1896:GLN:NE2 | 1:C:1906:PRO:O | 2.21 | 0.65 |
| 1:C:2585:LEU:HD13 | 1:C:2706:PHE:CE2 | 2.31 | 0.65 |
| 1:D:737:PHE:O | 1:D:829:ILE:N | 2.27 | 0.65 |
| 1:D:2709:HIS:HA | 1:D:2712:VAL:HG12 | 1.78 | 0.65 |
| 1:E:636:ILE:H | 1:E:636:ILE:HD12 | 1.61 | 0.65 |
| 1:E:2796:ARG:O | 1:E:2796:ARG:NH1 | 2.30 | 0.65 |
| 1:F:2287:HIS:HE1 | 1:F:2432:LEU:HB2 | 1.61 | 0.65 |
| 1:G:3211:ASP:HB2 | 1:G:3309:ALA:HB2 | 1.77 | 0.65 |
| 1:H:256:ARG:O | 1:H:265:ARG:NH1 | 2.28 | 0.65 |
| 1:H:1743:HIS:HD2 | 1:H:1885:HIS:HD2 | 1.42 | 0.65 |
| 1:H:2806:PHE:CE2 | 1:H:2892:PRO:HB3 | 2.31 | 0.65 |
| 1:I:471:HIS:NE2 | 1:I:489:CYS:SG | 2.70 | 0.65 |
| 1:J:1763:ILE:HD12 | 1:J:1764:PRO:HD2 | 1.78 | 0.65 |
| 1:J:2709:HIS:HA | 1:J:2712:VAL:HG22 | 1.78 | 0.65 |
| 1:K:836:HIS:CE1 | 1:K:838:GLU:HB3 | 2.30 | 0.65 |
| 1:M:1359:PRO:HD2 | 1:M:1362:ILE:HD11 | 1.79 | 0.65 |
| 1:N:313:PHE:CE2 | 1:N:406:PRO:HB3 | 2.31 | 0.65 |
| 1:O:2088:PRO:O | 1:O:2090:ASN:N | 2.29 | 0.65 |
| 1:Q:512:LYS:HA | 1:Q:516:LEU:HB2 | 1.77 | 0.65 |
| 1:Q:1689:ARG:NE | 1:Q:1786:ASP:OD1 | 2.27 | 0.65 |
| 1:Q:2534:ALA:HA | 1:Q:2537:GLN:HE22 | 1.61 | 0.65 |
| 1:Q:3020:LEU:HB3 | 1:Q:3024:LEU:HD11 | 1.78 | 0.65 |
| 1:R:846:HIS:HB3 | 1:R:1121:TYR:HA | 1.78 | 0.65 |
| 1:R:2311:GLU:O | 1:R:2315:ARG:NH1 | 2.28 | 0.65 |
| 1:T:3266:VAL:HG21 | 1:T:3283:PHE:HE2 | 1.61 | 0.65 |
| 1:A:593:ALA:HA | 1:A:605:GLN:HG3 | 1.77 | 0.65 |
| 1:B:337:GLN:NE2 | 1:I:1575:ILE:O | 2.24 | 0.65 |
| 1:C:2001:CYS:HA | 1:C:2007:CYS:HB3 | 1.78 | 0.65 |
| 1:E:799:LYS:N | 1:E:802:ASP:OD2 | 2.30 | 0.65 |
| 1:E:2226:ARG:O | 1:H:113:LYS:NZ | 2.22 | 0.65 |
| 1:E:2977:CYS:HA | 1:E:2987:TRP:HZ3 | 1.60 | 0.65 |
| 1:F:2232:LEU:HD12 | 1:F:2274:LEU:HB3 | 1.79 | 0.65 |
| 1:G:1931:LEU:HD23 | 1:H:2102:ARG:HA | 1.77 | 0.65 |
| 1:H:1349:TRP:O | 1:H:1463:ASN:ND2 | 2.28 | 0.65 |
| 1:H:2665:ARG:O | 1:H:2723:GLN:NE2 | 2.29 | 0.65 |
| 1:H:3113:PRO:HA | 1:H:3116:MET:HE2 | 1.79 | 0.65 |
| 1:K:126:PHE:O | 1:K:143:ARG:NH1 | 2.28 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:L:2985:PRO:HB2 | 1:L:2989:ARG:HH21 | 1.62 | 0.65 |
| 1:M:1919:PRO:HB2 | 1:M:1924:SER:HB2 | 1.78 | 0.65 |
| 1:P:1546:VAL:HA | 1:P:1549:ARG:HG2 | 1.78 | 0.65 |
| 1:Q:454:ARG:NH2 | 1:Q:514:ARG:O | 2.29 | 0.65 |
| 1:T:1880:ILE:HA | 1:T:1883:LEU:HD12 | 1.78 | 0.65 |
| 1:T:2313:GLN:HG2 | 1:T:2320:TYR:HB3 | 1.78 | 0.65 |
| 1:A:1395:ASP:HB3 | 1:A:1439:GLY:HA3 | 1.78 | 0.65 |
| 1:B:1012:CYS:SG | 1:B:1196:ARG:NH1 | 2.68 | 0.65 |
| 1:C:3171:ASN:HA | 1:C:3176:GLN:HE22 | 1.60 | 0.65 |
| 1:D:673:GLU:O | 1:D:695:ARG:NH2 | 2.23 | 0.65 |
| 1:E:613:PRO:HB2 | 1:E:640:HIS:CE1 | 2.31 | 0.65 |
| 1:E:738:VAL:HG23 | 1:E:789:ILE:HD13 | 1.76 | 0.65 |
| 1:F:1646:GLU:OE1 | 1:F:1648:SER:OG | 2.10 | 0.65 |
| 1:G:844:GLU:OE1 | 1:G:926:ARG:NH2 | 2.29 | 0.65 |
| 1:H:2639:ARG:HD3 | 1:H:2641:GLN:HE22 | 1.59 | 0.65 |
| 1:I:512:LYS:HA | 1:I:516:LEU:HB2 | 1.77 | 0.65 |
| 1:I:2602:ASP:HA | 1:I:2711:ASN:HD21 | 1.62 | 0.65 |
| 1:K:437:VAL:HG12 | 1:K:521:PRO:HB2 | 1.79 | 0.65 |
| 1:O:2551:HIS:HB2 | 1:O:2581:PHE:HE1 | 1.62 | 0.65 |
| 1:O:3214:TYR:HD1 | 1:O:3265:ASP:HA | 1.62 | 0.65 |
| 1:Q:2148:LEU:HB3 | 1:Q:2151:VAL:HG11 | 1.77 | 0.65 |
| 1:Q:2509:SER:O | 1:Q:3138:ARG:NH2 | 2.30 | 0.65 |
| 1:R:2775:GLN:NE2 | 1:R:2776:TYR:O | 2.28 | 0.65 |
| 1:B:598:ASP:HB3 | 1:B:601:ASP:HB3 | 1.77 | 0.65 |
| 1:B:905:HIS:HA | 1:B:910:PHE:HD2 | 1.60 | 0.65 |
| 1:D:74:VAL:HA | 1:D:77:LEU:HD23 | 1.79 | 0.65 |
| 1:D:3208:ARG:HH12 | 1:D:3310:ASN:HA | 1.62 | 0.65 |
| 1:E:2155:PRO:HB2 | 1:E:2159:ARG:HH22 | 1.61 | 0.65 |
| 1:E:3020:LEU:HB3 | 1:E:3024:LEU:HD11 | 1.79 | 0.65 |
| 1:F:1049:PHE:O | 1:F:1053:HIS:ND1 | 2.30 | 0.65 |
| 1:F:2809:GLN:NE2 | 1:F:2845:TRP:O | 2.29 | 0.65 |
| 1:G:714:GLN:OE1 | 1:G:718:MET:N | 2.28 | 0.65 |
| 1:H:1492:MET:HA | 1:H:1516:PRO:HG2 | 1.79 | 0.65 |
| 1:I:711:ASP:OD1 | 1:I:712:ASN:N | 2.29 | 0.65 |
| 1:J:1492:MET:HA | 1:J:1516:PRO:HG2 | 1.79 | 0.65 |
| 1:K:3157:PHE:O | 1:K:3163:ASN:ND2 | 2.29 | 0.65 |
| 1:M:1195:ASP:HB2 | 1:N:2441:LEU:HD21 | 1.78 | 0.65 |
| 1:M:3317:ILE:HG12 | 1:M:3339:ARG:HB3 | 1.76 | 0.65 |
| 1:P:1769:VAL:O | 1:P:1828:ASN:ND2 | 2.29 | 0.65 |
| 1:R:1743:HIS:HD2 | 1:R:1885:HIS:HD2 | 1.44 | 0.65 |
| 1:D:2809:GLN:NE2 | 1:D:2845:TRP:O | 2.30 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:G:2056:ARG:NH1 | 1:G:2061:SER:O | 2.29 | 0.65 |
| 1:I:1448:LEU:HD21 | 1:I:1596:LEU:HD21 | 1.78 | 0.65 |
| 1:J:2149:HIS:HA | 1:J:2154:PHE:HD2 | 1.61 | 0.65 |
| 1:L:1677:ARG:NH2 | 1:L:1751:GLU:OE1 | 2.29 | 0.65 |
| 1:L:3037:ILE:HG22 | 1:L:3042:HIS:H | 1.62 | 0.65 |
| 1:N:328:VAL:HG12 | 1:N:386:VAL:HG22 | 1.78 | 0.65 |
| 1:O:514:ARG:HH12 | 1:O:1343:ALA:HA | 1.62 | 0.65 |
| 1:Q:881:ILE:HA | 1:Q:884:PHE:HD2 | 1.60 | 0.65 |
| 1:R:509:ASP:OD1 | 1:R:510:ALA:N | 2.29 | 0.65 |
| 1:R:3398:GLN:OE1 | 1:R:3400:THR:OG1 | 2.15 | 0.65 |
| 1:T:1839:GLU:HA | 1:T:1902:ARG:HH22 | 1.61 | 0.65 |
| 1:A:1400:LEU:HD21 | 1:A:1436:LEU:HB3 | 1.78 | 0.65 |
| 1:B:2809:GLN:NE2 | 1:B:2845:TRP:O | 2.30 | 0.65 |
| 1:B:3383:PRO:HA | 1:B:3406:ILE:HB | 1.78 | 0.65 |
| 1:B:3392:ASN:HB3 | 1:B:3395:ARG:HG2 | 1.79 | 0.65 |
| 1:D:1089:GLN:HE22 | 1:D:1092:ALA:HB3 | 1.61 | 0.65 |
| 1:F:2709:HIS:HA | 1:F:2712:VAL:HG22 | 1.79 | 0.65 |
| 1:G:3390:SER:HB3 | 1:G:3395:ARG:HG3 | 1.78 | 0.65 |
| 1:H:1672:GLU:HG3 | 1:H:1673:ARG:HG2 | 1.79 | 0.65 |
| 1:M:1854:HIS:HD2 | 1:M:1888:THR:HG21 | 1.61 | 0.65 |
| 1:O:613:PRO:HB2 | 1:O:640:HIS:CE1 | 2.32 | 0.65 |
| 1:O:2580:LEU:HA | 1:O:2583:VAL:HG12 | 1.79 | 0.65 |
| 1:Q:654:LEU:HD21 | 1:Q:658:ARG:HH21 | 1.61 | 0.65 |
| 1:Q:2130:HIS:NE2 | 1:Q:2147:CYS:SG | 2.69 | 0.65 |
| 1:Q:2462:ASN:O | 1:R:1085:ARG:NH1 | 2.29 | 0.65 |
| 1:Q:2805:ASN:HB3 | 1:Q:2850:LEU:HD21 | 1.79 | 0.65 |
| 1:R:727:ILE:HG22 | 1:R:730:ARG:HH21 | 1.61 | 0.65 |
| 1:S:956:VAL:HA | 1:S:963:PRO:HA | 1.78 | 0.65 |
| 1:A:2059:ASN:OD1 | 1:A:2060:GLY:N | 2.30 | 0.65 |
| 1:C:465:GLN:HG2 | 1:C:560:ALA:HB2 | 1.79 | 0.65 |
| 1:C:471:HIS:NE2 | 1:C:489:CYS:SG | 2.70 | 0.65 |
| 1:C:2534:ALA:HA | 1:C:2537:GLN:HE22 | 1.60 | 0.65 |
| 1:E:3390:SER:HB3 | 1:E:3395:ARG:HG3 | 1.79 | 0.65 |
| 1:F:5:ARG:HH21 | 1:F:90:GLY:HA3 | 1.62 | 0.65 |
| 1:F:2806:PHE:CE1 | 1:F:2892:PRO:HB3 | 2.32 | 0.65 |
| 1:G:31:THR:OG1 | 1:G:32:VAL:N | 2.29 | 0.65 |
| 1:H:23:LEU:HD21 | 1:H:124:SER:HB2 | 1.79 | 0.65 |
| 1:H:97:THR:OG1 | 1:H:98:LYS:NZ | 2.30 | 0.65 |
| 1:I:937:TRP:O | 1:I:1055:ASN:ND2 | 2.30 | 0.65 |
| 1:J:97:THR:OG1 | 1:J:98:LYS:NZ | 2.29 | 0.65 |
| 1:J:2311:GLU:O | 1:J:2315:ARG:NH1 | 2.30 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:J:3131:THR:HA | 1:J:3134:LYS:HZ3 | 1.62 | 0.65 |
| 1:K:1689:ARG:NE | 1:K:1786:ASP:OD1 | 2.26 | 0.65 |
| 1:K:1786:ASP:OD2 | 1:K:1789:LEU:N | 2.26 | 0.65 |
| 1:K:1931:LEU:HD23 | 1:L:2102:ARG:HA | 1.77 | 0.65 |
| 1:K:2960:HIS:HE1 | 1:K:3119:HIS:HE1 | 1.43 | 0.65 |
| 1:L:94:TRP:O | 1:L:218:ASN:ND2 | 2.29 | 0.65 |
| 1:L:1149:VAL:HG11 | 1:L:1206:LEU:HD13 | 1.78 | 0.65 |
| 1:L:2752:ASN:HD21 | 1:L:2757:ILE:HG13 | 1.61 | 0.65 |
| 1:M:1026:HIS:HD2 | 1:M:1184:LEU:HD11 | 1.61 | 0.65 |
| 1:N:1116:GLU:HA | 1:N:1120:GLN:HA | 1.79 | 0.65 |
| 1:O:75:VAL:HG21 | 1:O:279:LEU:HD12 | 1.78 | 0.65 |
| 1:Q:731:ARG:HG2 | 1:Q:735:ARG:HH22 | 1.61 | 0.65 |
| 1:S:1359:PRO:HD2 | 1:S:1362:ILE:HD11 | 1.79 | 0.65 |
| 1:S:1362:ILE:HD13 | 1:S:1456:LEU:HD11 | 1.78 | 0.65 |
| 1:S:3133:GLN:NE2 | 1:S:3138:ARG:O | 2.30 | 0.65 |
| 1:T:597:ARG:HH22 | 1:T:655:GLN:HA | 1.62 | 0.65 |
| 1:A:3074:GLU:HB3 | 1:A:3080:PHE:CE1 | 2.32 | 0.65 |
| 1:B:450:GLN:O | 1:B:454:ARG:HG2 | 1.96 | 0.65 |
| 1:B:2194:PHE:HD1 | 1:B:2212:PHE:HB3 | 1.62 | 0.65 |
| 1:C:1802:ILE:HD12 | 1:C:1805:GLU:HB2 | 1.79 | 0.65 |
| 1:C:2674:TYR:OH | 1:C:2712:VAL:O | 2.14 | 0.65 |
| 1:D:1448:LEU:HD21 | 1:D:1596:LEU:HG | 1.79 | 0.65 |
| 1:D:2876:ILE:HB | 1:D:2884:LEU:HB2 | 1.79 | 0.65 |
| 1:G:855:THR:HG22 | 1:G:858:GLN:HE22 | 1.62 | 0.65 |
| 1:G:2027:ASP:OD2 | 1:G:2028:ARG:NH1 | 2.30 | 0.65 |
| 1:G:2858:VAL:HA | 1:G:2861:GLN:HG2 | 1.77 | 0.65 |
| 1:H:614:HIS:HA | 1:H:625:LEU:HG | 1.79 | 0.65 |
| 1:I:2970:ALA:O | 1:I:2973:ARG:NH1 | 2.28 | 0.65 |
| 1:J:188:ILE:HG21 | 1:J:215:HIS:NE2 | 2.11 | 0.65 |
| 1:J:2824:ALA:HB2 | 1:J:2869:VAL:HG23 | 1.78 | 0.65 |
| 1:K:854:LEU:HD12 | 1:K:858:GLN:HG3 | 1.78 | 0.65 |
| 1:K:2348:THR:OG1 | 1:K:2349:ARG:NH1 | 2.30 | 0.65 |
| 1:N:3321:LEU:O | 1:N:3395:ARG:NH2 | 2.29 | 0.65 |
| 1:O:2462:ASN:O | 1:P:1085:ARG:NH1 | 2.30 | 0.65 |
| 1:P:2159:ARG:NE | 1:P:2303:ASP:OD1 | 2.24 | 0.65 |
| 1:Q:844:GLU:OE1 | 1:Q:926:ARG:NH2 | 2.29 | 0.65 |
| 1:R:2712:VAL:HA | 1:R:2715:GLN:HE21 | 1.62 | 0.65 |
| 1:A:3307:ARG:NH1 | 1:A:3312:ASP:O | 2.30 | 0.65 |
| 1:B:913:TRP:NE1 | 1:B:1089:GLN:O | 2.29 | 0.65 |
| 1:C:63:MET:HB3 | 1:C:246:LEU:HD21 | 1.79 | 0.65 |
| 1:C:1571:VAL:O | 1:C:1592:SER:OG | 2.15 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:E:55:ARG:NH2 | 1:E:56:VAL:O | 2.29 | 0.65 |
| 1:G:2686:GLY:HA2 | 1:G:2693:MET:HB3 | 1.78 | 0.65 |
| 1:H:1844:CYS:SG | 1:H:2028:ARG:NH1 | 2.68 | 0.65 |
| 1:K:1420:CYS:HB2 | 1:K:1608:ARG:HH21 | 1.62 | 0.65 |
| 1:K:3128:ILE:HG22 | 1:K:3190:LEU:HD22 | 1.78 | 0.65 |
| 1:L:474:PRO:HB2 | 1:L:476:ARG:HH22 | 1.60 | 0.65 |
| 1:L:1714:HIS:NE2 | 1:L:1732:CYS:SG | 2.70 | 0.65 |
| 1:O:3386:TYR:HB2 | 1:O:3404:ILE:HG22 | 1.78 | 0.65 |
| 1:S:1286:MET:HG3 | 1:S:1292:PHE:HB2 | 1.78 | 0.65 |
| 1:S:3334:ARG:NH1 | 1:S:3407:ASP:OD1 | 2.29 | 0.65 |
| 1:T:696:PRO:HA | 1:T:699:ILE:HD13 | 1.77 | 0.65 |
| 1:B:1560:PHE:HZ | 1:B:1573:LEU:HD11 | 1.60 | 0.64 |
| 1:B:1710:LEU:HD13 | 1:B:1750:PHE:CE1 | 2.31 | 0.64 |
| 1:B:2370:MET:HE1 | 1:B:2377:LEU:HB3 | 1.77 | 0.64 |
| 1:C:881:ILE:HA | 1:C:884:PHE:HD2 | 1.62 | 0.64 |
| 1:C:1082:ALA:HB2 | 1:D:2491:ILE:HG13 | 1.78 | 0.64 |
| 1:D:256:ARG:O | 1:D:265:ARG:NH1 | 2.28 | 0.64 |
| 1:D:1012:CYS:O | 1:D:1196:ARG:NH1 | 2.31 | 0.64 |
| 1:G:2091:ARG:HH21 | 1:G:2364:ASN:HD21 | 1.43 | 0.64 |
| 1:G:2780:ASN:OD1 | 1:G:2781:PHE:N | 2.30 | 0.64 |
| 1:H:1149:VAL:HG11 | 1:H:1206:LEU:HD13 | 1.79 | 0.64 |
| 1:H:2674:TYR:HE2 | 1:H:2715:GLN:HE21 | 1.45 | 0.64 |
| 1:I:1689:ARG:NE | 1:I:1786:ASP:OD1 | 2.26 | 0.64 |
| 1:I:2393:VAL:H | 1:I:2447:THR:HG22 | 1.61 | 0.64 |
| 1:J:31:THR:O | 1:J:36:GLN:NE2 | 2.28 | 0.64 |
| 1:J:1100:ASP:O | 1:J:1104:ARG:NH1 | 2.29 | 0.64 |
| 1:J:1153:PHE:HB2 | 1:J:1198:PHE:HD2 | 1.60 | 0.64 |
| 1:J:1677:ARG:NH1 | 1:J:1763:ILE:O | 2.27 | 0.64 |
| 1:L:846:HIS:HB3 | 1:L:1121:TYR:HA | 1.78 | 0.64 |
| 1:L:1011:PHE:HA | 1:L:1063:TRP:HH2 | 1.62 | 0.64 |
| 1:N:1978:LYS:HA | 1:N:2078:LYS:HZ3 | 1.62 | 0.64 |
| 1:O:1744:ARG:NH1 | 1:O:1944:VAL:O | 2.30 | 0.64 |
| 1:O:3036:GLN:OE1 | 1:O:3043:GLN:NE2 | 2.30 | 0.64 |
| 1:P:744:ASN:HD21 | 1:P:778:PRO:HA | 1.61 | 0.64 |
| 1:P:1222:SER:HB3 | 1:P:1230:LYS:HZ1 | 1.62 | 0.64 |
| 1:P:2113:ASP:OD1 | 1:P:2114:LEU:N | 2.29 | 0.64 |
| 1:P:2938:ARG:NH2 | 1:P:3029:ASN:OD1 | 2.28 | 0.64 |
| 1:Q:109:GLU:O | 1:Q:123:ASN:ND2 | 2.27 | 0.64 |
| 1:Q:1161:SER:OG | 1:Q:1185:GLY:N | 2.29 | 0.64 |
| 1:R:1055:ASN:HA | 1:R:1058:ARG:HG3 | 1.78 | 0.64 |
| 1:S:2234:LYS:HG3 | 1:S:2243:VAL:HG11 | 1.79 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:T:247:PHE:HB3 | 1:T:271:LYS:HD2 | 1.78 | 0.64 |
| 1:T:2353:LEU:HD13 | 1:T:2355:LYS:HB2 | 1.78 | 0.64 |
| 1:A:799:LYS:N | 1:A:802:ASP:OD1 | 2.30 | 0.64 |
| 1:C:1025:ILE:HD12 | 1:C:1028:LEU:HD23 | 1.79 | 0.64 |
| 1:C:2313:GLN:HG2 | 1:C:2320:TYR:HB3 | 1.79 | 0.64 |
| 1:D:499:TRP:NE1 | 1:D:676:LYS:O | 2.29 | 0.64 |
| 1:D:1677:ARG:NH1 | 1:D:1763:ILE:O | 2.29 | 0.64 |
| 1:E:2059:ASN:OD1 | 1:E:2060:GLY:N | 2.30 | 0.64 |
| 1:F:1770:ASN:HB2 | 1:F:1772:GLN:HE22 | 1.62 | 0.64 |
| 1:G:2674:TYR:HE1 | 1:G:2712:VAL:HG13 | 1.62 | 0.64 |
| 1:H:1420:CYS:SG | 1:H:1485:SER:OG | 2.54 | 0.64 |
| 1:H:2243:VAL:HG23 | 1:H:2244:LEU:HD12 | 1.79 | 0.64 |
| 1:H:3127:GLN:HE22 | 1:H:3190:LEU:HD21 | 1.61 | 0.64 |
| 1:I:1328:LEU:HB3 | 1:I:1499:PHE:HE2 | 1.61 | 0.64 |
| 1:I:2509:SER:O | 1:I:3138:ARG:NH1 | 2.29 | 0.64 |
| 1:L:3276:ASN:ND2 | 1:L:3279:SER:OG | 2.30 | 0.64 |
| 1:M:471:HIS:NE2 | 1:M:489:CYS:SG | 2.70 | 0.64 |
| 1:N:994:ARG:HE | 1:N:995:LEU:H | 1.45 | 0.64 |
| 1:N:1492:MET:HB3 | 1:N:1517:ILE:HG12 | 1.80 | 0.64 |
| 1:N:2159:ARG:NE | 1:N:2303:ASP:OD1 | 2.27 | 0.64 |
| 1:O:596:GLN:HG2 | 1:O:605:GLN:HE22 | 1.62 | 0.64 |
| 1:O:1037:MET:HA | 1:O:1043:THR:HA | 1.79 | 0.64 |
| 1:O:1178:GLU:HG3 | 1:O:1205:ILE:HG12 | 1.79 | 0.64 |
| 1:O:2248:VAL:HG13 | 1:O:2249:LEU:HD12 | 1.79 | 0.64 |
| 1:P:2337:PHE:O | 1:P:2349:ARG:NH2 | 2.29 | 0.64 |
| 1:P:3276:ASN:ND2 | 1:P:3279:SER:OG | 2.30 | 0.64 |
| 1:Q:1316:VAL:HG11 | 1:Q:1321:VAL:HG23 | 1.77 | 0.64 |
| 1:Q:2056:ARG:NH1 | 1:Q:2057:ALA:O | 2.31 | 0.64 |
| 1:R:3008:ILE:HD13 | 1:R:3116:MET:HB3 | 1.79 | 0.64 |
| 1:S:454:ARG:NH2 | 1:S:514:ARG:O | 2.30 | 0.64 |
| 1:A:1539:THR:HG23 | 1:A:1541:PRO:HD2 | 1.79 | 0.64 |
| 1:B:674:LEU:HG | 1:B:676:LYS:HE3 | 1.79 | 0.64 |
| 1:B:2113:ASP:OD1 | 1:B:2114:LEU:N | 2.28 | 0.64 |
| 1:D:645:ASP:OD1 | 1:D:710:TYR:OH | 2.12 | 0.64 |
| 1:D:696:PRO:HA | 1:D:699:ILE:HD13 | 1.80 | 0.64 |
| 1:E:903:CYS:O | 1:E:905:HIS:ND1 | 2.28 | 0.64 |
| 1:E:956:VAL:HA | 1:E:963:PRO:HA | 1.78 | 0.64 |
| 1:E:2119:THR:HG22 | 1:E:2120:LYS:H | 1.61 | 0.64 |
| 1:E:3056:ARG:NH1 | 1:E:3058:GLN:OE1 | 2.30 | 0.64 |
| 1:E:3072:LEU:HD23 | 1:E:3129:TRP:HD1 | 1.63 | 0.64 |
| 1:F:450:GLN:O | 1:F:454:ARG:HG2 | 1.97 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:G:2669:ASN:HA | 1:G:2672:VAL:HG12 | 1.78 | 0.64 |
| 1:H:986:LEU:HD11 | 1:H:1028:LEU:HB3 | 1.79 | 0.64 |
| 1:J:523:TRP:HB3 | 1:J:639:LEU:HD13 | 1.79 | 0.64 |
| 1:J:2378:ASP:OD1 | 1:J:2379:GLU:N | 2.29 | 0.64 |
| 1:L:97:THR:OG1 | 1:L:98:LYS:NZ | 2.30 | 0.64 |
| 1:L:473:LEU:H | 1:L:629:HIS:HB3 | 1.62 | 0.64 |
| 1:N:808:LEU:HB2 | 1:N:820:GLU:HG3 | 1.80 | 0.64 |
| 1:N:907:MET:HG2 | 1:N:909:VAL:H | 1.63 | 0.64 |
| 1:O:731:ARG:HA | 1:O:735:ARG:HH12 | 1.62 | 0.64 |
| 1:Q:854:LEU:HD12 | 1:Q:858:GLN:HG3 | 1.80 | 0.64 |
| 1:Q:1448:LEU:HD11 | 1:Q:1596:LEU:HD21 | 1.80 | 0.64 |
| 1:Q:1802:ILE:HD12 | 1:Q:1805:GLU:HB2 | 1.79 | 0.64 |
| 1:R:2313:GLN:NE2 | 1:R:2318:LEU:O | 2.30 | 0.64 |
| 1:R:2542:ARG:HD3 | 1:R:2591:LEU:HD23 | 1.78 | 0.64 |
| 1:A:2393:VAL:H | 1:A:2447:THR:HG22 | 1.60 | 0.64 |
| 1:C:109:GLU:O | 1:C:123:ASN:ND2 | 2.28 | 0.64 |
| 1:C:3260:ARG:HE | 1:C:3261:VAL:H | 1.45 | 0.64 |
| 1:F:1448:LEU:HD21 | 1:F:1596:LEU:HG | 1.79 | 0.64 |
| 1:F:2666:ASP:OD1 | 1:F:2667:TYR:N | 2.30 | 0.64 |
| 1:G:44:GLU:HG3 | 1:G:135:MET:HE1 | 1.79 | 0.64 |
| 1:G:1963:ILE:HG23 | 1:G:1967:LEU:HD23 | 1.79 | 0.64 |
| 1:J:111:ILE:HG23 | 1:J:122:LYS:HB2 | 1.80 | 0.64 |
| 1:J:3156:PRO:HB2 | 1:J:3162:LYS:HG3 | 1.77 | 0.64 |
| 1:K:956:VAL:HA | 1:K:963:PRO:HA | 1.77 | 0.64 |
| 1:L:920:GLN:OE1 | 1:L:1103:THR:OG1 | 2.11 | 0.64 |
| 1:L:1865:LYS:HE3 | 1:L:1867:HIS:H | 1.62 | 0.64 |
| 1:L:3131:THR:HA | 1:L:3134:LYS:HE3 | 1.79 | 0.64 |
| 1:M:1978:LYS:NZ | 1:M:1979:SER:O | 2.28 | 0.64 |
| 1:M:3089:ASN:HD21 | 1:M:3248:LEU:H | 1.44 | 0.64 |
| 1:P:5:ARG:HG3 | 1:P:283:TYR:HA | 1.79 | 0.64 |
| 1:P:23:LEU:HD21 | 1:P:124:SER:HB2 | 1.79 | 0.64 |
| 1:P:501:ARG:NH1 | 1:P:708:TYR:OH | 2.30 | 0.64 |
| 1:P:1433:LEU:HD11 | 1:P:1460:HIS:CD2 | 2.32 | 0.64 |
| 1:Q:3046:ARG:NH2 | 1:Q:3112:ASP:OD2 | 2.31 | 0.64 |
| 1:Q:3227:THR:OG1 | 1:Q:3245:PHE:O | 2.12 | 0.64 |
| 1:R:3213:VAL:HG21 | 1:R:3270:LEU:HD12 | 1.79 | 0.64 |
| 1:S:1026:HIS:HD2 | 1:S:1184:LEU:HD11 | 1.61 | 0.64 |
| 1:T:188:ILE:HG21 | 1:T:215:HIS:NE2 | 2.13 | 0.64 |
| 1:T:3351:VAL:HG23 | 1:T:3390:SER:HA | 1.80 | 0.64 |
| 1:A:3385:ASP:O | 1:B:3148:ARG:NH2 | 2.30 | 0.64 |
| 1:B:978:THR:HB | 1:B:1036:SER:HA | 1.78 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:2085:GLN:HE22 | 1:C:2088:PRO:HD2 | 1.63 | 0.64 |
| 1:D:1154:MET:HE1 | 1:D:1197:LEU:HD23 | 1.78 | 0.64 |
| 1:E:836:HIS:CD2 | 1:S:277:ARG:HD2 | 2.32 | 0.64 |
| 1:G:259:ASN:O | 1:G:265:ARG:NH2 | 2.30 | 0.64 |
| 1:G:1033:GLU:O | 1:G:1036:SER:OG | 2.16 | 0.64 |
| 1:I:949:ILE:HG23 | 1:I:950:VAL:HG13 | 1.79 | 0.64 |
| 1:I:1786:ASP:OD2 | 1:I:1789:LEU:N | 2.27 | 0.64 |
| 1:I:2601:TRP:O | 1:I:2711:ASN:ND2 | 2.30 | 0.64 |
| 1:J:1204:ASP:OD1 | 1:J:1205:ILE:N | 2.30 | 0.64 |
| 1:J:1501:ASP:HB3 | 1:J:1504:GLN:HB2 | 1.78 | 0.64 |
| 1:J:1847:GLU:HA | 1:J:1850:PHE:HB3 | 1.80 | 0.64 |
| 1:K:1588:HIS:ND1 | 1:N:337:GLN:OE1 | 2.29 | 0.64 |
| 1:K:2025:SER:O | 1:L:1651:ARG:NH2 | 2.31 | 0.64 |
| 1:M:2508:VAL:O | 1:M:2515:LYS:NZ | 2.31 | 0.64 |
| 1:M:2780:ASN:OD1 | 1:M:2781:PHE:N | 2.30 | 0.64 |
| 1:N:1088:LEU:HD22 | 1:N:1109:PRO:HG3 | 1.80 | 0.64 |
| 1:N:3008:ILE:HG21 | 1:N:3116:MET:HB3 | 1.79 | 0.64 |
| 1:O:593:ALA:HA | 1:O:605:GLN:HG3 | 1.79 | 0.64 |
| 1:O:605:GLN:HA | 1:O:608:VAL:HG12 | 1.78 | 0.64 |
| 1:O:1708:GLN:HE21 | 1:O:1803:ALA:HB2 | 1.61 | 0.64 |
| 1:P:3047:ASP:HB2 | 1:P:3097:GLY:HA3 | 1.79 | 0.64 |
| 1:Q:471:HIS:NE2 | 1:Q:489:CYS:SG | 2.70 | 0.64 |
| 1:T:111:ILE:HG23 | 1:T:122:LYS:HB2 | 1.80 | 0.64 |
| 1:T:1576:CYS:N | 1:T:1632:ASP:O | 2.31 | 0.64 |
| 1:T:2126:LEU:HD21 | 1:T:2165:VAL:HG12 | 1.80 | 0.64 |
| 1:B:97:THR:OG1 | 1:B:98:LYS:NZ | 2.31 | 0.64 |
| 1:B:2251:VAL:HG22 | 1:B:2263:GLN:HG3 | 1.80 | 0.64 |
| 1:B:3113:PRO:HA | 1:B:3116:MET:HE2 | 1.79 | 0.64 |
| 1:D:24:ARG:HD3 | 1:D:123:ASN:HA | 1.79 | 0.64 |
| 1:D:2191:PRO:HG2 | 1:D:2194:PHE:HD2 | 1.61 | 0.64 |
| 1:H:1714:HIS:NE2 | 1:H:1732:CYS:SG | 2.71 | 0.64 |
| 1:H:2469:LEU:HD11 | 1:H:2489:PRO:HG2 | 1.79 | 0.64 |
| 1:J:1086:LYS:HZ1 | 1:J:1089:GLN:HE21 | 1.44 | 0.64 |
| 1:L:1349:TRP:O | 1:L:1463:ASN:ND2 | 2.30 | 0.64 |
| 1:M:2018:GLY:N | 1:M:2021:GLU:OE2 | 2.30 | 0.64 |
| 1:M:2085:GLN:HE22 | 1:M:2088:PRO:HD2 | 1.61 | 0.64 |
| 1:O:2709:HIS:HA | 1:O:2712:VAL:HG12 | 1.78 | 0.64 |
| 1:P:2865:ARG:HD3 | 1:P:2867:ASP:H | 1.63 | 0.64 |
| 1:Q:613:PRO:HA | 1:Q:616:LEU:HB3 | 1.80 | 0.64 |
| 1:Q:1756:ARG:HH22 | 1:R:2175:THR:HB | 1.61 | 0.64 |
| 1:R:23:LEU:HD21 | 1:R:124:SER:HB2 | 1.78 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:R:524:ASP:OD2 | 1:R:527:ARG:NH1 | 2.31 | 0.64 |
| 1:R:1319:SER:OG | 1:R:1320:ALA:N | 2.30 | 0.64 |
| 1:S:1744:ARG:NH1 | 1:S:1944:VAL:O | 2.31 | 0.64 |
| 1:S:2114:LEU:HG | 1:S:2123:TRP:HB2 | 1.80 | 0.64 |
| 1:T:2757:ILE:O | 1:T:2761:ALA:HB2 | 1.97 | 0.64 |
| 1:A:1413:ALA:HB1 | 1:A:1425:GLN:HG3 | 1.79 | 0.64 |
| 1:A:2534:ALA:O | 1:A:2538:GLN:NE2 | 2.29 | 0.64 |
| 1:C:2130:HIS:NE2 | 1:C:2147:CYS:SG | 2.71 | 0.64 |
| 1:C:3020:LEU:HB3 | 1:C:3024:LEU:HD11 | 1.78 | 0.64 |
| 1:E:854:LEU:HD12 | 1:E:858:GLN:HG3 | 1.79 | 0.64 |
| 1:G:1082:ALA:HB2 | 1:H:2491:ILE:HG12 | 1.79 | 0.64 |
| 1:J:1348:TYR:OH | 1:J:1466:ARG:NH1 | 2.31 | 0.64 |
| 1:J:2639:ARG:HD3 | 1:J:2641:GLN:HE22 | 1.62 | 0.64 |
| 1:K:1579:THR:OG1 | 1:K:1584:ARG:NH2 | 2.30 | 0.64 |
| 1:M:1914:GLU:OE2 | 1:N:1655:LEU:HD23 | 1.97 | 0.64 |
| 1:Q:1744:ARG:NH2 | 1:Q:1947:TYR:HB3 | 2.13 | 0.64 |
| 1:R:2921:VAL:HG11 | 1:R:3000:ARG:HH22 | 1.63 | 0.64 |
| 1:S:1214:ASN:O | 1:S:1216:ARG:NH2 | 2.30 | 0.64 |
| 1:S:1362:ILE:HG22 | 1:S:1380:PHE:HD2 | 1.63 | 0.64 |
| 1:A:1085:ARG:NH2 | 1:B:2463:ALA:O | 2.26 | 0.64 |
| 1:C:2046:ASP:HB2 | 1:D:1493:ARG:HH12 | 1.63 | 0.64 |
| 1:C:3227:THR:OG1 | 1:C:3245:PHE:O | 2.14 | 0.64 |
| 1:D:2149:HIS:HA | 1:D:2154:PHE:HD2 | 1.63 | 0.64 |
| 1:E:2926:VAL:HB | 1:E:3023:LEU:HD21 | 1.78 | 0.64 |
| 1:E:2929:LEU:HD22 | 1:E:2933:GLN:HG3 | 1.80 | 0.64 |
| 1:F:808:LEU:HB2 | 1:F:820:GLU:HG3 | 1.80 | 0.64 |
| 1:H:450:GLN:O | 1:H:454:ARG:HG2 | 1.97 | 0.64 |
| 1:H:1348:TYR:OH | 1:H:1466:ARG:NH1 | 2.31 | 0.64 |
| 1:I:2926:VAL:HB | 1:I:3023:LEU:HD21 | 1.79 | 0.64 |
| 1:J:2944:LEU:HA | 1:J:3002:LYS:HE2 | 1.79 | 0.64 |
| 1:J:3395:ARG:O | 1:J:3401:ARG:NH2 | 2.31 | 0.64 |
| 1:K:981:SER:OG | 1:K:1030:GLY:O | 2.15 | 0.64 |
| 1:L:1626:ASP:OD1 | 1:L:1627:SER:N | 2.31 | 0.64 |
| 1:N:247:PHE:O | 1:N:271:LYS:NZ | 2.30 | 0.64 |
| 1:N:450:GLN:O | 1:N:454:ARG:HG2 | 1.98 | 0.64 |
| 1:N:1100:ASP:O | 1:N:1104:ARG:NH1 | 2.31 | 0.64 |
| 1:N:1143:ARG:HB3 | 1:N:1148:ARG:HH22 | 1.61 | 0.64 |
| 1:O:3289:LYS:HD2 | 1:O:3291:ASN:HD22 | 1.63 | 0.64 |
| 1:P:1837:ALA:HA | 1:P:1849:GLN:HE21 | 1.61 | 0.64 |
| 1:Q:259:ASN:ND2 | 1:Q:264:THR:OG1 | 2.31 | 0.64 |
| 1:Q:1156:HIS:HB3 | 1:Q:1193:GLN:HE22 | 1.62 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:R:1546:VAL:HA | 1:R:1549:ARG:HG2 | 1.78 | 0.64 |
| 1:T:673:GLU:O | 1:T:695:ARG:NH2 | 2.27 | 0.64 |
| 1:T:2336:PRO:HB2 | 1:T:2342:LEU:HD12 | 1.79 | 0.64 |
| 1:A:1651:ARG:NH2 | 1:B:2025:SER:O | 2.31 | 0.64 |
| 1:B:735:ARG:HB3 | 1:B:831:GLU:HB3 | 1.78 | 0.64 |
| 1:C:1284:ARG:NH2 | 1:C:1377:SER:O | 2.31 | 0.64 |
| 1:C:2820:ASP:OD1 | 1:C:2831:ALA:N | 2.31 | 0.64 |
| 1:E:1161:SER:OG | 1:E:1185:GLY:N | 2.24 | 0.64 |
| 1:E:2586:GLU:O | 1:E:2590:THR:OG1 | 2.16 | 0.64 |
| 1:E:2623:GLU:N | 1:E:2623:GLU:OE1 | 2.31 | 0.64 |
| 1:F:1089:GLN:HE22 | 1:F:1092:ALA:HB3 | 1.63 | 0.64 |
| 1:H:3032:PHE:HA | 1:H:3113:PRO:HG2 | 1.80 | 0.64 |
| 1:J:3276:ASN:ND2 | 1:J:3279:SER:OG | 2.31 | 0.64 |
| 1:K:3133:GLN:NE2 | 1:K:3138:ARG:O | 2.29 | 0.64 |
| 1:L:2149:HIS:HA | 1:L:2154:PHE:HD2 | 1.63 | 0.64 |
| 1:M:1328:LEU:HB3 | 1:M:1499:PHE:CE2 | 2.33 | 0.64 |
| 1:N:605:GLN:HE22 | 1:N:786:LYS:H | 1.45 | 0.64 |
| 1:N:887:GLN:HE22 | 1:N:889:ASN:HB2 | 1.63 | 0.64 |
| 1:N:2194:PHE:CD1 | 1:N:2212:PHE:HB3 | 2.33 | 0.64 |
| 1:O:1651:ARG:NH1 | 1:P:2025:SER:O | 2.31 | 0.64 |
| 1:P:230:GLN:NE2 | 1:P:236:THR:O | 2.31 | 0.64 |
| 1:P:2979:HIS:HA | 1:P:2984:PHE:HD2 | 1.63 | 0.64 |
| 1:Q:527:ARG:HD3 | 1:Q:528:PRO:HD2 | 1.80 | 0.64 |
| 1:Q:3008:ILE:HD11 | 1:Q:3117:ILE:HG22 | 1.80 | 0.64 |
| 1:R:2988:HIS:HA | 1:R:2991:LEU:HD12 | 1.79 | 0.64 |
| 1:T:221:ARG:HE | 1:T:283:TYR:HD2 | 1.46 | 0.64 |
| 1:A:109:GLU:O | 1:A:123:ASN:ND2 | 2.30 | 0.64 |
| 1:A:718:MET:HE1 | 1:A:723:LEU:HA | 1.80 | 0.64 |
| 1:A:1225:ASP:OD1 | 1:A:1229:LYS:N | 2.30 | 0.64 |
| 1:A:2488:LYS:HD2 | 1:A:2489:PRO:HD2 | 1.78 | 0.64 |
| 1:B:1433:LEU:HD11 | 1:B:1460:HIS:CD2 | 2.33 | 0.64 |
| 1:B:3382:GLU:O | 1:B:3386:TYR:OH | 2.12 | 0.64 |
| 1:C:1583:GLU:OE2 | 1:F:327:LYS:NZ | 2.29 | 0.64 |
| 1:E:159:THR:HG23 | 1:E:162:PHE:H | 1.62 | 0.64 |
| 1:E:2018:GLY:N | 1:E:2021:GLU:OE2 | 2.26 | 0.64 |
| 1:J:2159:ARG:NE | 1:J:2303:ASP:OD1 | 2.25 | 0.64 |
| 1:N:1154:MET:HE1 | 1:N:1197:LEU:HD23 | 1.80 | 0.64 |
| 1:Q:1325:TRP:HE1 | 1:Q:1498:PRO:HG3 | 1.62 | 0.64 |
| 1:Q:3052:LEU:O | 1:Q:3055:ARG:NH2 | 2.31 | 0.64 |
| 1:C:38:LEU:O | 1:C:73:TYR:OH | 2.15 | 0.63 |
| 1:C:3036:GLN:OE1 | 1:C:3043:GLN:NE2 | 2.31 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:D:2806:PHE:HE1 | 1:D:2892:PRO:HB3 | 1.61 | 0.63 |
| 1:E:3307:ARG:NH1 | 1:E:3312:ASP:O | 2.31 | 0.63 |
| 1:F:3276:ASN:ND2 | 1:F:3279:SER:OG | 2.32 | 0.63 |
| 1:G:126:PHE:O | 1:G:143:ARG:NH2 | 2.31 | 0.63 |
| 1:G:1535:PHE:N | 1:G:1538:TRP:O | 2.28 | 0.63 |
| 1:H:2709:HIS:HA | 1:H:2712:VAL:HG22 | 1.79 | 0.63 |
| 1:J:3270:LEU:HG | 1:J:3275:LEU:HB2 | 1.79 | 0.63 |
| 1:K:55:ARG:NH2 | 1:K:56:VAL:O | 2.31 | 0.63 |
| 1:L:2055:LEU:HB2 | 1:L:2063:LEU:HB2 | 1.78 | 0.63 |
| 1:M:2805:ASN:HB3 | 1:M:2850:LEU:HD21 | 1.80 | 0.63 |
| 1:N:475:ALA:HB3 | 1:N:485:ARG:HB3 | 1.78 | 0.63 |
| 1:O:915:ARG:NH1 | 1:O:1057:ASP:OD1 | 2.31 | 0.63 |
| 1:O:2018:GLY:N | 1:O:2021:GLU:OE2 | 2.29 | 0.63 |
| 1:O:2959:PHE:HE1 | 1:O:3162:LYS:HE2 | 1.63 | 0.63 |
| 1:Q:434:ARG:HD2 | 1:Q:710:TYR:HE1 | 1.61 | 0.63 |
| 1:Q:1151:ALA:HB2 | 1:Q:1202:ILE:HD11 | 1.80 | 0.63 |
| 1:B:23:LEU:HD21 | 1:B:124:SER:HB2 | 1.81 | 0.63 |
| 1:B:272:SER:O | 1:B:278:GLN:NE2 | 2.31 | 0.63 |
| 1:B:2243:VAL:HG23 | 1:B:2244:LEU:HD12 | 1.80 | 0.63 |
| 1:C:437:VAL:HG12 | 1:C:521:PRO:HB2 | 1.80 | 0.63 |
| 1:C:2970:ALA:O | 1:C:2973:ARG:NH2 | 2.31 | 0.63 |
| 1:D:2867:ASP:O | 1:E:2741:ARG:NH1 | 2.32 | 0.63 |
| 1:F:247:PHE:HB3 | 1:F:271:LYS:HD2 | 1.80 | 0.63 |
| 1:F:2752:ASN:HD21 | 1:F:2757:ILE:HG13 | 1.63 | 0.63 |
| 1:G:2088:PRO:HD2 | 1:G:2366:ARG:HH12 | 1.63 | 0.63 |
| 1:G:2532:LEU:HD23 | 1:G:2621:PRO:HG2 | 1.80 | 0.63 |
| 1:I:109:GLU:O | 1:I:123:ASN:ND2 | 2.26 | 0.63 |
| 1:I:1195:ASP:HB2 | 1:J:2441:LEU:HD21 | 1.81 | 0.63 |
| 1:I:2637:SER:HB2 | 1:I:2687:GLY:HA3 | 1.78 | 0.63 |
| 1:I:2817:VAL:HG22 | 1:I:2876:ILE:HG22 | 1.81 | 0.63 |
| 1:J:2414:GLN:HE22 | 1:J:2453:LEU:HD22 | 1.62 | 0.63 |
| 1:K:309:ALA:H | 1:K:370:SER:HG | 1.46 | 0.63 |
| 1:L:2964:LYS:NZ | 1:L:2973:ARG:O | 2.26 | 0.63 |
| 1:N:254:PHE:HD2 | 1:N:264:THR:HB | 1.63 | 0.63 |
| 1:P:1743:HIS:HD2 | 1:P:1885:HIS:HD2 | 1.46 | 0.63 |
| 1:P:1932:ASP:OD2 | 1:P:1935:THR:N | 2.27 | 0.63 |
| 1:Q:1380:PHE:O | 1:Q:1394:ARG:NH2 | 2.27 | 0.63 |
| 1:Q:1773:ASN:OD1 | 1:Q:1774:SER:N | 2.30 | 0.63 |
| 1:R:3382:GLU:O | 1:R:3386:TYR:OH | 2.15 | 0.63 |
| 1:B:1012:CYS:O | 1:B:1196:ARG:NH1 | 2.30 | 0.63 |
| 1:B:1222:SER:HB3 | 1:B:1230:LYS:HZ1 | 1.63 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:D:2921:VAL:HG11 | 1:D:3000:ARG:HH22 | 1.63 | 0.63 |
| 1:D:3124:ARG:O | 1:D:3128:ILE:HG12 | 1.98 | 0.63 |
| 1:D:3289:LYS:HG2 | 1:D:3293:GLU:HB3 | 1.78 | 0.63 |
| 1:F:245:GLU:HA | 1:F:248:ARG:HD2 | 1.80 | 0.63 |
| 1:F:1763:ILE:HD12 | 1:F:1764:PRO:HD2 | 1.79 | 0.63 |
| 1:I:248:ARG:NH1 | 1:I:802:ASP:O | 2.32 | 0.63 |
| 1:J:887:GLN:HE22 | 1:J:889:ASN:HB2 | 1.62 | 0.63 |
| 1:J:3324:ASN:OD1 | 1:J:3395:ARG:NH2 | 2.31 | 0.63 |
| 1:K:44:GLU:HG3 | 1:K:135:MET:HE1 | 1.79 | 0.63 |
| 1:L:1785:ARG:NH1 | 1:L:1786:ASP:O | 2.31 | 0.63 |
| 1:M:2027:ASP:OD2 | 1:M:2028:ARG:NH1 | 2.31 | 0.63 |
| 1:M:2529:LYS:O | 1:M:2533:ARG:HG2 | 1.97 | 0.63 |
| 1:N:43:GLY:O | 1:N:46:SER:OG | 2.16 | 0.63 |
| 1:N:673:GLU:O | 1:N:695:ARG:NH2 | 2.25 | 0.63 |
| 1:N:1204:ASP:OD1 | 1:N:1205:ILE:N | 2.29 | 0.63 |
| 1:N:1809:VAL:HG22 | 1:N:1811:ARG:HH12 | 1.62 | 0.63 |
| 1:O:2254:GLN:N | 1:O:2254:GLN:OE1 | 2.30 | 0.63 |
| 1:O:2587:ARG:HH22 | 1:O:2753:PRO:HB2 | 1.62 | 0.63 |
| 1:P:1012:CYS:SG | 1:P:1196:ARG:NH1 | 2.71 | 0.63 |
| 1:Q:1225:ASP:OD1 | 1:Q:1229:LYS:N | 2.31 | 0.63 |
| 1:Q:2443:LYS:HZ2 | 1:Q:2492:ILE:HD11 | 1.63 | 0.63 |
| 1:S:650:ILE:HG22 | 1:S:713:LEU:HD12 | 1.80 | 0.63 |
| 1:S:2623:GLU:OE1 | 1:S:2623:GLU:N | 2.28 | 0.63 |
| 1:S:3064:LEU:O | 1:S:3067:GLN:NE2 | 2.31 | 0.63 |
| 1:B:1769:VAL:O | 1:B:1828:ASN:ND2 | 2.31 | 0.63 |
| 1:B:2313:GLN:HG2 | 1:B:2320:TYR:HB3 | 1.80 | 0.63 |
| 1:D:325:ARG:HH21 | 1:D:391:TYR:HE1 | 1.47 | 0.63 |
| 1:E:893:SER:OG | 1:E:895:ASP:OD1 | 2.15 | 0.63 |
| 1:E:1338:LEU:HD21 | 1:E:1345:SER:HA | 1.80 | 0.63 |
| 1:F:2113:ASP:OD1 | 1:F:2114:LEU:N | 2.31 | 0.63 |
| 1:G:1830:LEU:HG | 1:G:1834:PHE:HE2 | 1.64 | 0.63 |
| 1:I:2152:PRO:O | 1:I:2257:TYR:OH | 2.16 | 0.63 |
| 1:I:2926:VAL:HG12 | 1:I:3009:PRO:HB2 | 1.79 | 0.63 |
| 1:J:36:GLN:NE2 | 1:J:37:ASN:OD1 | 2.32 | 0.63 |
| 1:J:244:VAL:HG22 | 1:J:828:ILE:HG21 | 1.80 | 0.63 |
| 1:L:105:ARG:HA | 1:L:108:GLN:HE22 | 1.63 | 0.63 |
| 1:L:1501:ASP:HB3 | 1:L:1504:GLN:HB2 | 1.80 | 0.63 |
| 1:N:540:THR:HG22 | 1:N:551:HIS:HA | 1.80 | 0.63 |
| 1:N:3196:SER:OG | 1:N:3199:GLU:OE1 | 2.17 | 0.63 |
| 1:P:1086:LYS:NZ | 1:P:1087:PRO:O | 2.30 | 0.63 |
| 1:P:1087:PRO:HA | 1:P:1109:PRO:HD3 | 1.80 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:Q:1732:CYS:O | 1:Q:1734:HIS:ND1 | 2.27 | 0.63 |
| 1:Q:1919:PRO:O | 1:Q:1921:LYS:NZ | 2.31 | 0.63 |
| 1:Q:3149:ASN:OD1 | 1:Q:3152:ARG:NH2 | 2.29 | 0.63 |
| 1:T:331:HIS:CE1 | 1:T:672:HIS:HB3 | 2.33 | 0.63 |
| 1:T:2812:LYS:HG2 | 1:T:2840:PRO:HA | 1.79 | 0.63 |
| 1:A:2579:ARG:NH1 | 1:A:2774:TYR:OH | 2.31 | 0.63 |
| 1:C:64:ALA:O | 1:C:174:TYR:OH | 2.16 | 0.63 |
| 1:D:2232:LEU:HD12 | 1:D:2274:LEU:HB3 | 1.78 | 0.63 |
| 1:E:2994:GLN:OE1 | 1:E:3165:ASN:ND2 | 2.31 | 0.63 |
| 1:G:2535:VAL:HG22 | 1:G:2592:GLN:HE21 | 1.62 | 0.63 |
| 1:H:105:ARG:HA | 1:H:108:GLN:HE22 | 1.62 | 0.63 |
| 1:H:1058:ARG:NH1 | 1:H:1125:ASP:O | 2.31 | 0.63 |
| 1:H:2806:PHE:HE2 | 1:H:2892:PRO:HB3 | 1.64 | 0.63 |
| 1:J:1049:PHE:O | 1:J:1053:HIS:ND1 | 2.31 | 0.63 |
| 1:J:3218:VAL:HG23 | 1:J:3261:VAL:HG13 | 1.80 | 0.63 |
| 1:K:2656:ARG:HD2 | 1:K:2656:ARG:H | 1.63 | 0.63 |
| 1:L:1718:PRO:HG2 | 1:L:1728:ARG:HB3 | 1.79 | 0.63 |
| 1:L:2336:PRO:HB2 | 1:L:2342:LEU:HD12 | 1.80 | 0.63 |
| 1:N:1710:LEU:HD22 | 1:N:1750:PHE:HE1 | 1.64 | 0.63 |
| 1:N:3342:SER:OG | 1:N:3344:VAL:O | 2.17 | 0.63 |
| 1:Q:259:ASN:O | 1:Q:265:ARG:NH2 | 2.31 | 0.63 |
| 1:R:848:ARG:H | 1:R:1123:TYR:HA | 1.64 | 0.63 |
| 1:R:2481:LEU:HD21 | 3:uA:1:NAG:H62 | 1.80 | 0.63 |
| 1:S:2398:LEU:HB3 | 1:S:2441:LEU:HD22 | 1.79 | 0.63 |
| 1:S:2641:GLN:NE2 | 1:S:2645:ASP:OD1 | 2.31 | 0.63 |
| 1:A:1785:ARG:NH1 | 1:A:1790:ASP:OD1 | 2.32 | 0.63 |
| 1:A:2533:ARG:NH1 | 1:A:2619:ASP:O | 2.30 | 0.63 |
| 1:A:2817:VAL:HG22 | 1:A:2876:ILE:HG22 | 1.80 | 0.63 |
| 1:B:1965:ALA:HA | 1:B:1968:LEU:HB2 | 1.81 | 0.63 |
| 1:C:307:GLU:O | 1:C:308:ARG:NE | 2.30 | 0.63 |
| 1:C:1037:MET:HA | 1:C:1043:THR:HA | 1.81 | 0.63 |
| 1:C:1710:LEU:HB3 | 1:C:1750:PHE:HE1 | 1.64 | 0.63 |
| 1:C:3142:TYR:OH | 1:C:3144:ARG:NH1 | 2.30 | 0.63 |
| 1:D:722:GLN:NE2 | 1:D:932:ASP:OD1 | 2.32 | 0.63 |
| 1:E:2970:ALA:O | 1:E:2973:ARG:NH1 | 2.32 | 0.63 |
| 1:F:244:VAL:HG22 | 1:F:828:ILE:HG21 | 1.80 | 0.63 |
| 1:F:1728:ARG:NH2 | 4:H:3501:NAG:O7 | 2.31 | 0.63 |
| 1:F:2055:LEU:HB2 | 1:F:2063:LEU:HB2 | 1.81 | 0.63 |
| 1:G:3352:LYS:HB3 | 1:G:3371:ASN:HB3 | 1.81 | 0.63 |
| 1:H:247:PHE:O | 1:H:271:LYS:NZ | 2.31 | 0.63 |
| 1:J:2551:HIS:HB2 | 1:J:2700:ALA:HB2 | 1.79 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:J:3213:VAL:HG21 | 1:J:3270:LEU:HD13 | 1.80 | 0.63 |
| 1:K:31:THR:OG1 | 1:K:32:VAL:N | 2.31 | 0.63 |
| 1:K:1151:ALA:HB2 | 1:K:1202:ILE:HD11 | 1.80 | 0.63 |
| 1:K:2667:TYR:O | 1:K:2671:GLU:HG3 | 1.99 | 0.63 |
| 1:K:3385:ASP:OD2 | 1:K:3403:GLN:NE2 | 2.32 | 0.63 |
| 1:M:559:VAL:N | 1:M:564:GLU:O | 2.31 | 0.63 |
| 1:M:2509:SER:O | 1:M:3138:ARG:NH1 | 2.32 | 0.63 |
| 1:N:671:THR:O | 1:N:695:ARG:NH2 | 2.31 | 0.63 |
| 1:N:913:TRP:HD1 | 1:N:1088:LEU:HD12 | 1.63 | 0.63 |
| 1:O:1646:GLU:OE1 | 1:R:483:ARG:NH2 | 2.31 | 0.63 |
| 1:Q:38:LEU:O | 1:Q:73:TYR:OH | 2.17 | 0.63 |
| 1:Q:1070:ARG:HH12 | 1:Q:1137:GLN:HE22 | 1.46 | 0.63 |
| 1:Q:3125:ILE:HA | 1:Q:3128:ILE:HG12 | 1.80 | 0.63 |
| 1:R:221:ARG:NH1 | 1:R:285:ASP:O | 2.32 | 0.63 |
| 1:S:126:PHE:O | 1:S:143:ARG:NH2 | 2.32 | 0.63 |
| 1:S:512:LYS:HA | 1:S:516:LEU:HB2 | 1.81 | 0.63 |
| 1:S:1070:ARG:HH12 | 1:S:1137:GLN:HE22 | 1.46 | 0.63 |
| 1:S:1225:ASP:OD1 | 1:S:1229:LYS:N | 2.31 | 0.63 |
| 1:S:2980:GLY:HA2 | 1:S:3258:TYR:HE1 | 1.62 | 0.63 |
| 1:T:362:ASN:HB2 | 1:T:784:LEU:HD21 | 1.81 | 0.63 |
| 3:4A:1:NAG:H4 | 3:4A:2:NAG:N2 | 2.13 | 0.63 |
| 1:A:50:LYS:HG3 | 1:A:52:ASP:H | 1.62 | 0.63 |
| 1:A:2105:MET:HA | 1:A:2108:LYS:HG2 | 1.79 | 0.63 |
| 1:E:1756:ARG:HG3 | 1:F:2089:PRO:HG2 | 1.81 | 0.63 |
| 1:E:2990:LEU:HA | 1:E:2993:VAL:HG12 | 1.80 | 0.63 |
| 1:E:3125:ILE:HA | 1:E:3128:ILE:HG12 | 1.81 | 0.63 |
| 1:F:313:PHE:HB3 | 1:F:315:LEU:HD23 | 1.81 | 0.63 |
| 1:F:514:ARG:HH12 | 1:F:1341:GLY:HA2 | 1.63 | 0.63 |
| 1:F:737:PHE:N | 1:F:829:ILE:O | 2.30 | 0.63 |
| 1:H:244:VAL:HG23 | 1:H:248:ARG:HE | 1.64 | 0.63 |
| 1:H:1720:CYS:SG | 1:H:1731:CYS:N | 2.71 | 0.63 |
| 1:J:313:PHE:CE2 | 1:J:406:PRO:HB3 | 2.33 | 0.63 |
| 1:J:1192:TRP:HZ3 | 1:J:1194:TYR:HB2 | 1.64 | 0.63 |
| 1:K:454:ARG:NH2 | 1:K:514:ARG:O | 2.30 | 0.63 |
| 1:M:799:LYS:N | 1:M:802:ASP:OD2 | 2.31 | 0.63 |
| 1:M:2547:ILE:HD12 | 1:M:2585:LEU:HD22 | 1.81 | 0.63 |
| 1:O:512:LYS:HA | 1:O:516:LEU:HB2 | 1.79 | 0.63 |
| 1:O:2105:MET:HA | 1:O:2108:LYS:HG2 | 1.81 | 0.63 |
| 1:P:2408:VAL:HG22 | 1:P:2473:ILE:HG22 | 1.80 | 0.63 |
| 1:R:105:ARG:HG2 | 1:R:105:ARG:HH11 | 1.63 | 0.63 |
| 1:S:1689:ARG:NE | 1:S:1786:ASP:OD1 | 2.29 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:S:2096:ILE:HD13 | 1:S:2179:PRO:HG2 | 1.78 | 0.63 |
| 1:S:2579:ARG:NE | 1:S:2774:TYR:OH | 2.26 | 0.63 |
| 1:A:527:ARG:NH1 | 1:A:528:PRO:O | 2.31 | 0.63 |
| 1:B:1415:GLU:HA | 1:B:1547:LEU:HD21 | 1.80 | 0.63 |
| 1:D:1319:SER:OG | 1:D:1320:ALA:N | 2.32 | 0.63 |
| 1:D:3234:PRO:HG2 | 1:D:3237:GLY:HA3 | 1.79 | 0.63 |
| 1:E:612:LEU:HD21 | 1:E:768:LEU:HD12 | 1.80 | 0.63 |
| 1:F:105:ARG:HA | 1:F:108:GLN:HE22 | 1.64 | 0.63 |
| 1:F:1011:PHE:HA | 1:F:1063:TRP:HH2 | 1.64 | 0.63 |
| 1:G:109:GLU:O | 1:G:123:ASN:ND2 | 2.24 | 0.63 |
| 1:I:454:ARG:HH21 | 1:I:514:ARG:HB3 | 1.63 | 0.63 |
| 1:I:3307:ARG:NH1 | 1:I:3312:ASP:O | 2.31 | 0.63 |
| 1:K:2090:ASN:ND2 | 1:K:2175:THR:O | 2.32 | 0.63 |
| 1:K:2542:ARG:HH11 | 1:K:2588:ALA:HA | 1.63 | 0.63 |
| 1:L:996:THR:HG23 | 1:L:999:ALA:H | 1.64 | 0.63 |
| 1:L:1431:ASN:OD1 | 1:L:1594:SER:OG | 2.17 | 0.63 |
| 1:M:2258:CYS:HB2 | 1:M:2440:ARG:HH22 | 1.61 | 0.63 |
| 1:M:2286:LEU:HD12 | 1:M:2429:GLY:HA2 | 1.81 | 0.63 |
| 1:N:1546:VAL:HA | 1:N:1549:ARG:HG2 | 1.80 | 0.63 |
| 1:N:3047:ASP:HB2 | 1:N:3097:GLY:HA3 | 1.81 | 0.63 |
| 1:O:1225:ASP:OD1 | 1:O:1229:LYS:N | 2.31 | 0.63 |
| 1:O:3395:ARG:NE | 1:O:3398:GLN:OE1 | 2.31 | 0.63 |
| 1:Q:1426:PHE:HZ | 1:Q:1464:VAL:HG13 | 1.63 | 0.63 |
| 1:Q:1931:LEU:HD23 | 1:R:2102:ARG:HA | 1.80 | 0.63 |
| 1:Q:3100:THR:HA | 1:Q:3290:TYR:HE2 | 1.64 | 0.63 |
| 1:C:915:ARG:NH1 | 1:C:1057:ASP:OD2 | 2.32 | 0.63 |
| 1:C:1325:TRP:HE1 | 1:C:1498:PRO:HG3 | 1.63 | 0.63 |
| 1:C:3008:ILE:HD11 | 1:C:3117:ILE:HG22 | 1.79 | 0.63 |
| 1:D:3398:GLN:OE1 | 1:D:3400:THR:OG1 | 2.16 | 0.63 |
| 1:E:1214:ASN:O | 1:E:1216:ARG:NH2 | 2.32 | 0.63 |
| 1:F:3392:ASN:HB3 | 1:F:3395:ARG:HG2 | 1.81 | 0.63 |
| 1:H:2542:ARG:HD2 | 1:H:2591:LEU:HD23 | 1.80 | 0.63 |
| 1:I:1730:ALA:N | 1:I:2020:ALA:O | 2.32 | 0.63 |
| 1:K:3386:TYR:HB2 | 1:K:3404:ILE:HG22 | 1.81 | 0.63 |
| 1:L:1348:TYR:OH | 1:L:1466:ARG:NH1 | 2.31 | 0.63 |
| 1:M:1082:ALA:HB2 | 1:N:2491:ILE:HG13 | 1.81 | 0.63 |
| 1:O:2805:ASN:HB3 | 1:O:2850:LEU:HD21 | 1.81 | 0.63 |
| 1:O:3089:ASN:HD21 | 1:O:3248:LEU:H | 1.46 | 0.63 |
| 1:P:244:VAL:HG22 | 1:P:828:ILE:HG21 | 1.81 | 0.63 |
| 1:P:1012:CYS:O | 1:P:1196:ARG:NH1 | 2.32 | 0.63 |
| 1:R:2806:PHE:CE1 | 1:R:2892:PRO:HB3 | 2.32 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:S:949:ILE:HG23 | 1:S:950:VAL:HG13 | 1.81 | 0.63 |
| 1:T:737:PHE:HB2 | 1:T:829:ILE:HB | 1.80 | 0.63 |
| 1:A:2348:THR:OG1 | 1:A:2349:ARG:NH1 | 2.32 | 0.62 |
| 1:A:3289:LYS:HD2 | 1:A:3291:ASN:HD22 | 1.63 | 0.62 |
| 1:C:2567:CYS:O | 1:C:2569:HIS:ND1 | 2.32 | 0.62 |
| 1:D:2313:GLN:HG2 | 1:D:2320:TYR:HB3 | 1.81 | 0.62 |
| 1:F:2194:PHE:HD1 | 1:F:2212:PHE:HB3 | 1.64 | 0.62 |
| 1:I:981:SER:OG | 1:I:1030:GLY:O | 2.15 | 0.62 |
| 1:I:2654:PHE:HA | 1:I:2657:GLN:NE2 | 2.14 | 0.62 |
| 1:I:3395:ARG:NE | 1:I:3398:GLN:OE1 | 2.30 | 0.62 |
| 1:J:3:LEU:HD13 | 1:J:78:GLU:HG2 | 1.81 | 0.62 |
| 1:J:1089:GLN:HE22 | 1:J:1092:ALA:HB3 | 1.63 | 0.62 |
| 1:J:1769:VAL:O | 1:J:1828:ASN:ND2 | 2.32 | 0.62 |
| 1:K:855:THR:H | 1:K:858:GLN:NE2 | 1.97 | 0.62 |
| 1:L:3048:VAL:HG23 | 1:L:3052:LEU:HD22 | 1.81 | 0.62 |
| 1:M:953:GLU:O | 1:M:966:ASN:N | 2.27 | 0.62 |
| 1:M:2200:TYR:OH | 1:M:2205:ASP:OD1 | 2.15 | 0.62 |
| 1:O:2286:LEU:HD12 | 1:O:2429:GLY:HA2 | 1.81 | 0.62 |
| 1:Q:2674:TYR:OH | 1:Q:2712:VAL:O | 2.16 | 0.62 |
| 1:R:981:SER:HB3 | 1:R:1031:GLY:HA3 | 1.80 | 0.62 |
| 1:S:2248:VAL:HG13 | 1:S:2249:LEU:HD12 | 1.80 | 0.62 |
| 1:T:1012:CYS:SG | 1:T:1196:ARG:NH1 | 2.71 | 0.62 |
| 3:c:1:NAG:HO3 | 3:c:2:NAG:HO6 | 1.47 | 0.62 |
| 1:C:555:PHE:HA | 1:C:568:ARG:HH22 | 1.64 | 0.62 |
| 1:C:1144:GLN:OE1 | 1:C:1148:ARG:NH1 | 2.32 | 0.62 |
| 1:D:671:THR:O | 1:D:695:ARG:NH2 | 2.32 | 0.62 |
| 1:D:808:LEU:HB2 | 1:D:820:GLU:HG3 | 1.80 | 0.62 |
| 1:E:1082:ALA:HB2 | 1:F:2491:ILE:HG13 | 1.81 | 0.62 |
| 1:E:1328:LEU:HB3 | 1:E:1499:PHE:CE2 | 2.33 | 0.62 |
| 1:E:3089:ASN:HD21 | 1:E:3248:LEU:H | 1.47 | 0.62 |
| 1:F:2513:VAL:HG21 | 1:F:2515:LYS:HZ2 | 1.64 | 0.62 |
| 1:G:2313:GLN:HG2 | 1:G:2320:TYR:HB3 | 1.81 | 0.62 |
| 1:H:248:ARG:NH1 | 1:H:802:ASP:O | 2.32 | 0.62 |
| 1:H:3152:ARG:HH11 | 1:H:3153:PRO:HD2 | 1.63 | 0.62 |
| 1:H:3383:PRO:HA | 1:H:3406:ILE:HB | 1.81 | 0.62 |
| 1:I:1584:ARG:NH2 | 1:I:1585:ASN:O | 2.31 | 0.62 |
| 1:I:2164:GLN:HE22 | 1:I:2348:THR:HG21 | 1.63 | 0.62 |
| 1:J:3010:TYR:OH | 1:J:3189:ASN:ND2 | 2.32 | 0.62 |
| 1:K:1225:ASP:OD1 | 1:K:1229:LYS:N | 2.32 | 0.62 |
| 1:K:2639:ARG:HD3 | 1:K:2640:PRO:HD2 | 1.81 | 0.62 |
| 1:O:221:ARG:NH2 | 1:O:287:SER:O | 2.32 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:O:2590:THR:HA | 1:O:2594:ALA:HB3 | 1.81 | 0.62 |
| 1:P:450:GLN:O | 1:P:454:ARG:HG2 | 2.00 | 0.62 |
| 1:P:749:ALA:HB1 | 1:P:810:ILE:HD11 | 1.81 | 0.62 |
| 1:R:499:TRP:NE1 | 1:R:676:LYS:O | 2.32 | 0.62 |
| 1:S:854:LEU:HD12 | 1:S:858:GLN:HG3 | 1.81 | 0.62 |
| 1:T:581:GLY:H | 1:T:856:ARG:NH2 | 1.96 | 0.62 |
| 1:T:1809:VAL:HG22 | 1:T:1811:ARG:HH12 | 1.64 | 0.62 |
| 1:C:2059:ASN:OD1 | 1:C:2060:GLY:N | 2.32 | 0.62 |
| 1:C:2534:ALA:O | 1:C:2538:GLN:NE2 | 2.28 | 0.62 |
| 1:C:2542:ARG:HH12 | 1:C:2591:LEU:HB2 | 1.62 | 0.62 |
| 1:C:3089:ASN:HD21 | 1:C:3248:LEU:H | 1.47 | 0.62 |
| 1:D:2041:LYS:HG3 | 1:D:2043:LEU:HD23 | 1.82 | 0.62 |
| 1:E:594:LEU:O | 1:E:597:ARG:NH2 | 2.29 | 0.62 |
| 1:E:1522:TYR:HA | 1:E:1526:PHE:HD2 | 1.65 | 0.62 |
| 1:E:2780:ASN:OD1 | 1:E:2781:PHE:N | 2.33 | 0.62 |
| 1:G:2130:HIS:NE2 | 1:G:2147:CYS:SG | 2.72 | 0.62 |
| 1:H:885:HIS:HD1 | 1:H:1044:ALA:HB2 | 1.64 | 0.62 |
| 1:H:2219:GLU:O | 1:H:2221:LYS:NZ | 2.32 | 0.62 |
| 1:I:259:ASN:O | 1:I:265:ARG:NH2 | 2.32 | 0.62 |
| 1:I:939:TRP:HA | 1:I:943:MET:HE1 | 1.81 | 0.62 |
| 1:I:3072:LEU:HD23 | 1:I:3129:TRP:HD1 | 1.63 | 0.62 |
| 1:J:524:ASP:OD2 | 1:J:527:ARG:NH1 | 2.33 | 0.62 |
| 1:K:1830:LEU:HG | 1:K:1834:PHE:HE2 | 1.64 | 0.62 |
| 1:K:2509:SER:O | 1:K:3138:ARG:NH1 | 2.32 | 0.62 |
| 1:M:2817:VAL:HG22 | 1:M:2876:ILE:HG22 | 1.81 | 0.62 |
| 1:N:1501:ASP:HB3 | 1:N:1504:GLN:HB2 | 1.81 | 0.62 |
| 1:N:2111:LEU:HD13 | 1:N:2212:PHE:HE1 | 1.64 | 0.62 |
| 1:R:435:LYS:HG2 | 1:R:436:ASP:H | 1.63 | 0.62 |
| 1:R:1149:VAL:HG11 | 1:R:1206:LEU:HD13 | 1.81 | 0.62 |
| 1:R:1222:SER:HA | 1:R:1233:SER:HB3 | 1.80 | 0.62 |
| 1:R:1415:GLU:HA | 1:R:1547:LEU:HD21 | 1.81 | 0.62 |
| 1:R:2283:LEU:HD21 | 1:R:2292:ASP:HB3 | 1.81 | 0.62 |
| 1:R:3276:ASN:ND2 | 1:R:3279:SER:OG | 2.32 | 0.62 |
| 1:S:1913:LEU:HA | 1:S:1916:MET:HG2 | 1.81 | 0.62 |
| 1:T:1448:LEU:HD21 | 1:T:1596:LEU:HG | 1.81 | 0.62 |
| 1:A:2868:SER:O | 1:J:2741:ARG:NH1 | 2.32 | 0.62 |
| 1:B:221:ARG:NH1 | 1:B:285:ASP:O | 2.32 | 0.62 |
| 1:D:1919:PRO:HB2 | 1:D:1924:SER:HB2 | 1.82 | 0.62 |
| 1:E:574:LEU:HB3 | 1:E:616:LEU:HD21 | 1.81 | 0.62 |
| 1:E:1733:VAL:HG13 | 1:E:1736:MET:HE2 | 1.81 | 0.62 |
| 1:E:2001:CYS:HA | 1:E:2007:CYS:HB3 | 1.81 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:F:1905:ASP:HB3 | 1:F:1908:GLU:HB2 | 1.81 | 0.62 |
| 1:F:2985:PRO:HB2 | 1:F:2989:ARG:HH21 | 1.65 | 0.62 |
| 1:F:3300:ALA:HA | 1:F:3325:LYS:HG3 | 1.80 | 0.62 |
| 1:G:3213:VAL:HG23 | 1:G:3306:SER:HB2 | 1.81 | 0.62 |
| 1:H:2313:GLN:NE2 | 1:H:2318:LEU:O | 2.28 | 0.62 |
| 1:I:2780:ASN:OD1 | 1:I:2781:PHE:N | 2.33 | 0.62 |
| 1:I:3089:ASN:HD21 | 1:I:3248:LEU:H | 1.47 | 0.62 |
| 1:J:2626:GLU:HB2 | 1:J:2633:LYS:HD3 | 1.82 | 0.62 |
| 1:J:3342:SER:OG | 1:J:3344:VAL:O | 2.17 | 0.62 |
| 1:K:409:VAL:HG13 | 1:K:666:CYS:HA | 1.81 | 0.62 |
| 1:K:2780:ASN:OD1 | 1:K:2781:PHE:N | 2.31 | 0.62 |
| 1:M:2148:LEU:HB3 | 1:M:2151:VAL:HG11 | 1.80 | 0.62 |
| 1:M:3289:LYS:HD2 | 1:M:3291:ASN:HD22 | 1.63 | 0.62 |
| 1:N:524:ASP:OD2 | 1:N:527:ARG:NH1 | 2.32 | 0.62 |
| 1:O:2805:ASN:ND2 | 1:O:2852:GLN:OE1 | 2.32 | 0.62 |
| 1:P:1919:PRO:HB2 | 1:P:1924:SER:HB2 | 1.81 | 0.62 |
| 1:Q:1417:THR:O | 1:Q:1475:GLN:NE2 | 2.32 | 0.62 |
| 1:Q:3364:SER:HB2 | 1:R:3255:PRO:HB2 | 1.80 | 0.62 |
| 1:R:845:LEU:HD22 | 1:R:926:ARG:HD3 | 1.80 | 0.62 |
| 1:S:471:HIS:NE2 | 1:S:489:CYS:SG | 2.72 | 0.62 |
| 1:S:981:SER:OG | 1:S:1030:GLY:O | 2.16 | 0.62 |
| 1:S:3125:ILE:HA | 1:S:3128:ILE:HG12 | 1.81 | 0.62 |
| 1:B:2316:ARG:HG2 | 1:B:2318:LEU:HG | 1.80 | 0.62 |
| 1:B:2622:PHE:O | 1:B:2636:ARG:NH2 | 2.31 | 0.62 |
| 1:C:1586:CYS:HA | 1:F:337:GLN:HG3 | 1.81 | 0.62 |
| 1:E:1646:GLU:OE1 | 1:H:483:ARG:NH2 | 2.33 | 0.62 |
| 1:F:2337:PHE:O | 1:F:2349:ARG:NH2 | 2.31 | 0.62 |
| 1:F:2567:CYS:O | 1:F:2569:HIS:ND1 | 2.33 | 0.62 |
| 1:G:1756:ARG:HH12 | 1:H:2175:THR:HB | 1.65 | 0.62 |
| 1:G:2724:ARG:NH1 | 1:G:2730:TYR:OH | 2.32 | 0.62 |
| 1:H:996:THR:HG23 | 1:H:999:ALA:H | 1.64 | 0.62 |
| 1:I:277:ARG:HH21 | 1:O:836:HIS:CD2 | 2.18 | 0.62 |
| 1:J:808:LEU:HB2 | 1:J:820:GLU:HG3 | 1.80 | 0.62 |
| 1:J:2988:HIS:HA | 1:J:2991:LEU:HD12 | 1.82 | 0.62 |
| 1:K:767:LYS:HE2 | 1:K:767:LYS:HA | 1.82 | 0.62 |
| 1:L:1272:SER:N | 1:L:1275:GLU:OE2 | 2.31 | 0.62 |
| 1:L:2064:SER:HG | 1:L:2066:SER:HG | 1.48 | 0.62 |
| 1:M:903:CYS:O | 1:M:905:HIS:ND1 | 2.33 | 0.62 |
| 1:M:2674:TYR:OH | 1:M:2712:VAL:O | 2.16 | 0.62 |
| 1:N:1862:GLY:HA3 | 1:N:1870:ALA:HB2 | 1.81 | 0.62 |
| 1:O:24:ARG:NH2 | 1:O:123:ASN:HA | 2.14 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:O:1395:ASP:HB3 | 1:O:1439:GLY:HA3 | 1.81 | 0.62 |
| 1:P:1049:PHE:O | 1:P:1053:HIS:ND1 | 2.27 | 0.62 |
| 1:P:2720:GLN:HE22 | 1:P:2730:TYR:HB2 | 1.64 | 0.62 |
| 1:Q:126:PHE:O | 1:Q:143:ARG:NH2 | 2.32 | 0.62 |
| 1:Q:767:LYS:HE2 | 1:Q:767:LYS:HA | 1.80 | 0.62 |
| 1:T:182:GLU:O | 1:T:186:ASN:ND2 | 2.33 | 0.62 |
| 1:T:1049:PHE:O | 1:T:1053:HIS:ND1 | 2.33 | 0.62 |
| 1:A:2872:PHE:HD2 | 1:A:2892:PRO:HG2 | 1.65 | 0.62 |
| 1:B:362:ASN:HB2 | 1:B:784:LEU:HD21 | 1.82 | 0.62 |
| 1:B:1254:ILE:HG23 | 1:B:1256:LYS:H | 1.65 | 0.62 |
| 1:C:512:LYS:HA | 1:C:516:LEU:HB2 | 1.80 | 0.62 |
| 1:C:2805:ASN:HB3 | 1:C:2850:LEU:HD21 | 1.81 | 0.62 |
| 1:C:3390:SER:HB3 | 1:C:3395:ARG:HG3 | 1.80 | 0.62 |
| 1:D:2113:ASP:OD1 | 1:D:2114:LEU:N | 2.32 | 0.62 |
| 1:D:2194:PHE:HD1 | 1:D:2212:PHE:HB3 | 1.63 | 0.62 |
| 1:D:3382:GLU:O | 1:D:3386:TYR:OH | 2.17 | 0.62 |
| 1:E:3289:LYS:HZ3 | 1:E:3293:GLU:HG2 | 1.65 | 0.62 |
| 1:G:2409:ARG:O | 1:G:2471:TYR:HA | 1.99 | 0.62 |
| 1:H:1993:SER:HB2 | 1:H:2058:LEU:HD11 | 1.82 | 0.62 |
| 1:H:2336:PRO:HB2 | 1:H:2342:LEU:HD12 | 1.80 | 0.62 |
| 1:I:50:LYS:HE2 | 1:I:357:MET:HG3 | 1.80 | 0.62 |
| 1:I:926:ARG:NH2 | 1:I:931:GLN:O | 2.28 | 0.62 |
| 1:I:1359:PRO:HD2 | 1:I:1362:ILE:HD11 | 1.81 | 0.62 |
| 1:I:2095:GLU:HB3 | 1:I:2098:HIS:CD2 | 2.34 | 0.62 |
| 1:I:2251:VAL:HG22 | 1:I:2263:GLN:HB3 | 1.82 | 0.62 |
| 1:I:2345:ASN:HD22 | 1:I:2348:THR:HG23 | 1.65 | 0.62 |
| 1:J:938:ASP:OD1 | 1:J:1055:ASN:ND2 | 2.33 | 0.62 |
| 1:K:1899:GLN:NE2 | 1:K:1904:HIS:HB2 | 2.14 | 0.62 |
| 1:K:2517:ILE:HD11 | 1:K:2601:TRP:HD1 | 1.64 | 0.62 |
| 1:L:787:VAL:HG23 | 1:L:789:ILE:HD11 | 1.82 | 0.62 |
| 1:L:913:TRP:HD1 | 1:L:1088:LEU:HD12 | 1.65 | 0.62 |
| 1:L:1913:LEU:HA | 1:L:1916:MET:HG3 | 1.82 | 0.62 |
| 1:L:2159:ARG:NE | 1:L:2303:ASP:OD1 | 2.21 | 0.62 |
| 1:M:437:VAL:HG12 | 1:M:521:PRO:HB2 | 1.81 | 0.62 |
| 1:N:696:PRO:HA | 1:N:699:ILE:HD13 | 1.80 | 0.62 |
| 1:O:390:LEU:HD22 | 1:O:398:LEU:HB3 | 1.81 | 0.62 |
| 1:O:2996:GLU:OE2 | 1:O:3008:ILE:N | 2.31 | 0.62 |
| 1:Q:2780:ASN:OD1 | 1:Q:2781:PHE:N | 2.32 | 0.62 |
| 1:Q:2796:ARG:HH22 | 1:Q:2801:ARG:HE | 1.48 | 0.62 |
| 1:Q:3064:LEU:O | 1:Q:3067:GLN:NE2 | 2.33 | 0.62 |
| 1:S:3260:ARG:HE | 1:S:3261:VAL:H | 1.47 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:T:905:HIS:HA | 1:T:910:PHE:HD2 | 1.65 | 0.62 |
| 1:A:1067:GLN:NE2 | 1:A:1072:LEU:HB2 | 2.15 | 0.62 |
| 1:A:2567:CYS:SG | 1:A:2578:HIS:NE2 | 2.73 | 0.62 |
| 1:A:2734:ASN:ND2 | 1:J:2896:PHE:O | 2.33 | 0.62 |
| 1:B:2448:ASP:OD1 | 1:B:2449:THR:N | 2.33 | 0.62 |
| 1:E:1156:HIS:HB3 | 1:E:1193:GLN:HE22 | 1.65 | 0.62 |
| 1:E:1814:LYS:HD2 | 1:E:1860:TRP:CZ3 | 2.34 | 0.62 |
| 1:F:188:ILE:HG13 | 1:F:191:LEU:HD23 | 1.80 | 0.62 |
| 1:H:887:GLN:HE22 | 1:H:889:ASN:HB2 | 1.64 | 0.62 |
| 1:H:1750:PHE:HD2 | 1:H:1882:LEU:HD11 | 1.65 | 0.62 |
| 1:H:2622:PHE:O | 1:H:2636:ARG:NH2 | 2.32 | 0.62 |
| 1:I:1674:ARG:HD2 | 1:I:1954:GLU:HG2 | 1.81 | 0.62 |
| 1:I:2777:ASP:O | 1:I:3137:HIS:NE2 | 2.33 | 0.62 |
| 1:J:1539:THR:HG22 | 1:J:1542:GLN:HE22 | 1.64 | 0.62 |
| 1:K:3339:ARG:NH2 | 1:K:3376:ASP:O | 2.33 | 0.62 |
| 1:L:144:ALA:HB3 | 1:L:194:GLY:HA3 | 1.82 | 0.62 |
| 1:L:501:ARG:NE | 1:L:645:ASP:OD2 | 2.27 | 0.62 |
| 1:L:954:THR:HG22 | 1:L:965:PRO:HA | 1.82 | 0.62 |
| 1:L:3382:GLU:O | 1:L:3386:TYR:OH | 2.17 | 0.62 |
| 1:N:256:ARG:O | 1:N:265:ARG:NH1 | 2.32 | 0.62 |
| 1:N:2232:LEU:HD12 | 1:N:2274:LEU:HB3 | 1.82 | 0.62 |
| 1:N:2923:ARG:NH1 | 1:N:3007:GLY:O | 2.31 | 0.62 |
| 1:P:221:ARG:HE | 1:P:283:TYR:HD2 | 1.47 | 0.62 |
| 1:Q:1577:VAL:HG22 | 1:T:337:GLN:HG2 | 1.82 | 0.62 |
| 1:R:1514:SER:OG | 1:R:1515:ARG:NH2 | 2.33 | 0.62 |
| 1:S:307:GLU:O | 1:S:308:ARG:NE | 2.32 | 0.62 |
| 1:S:738:VAL:HG23 | 1:S:789:ILE:HD13 | 1.80 | 0.62 |
| 1:S:2664:GLN:HE21 | 1:S:2670:PHE:HA | 1.63 | 0.62 |
| 1:T:938:ASP:OD1 | 1:T:1055:ASN:ND2 | 2.33 | 0.62 |
| 1:T:2666:ASP:OD1 | 1:T:2667:TYR:N | 2.32 | 0.62 |
| 1:A:2080:ARG:HG3 | 1:A:2314:LYS:HE3 | 1.81 | 0.62 |
| 1:B:172:ASP:OD1 | 1:B:173:ASP:N | 2.31 | 0.62 |
| 1:B:435:LYS:HG2 | 1:B:436:ASP:H | 1.63 | 0.62 |
| 1:B:744:ASN:HD21 | 1:B:778:PRO:HA | 1.63 | 0.62 |
| 1:B:2630:LEU:HD11 | 1:B:2698:TYR:HE1 | 1.63 | 0.62 |
| 1:C:460:SER:O | 1:C:1371:ARG:NH1 | 2.30 | 0.62 |
| 1:C:2232:LEU:HB2 | 1:C:2274:LEU:HD11 | 1.82 | 0.62 |
| 1:C:3395:ARG:NE | 1:C:3398:GLN:OE1 | 2.31 | 0.62 |
| 1:D:2112:ARG:O | 1:D:2116:LYS:NZ | 2.32 | 0.62 |
| 1:E:838:GLU:OE1 | 1:S:2:SER:N | 2.33 | 0.62 |
| 1:E:1773:ASN:OD1 | 1:E:1774:SER:N | 2.32 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:H:2579:ARG:NH1 | 1:H:2766:ALA:O | 2.32 | 0.62 |
| 1:I:1919:PRO:O | 1:I:1921:LYS:NZ | 2.31 | 0.62 |
| 1:K:1033:GLU:O | 1:K:1036:SER:OG | 2.17 | 0.62 |
| 1:K:1400:LEU:HD11 | 1:K:1436:LEU:HB3 | 1.82 | 0.62 |
| 1:K:1919:PRO:O | 1:K:1921:LYS:NZ | 2.31 | 0.62 |
| 1:L:885:HIS:HD1 | 1:L:1044:ALA:HB2 | 1.65 | 0.62 |
| 1:L:1012:CYS:O | 1:L:1196:ARG:NH1 | 2.33 | 0.62 |
| 1:M:55:ARG:NH2 | 1:M:56:VAL:O | 2.32 | 0.62 |
| 1:N:2587:ARG:HH22 | 1:N:2753:PRO:HG2 | 1.65 | 0.62 |
| 1:P:2568:HIS:C | 1:P:2569:HIS:HD1 | 2.08 | 0.62 |
| 1:Q:1447:SER:OG | 1:Q:1449:ASP:OD1 | 2.17 | 0.62 |
| 1:Q:2750:ASP:HA | 1:Q:2758:ARG:HH11 | 1.65 | 0.62 |
| 1:Q:3157:PHE:O | 1:Q:3163:ASN:ND2 | 2.32 | 0.62 |
| 1:S:159:THR:HG23 | 1:S:162:PHE:H | 1.63 | 0.62 |
| 1:T:1722:TYR:HD2 | 1:T:1725:ALA:HB2 | 1.64 | 0.62 |
| 1:A:1272:SER:HG | 1:A:1275:GLU:CD | 2.07 | 0.62 |
| 1:A:3334:ARG:HH21 | 1:A:3406:ILE:HG23 | 1.64 | 0.62 |
| 1:B:526:THR:OG1 | 1:B:527:ARG:NH1 | 2.32 | 0.62 |
| 1:B:981:SER:HB3 | 1:B:1031:GLY:HA3 | 1.82 | 0.62 |
| 1:B:2413:CYS:SG | 1:B:2470:ARG:NH2 | 2.71 | 0.62 |
| 1:D:1433:LEU:HD11 | 1:D:1460:HIS:CD2 | 2.34 | 0.62 |
| 1:F:655:GLN:HG2 | 1:F:662:TYR:HB3 | 1.81 | 0.62 |
| 1:F:1924:SER:O | 1:F:1936:LYS:NZ | 2.32 | 0.62 |
| 1:F:2988:HIS:HA | 1:F:2991:LEU:HD12 | 1.81 | 0.62 |
| 1:H:445:VAL:HG12 | 1:H:449:ARG:HH21 | 1.63 | 0.62 |
| 1:I:559:VAL:N | 1:I:564:GLU:O | 2.31 | 0.62 |
| 1:I:646:ARG:NH2 | 1:I:712:ASN:O | 2.33 | 0.62 |
| 1:J:23:LEU:HD21 | 1:J:124:SER:HB2 | 1.80 | 0.62 |
| 1:K:1122:HIS:ND1 | 1:K:1123:TYR:O | 2.30 | 0.62 |
| 1:K:1641:ASN:OD1 | 2:KA:1:NAG:N2 | 2.32 | 0.62 |
| 1:L:1142:HIS:HE1 | 1:L:1524:ASN:HA | 1.65 | 0.62 |
| 1:L:2219:GLU:O | 1:L:2221:LYS:NZ | 2.33 | 0.62 |
| 1:M:1214:ASN:O | 1:M:1216:ARG:NH2 | 2.32 | 0.62 |
| 1:M:1556:LEU:HD11 | 1:M:1655:LEU:HD21 | 1.82 | 0.62 |
| 1:M:1865:LYS:HB3 | 1:M:1868:SER:HB3 | 1.80 | 0.62 |
| 1:N:24:ARG:HD3 | 1:N:123:ASN:HA | 1.81 | 0.62 |
| 1:O:2510:GLY:HA3 | 1:O:2513:VAL:HB | 1.80 | 0.62 |
| 1:P:3113:PRO:HA | 1:P:3116:MET:HE2 | 1.81 | 0.62 |
| 1:Q:613:PRO:HB2 | 1:Q:640:HIS:CE1 | 2.34 | 0.62 |
| 1:Q:857:GLU:N | 1:Q:857:GLU:OE1 | 2.30 | 0.62 |
| 1:Q:903:CYS:O | 1:Q:905:HIS:ND1 | 2.33 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:Q:915:ARG:HH22 | 1:Q:1115:TYR:HB3 | 1.62 | 0.62 |
| 1:Q:1397:GLN:NE2 | 1:Q:1399:GLU:OE2 | 2.26 | 0.62 |
| 1:R:1086:LYS:NZ | 1:R:1087:PRO:O | 2.32 | 0.62 |
| 1:R:1154:MET:HE1 | 1:R:1197:LEU:HD23 | 1.82 | 0.62 |
| 1:S:1919:PRO:O | 1:S:1921:LYS:NZ | 2.32 | 0.62 |
| 1:S:3089:ASN:HD21 | 1:S:3248:LEU:H | 1.46 | 0.62 |
| 1:T:2970:ALA:O | 1:T:2973:ARG:NE | 2.29 | 0.62 |
| 1:A:2114:LEU:HG | 1:A:2123:TRP:HB2 | 1.80 | 0.62 |
| 1:A:2251:VAL:HG22 | 1:A:2263:GLN:HB3 | 1.81 | 0.62 |
| 1:C:584:THR:HG23 | 1:C:587:PHE:H | 1.64 | 0.62 |
| 1:C:1858:HIS:HA | 1:C:1869:MET:HE1 | 1.79 | 0.62 |
| 1:C:2174:SER:O | 1:D:1757:ARG:NH2 | 2.33 | 0.62 |
| 1:C:2959:PHE:HE1 | 1:C:3162:LYS:HE2 | 1.64 | 0.62 |
| 1:D:1531:ASP:OD1 | 1:D:1532:THR:N | 2.32 | 0.62 |
| 1:F:673:GLU:O | 1:F:695:ARG:NH2 | 2.27 | 0.62 |
| 1:F:2970:ALA:O | 1:F:2973:ARG:NE | 2.30 | 0.62 |
| 1:G:454:ARG:NH2 | 1:G:514:ARG:O | 2.33 | 0.62 |
| 1:G:650:ILE:HG22 | 1:G:713:LEU:HD12 | 1.81 | 0.62 |
| 1:G:2585:LEU:HD22 | 1:G:2706:PHE:HE1 | 1.65 | 0.62 |
| 1:H:981:SER:HB3 | 1:H:1031:GLY:HA3 | 1.82 | 0.62 |
| 1:I:1466:ARG:NH2 | 1:I:1534:ASN:O | 2.32 | 0.62 |
| 1:I:2059:ASN:OD1 | 1:I:2060:GLY:N | 2.33 | 0.62 |
| 1:J:662:TYR:HE2 | 1:J:700:TYR:HB3 | 1.64 | 0.62 |
| 1:K:903:CYS:O | 1:K:905:HIS:ND1 | 2.29 | 0.62 |
| 1:M:1571:VAL:O | 1:M:1592:SER:OG | 2.14 | 0.62 |
| 1:M:2421:ARG:HH22 | 1:M:2424:ALA:HB2 | 1.65 | 0.62 |
| 1:N:3127:GLN:HE22 | 1:N:3190:LEU:HD22 | 1.63 | 0.62 |
| 1:P:506:GLN:NE2 | 1:P:690:THR:OG1 | 2.33 | 0.62 |
| 1:Q:938:ASP:OD2 | 1:Q:1058:ARG:NH2 | 2.33 | 0.62 |
| 1:Q:1539:THR:HG23 | 1:Q:1541:PRO:HD2 | 1.81 | 0.62 |
| 1:R:182:GLU:O | 1:R:186:ASN:ND2 | 2.33 | 0.62 |
| 1:S:1448:LEU:HB3 | 1:S:1596:LEU:HD11 | 1.80 | 0.62 |
| 1:S:3395:ARG:HH21 | 1:S:3398:GLN:HE22 | 1.48 | 0.62 |
| 1:T:2589:LEU:O | 1:T:2592:GLN:NE2 | 2.29 | 0.62 |
| 1:A:1417:THR:O | 1:A:1475:GLN:NE2 | 2.32 | 0.61 |
| 1:B:3037:ILE:HG22 | 1:B:3042:HIS:H | 1.63 | 0.61 |
| 1:C:903:CYS:O | 1:C:905:HIS:ND1 | 2.32 | 0.61 |
| 1:D:378:LYS:NZ | 1:D:383:ASP:O | 2.32 | 0.61 |
| 1:D:2979:HIS:HA | 1:D:2984:PHE:HD2 | 1.63 | 0.61 |
| 1:F:1100:ASP:O | 1:F:1104:ARG:NH1 | 2.33 | 0.61 |
| 1:F:3139:SER:HB3 | 1:F:3142:TYR:HB3 | 1.83 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:G:2915:PRO:HA | 1:G:2917:LYS:HZ2 | 1.65 | 0.61 |
| 1:I:2729:ASP:OD1 | 1:I:2916:THR:OG1 | 2.18 | 0.61 |
| 1:J:2923:ARG:HE | 1:J:2924:TYR:H | 1.47 | 0.61 |
| 1:K:714:GLN:OE1 | 1:K:718:MET:N | 2.30 | 0.61 |
| 1:K:1802:ILE:HD12 | 1:K:1805:GLU:HB2 | 1.81 | 0.61 |
| 1:K:2641:GLN:NE2 | 1:K:2645:ASP:OD1 | 2.33 | 0.61 |
| 1:K:2820:ASP:OD1 | 1:K:2831:ALA:N | 2.31 | 0.61 |
| 1:L:475:ALA:HB3 | 1:L:485:ARG:HB3 | 1.81 | 0.61 |
| 1:L:1353:GLN:NE2 | 1:L:1536:ASN:OD1 | 2.32 | 0.61 |
| 1:L:1546:VAL:HA | 1:L:1549:ARG:HG2 | 1.82 | 0.61 |
| 1:M:1854:HIS:CD2 | 1:M:1888:THR:HG21 | 2.34 | 0.61 |
| 1:M:2095:GLU:HB3 | 1:M:2098:HIS:HD2 | 1.65 | 0.61 |
| 1:N:1750:PHE:HD2 | 1:N:1882:LEU:HD11 | 1.65 | 0.61 |
| 1:N:2848:ASP:OD1 | 1:N:2849:ARG:N | 2.33 | 0.61 |
| 1:N:3351:VAL:HG23 | 1:N:3390:SER:HA | 1.80 | 0.61 |
| 1:O:307:GLU:O | 1:O:308:ARG:NE | 2.33 | 0.61 |
| 1:O:525:TRP:CD1 | 1:O:643:ASN:HD22 | 2.18 | 0.61 |
| 1:O:2962:ALA:HB2 | 1:O:3107:GLU:HG2 | 1.82 | 0.61 |
| 1:P:996:THR:HG23 | 1:P:999:ALA:H | 1.65 | 0.61 |
| 1:P:1415:GLU:OE2 | 1:P:1555:ARG:NH2 | 2.33 | 0.61 |
| 1:Q:2085:GLN:HE22 | 1:Q:2088:PRO:HD2 | 1.64 | 0.61 |
| 1:Q:2669:ASN:OD1 | 1:Q:2849:ARG:NE | 2.33 | 0.61 |
| 1:T:313:PHE:HB3 | 1:T:315:LEU:HD23 | 1.82 | 0.61 |
| 1:A:1328:LEU:HB3 | 1:A:1499:PHE:CE2 | 2.33 | 0.61 |
| 1:A:2315:ARG:HD3 | 1:A:2377:LEU:HD13 | 1.81 | 0.61 |
| 1:B:94:TRP:O | 1:B:218:ASN:ND2 | 2.33 | 0.61 |
| 1:C:69:TRP:HD1 | 1:C:251:LEU:HD12 | 1.65 | 0.61 |
| 1:C:2780:ASN:OD1 | 1:C:2781:PHE:N | 2.33 | 0.61 |
| 1:D:3058:GLN:N | 1:D:3061:LEU:O | 2.30 | 0.61 |
| 1:E:2254:GLN:OE1 | 1:E:2254:GLN:N | 2.30 | 0.61 |
| 1:F:2865:ARG:HG2 | 1:F:2866:PRO:HD2 | 1.82 | 0.61 |
| 1:F:3156:PRO:HB2 | 1:F:3162:LYS:HG3 | 1.82 | 0.61 |
| 1:G:2778:ASP:OD1 | 1:G:2779:LEU:N | 2.33 | 0.61 |
| 1:G:3052:LEU:O | 1:G:3055:ARG:NH2 | 2.31 | 0.61 |
| 1:G:3289:LYS:HD2 | 1:G:3291:ASN:HD22 | 1.65 | 0.61 |
| 1:H:2616:ASP:OD1 | 1:H:2617:LYS:N | 2.32 | 0.61 |
| 1:H:2991:LEU:HA | 1:H:2994:GLN:HE21 | 1.65 | 0.61 |
| 1:I:1417:THR:O | 1:I:1475:GLN:NE2 | 2.32 | 0.61 |
| 1:I:1723:PRO:HA | 1:I:1728:ARG:HH22 | 1.64 | 0.61 |
| 1:I:2095:GLU:HB3 | 1:I:2098:HIS:HD2 | 1.65 | 0.61 |
| 1:K:527:ARG:HD3 | 1:K:528:PRO:HD2 | 1.81 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:K:1570:ASP:HB2 | 1:K:1638:ARG:HB3 | 1.81 | 0.61 |
| 1:K:2000:VAL:HG12 | 1:K:2051:VAL:HG22 | 1.82 | 0.61 |
| 1:L:2595:ARG:HG3 | 1:L:2596:VAL:HG13 | 1.83 | 0.61 |
| 1:O:1770:ASN:OD1 | 1:O:1772:GLN:NE2 | 2.32 | 0.61 |
| 1:P:1285:ARG:O | 1:P:1340:ARG:NH1 | 2.33 | 0.61 |
| 1:P:3008:ILE:HG21 | 1:P:3116:MET:HB3 | 1.82 | 0.61 |
| 1:Q:460:SER:O | 1:Q:1371:ARG:NH1 | 2.34 | 0.61 |
| 1:Q:2348:THR:OG1 | 1:Q:2349:ARG:NH1 | 2.32 | 0.61 |
| 1:R:1019:GLU:HA | 1:R:1022:HIS:CD2 | 2.36 | 0.61 |
| 1:R:2636:ARG:NH2 | 1:R:2702:ASP:OD1 | 2.31 | 0.61 |
| 1:S:2508:VAL:O | 1:S:2515:LYS:NZ | 2.34 | 0.61 |
| 1:T:48:CYS:H | 1:T:58:CYS:HB2 | 1.65 | 0.61 |
| 1:T:808:LEU:HB2 | 1:T:820:GLU:HG3 | 1.82 | 0.61 |
| 1:T:3010:TYR:OH | 1:T:3188:ASP:OD1 | 2.14 | 0.61 |
| 1:T:3032:PHE:HA | 1:T:3113:PRO:HG2 | 1.81 | 0.61 |
| 1:A:1914:GLU:OE1 | 1:B:1655:LEU:N | 2.23 | 0.61 |
| 1:C:159:THR:HG23 | 1:C:162:PHE:H | 1.64 | 0.61 |
| 1:C:767:LYS:HE2 | 1:C:767:LYS:HA | 1.81 | 0.61 |
| 1:C:1265:ARG:NH2 | 1:C:1331:ASP:OD2 | 2.33 | 0.61 |
| 1:C:1362:ILE:HD13 | 1:C:1456:LEU:HD11 | 1.83 | 0.61 |
| 1:D:230:GLN:NE2 | 1:D:236:THR:O | 2.30 | 0.61 |
| 1:D:474:PRO:HB2 | 1:D:476:ARG:HH22 | 1.65 | 0.61 |
| 1:D:503:PHE:HA | 1:D:678:PHE:HE1 | 1.65 | 0.61 |
| 1:D:507:VAL:HG21 | 1:D:638:ILE:HD11 | 1.82 | 0.61 |
| 1:D:3131:THR:HA | 1:D:3134:LYS:HE3 | 1.81 | 0.61 |
| 1:D:3287:LEU:HB3 | 1:D:3295:LEU:HB3 | 1.81 | 0.61 |
| 1:F:569:GLN:HB3 | 1:F:619:GLY:HA3 | 1.80 | 0.61 |
| 1:F:3114:PHE:HA | 1:F:3117:ILE:HG12 | 1.82 | 0.61 |
| 1:G:1689:ARG:NE | 1:G:1786:ASP:OD2 | 2.32 | 0.61 |
| 1:G:1919:PRO:O | 1:G:1921:LYS:NZ | 2.33 | 0.61 |
| 1:H:331:HIS:CE1 | 1:H:672:HIS:HB3 | 2.35 | 0.61 |
| 1:H:1431:ASN:OD1 | 1:H:1594:SER:OG | 2.16 | 0.61 |
| 1:H:3260:ARG:NH2 | 1:H:3407:ASP:OD2 | 2.33 | 0.61 |
| 1:I:1362:ILE:HD13 | 1:I:1456:LEU:HD11 | 1.80 | 0.61 |
| 1:J:905:HIS:HA | 1:J:910:PHE:HD2 | 1.65 | 0.61 |
| 1:J:2970:ALA:O | 1:J:2973:ARG:NE | 2.30 | 0.61 |
| 1:K:1312:VAL:HG22 | 1:K:1313:ALA:H | 1.66 | 0.61 |
| 1:K:1362:ILE:HD12 | 1:K:1380:PHE:HB3 | 1.81 | 0.61 |
| 1:K:1607:ASP:OD1 | 1:K:1608:ARG:N | 2.33 | 0.61 |
| 1:L:914:HIS:O | 1:L:918:THR:HG23 | 1.99 | 0.61 |
| 1:L:1153:PHE:HB2 | 1:L:1198:PHE:HD2 | 1.65 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:M:512:LYS:HA | 1:M:516:LEU:HB2 | 1.82 | 0.61 |
| 1:M:605:GLN:HA | 1:M:608:VAL:HG12 | 1.82 | 0.61 |
| 1:M:667:ALA:HB1 | 1:M:670:MET:HB3 | 1.83 | 0.61 |
| 1:M:1195:ASP:OD2 | 1:M:1196:ARG:NH1 | 2.33 | 0.61 |
| 1:M:2056:ARG:NH1 | 1:M:2057:ALA:O | 2.33 | 0.61 |
| 1:N:2610:LEU:HG | 1:N:2614:LEU:HD23 | 1.82 | 0.61 |
| 1:O:2118:GLY:HA2 | 1:O:2124:GLN:HE22 | 1.64 | 0.61 |
| 1:P:2311:GLU:O | 1:P:2315:ARG:NH1 | 2.33 | 0.61 |
| 1:P:3131:THR:HA | 1:P:3134:LYS:HE3 | 1.81 | 0.61 |
| 1:Q:1583:GLU:N | 1:T:340:SER:O | 2.34 | 0.61 |
| 1:Q:1896:GLN:NE2 | 1:Q:1906:PRO:O | 2.28 | 0.61 |
| 1:Q:2096:ILE:HD13 | 1:Q:2179:PRO:HG2 | 1.82 | 0.61 |
| 1:R:913:TRP:HD1 | 1:R:1088:LEU:HD12 | 1.66 | 0.61 |
| 1:S:2155:PRO:HB2 | 1:S:2159:ARG:HH22 | 1.65 | 0.61 |
| 1:S:2509:SER:O | 1:S:3138:ARG:NH2 | 2.33 | 0.61 |
| 1:S:2959:PHE:HE1 | 1:S:3162:LYS:HE2 | 1.66 | 0.61 |
| 1:S:3312:ASP:OD2 | 1:S:3313:TYR:N | 2.34 | 0.61 |
| 1:T:958:PRO:HA | 1:T:961:ASN:HA | 1.83 | 0.61 |
| 1:T:1946:ASP:HB3 | 1:T:1950:HIS:HD2 | 1.64 | 0.61 |
| 1:A:307:GLU:O | 1:A:308:ARG:NE | 2.33 | 0.61 |
| 1:B:465:GLN:NE2 | 1:B:558:PRO:O | 2.28 | 0.61 |
| 1:B:1714:HIS:NE2 | 1:B:1732:CYS:SG | 2.73 | 0.61 |
| 1:B:1763:ILE:HD12 | 1:B:1764:PRO:HD2 | 1.81 | 0.61 |
| 1:B:3360:LEU:HD12 | 1:B:3387:PHE:HB3 | 1.83 | 0.61 |
| 1:C:1494:GLN:NE2 | 1:C:1500:ASN:OD1 | 2.34 | 0.61 |
| 1:C:2470:ARG:NH2 | 1:C:2471:TYR:O | 2.33 | 0.61 |
| 1:F:2159:ARG:NE | 1:F:2303:ASP:OD1 | 2.24 | 0.61 |
| 1:G:55:ARG:NH2 | 1:G:56:VAL:O | 2.33 | 0.61 |
| 1:I:55:ARG:NH2 | 1:I:56:VAL:O | 2.33 | 0.61 |
| 1:J:105:ARG:O | 1:J:105:ARG:NH1 | 2.33 | 0.61 |
| 1:J:2439:ASP:OD2 | 1:J:2440:ARG:NH1 | 2.33 | 0.61 |
| 1:L:719:THR:H | 1:L:722:GLN:NE2 | 1.98 | 0.61 |
| 1:L:757:PRO:HB2 | 1:L:760:GLY:H | 1.63 | 0.61 |
| 1:L:2666:ASP:OD1 | 1:L:2667:TYR:N | 2.32 | 0.61 |
| 1:M:1684:THR:OG1 | 1:M:1687:GLU:OE1 | 2.17 | 0.61 |
| 1:M:1931:LEU:HD23 | 1:N:2102:ARG:HA | 1.82 | 0.61 |
| 1:M:3020:LEU:HB3 | 1:M:3024:LEU:HD11 | 1.82 | 0.61 |
| 1:N:3398:GLN:OE1 | 1:N:3400:THR:OG1 | 2.17 | 0.61 |
| 1:O:2256:ASP:OD2 | 1:O:2440:ARG:NH2 | 2.33 | 0.61 |
| 1:O:2780:ASN:OD1 | 1:O:2781:PHE:N | 2.32 | 0.61 |
| 1:P:2251:VAL:HG22 | 1:P:2263:GLN:HG3 | 1.82 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:P:2741:ARG:NH1 | 1:Q:2868:SER:O | 2.33 | 0.61 |
| 1:Q:33:ASN:HB3 | 1:Q:80:LYS:HD2 | 1.81 | 0.61 |
| 1:R:527:ARG:O | 1:R:530:THR:OG1 | 2.19 | 0.61 |
| 1:R:1040:LEU:HD21 | 1:R:1184:LEU:HD21 | 1.82 | 0.61 |
| 1:S:390:LEU:HD22 | 1:S:398:LEU:HB3 | 1.81 | 0.61 |
| 1:S:1085:ARG:NH1 | 1:T:2462:ASN:O | 2.33 | 0.61 |
| 1:S:2348:THR:OG1 | 1:S:2349:ARG:NH1 | 2.33 | 0.61 |
| 1:T:654:LEU:HD13 | 1:T:723:LEU:HD11 | 1.81 | 0.61 |
| 1:A:1583:GLU:OE2 | 1:D:327:LYS:NZ | 2.33 | 0.61 |
| 1:B:735:ARG:HH22 | 1:B:790:THR:H | 1.48 | 0.61 |
| 1:C:1743:HIS:HD2 | 1:C:1885:HIS:CD2 | 2.18 | 0.61 |
| 1:C:2254:GLN:N | 1:C:2254:GLN:OE1 | 2.32 | 0.61 |
| 1:D:2393:VAL:HG11 | 1:D:2450:LEU:HD12 | 1.81 | 0.61 |
| 1:D:2720:GLN:HE22 | 1:D:2730:TYR:HB2 | 1.66 | 0.61 |
| 1:F:671:THR:O | 1:F:695:ARG:NH2 | 2.33 | 0.61 |
| 1:G:2695:THR:OG1 | 1:G:2697:GLU:OE1 | 2.17 | 0.61 |
| 1:H:737:PHE:HB2 | 1:H:829:ILE:HB | 1.83 | 0.61 |
| 1:H:2567:CYS:O | 1:H:2569:HIS:ND1 | 2.34 | 0.61 |
| 1:I:605:GLN:HA | 1:I:608:VAL:HG12 | 1.81 | 0.61 |
| 1:I:1240:THR:HA | 1:J:2328:ASN:HD21 | 1.66 | 0.61 |
| 1:J:1978:LYS:HA | 1:J:2078:LYS:HZ1 | 1.65 | 0.61 |
| 1:J:3085:GLU:O | 1:J:3089:ASN:ND2 | 2.32 | 0.61 |
| 1:K:482:ALA:O | 1:K:485:ARG:NH2 | 2.34 | 0.61 |
| 1:K:654:LEU:HD21 | 1:K:658:ARG:HH21 | 1.64 | 0.61 |
| 1:K:1494:GLN:NE2 | 1:K:1500:ASN:OD1 | 2.34 | 0.61 |
| 1:K:2001:CYS:HA | 1:K:2007:CYS:HB3 | 1.82 | 0.61 |
| 1:L:188:ILE:HG21 | 1:L:215:HIS:NE2 | 2.16 | 0.61 |
| 1:L:405:ARG:NH1 | 1:L:406:PRO:O | 2.33 | 0.61 |
| 1:M:1037:MET:HA | 1:M:1043:THR:HA | 1.81 | 0.61 |
| 1:M:1417:THR:O | 1:M:1475:GLN:NE2 | 2.30 | 0.61 |
| 1:M:1626:ASP:OD1 | 1:M:1627:SER:N | 2.33 | 0.61 |
| 1:M:1674:ARG:HD2 | 1:M:1954:GLU:HG2 | 1.83 | 0.61 |
| 1:N:297:TYR:O | 1:N:300:LEU:HG | 2.01 | 0.61 |
| 1:N:1222:SER:HA | 1:N:1233:SER:HB3 | 1.82 | 0.61 |
| 1:N:3018:LYS:HA | 1:N:3055:ARG:HH12 | 1.65 | 0.61 |
| 1:Q:584:THR:HG23 | 1:Q:587:PHE:H | 1.66 | 0.61 |
| 1:Q:939:TRP:HE1 | 1:Q:998:ILE:HG21 | 1.65 | 0.61 |
| 1:Q:1900:ARG:O | 1:Q:1900:ARG:NH1 | 2.33 | 0.61 |
| 1:R:925:LEU:HD22 | 1:R:928:LYS:HZ3 | 1.65 | 0.61 |
| 1:R:1490:ASN:OD1 | 1:R:1493:ARG:NH2 | 2.25 | 0.61 |
| 1:R:3082:VAL:O | 1:R:3086:MET:HG2 | 2.00 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:S:881:ILE:HA | 1:S:884:PHE:HD2 | 1.65 | 0.61 |
| 1:S:1161:SER:OG | 1:S:1185:GLY:N | 2.30 | 0.61 |
| 1:T:719:THR:H | 1:T:722:GLN:NE2 | 1.99 | 0.61 |
| 1:A:159:THR:HG23 | 1:A:162:PHE:H | 1.66 | 0.61 |
| 1:A:2254:GLN:N | 1:A:2254:GLN:OE1 | 2.32 | 0.61 |
| 1:B:1153:PHE:HB2 | 1:B:1198:PHE:HD2 | 1.63 | 0.61 |
| 1:C:728:ASP:OD1 | 1:C:836:HIS:ND1 | 2.32 | 0.61 |
| 1:C:758:LYS:NZ | 1:C:803:GLU:OE2 | 2.34 | 0.61 |
| 1:C:1623:LEU:HD23 | 1:D:2785:THR:HG21 | 1.82 | 0.61 |
| 1:D:71:ARG:NH1 | 1:D:273:LEU:O | 2.32 | 0.61 |
| 1:D:81:LEU:HD12 | 1:D:86:LEU:HD13 | 1.81 | 0.61 |
| 1:D:331:HIS:NE2 | 1:D:672:HIS:O | 2.34 | 0.61 |
| 1:E:2959:PHE:HE1 | 1:E:3162:LYS:HE2 | 1.66 | 0.61 |
| 1:G:953:GLU:HG3 | 1:G:954:THR:HG23 | 1.82 | 0.61 |
| 1:G:1571:VAL:O | 1:G:1592:SER:OG | 2.16 | 0.61 |
| 1:G:1865:LYS:HZ1 | 1:G:1867:HIS:HB2 | 1.66 | 0.61 |
| 1:G:3157:PHE:O | 1:G:3163:ASN:ND2 | 2.33 | 0.61 |
| 1:H:613:PRO:HA | 1:H:616:LEU:HB2 | 1.82 | 0.61 |
| 1:H:741:HIS:HE1 | 1:H:780:ASN:HD21 | 1.46 | 0.61 |
| 1:J:2138:SER:OG | 1:J:2143:LYS:NZ | 2.33 | 0.61 |
| 1:K:559:VAL:N | 1:K:564:GLU:O | 2.33 | 0.61 |
| 1:K:2130:HIS:NE2 | 1:K:2147:CYS:SG | 2.74 | 0.61 |
| 1:L:2876:ILE:HB | 1:L:2884:LEU:HB2 | 1.81 | 0.61 |
| 1:M:2108:LYS:HG3 | 1:M:2112:ARG:HH12 | 1.64 | 0.61 |
| 1:N:23:LEU:HD23 | 1:N:123:ASN:HD21 | 1.64 | 0.61 |
| 1:N:869:LEU:HD23 | 1:N:925:LEU:HD11 | 1.83 | 0.61 |
| 1:N:905:HIS:HA | 1:N:910:PHE:HD2 | 1.65 | 0.61 |
| 1:O:2488:LYS:HD2 | 1:O:2489:PRO:HD2 | 1.83 | 0.61 |
| 1:O:3280:ASN:OD1 | 1:O:3341:HIS:NE2 | 2.32 | 0.61 |
| 1:Q:2159:ARG:NH1 | 1:Q:2303:ASP:OD1 | 2.33 | 0.61 |
| 1:R:808:LEU:HB2 | 1:R:820:GLU:HG3 | 1.83 | 0.61 |
| 1:S:2986:HIS:HB3 | 1:S:3177:ILE:HD13 | 1.81 | 0.61 |
| 1:A:2651:GLU:HG3 | 1:A:2656:ARG:HH12 | 1.66 | 0.61 |
| 1:B:1232:SER:OG | 1:B:1234:GLU:OE1 | 2.19 | 0.61 |
| 1:B:2988:HIS:HA | 1:B:2991:LEU:HD12 | 1.83 | 0.61 |
| 1:B:3276:ASN:ND2 | 1:B:3279:SER:OG | 2.33 | 0.61 |
| 1:B:3350:ASN:OD1 | 1:B:3351:VAL:N | 2.34 | 0.61 |
| 1:C:1815:ARG:HD2 | 1:C:1818:LEU:HD11 | 1.83 | 0.61 |
| 1:D:313:PHE:CE1 | 1:D:406:PRO:HB3 | 2.36 | 0.61 |
| 1:D:459:THR:OG1 | 1:D:1285:ARG:NH1 | 2.34 | 0.61 |
| 1:D:1742:TRP:HD1 | 1:D:1920:LEU:HD12 | 1.65 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:D:2542:ARG:HD3 | 1:D:2591:LEU:HD23 | 1.83 | 0.61 |
| 1:E:259:ASN:O | 1:E:265:ARG:NH2 | 2.34 | 0.61 |
| 1:E:1166:LEU:HD22 | 1:E:1200:TYR:HD2 | 1.64 | 0.61 |
| 1:E:2313:GLN:HG2 | 1:E:2320:TYR:HB3 | 1.82 | 0.61 |
| 1:F:3058:GLN:NE2 | 1:F:3268:ASP:OD2 | 2.34 | 0.61 |
| 1:F:3324:ASN:OD1 | 1:F:3398:GLN:NE2 | 2.32 | 0.61 |
| 1:G:1266:ARG:NH2 | 1:G:1270:ASP:OD1 | 2.33 | 0.61 |
| 1:G:2000:VAL:HG12 | 1:G:2051:VAL:HG22 | 1.83 | 0.61 |
| 1:H:1546:VAL:HA | 1:H:1549:ARG:HG2 | 1.83 | 0.61 |
| 1:J:313:PHE:HE2 | 1:J:406:PRO:HB3 | 1.65 | 0.61 |
| 1:K:159:THR:HG23 | 1:K:162:PHE:H | 1.66 | 0.61 |
| 1:K:1855:ASN:HD21 | 1:K:2015:VAL:HA | 1.66 | 0.61 |
| 1:K:2446:ILE:HD11 | 1:K:2491:ILE:HD11 | 1.83 | 0.61 |
| 1:L:499:TRP:NE1 | 1:L:676:LYS:O | 2.34 | 0.61 |
| 1:L:3052:LEU:O | 1:L:3055:ARG:NH1 | 2.29 | 0.61 |
| 1:M:2600:TYR:OH | 1:M:2714:ARG:NH1 | 2.33 | 0.61 |
| 1:M:3284:GLN:HE22 | 1:M:3286:THR:HG23 | 1.64 | 0.61 |
| 1:N:698:ASN:ND2 | 1:N:705:GLU:OE2 | 2.33 | 0.61 |
| 1:N:2988:HIS:HA | 1:N:2991:LEU:HD12 | 1.81 | 0.61 |
| 1:O:1417:THR:O | 1:O:1475:GLN:NE2 | 2.34 | 0.61 |
| 1:O:1872:LEU:HD21 | 1:O:2016:LEU:HD13 | 1.82 | 0.61 |
| 1:Q:2313:GLN:HG2 | 1:Q:2320:TYR:HB3 | 1.83 | 0.61 |
| 1:R:925:LEU:HD13 | 1:R:928:LYS:HE2 | 1.82 | 0.61 |
| 1:R:2979:HIS:HA | 1:R:2984:PHE:HD2 | 1.66 | 0.61 |
| 1:T:2416:ASN:ND2 | 1:T:2418:LYS:O | 2.32 | 0.61 |
| 1:D:2806:PHE:CE1 | 1:D:2892:PRO:HB3 | 2.36 | 0.61 |
| 1:E:2056:ARG:NH1 | 1:E:2057:ALA:O | 2.34 | 0.61 |
| 1:F:180:GLN:HE22 | 1:F:366:HIS:HB2 | 1.66 | 0.61 |
| 1:F:719:THR:H | 1:F:722:GLN:NE2 | 1.99 | 0.61 |
| 1:F:1012:CYS:SG | 1:F:1196:ARG:NH1 | 2.74 | 0.61 |
| 1:F:1713:PHE:HE1 | 1:F:1929:TYR:HB3 | 1.66 | 0.61 |
| 1:F:2630:LEU:HD11 | 1:F:2698:TYR:HE1 | 1.66 | 0.61 |
| 1:F:3213:VAL:HG11 | 1:F:3270:LEU:HD12 | 1.83 | 0.61 |
| 1:G:3133:GLN:HE21 | 1:G:3138:ARG:HB3 | 1.66 | 0.61 |
| 1:H:297:TYR:O | 1:H:300:LEU:HG | 2.00 | 0.61 |
| 1:H:905:HIS:HA | 1:H:910:PHE:HD2 | 1.65 | 0.61 |
| 1:H:939:TRP:CZ3 | 1:H:1052:HIS:HA | 2.35 | 0.61 |
| 1:H:1142:HIS:HE1 | 1:H:1524:ASN:HA | 1.66 | 0.61 |
| 1:H:2138:SER:OG | 1:H:2143:LYS:NZ | 2.34 | 0.61 |
| 1:H:3276:ASN:ND2 | 1:H:3279:SER:OG | 2.33 | 0.61 |
| 1:H:3395:ARG:NE | 1:H:3400:THR:OG1 | 2.33 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:I:1890:ARG:NH2 | 1:I:1959:GLU:O | 2.34 | 0.61 |
| 1:J:247:PHE:HB3 | 1:J:271:LYS:HD2 | 1.80 | 0.61 |
| 1:J:580:TYR:HE2 | 1:J:959:GLU:HB3 | 1.65 | 0.61 |
| 1:J:1963:ILE:HG23 | 1:J:1968:LEU:HD11 | 1.81 | 0.61 |
| 1:J:2194:PHE:CD1 | 1:J:2212:PHE:HB3 | 2.36 | 0.61 |
| 1:J:2264:PHE:HZ | 1:J:2302:VAL:HG13 | 1.63 | 0.61 |
| 1:K:1914:GLU:OE2 | 1:L:1655:LEU:HD23 | 2.01 | 0.61 |
| 1:K:2930:SER:H | 1:K:2933:GLN:NE2 | 1.97 | 0.61 |
| 1:K:3226:ALA:HA | 1:K:3289:LYS:HA | 1.82 | 0.61 |
| 1:L:1015:GLU:N | 1:L:1015:GLU:OE1 | 2.33 | 0.61 |
| 1:M:1007:GLU:HB3 | 1:M:1140:ILE:HG12 | 1.83 | 0.61 |
| 1:N:3131:THR:HA | 1:N:3134:LYS:HE3 | 1.81 | 0.61 |
| 1:O:2755:ASP:OD1 | 1:O:2758:ARG:NH2 | 2.32 | 0.61 |
| 1:P:1154:MET:HE1 | 1:P:1197:LEU:HD23 | 1.83 | 0.61 |
| 1:P:2630:LEU:HD11 | 1:P:2698:TYR:HE1 | 1.66 | 0.61 |
| 1:Q:738:VAL:HG23 | 1:Q:789:ILE:HD13 | 1.83 | 0.61 |
| 1:Q:1426:PHE:CZ | 1:Q:1464:VAL:HG13 | 2.36 | 0.61 |
| 1:Q:2088:PRO:HD2 | 1:Q:2366:ARG:HH21 | 1.66 | 0.61 |
| 1:R:741:HIS:HE1 | 1:R:780:ASN:HD21 | 1.49 | 0.61 |
| 1:T:23:LEU:HD21 | 1:T:124:SER:HB2 | 1.83 | 0.61 |
| 1:T:554:PHE:O | 1:T:568:ARG:NH2 | 2.34 | 0.61 |
| 1:T:1086:LYS:NZ | 1:T:1087:PRO:O | 2.33 | 0.61 |
| 1:T:1431:ASN:OD1 | 1:T:1594:SER:OG | 2.18 | 0.61 |
| 1:T:2709:HIS:HA | 1:T:2712:VAL:HG22 | 1.82 | 0.61 |
| 1:T:2984:PHE:O | 1:T:2988:HIS:ND1 | 2.32 | 0.61 |
| 1:T:3122:ILE:HA | 1:T:3125:ILE:HG12 | 1.82 | 0.61 |
| 1:A:275:SER:HB3 | 1:A:278:GLN:HE22 | 1.65 | 0.61 |
| 1:A:1100:ASP:O | 1:A:1104:ARG:NH1 | 2.34 | 0.61 |
| 1:A:1515:ARG:HB2 | 1:A:1518:ASP:HB2 | 1.83 | 0.61 |
| 1:A:1757:ARG:NH1 | 1:B:2174:SER:O | 2.34 | 0.61 |
| 1:A:2056:ARG:NH1 | 1:A:2057:ALA:O | 2.34 | 0.61 |
| 1:A:3390:SER:HB3 | 1:A:3395:ARG:HG3 | 1.81 | 0.61 |
| 1:B:110:PRO:HD3 | 1:I:2197:GLN:HG3 | 1.83 | 0.61 |
| 1:B:958:PRO:HA | 1:B:961:ASN:HA | 1.83 | 0.61 |
| 1:B:1539:THR:HG22 | 1:B:1542:GLN:NE2 | 2.15 | 0.61 |
| 1:B:2979:HIS:HA | 1:B:2984:PHE:HD2 | 1.64 | 0.61 |
| 1:C:613:PRO:HB2 | 1:C:640:HIS:CE1 | 2.36 | 0.61 |
| 1:C:1380:PHE:O | 1:C:1394:ARG:NH2 | 2.33 | 0.61 |
| 1:C:1549:ARG:NH2 | 1:D:2509:SER:O | 2.33 | 0.61 |
| 1:D:450:GLN:O | 1:D:454:ARG:HG2 | 2.01 | 0.61 |
| 1:D:2867:ASP:HB3 | 1:E:2741:ARG:HH12 | 1.65 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:E:2118:GLY:HA2 | 1:E:2124:GLN:HE22 | 1.65 | 0.61 |
| 1:F:2149:HIS:HA | 1:F:2154:PHE:HD2 | 1.66 | 0.61 |
| 1:F:2850:LEU:HD11 | 1:G:2848:ASP:HB2 | 1.81 | 0.61 |
| 1:H:738:VAL:HG23 | 1:H:789:ILE:HG13 | 1.83 | 0.61 |
| 1:H:2448:ASP:OD1 | 1:H:2449:THR:N | 2.33 | 0.61 |
| 1:H:2988:HIS:HA | 1:H:2991:LEU:HD12 | 1.81 | 0.61 |
| 1:I:2085:GLN:HE22 | 1:I:2088:PRO:HD2 | 1.65 | 0.61 |
| 1:I:3088:HIS:CD2 | 1:I:3122:ILE:HG13 | 2.35 | 0.61 |
| 1:K:2727:GLY:O | 1:K:2914:GLN:NE2 | 2.32 | 0.61 |
| 1:K:3390:SER:HB3 | 1:K:3395:ARG:HG3 | 1.82 | 0.61 |
| 1:L:2511:ILE:HD12 | 1:L:2773:ASN:HB2 | 1.82 | 0.61 |
| 1:L:2950:PRO:HD2 | 1:L:2951:ASN:H | 1.65 | 0.61 |
| 1:M:2000:VAL:HG12 | 1:M:2051:VAL:HG22 | 1.83 | 0.61 |
| 1:N:1055:ASN:HA | 1:N:1058:ARG:HG3 | 1.83 | 0.61 |
| 1:N:2055:LEU:HB2 | 1:N:2063:LEU:HB2 | 1.81 | 0.61 |
| 1:N:2970:ALA:O | 1:N:2973:ARG:NE | 2.30 | 0.61 |
| 1:N:2984:PHE:O | 1:N:2988:HIS:ND1 | 2.32 | 0.61 |
| 1:N:3276:ASN:ND2 | 1:N:3279:SER:OG | 2.33 | 0.61 |
| 1:O:357:MET:HE3 | 1:O:358:PRO:HD2 | 1.83 | 0.61 |
| 1:P:143:ARG:NH2 | 1:P:209:ASP:OD2 | 2.34 | 0.61 |
| 1:P:2151:VAL:HB | 1:P:2329:TYR:HE2 | 1.64 | 0.61 |
| 1:Q:3390:SER:HB3 | 1:Q:3395:ARG:HG3 | 1.82 | 0.61 |
| 1:R:378:LYS:NZ | 1:R:383:ASP:O | 2.33 | 0.61 |
| 1:S:2273:TYR:HB2 | 1:S:2428:LEU:HD11 | 1.82 | 0.61 |
| 1:S:3056:ARG:NH1 | 1:S:3058:GLN:OE1 | 2.34 | 0.61 |
| 1:S:3072:LEU:HD23 | 1:S:3129:TRP:HD1 | 1.65 | 0.61 |
| 1:T:1999:LYS:NZ | 1:T:2009:ASP:OD1 | 2.34 | 0.61 |
| 1:T:2149:HIS:HA | 1:T:2154:PHE:HD2 | 1.66 | 0.61 |
| 1:A:2409:ARG:O | 1:A:2471:TYR:HA | 2.01 | 0.61 |
| 1:D:913:TRP:HD1 | 1:D:1088:LEU:HD12 | 1.66 | 0.61 |
| 1:E:313:PHE:HZ | 1:E:326:ILE:HD13 | 1.65 | 0.61 |
| 1:E:471:HIS:NE2 | 1:E:489:CYS:SG | 2.74 | 0.61 |
| 1:G:540:THR:HG22 | 1:G:551:HIS:HA | 1.83 | 0.61 |
| 1:G:2454:HIS:O | 1:G:2456:ARG:NH1 | 2.34 | 0.61 |
| 1:H:2137:PRO:HD2 | 1:H:2143:LYS:HE2 | 1.81 | 0.61 |
| 1:I:341:HIS:NE2 | 1:I:343:GLU:OE2 | 2.34 | 0.61 |
| 1:I:1978:LYS:NZ | 1:I:1979:SER:O | 2.29 | 0.61 |
| 1:I:2325:CYS:HA | 1:J:1242:VAL:HG13 | 1.82 | 0.61 |
| 1:I:2621:PRO:HD2 | 1:I:2622:PHE:HD1 | 1.65 | 0.61 |
| 1:J:727:ILE:HG22 | 1:J:730:ARG:HH21 | 1.65 | 0.61 |
| 1:J:2616:ASP:OD1 | 1:J:2617:LYS:N | 2.34 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:J:2661:ALA:HA | 1:J:2664:GLN:HE22 | 1.65 | 0.61 |
| 1:J:3037:ILE:HG22 | 1:J:3042:HIS:H | 1.66 | 0.61 |
| 1:K:738:VAL:HG23 | 1:K:789:ILE:HD13 | 1.83 | 0.61 |
| 1:K:2345:ASN:HD22 | 1:K:2348:THR:HG23 | 1.66 | 0.61 |
| 1:K:2460:VAL:HG12 | 1:K:2467:PHE:HZ | 1.65 | 0.61 |
| 1:K:3289:LYS:HB3 | 1:K:3295:LEU:HD11 | 1.81 | 0.61 |
| 1:L:714:GLN:HE22 | 1:L:719:THR:HB | 1.65 | 0.61 |
| 1:L:1009:THR:HG22 | 1:L:1070:ARG:HH12 | 1.66 | 0.61 |
| 1:M:2095:GLU:HB3 | 1:M:2098:HIS:CD2 | 2.36 | 0.61 |
| 1:O:1539:THR:HG23 | 1:O:1541:PRO:HD2 | 1.83 | 0.61 |
| 1:P:248:ARG:NH1 | 1:P:802:ASP:O | 2.33 | 0.61 |
| 1:R:1100:ASP:O | 1:R:1104:ARG:NH1 | 2.33 | 0.61 |
| 1:S:20:GLU:O | 1:S:24:ARG:HD3 | 2.01 | 0.61 |
| 1:S:1654:SER:OG | 1:S:1655:LEU:N | 2.34 | 0.61 |
| 1:T:2587:ARG:HH22 | 1:T:2753:PRO:HG2 | 1.65 | 0.61 |
| 1:A:1495:PRO:HG3 | 1:A:1515:ARG:HD3 | 1.83 | 0.60 |
| 1:A:2110:ALA:HB1 | 1:A:2172:HIS:HB3 | 1.83 | 0.60 |
| 1:B:180:GLN:OE1 | 1:B:366:HIS:N | 2.26 | 0.60 |
| 1:B:2583:VAL:HG21 | 1:B:2772:PHE:HD2 | 1.66 | 0.60 |
| 1:C:949:ILE:HG23 | 1:C:950:VAL:HG13 | 1.81 | 0.60 |
| 1:C:2348:THR:OG1 | 1:C:2349:ARG:NH1 | 2.33 | 0.60 |
| 1:E:111:ILE:HG13 | 1:H:2214:ARG:HH21 | 1.65 | 0.60 |
| 1:F:1272:SER:N | 1:F:1275:GLU:OE2 | 2.33 | 0.60 |
| 1:G:183:VAL:HG21 | 1:G:365:TYR:CE1 | 2.36 | 0.60 |
| 1:H:188:ILE:HG21 | 1:H:215:HIS:NE2 | 2.15 | 0.60 |
| 1:H:2251:VAL:HG22 | 1:H:2263:GLN:HG3 | 1.82 | 0.60 |
| 1:H:3084:PHE:HD2 | 1:H:3122:ILE:HD11 | 1.66 | 0.60 |
| 1:I:1981:ALA:H | 1:I:2035:THR:HG1 | 1.49 | 0.60 |
| 1:I:2056:ARG:NH1 | 1:I:2057:ALA:O | 2.33 | 0.60 |
| 1:I:3064:LEU:O | 1:I:3067:GLN:NE2 | 2.34 | 0.60 |
| 1:K:2108:LYS:HG3 | 1:K:2112:ARG:HH12 | 1.66 | 0.60 |
| 1:K:2741:ARG:NH1 | 1:T:2866:PRO:O | 2.34 | 0.60 |
| 1:K:2962:ALA:HB2 | 1:K:3107:GLU:HG2 | 1.83 | 0.60 |
| 1:K:2989:ARG:NH1 | 1:K:3177:ILE:O | 2.34 | 0.60 |
| 1:M:231:LYS:HD3 | 1:M:237:TYR:CE1 | 2.35 | 0.60 |
| 1:M:1588:HIS:ND1 | 1:P:337:GLN:OE1 | 2.34 | 0.60 |
| 1:N:569:GLN:HB3 | 1:N:619:GLY:HA3 | 1.82 | 0.60 |
| 1:N:1015:GLU:N | 1:N:1015:GLU:OE1 | 2.34 | 0.60 |
| 1:N:1898:LEU:HD21 | 1:N:1965:ALA:HB1 | 1.83 | 0.60 |
| 1:P:526:THR:OG1 | 1:P:527:ARG:NH1 | 2.34 | 0.60 |
| 1:P:2112:ARG:O | 1:P:2116:LYS:NZ | 2.31 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:T:1472:GLN:NE2 | 1:T:1482:ASP:OD2 | 2.34 | 0.60 |
| 1:B:1285:ARG:O | 1:B:1340:ARG:NH1 | 2.34 | 0.60 |
| 1:B:2919:LYS:HD3 | 1:B:3184:HIS:HB2 | 1.83 | 0.60 |
| 1:D:221:ARG:HE | 1:D:283:TYR:HD2 | 1.47 | 0.60 |
| 1:E:1225:ASP:OD1 | 1:E:1229:LYS:N | 2.34 | 0.60 |
| 1:E:1899:GLN:HE22 | 1:E:1906:PRO:HA | 1.67 | 0.60 |
| 1:E:2348:THR:OG1 | 1:E:2349:ARG:NH1 | 2.33 | 0.60 |
| 1:G:527:ARG:HD3 | 1:G:528:PRO:HD2 | 1.83 | 0.60 |
| 1:G:3133:GLN:NE2 | 1:G:3138:ARG:O | 2.34 | 0.60 |
| 1:G:3191:ASN:OD1 | 1:G:3195:HIS:N | 2.33 | 0.60 |
| 1:I:1214:ASN:O | 1:I:1216:ARG:NH2 | 2.34 | 0.60 |
| 1:I:2248:VAL:HG13 | 1:I:2249:LEU:HD12 | 1.83 | 0.60 |
| 1:J:1777:ALA:HB1 | 1:J:1781:GLU:HG3 | 1.83 | 0.60 |
| 1:L:1098:ASN:HB2 | 1:L:1104:ARG:HD3 | 1.83 | 0.60 |
| 1:L:2041:LYS:HG3 | 1:L:2043:LEU:HD23 | 1.82 | 0.60 |
| 1:L:2745:GLU:OE1 | 1:L:2749:TRP:NE1 | 2.34 | 0.60 |
| 1:M:2:SER:N | 1:M:280:GLY:O | 2.33 | 0.60 |
| 1:M:1433:LEU:HD11 | 1:M:1460:HIS:CE1 | 2.35 | 0.60 |
| 1:M:2248:VAL:HG13 | 1:M:2249:LEU:HD12 | 1.83 | 0.60 |
| 1:M:2529:LYS:HB3 | 1:M:2533:ARG:HH21 | 1.66 | 0.60 |
| 1:N:313:PHE:HE2 | 1:N:406:PRO:HB3 | 1.65 | 0.60 |
| 1:O:2348:THR:OG1 | 1:O:2349:ARG:NH1 | 2.33 | 0.60 |
| 1:O:3020:LEU:HB3 | 1:O:3024:LEU:HD11 | 1.82 | 0.60 |
| 1:P:1319:SER:OG | 1:P:1320:ALA:N | 2.34 | 0.60 |
| 1:P:2370:MET:HE1 | 1:P:2377:LEU:HB3 | 1.83 | 0.60 |
| 1:Q:2409:ARG:O | 1:Q:2471:TYR:HA | 2.01 | 0.60 |
| 1:R:3218:VAL:HG23 | 1:R:3261:VAL:HG13 | 1.83 | 0.60 |
| 1:T:1946:ASP:HB3 | 1:T:1950:HIS:CD2 | 2.36 | 0.60 |
| 1:T:3080:PHE:HA | 1:T:3083:GLN:HE22 | 1.66 | 0.60 |
| 1:A:231:LYS:HD3 | 1:A:237:TYR:HE1 | 1.66 | 0.60 |
| 1:A:1583:GLU:N | 1:D:340:SER:O | 2.35 | 0.60 |
| 1:B:1086:LYS:NZ | 1:B:1087:PRO:O | 2.33 | 0.60 |
| 1:B:1349:TRP:O | 1:B:1463:ASN:ND2 | 2.34 | 0.60 |
| 1:B:1963:ILE:HG23 | 1:B:1968:LEU:HD11 | 1.81 | 0.60 |
| 1:D:1012:CYS:SG | 1:D:1196:ARG:NH1 | 2.71 | 0.60 |
| 1:E:331:HIS:CD2 | 1:E:332:ASP:H | 2.19 | 0.60 |
| 1:F:3038:LYS:O | 1:F:3041:GLN:NE2 | 2.35 | 0.60 |
| 1:G:1495:PRO:HA | 1:G:1516:PRO:HD3 | 1.83 | 0.60 |
| 1:G:2108:LYS:HG3 | 1:G:2112:ARG:HH12 | 1.66 | 0.60 |
| 1:G:3154:LEU:H | 1:G:3172:SER:HB2 | 1.65 | 0.60 |
| 1:I:2048:ALA:HA | 1:J:1493:ARG:HH21 | 1.66 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:J:435:LYS:NZ | 1:J:439:THR:OG1 | 2.35 | 0.60 |
| 1:L:737:PHE:HB2 | 1:L:829:ILE:HB | 1.82 | 0.60 |
| 1:L:1222:SER:HB3 | 1:L:1230:LYS:HZ1 | 1.66 | 0.60 |
| 1:M:3226:ALA:HA | 1:M:3289:LYS:HA | 1.83 | 0.60 |
| 1:N:1087:PRO:HA | 1:N:1109:PRO:HD3 | 1.83 | 0.60 |
| 1:N:1192:TRP:HZ3 | 1:N:1194:TYR:HB2 | 1.66 | 0.60 |
| 1:N:3037:ILE:HG22 | 1:N:3042:HIS:H | 1.66 | 0.60 |
| 1:O:3307:ARG:NH1 | 1:O:3312:ASP:O | 2.34 | 0.60 |
| 1:P:2448:ASP:OD1 | 1:P:2449:THR:N | 2.33 | 0.60 |
| 1:R:473:LEU:H | 1:R:629:HIS:HB3 | 1.65 | 0.60 |
| 1:T:248:ARG:NH1 | 1:T:802:ASP:O | 2.34 | 0.60 |
| 1:T:447:GLU:HA | 1:T:450:GLN:HE21 | 1.67 | 0.60 |
| 1:T:527:ARG:O | 1:T:530:THR:OG1 | 2.19 | 0.60 |
| 1:T:580:TYR:HE2 | 1:T:959:GLU:HB3 | 1.65 | 0.60 |
| 1:T:1492:MET:N | 1:T:1492:MET:SD | 2.74 | 0.60 |
| 1:T:1713:PHE:HE1 | 1:T:1929:TYR:HB3 | 1.66 | 0.60 |
| 1:T:3113:PRO:HA | 1:T:3116:MET:HE2 | 1.83 | 0.60 |
| 1:A:454:ARG:NH2 | 1:A:514:ARG:O | 2.34 | 0.60 |
| 1:A:1587:ASN:OD1 | 1:D:337:GLN:N | 2.34 | 0.60 |
| 1:B:2111:LEU:HD13 | 1:B:2212:PHE:HE1 | 1.66 | 0.60 |
| 1:B:2149:HIS:HA | 1:B:2154:PHE:HD2 | 1.67 | 0.60 |
| 1:B:2542:ARG:HD3 | 1:B:2591:LEU:HD23 | 1.83 | 0.60 |
| 1:C:1417:THR:O | 1:C:1475:GLN:NE2 | 2.32 | 0.60 |
| 1:C:1671:THR:O | 1:C:1673:ARG:NH1 | 2.35 | 0.60 |
| 1:C:2586:GLU:O | 1:C:2590:THR:OG1 | 2.19 | 0.60 |
| 1:C:2929:LEU:HD22 | 1:C:2933:GLN:HG3 | 1.83 | 0.60 |
| 1:D:2283:LEU:HD21 | 1:D:2292:ASP:HB3 | 1.84 | 0.60 |
| 1:F:524:ASP:OD2 | 1:F:527:ARG:NH1 | 2.33 | 0.60 |
| 1:G:1531:ASP:OD1 | 1:G:1532:THR:N | 2.35 | 0.60 |
| 1:G:1715:ALA:HB1 | 1:G:1873:HIS:HA | 1.83 | 0.60 |
| 1:H:527:ARG:O | 1:H:530:THR:OG1 | 2.19 | 0.60 |
| 1:H:954:THR:HG22 | 1:H:965:PRO:HA | 1.82 | 0.60 |
| 1:H:2041:LYS:HG3 | 1:H:2043:LEU:HD23 | 1.84 | 0.60 |
| 1:I:159:THR:HG23 | 1:I:162:PHE:H | 1.67 | 0.60 |
| 1:I:881:ILE:HA | 1:I:884:PHE:HD2 | 1.64 | 0.60 |
| 1:J:230:GLN:NE2 | 1:J:236:THR:O | 2.34 | 0.60 |
| 1:J:2729:ASP:OD2 | 1:J:2732:SER:OG | 2.19 | 0.60 |
| 1:K:520:ILE:HD12 | 1:K:521:PRO:HD2 | 1.84 | 0.60 |
| 1:K:651:TRP:CZ3 | 1:K:655:GLN:HG3 | 2.37 | 0.60 |
| 1:K:2454:HIS:O | 1:K:2456:ARG:NH1 | 2.34 | 0.60 |
| 1:M:2570:GLY:HA2 | 1:M:2847:PHE:HE2 | 1.66 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:P:2791:GLU:OE1 | 1:P:2795:LYS:NZ | 2.31 | 0.60 |
| 1:R:256:ARG:O | 1:R:265:ARG:NH1 | 2.29 | 0.60 |
| 1:R:1088:LEU:HD22 | 1:R:1109:PRO:HG3 | 1.83 | 0.60 |
| 1:S:926:ARG:NH1 | 1:S:931:GLN:O | 2.34 | 0.60 |
| 1:S:2780:ASN:OD1 | 1:S:2781:PHE:N | 2.35 | 0.60 |
| 1:A:55:ARG:NH2 | 1:A:56:VAL:O | 2.35 | 0.60 |
| 1:A:3036:GLN:OE1 | 1:A:3043:GLN:NE2 | 2.34 | 0.60 |
| 1:C:613:PRO:HA | 1:C:616:LEU:HB3 | 1.83 | 0.60 |
| 1:D:1063:TRP:O | 1:D:1066:LEU:HG | 2.02 | 0.60 |
| 1:D:1222:SER:HA | 1:D:1233:SER:HB3 | 1.83 | 0.60 |
| 1:E:1465:ASP:OD2 | 1:E:1528:TYR:OH | 2.19 | 0.60 |
| 1:F:331:HIS:NE2 | 1:F:672:HIS:O | 2.33 | 0.60 |
| 1:F:698:ASN:ND2 | 1:F:705:GLU:OE2 | 2.24 | 0.60 |
| 1:F:1040:LEU:HD21 | 1:F:1184:LEU:HD11 | 1.84 | 0.60 |
| 1:G:2511:ILE:H | 1:G:2596:VAL:HG12 | 1.66 | 0.60 |
| 1:G:2666:ASP:OD2 | 1:G:2669:ASN:ND2 | 2.35 | 0.60 |
| 1:H:418:ASP:OD2 | 1:H:662:TYR:N | 2.33 | 0.60 |
| 1:I:1156:HIS:HB3 | 1:I:1193:GLN:HE22 | 1.65 | 0.60 |
| 1:I:2313:GLN:HG2 | 1:I:2320:TYR:HB3 | 1.83 | 0.60 |
| 1:I:2981:MET:SD | 1:I:2982:PRO:HD2 | 2.41 | 0.60 |
| 1:K:255:ASP:OD1 | 1:K:256:ARG:N | 2.35 | 0.60 |
| 1:K:1723:PRO:O | 1:K:1728:ARG:NH1 | 2.34 | 0.60 |
| 1:K:2190:LEU:HD21 | 1:K:2194:PHE:HD2 | 1.67 | 0.60 |
| 1:L:527:ARG:O | 1:L:530:THR:OG1 | 2.19 | 0.60 |
| 1:L:2253:GLU:OE2 | 1:L:2388:GLN:NE2 | 2.33 | 0.60 |
| 1:M:1583:GLU:OE2 | 1:P:327:LYS:NZ | 2.34 | 0.60 |
| 1:M:2001:CYS:HA | 1:M:2007:CYS:HB3 | 1.83 | 0.60 |
| 1:N:2112:ARG:HH11 | 1:N:2208:LEU:HD22 | 1.67 | 0.60 |
| 1:O:1518:ASP:OD1 | 1:O:1525:HIS:ND1 | 2.21 | 0.60 |
| 1:P:1100:ASP:O | 1:P:1104:ARG:NH1 | 2.34 | 0.60 |
| 1:P:2112:ARG:HE | 1:P:2116:LYS:HZ1 | 1.49 | 0.60 |
| 1:Q:1338:LEU:HD21 | 1:Q:1345:SER:HA | 1.83 | 0.60 |
| 1:R:737:PHE:O | 1:R:829:ILE:N | 2.30 | 0.60 |
| 1:R:1862:GLY:HA3 | 1:R:1870:ALA:HB2 | 1.82 | 0.60 |
| 1:R:2526:GLU:HA | 1:R:2529:LYS:HG2 | 1.83 | 0.60 |
| 1:S:55:ARG:NH2 | 1:S:56:VAL:O | 2.34 | 0.60 |
| 1:S:738:VAL:HG23 | 1:S:789:ILE:HG21 | 1.83 | 0.60 |
| 1:S:799:LYS:N | 1:S:802:ASP:OD2 | 2.35 | 0.60 |
| 1:S:3216:GLY:HA2 | 1:S:3262:TYR:O | 2.00 | 0.60 |
| 1:T:238:ASP:OD1 | 1:T:239:HIS:ND1 | 2.31 | 0.60 |
| 1:T:671:THR:O | 1:T:695:ARG:NH2 | 2.34 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:T:1769:VAL:O | 1:T:1828:ASN:ND2 | 2.34 | 0.60 |
| 1:B:182:GLU:O | 1:B:186:ASN:ND2 | 2.34 | 0.60 |
| 1:B:881:ILE:HD12 | 1:B:920:GLN:HE22 | 1.67 | 0.60 |
| 1:B:1009:THR:HA | 1:B:1070:ARG:HH22 | 1.66 | 0.60 |
| 1:B:1015:GLU:N | 1:B:1015:GLU:OE1 | 2.33 | 0.60 |
| 1:B:3159:TYR:O | 1:B:3169:ARG:NH1 | 2.35 | 0.60 |
| 1:D:3149:ASN:HA | 1:D:3152:ARG:HD3 | 1.83 | 0.60 |
| 1:E:569:GLN:HB3 | 1:E:619:GLY:HA3 | 1.83 | 0.60 |
| 1:F:5:ARG:HG3 | 1:F:283:TYR:HA | 1.83 | 0.60 |
| 1:F:221:ARG:HE | 1:F:283:TYR:HD2 | 1.48 | 0.60 |
| 1:H:221:ARG:NH1 | 1:H:285:ASP:O | 2.35 | 0.60 |
| 1:H:1086:LYS:NZ | 1:H:1087:PRO:O | 2.34 | 0.60 |
| 1:H:2149:HIS:HA | 1:H:2154:PHE:HD2 | 1.66 | 0.60 |
| 1:H:2326:ALA:HB1 | 1:H:2329:TYR:HB2 | 1.83 | 0.60 |
| 1:I:2980:GLY:HA2 | 1:I:3258:TYR:HE1 | 1.65 | 0.60 |
| 1:J:63:MET:SD | 1:J:64:ALA:N | 2.74 | 0.60 |
| 1:J:1743:HIS:HD2 | 1:J:1885:HIS:HD2 | 1.48 | 0.60 |
| 1:J:2152:PRO:HD2 | 1:J:2329:TYR:HD1 | 1.66 | 0.60 |
| 1:K:111:ILE:HD13 | 1:K:122:LYS:HA | 1.83 | 0.60 |
| 1:K:608:VAL:HG22 | 1:K:768:LEU:HD22 | 1.83 | 0.60 |
| 1:K:2409:ARG:O | 1:K:2471:TYR:HA | 2.02 | 0.60 |
| 1:K:2929:LEU:HD22 | 1:K:2933:GLN:HG3 | 1.84 | 0.60 |
| 1:K:3307:ARG:NH1 | 1:K:3312:ASP:O | 2.34 | 0.60 |
| 1:L:580:TYR:CG | 1:L:958:PRO:HG2 | 2.37 | 0.60 |
| 1:L:2251:VAL:HG22 | 1:L:2263:GLN:HG3 | 1.83 | 0.60 |
| 1:L:2579:ARG:NH1 | 1:L:2766:ALA:O | 2.34 | 0.60 |
| 1:L:2583:VAL:HG21 | 1:L:2772:PHE:HD2 | 1.67 | 0.60 |
| 1:M:1334:GLU:OE1 | 1:M:1346:VAL:HB | 2.00 | 0.60 |
| 1:M:2130:HIS:NE2 | 1:M:2147:CYS:SG | 2.75 | 0.60 |
| 1:M:2174:SER:O | 1:N:1757:ARG:NH2 | 2.33 | 0.60 |
| 1:M:2586:GLU:O | 1:M:2590:THR:OG1 | 2.18 | 0.60 |
| 1:O:2663:GLU:HA | 1:O:2793:ILE:HD11 | 1.82 | 0.60 |
| 1:O:2666:ASP:OD1 | 1:O:2669:ASN:ND2 | 2.34 | 0.60 |
| 1:O:3390:SER:HB3 | 1:O:3395:ARG:HG3 | 1.82 | 0.60 |
| 1:P:3392:ASN:HB3 | 1:P:3395:ARG:HG2 | 1.84 | 0.60 |
| 1:Q:508:GLU:OE1 | 1:Q:520:ILE:N | 2.33 | 0.60 |
| 1:Q:1586:CYS:HA | 1:T:337:GLN:OE1 | 2.02 | 0.60 |
| 1:Q:3200:ILE:HA | 1:Q:3203:ILE:HG22 | 1.84 | 0.60 |
| 1:R:2951:ASN:ND2 | 1:R:3001:ASP:OD2 | 2.34 | 0.60 |
| 1:T:1663:ASN:OD1 | 1:T:1665:GLN:NE2 | 2.33 | 0.60 |
| 1:T:2729:ASP:OD2 | 1:T:2732:SER:OG | 2.19 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:T:3276:ASN:ND2 | 1:T:3279:SER:OG | 2.34 | 0.60 |
| 1:A:854:LEU:HD12 | 1:A:858:GLN:HG3 | 1.84 | 0.60 |
| 1:A:1327:ARG:NH1 | 1:A:1465:ASP:OD1 | 2.35 | 0.60 |
| 1:B:1896:GLN:NE2 | 1:B:1906:PRO:O | 2.34 | 0.60 |
| 1:E:851:VAL:HG12 | 1:E:935:PRO:HB2 | 1.84 | 0.60 |
| 1:E:2883:GLN:NE2 | 1:E:2884:LEU:O | 2.35 | 0.60 |
| 1:F:1086:LYS:HZ3 | 1:F:1087:PRO:HD2 | 1.66 | 0.60 |
| 1:F:2979:HIS:HA | 1:F:2984:PHE:HD2 | 1.67 | 0.60 |
| 1:G:1646:GLU:OE1 | 1:J:483:ARG:NH1 | 2.33 | 0.60 |
| 1:I:2566:CYS:O | 1:I:2577:TRP:NE1 | 2.35 | 0.60 |
| 1:I:3203:ILE:HA | 1:I:3206:ASN:HB2 | 1.84 | 0.60 |
| 1:J:182:GLU:O | 1:J:186:ASN:ND2 | 2.34 | 0.60 |
| 1:J:247:PHE:O | 1:J:271:LYS:NZ | 2.34 | 0.60 |
| 1:L:2263:GLN:HE22 | 1:L:2443:LYS:H | 1.49 | 0.60 |
| 1:M:159:THR:HG23 | 1:M:162:PHE:H | 1.66 | 0.60 |
| 1:M:307:GLU:O | 1:M:308:ARG:NE | 2.33 | 0.60 |
| 1:O:1262:SER:OG | 1:O:1263:HIS:N | 2.35 | 0.60 |
| 1:P:2316:ARG:HG2 | 1:P:2318:LEU:HG | 1.84 | 0.60 |
| 1:P:2824:ALA:HB2 | 1:P:2869:VAL:HG23 | 1.83 | 0.60 |
| 1:Q:2353:LEU:HD13 | 1:Q:2355:LYS:HD3 | 1.83 | 0.60 |
| 1:S:50:LYS:HG3 | 1:S:52:ASP:H | 1.65 | 0.60 |
| 1:S:3081:GLU:HA | 1:S:3084:PHE:HB3 | 1.83 | 0.60 |
| 1:S:3390:SER:HB3 | 1:S:3395:ARG:HG3 | 1.83 | 0.60 |
| 1:T:1254:ILE:HG23 | 1:T:1256:LYS:H | 1.66 | 0.60 |
| 1:T:3225:SER:O | 1:T:3290:TYR:N | 2.34 | 0.60 |
| 1:T:3324:ASN:OD1 | 1:T:3395:ARG:NH2 | 2.35 | 0.60 |
| 1:A:2001:CYS:HA | 1:A:2007:CYS:HB3 | 1.84 | 0.60 |
| 1:A:2990:LEU:HD21 | 1:A:3177:ILE:HD12 | 1.84 | 0.60 |
| 1:B:1149:VAL:N | 1:B:1203:THR:OG1 | 2.32 | 0.60 |
| 1:B:1348:TYR:OH | 1:B:1466:ARG:NH1 | 2.34 | 0.60 |
| 1:B:3032:PHE:HA | 1:B:3113:PRO:HG2 | 1.84 | 0.60 |
| 1:C:844:GLU:OE1 | 1:C:926:ARG:NH2 | 2.33 | 0.60 |
| 1:D:1501:ASP:HB3 | 1:D:1504:GLN:HB2 | 1.84 | 0.60 |
| 1:E:2553:TYR:CD1 | 1:E:2554:PRO:HA | 2.36 | 0.60 |
| 1:F:2896:PHE:O | 1:G:2734:ASN:ND2 | 2.33 | 0.60 |
| 1:F:2938:ARG:NH2 | 1:F:3029:ASN:OD1 | 2.35 | 0.60 |
| 1:G:2872:PHE:HD2 | 1:G:2892:PRO:HG2 | 1.67 | 0.60 |
| 1:I:1249:THR:O | 1:I:1251:LYS:NZ | 2.29 | 0.60 |
| 1:I:1723:PRO:O | 1:I:1728:ARG:NH1 | 2.34 | 0.60 |
| 1:K:605:GLN:HA | 1:K:608:VAL:HG12 | 1.82 | 0.60 |
| 1:K:1161:SER:OG | 1:K:1185:GLY:N | 2.30 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:K:3096:GLY:HA3 | 1:K:3104:SER:HB3 | 1.83 | 0.60 |
| 1:L:256:ARG:O | 1:L:265:ARG:NH1 | 2.30 | 0.60 |
| 1:M:31:THR:OG1 | 1:M:32:VAL:N | 2.34 | 0.60 |
| 1:M:1144:GLN:HA | 1:M:1148:ARG:HH22 | 1.66 | 0.60 |
| 1:N:1362:ILE:HD13 | 1:N:1456:LEU:HD11 | 1.84 | 0.60 |
| 1:N:2824:ALA:HB2 | 1:N:2869:VAL:HG23 | 1.84 | 0.60 |
| 1:O:2251:VAL:HG22 | 1:O:2263:GLN:HB3 | 1.83 | 0.60 |
| 1:P:2991:LEU:HA | 1:P:2994:GLN:HE21 | 1.66 | 0.60 |
| 1:Q:2601:TRP:O | 1:Q:2711:ASN:ND2 | 2.35 | 0.60 |
| 1:R:2944:LEU:HA | 1:R:3002:LYS:HE2 | 1.84 | 0.60 |
| 1:S:2056:ARG:NH1 | 1:S:2057:ALA:O | 2.35 | 0.60 |
| 1:T:2614:LEU:HD21 | 1:T:2636:ARG:HH11 | 1.67 | 0.60 |
| 1:B:925:LEU:HD22 | 1:B:928:LYS:HZ3 | 1.66 | 0.60 |
| 1:B:1049:PHE:O | 1:B:1053:HIS:ND1 | 2.33 | 0.60 |
| 1:B:3038:LYS:O | 1:B:3041:GLN:NE2 | 2.34 | 0.60 |
| 1:C:851:VAL:HG12 | 1:C:935:PRO:HB2 | 1.84 | 0.60 |
| 1:C:1652:ARG:NH1 | 1:C:1653:PRO:O | 2.35 | 0.60 |
| 1:D:247:PHE:HB3 | 1:D:271:LYS:HD2 | 1.84 | 0.60 |
| 1:D:996:THR:HG23 | 1:D:999:ALA:H | 1.66 | 0.60 |
| 1:D:2111:LEU:HD13 | 1:D:2212:PHE:HE1 | 1.67 | 0.60 |
| 1:F:527:ARG:O | 1:F:530:THR:OG1 | 2.20 | 0.60 |
| 1:F:1769:VAL:O | 1:F:1828:ASN:ND2 | 2.35 | 0.60 |
| 1:G:520:ILE:HD12 | 1:G:521:PRO:HD2 | 1.83 | 0.60 |
| 1:G:838:GLU:OE1 | 1:Q:2:SER:N | 2.34 | 0.60 |
| 1:H:1019:GLU:HA | 1:H:1022:HIS:NE2 | 2.17 | 0.60 |
| 1:I:176:HIS:HE1 | 1:I:180:GLN:HE21 | 1.49 | 0.60 |
| 1:I:1626:ASP:OD1 | 1:I:1627:SER:N | 2.34 | 0.60 |
| 1:I:3284:GLN:HE22 | 1:I:3286:THR:HG23 | 1.67 | 0.60 |
| 1:J:3113:PRO:HA | 1:J:3116:MET:HE2 | 1.83 | 0.60 |
| 1:K:1865:LYS:HB3 | 1:K:1868:SER:HB3 | 1.83 | 0.60 |
| 1:L:43:GLY:O | 1:L:46:SER:OG | 2.20 | 0.60 |
| 1:L:297:TYR:O | 1:L:300:LEU:HG | 2.02 | 0.60 |
| 1:M:1632:ASP:HB3 | 1:N:1917:ARG:HH22 | 1.67 | 0.60 |
| 1:M:1730:ALA:N | 1:M:2020:ALA:O | 2.35 | 0.60 |
| 1:M:2994:GLN:OE1 | 1:M:3165:ASN:ND2 | 2.33 | 0.60 |
| 1:N:2745:GLU:OE1 | 1:N:2749:TRP:NE1 | 2.35 | 0.60 |
| 1:O:1316:VAL:HG11 | 1:O:1321:VAL:HG13 | 1.83 | 0.60 |
| 1:P:1011:PHE:HA | 1:P:1063:TRP:HH2 | 1.66 | 0.60 |
| 1:P:3122:ILE:HA | 1:P:3125:ILE:HG12 | 1.84 | 0.60 |
| 1:Q:376:LEU:HB3 | 1:Q:378:LYS:NZ | 2.17 | 0.60 |
| 1:Q:1351:TRP:HE1 | 1:Q:1460:HIS:HD2 | 1.47 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:R:735:ARG:HH22 | 1:R:790:THR:H | 1.49 | 0.60 |
| 1:R:1728:ARG:HH21 | 4:T:3501:NAG:H81 | 1.67 | 0.60 |
| 1:R:2338:ASN:OD1 | 1:R:2339:SER:N | 2.35 | 0.60 |
| 1:S:259:ASN:O | 1:S:265:ARG:NH2 | 2.35 | 0.60 |
| 1:S:711:ASP:OD1 | 1:S:712:ASN:N | 2.35 | 0.60 |
| 1:T:954:THR:HG22 | 1:T:965:PRO:HA | 1.82 | 0.60 |
| 1:A:31:THR:OG1 | 1:A:32:VAL:N | 2.33 | 0.60 |
| 1:A:854:LEU:HD12 | 1:A:858:GLN:HE21 | 1.66 | 0.60 |
| 1:C:1284:ARG:NH2 | 1:C:1376:GLU:OE1 | 2.35 | 0.60 |
| 1:C:1750:PHE:HD2 | 1:C:1882:LEU:HD11 | 1.67 | 0.60 |
| 1:E:275:SER:HB3 | 1:E:278:GLN:HE22 | 1.67 | 0.60 |
| 1:F:3131:THR:HA | 1:F:3134:LYS:HZ3 | 1.65 | 0.60 |
| 1:G:473:LEU:HD23 | 1:G:775:LYS:HZ1 | 1.67 | 0.60 |
| 1:H:244:VAL:HG22 | 1:H:828:ILE:HG21 | 1.84 | 0.60 |
| 1:I:2001:CYS:HA | 1:I:2007:CYS:HB3 | 1.84 | 0.60 |
| 1:K:2778:ASP:OD1 | 1:K:2779:LEU:N | 2.35 | 0.60 |
| 1:L:182:GLU:O | 1:L:186:ASN:ND2 | 2.34 | 0.60 |
| 1:L:1067:GLN:HG3 | 1:L:1070:ARG:HH21 | 1.67 | 0.60 |
| 1:M:881:ILE:HA | 1:M:884:PHE:HD2 | 1.67 | 0.60 |
| 1:M:2330:MET:HE1 | 1:M:2354:PRO:HG2 | 1.84 | 0.60 |
| 1:N:1004:LEU:O | 1:N:1008:GLN:NE2 | 2.35 | 0.60 |
| 1:N:3113:PRO:HA | 1:N:3116:MET:HE2 | 1.83 | 0.60 |
| 1:P:958:PRO:HA | 1:P:961:ASN:HA | 1.84 | 0.60 |
| 1:P:3229:ASN:H | 1:P:3286:THR:HG22 | 1.67 | 0.60 |
| 1:Q:937:TRP:O | 1:Q:1055:ASN:ND2 | 2.34 | 0.60 |
| 1:Q:2254:GLN:N | 1:Q:2254:GLN:OE1 | 2.35 | 0.60 |
| 1:Q:2820:ASP:OD1 | 1:Q:2831:ALA:N | 2.33 | 0.60 |
| 1:R:1652:ARG:HD3 | 1:R:1653:PRO:HD2 | 1.82 | 0.60 |
| 1:R:2394:PHE:HB2 | 1:R:2492:ILE:HB | 1.84 | 0.60 |
| 1:A:231:LYS:HD3 | 1:A:237:TYR:CE1 | 2.37 | 0.59 |
| 1:A:2994:GLN:OE1 | 1:A:3165:ASN:ND2 | 2.29 | 0.59 |
| 1:A:3046:ARG:NH2 | 1:A:3112:ASP:OD2 | 2.35 | 0.59 |
| 1:A:3088:HIS:O | 1:A:3092:HIS:ND1 | 2.34 | 0.59 |
| 1:B:3229:ASN:H | 1:B:3286:THR:HG22 | 1.67 | 0.59 |
| 1:C:1448:LEU:HA | 1:C:1451:SER:HB2 | 1.84 | 0.59 |
| 1:D:23:LEU:HD23 | 1:D:123:ASN:HD21 | 1.66 | 0.59 |
| 1:D:1169:CYS:HA | 1:D:1175:CYS:HA | 1.84 | 0.59 |
| 1:D:2387:HIS:HB3 | 1:D:2392:ARG:HH21 | 1.66 | 0.59 |
| 1:F:614:HIS:HA | 1:F:625:LEU:HG | 1.83 | 0.59 |
| 1:F:2720:GLN:HE22 | 1:F:2730:TYR:HB2 | 1.65 | 0.59 |
| 1:F:3270:LEU:HD22 | 1:F:3275:LEU:HB2 | 1.84 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:G:16:VAL:HG21 | 1:G:105:ARG:HH22 | 1.67 | 0.59 |
| 1:J:231:LYS:HB3 | 1:J:237:TYR:HE1 | 1.66 | 0.59 |
| 1:J:652:GLN:NE2 | 1:J:652:GLN:O | 2.35 | 0.59 |
| 1:J:1433:LEU:HD21 | 1:J:1460:HIS:NE2 | 2.17 | 0.59 |
| 1:K:2755:ASP:OD1 | 1:K:2758:ARG:NH2 | 2.35 | 0.59 |
| 1:K:2981:MET:SD | 1:K:2982:PRO:HD2 | 2.42 | 0.59 |
| 1:L:1433:LEU:HD21 | 1:L:1460:HIS:NE2 | 2.16 | 0.59 |
| 1:M:454:ARG:NH2 | 1:M:514:ARG:O | 2.35 | 0.59 |
| 1:N:1416:GLN:HE21 | 1:N:1422:PHE:HA | 1.66 | 0.59 |
| 1:O:1201:GLU:OE2 | 1:O:1203:THR:N | 2.32 | 0.59 |
| 1:O:1914:GLU:OE1 | 1:P:1655:LEU:HD23 | 2.01 | 0.59 |
| 1:O:2553:TYR:CD1 | 1:O:2554:PRO:HA | 2.37 | 0.59 |
| 1:O:2796:ARG:HH22 | 1:O:2801:ARG:HE | 1.49 | 0.59 |
| 1:P:696:PRO:HA | 1:P:699:ILE:HD13 | 1.82 | 0.59 |
| 1:P:1501:ASP:HB3 | 1:P:1504:GLN:HB2 | 1.84 | 0.59 |
| 1:Q:481:ASP:OD1 | 1:T:1644:TYR:N | 2.32 | 0.59 |
| 1:Q:2686:GLY:HA2 | 1:Q:2693:MET:HB3 | 1.84 | 0.59 |
| 1:R:461:VAL:HG12 | 1:R:1371:ARG:HB2 | 1.84 | 0.59 |
| 1:R:1153:PHE:O | 1:R:1198:PHE:HB3 | 2.02 | 0.59 |
| 1:R:2567:CYS:O | 1:R:2569:HIS:ND1 | 2.35 | 0.59 |
| 1:R:2970:ALA:O | 1:R:2973:ARG:NE | 2.29 | 0.59 |
| 1:S:574:LEU:HD23 | 1:S:616:LEU:HG | 1.83 | 0.59 |
| 1:S:2405:SER:HB3 | 1:S:2426:PHE:HE1 | 1.66 | 0.59 |
| 1:T:454:ARG:NH2 | 1:T:1338:LEU:HG | 2.17 | 0.59 |
| 1:T:934:LEU:HD12 | 1:T:935:PRO:HD2 | 1.84 | 0.59 |
| 1:A:2551:HIS:HB2 | 1:A:2581:PHE:CE1 | 2.37 | 0.59 |
| 1:B:737:PHE:N | 1:B:829:ILE:O | 2.28 | 0.59 |
| 1:B:738:VAL:HG23 | 1:B:789:ILE:HG13 | 1.83 | 0.59 |
| 1:B:2806:PHE:CE2 | 1:B:2892:PRO:HB3 | 2.37 | 0.59 |
| 1:B:2938:ARG:NH2 | 1:B:3029:ASN:OD1 | 2.34 | 0.59 |
| 1:C:50:LYS:HE2 | 1:C:357:MET:HG3 | 1.84 | 0.59 |
| 1:C:2383:GLU:O | 1:C:2387:HIS:ND1 | 2.35 | 0.59 |
| 1:D:182:GLU:O | 1:D:186:ASN:ND2 | 2.35 | 0.59 |
| 1:D:188:ILE:HG21 | 1:D:215:HIS:NE2 | 2.17 | 0.59 |
| 1:D:1322:PHE:HB3 | 1:D:1323:PRO:HD3 | 1.83 | 0.59 |
| 1:E:2674:TYR:OH | 1:E:2712:VAL:O | 2.19 | 0.59 |
| 1:G:1267:ASN:HB3 | 1:G:1269:GLN:HE21 | 1.67 | 0.59 |
| 1:G:2345:ASN:HD22 | 1:G:2348:THR:HG23 | 1.67 | 0.59 |
| 1:H:2393:VAL:HG11 | 1:H:2450:LEU:HD12 | 1.83 | 0.59 |
| 1:I:1828:ASN:OD1 | 1:I:1829:TRP:N | 2.36 | 0.59 |
| 1:I:2148:LEU:HB3 | 1:I:2151:VAL:HG11 | 1.83 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:J:540:THR:HG22 | 1:J:551:HIS:HA | 1.84 | 0.59 |
| 1:J:1365:ALA:HA | 1:J:1378:ASN:HB3 | 1.84 | 0.59 |
| 1:K:2056:ARG:NH1 | 1:K:2057:ALA:O | 2.35 | 0.59 |
| 1:L:1088:LEU:HD22 | 1:L:1109:PRO:HG3 | 1.83 | 0.59 |
| 1:L:1162:ALA:HB3 | 1:L:1183:ILE:HD11 | 1.83 | 0.59 |
| 1:L:1871:HIS:HE1 | 1:L:2018:GLY:HA3 | 1.65 | 0.59 |
| 1:L:2806:PHE:CE1 | 1:L:2892:PRO:HB3 | 2.37 | 0.59 |
| 1:M:1910:ASN:ND2 | 1:N:1657:PHE:O | 2.35 | 0.59 |
| 1:M:2551:HIS:HB2 | 1:M:2581:PHE:CE1 | 2.37 | 0.59 |
| 1:M:2778:ASP:OD1 | 1:M:2779:LEU:N | 2.35 | 0.59 |
| 1:N:1568:SER:N | 1:N:1597:GLY:O | 2.35 | 0.59 |
| 1:N:3082:VAL:O | 1:N:3086:MET:HG2 | 2.02 | 0.59 |
| 1:O:288:LEU:N | 1:O:291:LEU:O | 2.36 | 0.59 |
| 1:O:465:GLN:HG2 | 1:O:560:ALA:HB2 | 1.84 | 0.59 |
| 1:P:3038:LYS:O | 1:P:3041:GLN:NE2 | 2.35 | 0.59 |
| 1:P:3382:GLU:O | 1:P:3386:TYR:OH | 2.16 | 0.59 |
| 1:Q:2994:GLN:OE1 | 1:Q:3165:ASN:ND2 | 2.33 | 0.59 |
| 1:R:434:ARG:NH2 | 1:R:508:GLU:OE1 | 2.34 | 0.59 |
| 1:R:1169:CYS:HA | 1:R:1175:CYS:HA | 1.84 | 0.59 |
| 1:S:1240:THR:HA | 1:T:2328:ASN:HD21 | 1.68 | 0.59 |
| 1:S:2535:VAL:HG22 | 1:S:2592:GLN:HE21 | 1.66 | 0.59 |
| 1:S:3096:GLY:HA3 | 1:S:3104:SER:HB3 | 1.82 | 0.59 |
| 1:T:245:GLU:HA | 1:T:248:ARG:HD2 | 1.84 | 0.59 |
| 1:A:248:ARG:NH1 | 1:A:802:ASP:O | 2.35 | 0.59 |
| 1:A:1262:SER:OG | 1:A:1263:HIS:N | 2.34 | 0.59 |
| 1:A:1583:GLU:HB2 | 1:D:340:SER:HB3 | 1.83 | 0.59 |
| 1:A:2714:ARG:NH2 | 1:A:2778:ASP:O | 2.35 | 0.59 |
| 1:B:2191:PRO:HG2 | 1:B:2194:PHE:CD2 | 2.37 | 0.59 |
| 1:C:494:ALA:HB3 | 1:C:670:MET:HE3 | 1.84 | 0.59 |
| 1:C:520:ILE:HD12 | 1:C:521:PRO:HD2 | 1.84 | 0.59 |
| 1:C:605:GLN:HA | 1:C:608:VAL:HG12 | 1.84 | 0.59 |
| 1:F:1676:ILE:HG13 | 1:F:1761:VAL:HG23 | 1.84 | 0.59 |
| 1:F:2785:THR:OG1 | 1:F:2788:GLN:OE1 | 2.16 | 0.59 |
| 1:G:559:VAL:N | 1:G:564:GLU:O | 2.32 | 0.59 |
| 1:H:459:THR:OG1 | 1:H:1285:ARG:NH1 | 2.35 | 0.59 |
| 1:I:520:ILE:HD12 | 1:I:521:PRO:HD2 | 1.83 | 0.59 |
| 1:I:3200:ILE:HA | 1:I:3203:ILE:HG22 | 1.84 | 0.59 |
| 1:J:2745:GLU:OE1 | 1:J:2749:TRP:NE1 | 2.35 | 0.59 |
| 1:K:313:PHE:HZ | 1:K:326:ILE:HD13 | 1.67 | 0.59 |
| 1:K:2970:ALA:O | 1:K:2973:ARG:NH1 | 2.29 | 0.59 |
| 1:K:3105:THR:O | 1:K:3109:SER:HB3 | 2.02 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:L:1086:LYS:NZ | 1:L:1087:PRO:O | 2.34 | 0.59 |
| 1:L:2865:ARG:HD3 | 1:L:2867:ASP:H | 1.67 | 0.59 |
| 1:M:939:TRP:HA | 1:M:943:MET:HE1 | 1.83 | 0.59 |
| 1:M:2093:ARG:NH1 | 1:M:2177:ALA:O | 2.35 | 0.59 |
| 1:N:501:ARG:HH21 | 1:N:702:TYR:HB3 | 1.67 | 0.59 |
| 1:N:658:ARG:NH2 | 1:N:724:ASP:OD1 | 2.35 | 0.59 |
| 1:N:1040:LEU:HD21 | 1:N:1184:LEU:HD21 | 1.84 | 0.59 |
| 1:N:3058:GLN:N | 1:N:3061:LEU:O | 2.32 | 0.59 |
| 1:N:3085:GLU:O | 1:N:3089:ASN:ND2 | 2.35 | 0.59 |
| 1:O:881:ILE:HA | 1:O:884:PHE:HD2 | 1.66 | 0.59 |
| 1:O:2000:VAL:HG12 | 1:O:2051:VAL:HG22 | 1.83 | 0.59 |
| 1:P:473:LEU:H | 1:P:629:HIS:HB3 | 1.67 | 0.59 |
| 1:P:719:THR:H | 1:P:722:GLN:NE2 | 2.00 | 0.59 |
| 1:P:912:HIS:HE2 | 1:P:1113:PHE:HE1 | 1.49 | 0.59 |
| 1:P:2988:HIS:HA | 1:P:2991:LEU:HD12 | 1.84 | 0.59 |
| 1:P:3010:TYR:OH | 1:P:3189:ASN:OD1 | 2.17 | 0.59 |
| 1:P:3026:SER:OG | 1:P:3030:ASN:ND2 | 2.35 | 0.59 |
| 1:Q:2456:ARG:N | 1:Q:2459:ASP:OD2 | 2.36 | 0.59 |
| 1:Q:2663:GLU:HA | 1:Q:2793:ILE:HD11 | 1.84 | 0.59 |
| 1:R:244:VAL:HG23 | 1:R:248:ARG:HE | 1.67 | 0.59 |
| 1:R:757:PRO:HB2 | 1:R:760:GLY:H | 1.67 | 0.59 |
| 1:R:2745:GLU:OE1 | 1:R:2749:TRP:NE1 | 2.35 | 0.59 |
| 1:R:3234:PRO:HG2 | 1:R:3237:GLY:HA3 | 1.83 | 0.59 |
| 1:S:675:LEU:HD11 | 1:S:696:PRO:HG3 | 1.84 | 0.59 |
| 1:S:3200:ILE:HA | 1:S:3203:ILE:HG22 | 1.84 | 0.59 |
| 1:T:2616:ASP:OD1 | 1:T:2617:LYS:N | 2.35 | 0.59 |
| 1:A:1872:LEU:HD21 | 1:A:2016:LEU:HD13 | 1.84 | 0.59 |
| 1:B:1743:HIS:HD2 | 1:B:1885:HIS:CD2 | 2.18 | 0.59 |
| 1:B:2720:GLN:OE1 | 1:B:2730:TYR:HB2 | 2.01 | 0.59 |
| 1:C:1085:ARG:NH2 | 1:D:2462:ASN:O | 2.34 | 0.59 |
| 1:C:1931:LEU:HD23 | 1:D:2102:ARG:HA | 1.85 | 0.59 |
| 1:D:540:THR:HG22 | 1:D:551:HIS:HA | 1.85 | 0.59 |
| 1:D:1847:GLU:HA | 1:D:1850:PHE:HB3 | 1.85 | 0.59 |
| 1:D:3160:GLU:O | 1:D:3169:ARG:NH2 | 2.35 | 0.59 |
| 1:E:109:GLU:O | 1:E:123:ASN:ND2 | 2.23 | 0.59 |
| 1:E:711:ASP:OD1 | 1:E:712:ASN:ND2 | 2.35 | 0.59 |
| 1:F:1055:ASN:HA | 1:F:1058:ARG:HG3 | 1.84 | 0.59 |
| 1:F:2738:GLN:O | 1:F:2742:GLN:NE2 | 2.35 | 0.59 |
| 1:F:2741:ARG:NH1 | 1:G:2868:SER:O | 2.35 | 0.59 |
| 1:G:1518:ASP:OD1 | 1:G:1525:HIS:ND1 | 2.29 | 0.59 |
| 1:G:2261:GLU:HA | 1:G:2264:PHE:HD2 | 1.67 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:G:3200:ILE:HA | 1:G:3203:ILE:HG22 | 1.83 | 0.59 |
| 1:H:1019:GLU:HA | 1:H:1022:HIS:CD2 | 2.38 | 0.59 |
| 1:H:1809:VAL:HG22 | 1:H:1811:ARG:HH12 | 1.67 | 0.59 |
| 1:H:2111:LEU:HD13 | 1:H:2212:PHE:HE1 | 1.67 | 0.59 |
| 1:I:1085:ARG:NH1 | 1:J:2462:ASN:O | 2.35 | 0.59 |
| 1:I:2439:ASP:OD2 | 1:I:2440:ARG:NH1 | 2.36 | 0.59 |
| 1:I:2641:GLN:NE2 | 1:I:2645:ASP:OD1 | 2.35 | 0.59 |
| 1:I:3160:GLU:HA | 1:I:3169:ARG:HH22 | 1.66 | 0.59 |
| 1:J:1785:ARG:HH22 | 1:J:1790:ASP:HA | 1.67 | 0.59 |
| 1:J:2979:HIS:HA | 1:J:2984:PHE:HD2 | 1.67 | 0.59 |
| 1:J:3211:ASP:OD1 | 1:J:3309:ALA:N | 2.35 | 0.59 |
| 1:K:78:GLU:OE2 | 1:K:91:VAL:N | 2.18 | 0.59 |
| 1:K:594:LEU:O | 1:K:597:ARG:NH2 | 2.36 | 0.59 |
| 1:K:1588:HIS:O | 1:N:337:GLN:NE2 | 2.35 | 0.59 |
| 1:K:1684:THR:OG1 | 1:K:1687:GLU:OE1 | 2.17 | 0.59 |
| 1:L:188:ILE:HA | 1:L:191:LEU:HD12 | 1.83 | 0.59 |
| 1:L:231:LYS:HB3 | 1:L:237:TYR:HE2 | 1.67 | 0.59 |
| 1:M:1770:ASN:OD1 | 1:M:1772:GLN:NE2 | 2.36 | 0.59 |
| 1:M:2780:ASN:OD1 | 1:M:2784:LEU:N | 2.36 | 0.59 |
| 1:N:1560:PHE:HZ | 1:N:1573:LEU:HD11 | 1.66 | 0.59 |
| 1:N:2393:VAL:HG11 | 1:N:2450:LEU:HD12 | 1.84 | 0.59 |
| 1:N:2416:ASN:ND2 | 1:N:2418:LYS:O | 2.34 | 0.59 |
| 1:N:2785:THR:OG1 | 1:N:2788:GLN:OE1 | 2.19 | 0.59 |
| 1:O:2566:CYS:O | 1:O:2577:TRP:NE1 | 2.35 | 0.59 |
| 1:P:231:LYS:HB3 | 1:P:237:TYR:HE1 | 1.68 | 0.59 |
| 1:P:3321:LEU:O | 1:P:3395:ARG:NH2 | 2.35 | 0.59 |
| 1:R:1058:ARG:NH1 | 1:R:1125:ASP:O | 2.35 | 0.59 |
| 1:S:3304:VAL:HG23 | 1:S:3317:ILE:HB | 1.84 | 0.59 |
| 1:T:499:TRP:NE1 | 1:T:676:LYS:O | 2.34 | 0.59 |
| 1:A:730:ARG:HG3 | 1:A:735:ARG:HH22 | 1.67 | 0.59 |
| 1:A:2580:LEU:HA | 1:A:2583:VAL:HG12 | 1.84 | 0.59 |
| 1:B:655:GLN:HG2 | 1:B:662:TYR:HB3 | 1.83 | 0.59 |
| 1:C:2579:ARG:NH1 | 1:C:2774:TYR:OH | 2.35 | 0.59 |
| 1:C:2796:ARG:NH1 | 1:C:2796:ARG:O | 2.36 | 0.59 |
| 1:D:1698:LEU:HD21 | 1:D:1757:ARG:HG3 | 1.84 | 0.59 |
| 1:E:3036:GLN:OE1 | 1:E:3043:GLN:NE2 | 2.36 | 0.59 |
| 1:E:3339:ARG:NH2 | 1:E:3376:ASP:O | 2.35 | 0.59 |
| 1:F:3334:ARG:HD3 | 1:F:3409:GLU:HB2 | 1.85 | 0.59 |
| 1:G:1575:ILE:O | 1:J:337:GLN:NE2 | 2.35 | 0.59 |
| 1:G:1708:GLN:HE21 | 1:G:1803:ALA:HB2 | 1.67 | 0.59 |
| 1:G:2974:TYR:HB3 | 1:H:3367:PRO:HB2 | 1.83 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:G:3096:GLY:HA3 | 1:G:3104:SER:HB3 | 1.85 | 0.59 |
| 1:I:284:ASP:OD1 | 1:I:285:ASP:N | 2.35 | 0.59 |
| 1:I:1585:ASN:OD1 | 1:I:1586:CYS:N | 2.36 | 0.59 |
| 1:I:3026:SER:OG | 1:I:3030:ASN:ND2 | 2.35 | 0.59 |
| 1:J:934:LEU:HD12 | 1:J:935:PRO:HD2 | 1.84 | 0.59 |
| 1:J:2967:PRO:O | 1:J:2973:ARG:NH1 | 2.36 | 0.59 |
| 1:K:1195:ASP:HB2 | 1:L:2441:LEU:HD21 | 1.83 | 0.59 |
| 1:L:254:PHE:CD2 | 1:L:264:THR:HB | 2.33 | 0.59 |
| 1:M:2566:CYS:O | 1:M:2577:TRP:NE1 | 2.35 | 0.59 |
| 1:N:499:TRP:NE1 | 1:N:676:LYS:O | 2.36 | 0.59 |
| 1:N:1541:PRO:O | 1:N:1544:GLU:HG3 | 2.02 | 0.59 |
| 1:O:454:ARG:NH2 | 1:O:514:ARG:O | 2.34 | 0.59 |
| 1:O:2883:GLN:NE2 | 1:O:2884:LEU:O | 2.35 | 0.59 |
| 1:P:1254:ILE:HG23 | 1:P:1256:LYS:H | 1.67 | 0.59 |
| 1:P:2064:SER:HG | 1:P:2066:SER:HG | 1.51 | 0.59 |
| 1:Q:1623:LEU:HD23 | 1:R:2785:THR:HG21 | 1.85 | 0.59 |
| 1:Q:2778:ASP:OD1 | 1:Q:2779:LEU:N | 2.35 | 0.59 |
| 1:S:2443:LYS:HZ2 | 1:S:2492:ILE:HD11 | 1.68 | 0.59 |
| 1:S:2665:ARG:HH12 | 1:S:2726:ARG:HD2 | 1.67 | 0.59 |
| 1:S:3171:ASN:HA | 1:S:3176:GLN:HE22 | 1.67 | 0.59 |
| 1:T:1541:PRO:O | 1:T:1544:GLU:HG3 | 2.02 | 0.59 |
| 1:T:2138:SER:OG | 1:T:2143:LYS:NZ | 2.35 | 0.59 |
| 1:A:2338:ASN:OD1 | 1:A:2339:SER:N | 2.36 | 0.59 |
| 1:B:32:VAL:HA | 1:B:37:ASN:HD21 | 1.67 | 0.59 |
| 1:B:188:ILE:HD13 | 1:B:215:HIS:NE2 | 2.18 | 0.59 |
| 1:B:297:TYR:O | 1:B:300:LEU:HG | 2.03 | 0.59 |
| 1:B:2831:ALA:HA | 1:B:2858:VAL:HG11 | 1.84 | 0.59 |
| 1:C:711:ASP:OD1 | 1:C:712:ASN:N | 2.35 | 0.59 |
| 1:C:1251:LYS:HD2 | 1:C:1476:GLN:HE22 | 1.66 | 0.59 |
| 1:D:905:HIS:HA | 1:D:910:PHE:HD2 | 1.67 | 0.59 |
| 1:D:1153:PHE:HB2 | 1:D:1198:PHE:HD2 | 1.67 | 0.59 |
| 1:E:520:ILE:HD12 | 1:E:521:PRO:HD2 | 1.84 | 0.59 |
| 1:E:2114:LEU:HG | 1:E:2123:TRP:HB2 | 1.84 | 0.59 |
| 1:E:2234:LYS:HG3 | 1:E:2243:VAL:HG11 | 1.83 | 0.59 |
| 1:G:313:PHE:HZ | 1:G:326:ILE:HD13 | 1.68 | 0.59 |
| 1:I:2018:GLY:N | 1:I:2021:GLU:OE2 | 2.34 | 0.59 |
| 1:I:2533:ARG:NH1 | 1:I:2621:PRO:HD3 | 2.17 | 0.59 |
| 1:I:2994:GLN:OE1 | 1:I:3165:ASN:ND2 | 2.36 | 0.59 |
| 1:J:54:LYS:NZ | 1:J:355:ASN:OD1 | 2.30 | 0.59 |
| 1:J:1319:SER:OG | 1:J:1320:ALA:N | 2.34 | 0.59 |
| 1:J:1827:ASP:HA | 1:J:1831:TRP:CD1 | 2.38 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:K:307:GLU:O | 1:K:308:ARG:NE | 2.35 | 0.59 |
| 1:K:1415:GLU:OE1 | 1:K:1551:ARG:NH2 | 2.35 | 0.59 |
| 1:L:848:ARG:HB3 | 1:L:933:GLY:HA3 | 1.84 | 0.59 |
| 1:L:2979:HIS:HA | 1:L:2984:PHE:HD2 | 1.66 | 0.59 |
| 1:M:38:LEU:O | 1:M:73:TYR:OH | 2.16 | 0.59 |
| 1:M:313:PHE:HZ | 1:M:326:ILE:HD13 | 1.68 | 0.59 |
| 1:N:182:GLU:O | 1:N:186:ASN:ND2 | 2.35 | 0.59 |
| 1:O:755:ILE:HD11 | 1:O:763:TYR:HD2 | 1.67 | 0.59 |
| 1:O:903:CYS:O | 1:O:905:HIS:ND1 | 2.36 | 0.59 |
| 1:O:2114:LEU:HG | 1:O:2123:TRP:HB2 | 1.84 | 0.59 |
| 1:O:2273:TYR:HB2 | 1:O:2428:LEU:HD21 | 1.84 | 0.59 |
| 1:P:922:GLU:HG3 | 1:P:934:LEU:HB2 | 1.85 | 0.59 |
| 1:P:1041:ARG:NH2 | 1:P:1188:TYR:OH | 2.35 | 0.59 |
| 1:P:3360:LEU:HG | 1:P:3401:ARG:HD3 | 1.85 | 0.59 |
| 1:Q:69:TRP:HD1 | 1:Q:251:LEU:HD12 | 1.67 | 0.59 |
| 1:Q:307:GLU:O | 1:Q:308:ARG:NE | 2.35 | 0.59 |
| 1:Q:1388:THR:OG1 | 1:Q:1390:LYS:NZ | 2.36 | 0.59 |
| 1:Q:2962:ALA:HB2 | 1:Q:3107:GLU:HG2 | 1.84 | 0.59 |
| 1:R:1851:GLU:O | 1:R:1855:ASN:ND2 | 2.36 | 0.59 |
| 1:R:2112:ARG:HH11 | 1:R:2208:LEU:HD22 | 1.68 | 0.59 |
| 1:R:2113:ASP:OD1 | 1:R:2114:LEU:N | 2.35 | 0.59 |
| 1:R:2579:ARG:NH1 | 1:R:2766:ALA:O | 2.36 | 0.59 |
| 1:S:2797:ARG:HA | 1:S:2801:ARG:HH22 | 1.67 | 0.59 |
| 1:S:3395:ARG:NE | 1:S:3398:GLN:OE1 | 2.34 | 0.59 |
| 1:T:705:GLU:N | 1:T:705:GLU:OE1 | 2.36 | 0.59 |
| 1:A:1531:ASP:OD1 | 1:A:1532:THR:N | 2.35 | 0.59 |
| 1:A:1714:HIS:NE2 | 1:A:1732:CYS:SG | 2.76 | 0.59 |
| 1:A:2226:ARG:O | 1:D:113:LYS:NZ | 2.33 | 0.59 |
| 1:B:143:ARG:NH2 | 1:B:209:ASP:OD2 | 2.33 | 0.59 |
| 1:B:848:ARG:HD3 | 1:B:934:LEU:HB3 | 1.83 | 0.59 |
| 1:B:2393:VAL:HG11 | 1:B:2450:LEU:HD12 | 1.85 | 0.59 |
| 1:B:3084:PHE:HD1 | 1:B:3122:ILE:HD11 | 1.66 | 0.59 |
| 1:C:1413:ALA:HB1 | 1:C:1425:GLN:HG3 | 1.85 | 0.59 |
| 1:C:1756:ARG:NH2 | 1:D:2176:VAL:HG13 | 2.18 | 0.59 |
| 1:C:3056:ARG:NH1 | 1:C:3058:GLN:OE1 | 2.29 | 0.59 |
| 1:D:2138:SER:OG | 1:D:2143:LYS:NZ | 2.36 | 0.59 |
| 1:D:3132:LEU:HG | 1:D:3136:ARG:NH1 | 2.17 | 0.59 |
| 1:E:949:ILE:HG23 | 1:E:950:VAL:HG13 | 1.85 | 0.59 |
| 1:E:2088:PRO:O | 1:E:2090:ASN:N | 2.33 | 0.59 |
| 1:F:454:ARG:NH2 | 1:F:1338:LEU:HG | 2.17 | 0.59 |
| 1:F:1222:SER:HB3 | 1:F:1230:LYS:HZ1 | 1.66 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:G:277:ARG:NH2 | 1:Q:835:THR:OG1 | 2.35 | 0.59 |
| 1:G:3307:ARG:NH1 | 1:G:3312:ASP:O | 2.35 | 0.59 |
| 1:I:31:THR:OG1 | 1:I:32:VAL:N | 2.35 | 0.59 |
| 1:J:613:PRO:HA | 1:J:616:LEU:HB2 | 1.85 | 0.59 |
| 1:J:2919:LYS:HE3 | 1:J:3184:HIS:HB2 | 1.85 | 0.59 |
| 1:J:3077:TYR:HE1 | 1:J:3126:TRP:HE1 | 1.51 | 0.59 |
| 1:K:442:ASP:OD1 | 1:K:443:GLU:N | 2.35 | 0.59 |
| 1:L:3058:GLN:NE2 | 1:L:3268:ASP:OD2 | 2.36 | 0.59 |
| 1:N:1319:SER:OG | 1:N:1320:ALA:N | 2.36 | 0.59 |
| 1:O:2214:ARG:HH12 | 1:O:2216:TYR:HD2 | 1.51 | 0.59 |
| 1:P:1743:HIS:HD2 | 1:P:1885:HIS:CD2 | 2.20 | 0.59 |
| 1:R:312:SER:HB3 | 1:R:407:VAL:HG23 | 1.85 | 0.59 |
| 1:S:1294:LYS:O | 1:S:1297:SER:OG | 2.21 | 0.59 |
| 1:S:1433:LEU:HD11 | 1:S:1460:HIS:CD2 | 2.37 | 0.59 |
| 1:T:31:THR:O | 1:T:36:GLN:NE2 | 2.34 | 0.59 |
| 1:B:580:TYR:CG | 1:B:958:PRO:HG2 | 2.38 | 0.59 |
| 1:B:925:LEU:HD13 | 1:B:928:LYS:HE2 | 1.83 | 0.59 |
| 1:C:3289:LYS:HD2 | 1:C:3291:ASN:HD22 | 1.67 | 0.59 |
| 1:C:3395:ARG:HH21 | 1:C:3398:GLN:HE22 | 1.49 | 0.59 |
| 1:E:512:LYS:HA | 1:E:516:LEU:HB2 | 1.85 | 0.59 |
| 1:E:2200:TYR:OH | 1:E:2205:ASP:OD1 | 2.18 | 0.59 |
| 1:E:2456:ARG:N | 1:E:2459:ASP:OD2 | 2.36 | 0.59 |
| 1:F:46:SER:O | 1:F:55:ARG:NE | 2.34 | 0.59 |
| 1:F:913:TRP:CD1 | 1:F:1088:LEU:HD12 | 2.38 | 0.59 |
| 1:G:651:TRP:CZ3 | 1:G:655:GLN:HG3 | 2.38 | 0.59 |
| 1:G:2376:ASN:ND2 | 1:G:2379:GLU:OE2 | 2.35 | 0.59 |
| 1:H:505:VAL:HG21 | 1:H:706:LEU:HD12 | 1.84 | 0.59 |
| 1:H:1718:PRO:HG2 | 1:H:1728:ARG:HB3 | 1.84 | 0.59 |
| 1:I:38:LEU:O | 1:I:73:TYR:OH | 2.15 | 0.59 |
| 1:I:1632:ASP:HB3 | 1:J:1917:ARG:HH22 | 1.68 | 0.59 |
| 1:I:1651:ARG:NH2 | 1:J:2025:SER:O | 2.34 | 0.59 |
| 1:J:2865:ARG:HG2 | 1:J:2866:PRO:HD2 | 1.84 | 0.59 |
| 1:J:3351:VAL:HG23 | 1:J:3390:SER:HA | 1.83 | 0.59 |
| 1:K:646:ARG:HA | 1:K:710:TYR:HE2 | 1.67 | 0.59 |
| 1:K:1440:ARG:HH21 | 1:N:1368:PHE:HB3 | 1.67 | 0.59 |
| 1:K:2796:ARG:NH1 | 1:K:2796:ARG:O | 2.36 | 0.59 |
| 1:L:869:LEU:HD23 | 1:L:925:LEU:HD11 | 1.85 | 0.59 |
| 1:L:2551:HIS:HB2 | 1:L:2700:ALA:HB2 | 1.84 | 0.59 |
| 1:M:1896:GLN:NE2 | 1:M:1906:PRO:O | 2.29 | 0.59 |
| 1:O:229:LEU:HD21 | 1:O:296:LEU:HD11 | 1.84 | 0.59 |
| 1:O:1100:ASP:O | 1:O:1104:ARG:NH1 | 2.35 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:O:2044:SER:OG | 1:O:2046:ASP:OD1 | 2.16 | 0.59 |
| 1:P:32:VAL:HA | 1:P:37:ASN:HD21 | 1.68 | 0.59 |
| 1:P:182:GLU:O | 1:P:186:ASN:ND2 | 2.36 | 0.59 |
| 1:P:981:SER:HB3 | 1:P:1031:GLY:HA3 | 1.85 | 0.59 |
| 1:P:1348:TYR:OH | 1:P:1466:ARG:NH1 | 2.35 | 0.59 |
| 1:Q:1421:ASP:OD1 | 1:Q:1422:PHE:N | 2.35 | 0.59 |
| 1:R:2254:GLN:HE21 | 1:R:2260:PHE:HA | 1.67 | 0.59 |
| 1:R:2932:GLU:OE1 | 1:S:2939:ASN:ND2 | 2.35 | 0.59 |
| 1:S:711:ASP:OD1 | 1:S:712:ASN:ND2 | 2.36 | 0.59 |
| 1:S:854:LEU:HD12 | 1:S:858:GLN:HE21 | 1.67 | 0.59 |
| 1:T:1262:SER:OG | 1:T:1263:HIS:ND1 | 2.36 | 0.59 |
| 1:T:1599:GLU:OE2 | 1:T:1600:THR:OG1 | 2.20 | 0.59 |
| 1:T:2152:PRO:HD2 | 1:T:2329:TYR:HD2 | 1.68 | 0.59 |
| 1:T:3260:ARG:NH2 | 1:T:3407:ASP:OD2 | 2.34 | 0.59 |
| 1:A:465:GLN:HG2 | 1:A:560:ALA:HB2 | 1.83 | 0.59 |
| 1:A:481:ASP:OD1 | 1:D:1644:TYR:N | 2.35 | 0.59 |
| 1:A:520:ILE:HD12 | 1:A:521:PRO:HD2 | 1.85 | 0.59 |
| 1:B:2311:GLU:O | 1:B:2315:ARG:NH1 | 2.36 | 0.59 |
| 1:C:657:LYS:NZ | 1:C:720:ILE:O | 2.34 | 0.59 |
| 1:C:1426:PHE:HE1 | 1:C:1464:VAL:HG13 | 1.67 | 0.59 |
| 1:C:1782:PRO:O | 1:C:1795:ASN:N | 2.35 | 0.59 |
| 1:C:1835:LEU:HA | 1:C:1838:LEU:HD12 | 1.85 | 0.59 |
| 1:D:1086:LYS:HZ3 | 1:D:1087:PRO:HD2 | 1.67 | 0.59 |
| 1:D:2271:ILE:HD12 | 1:D:2298:HIS:NE2 | 2.17 | 0.59 |
| 1:E:310:LEU:HD23 | 1:E:366:HIS:HB3 | 1.84 | 0.59 |
| 1:E:2338:ASN:OD1 | 1:E:2339:SER:N | 2.35 | 0.59 |
| 1:F:493:MET:SD | 1:F:494:ALA:N | 2.74 | 0.59 |
| 1:F:580:TYR:HE2 | 1:F:959:GLU:HB3 | 1.67 | 0.59 |
| 1:F:1828:ASN:OD1 | 1:F:1831:TRP:N | 2.35 | 0.59 |
| 1:F:1851:GLU:O | 1:F:1855:ASN:ND2 | 2.35 | 0.59 |
| 1:F:2919:LYS:NZ | 1:F:3183:PHE:O | 2.32 | 0.59 |
| 1:F:3256:TRP:CD1 | 1:F:3256:TRP:H | 2.20 | 0.59 |
| 1:G:454:ARG:HH21 | 1:G:514:ARG:HB3 | 1.67 | 0.59 |
| 1:G:3386:TYR:HB2 | 1:G:3404:ILE:HG22 | 1.85 | 0.59 |
| 1:H:111:ILE:HG23 | 1:H:122:LYS:HB2 | 1.84 | 0.59 |
| 1:H:1599:GLU:OE2 | 1:H:1600:THR:OG1 | 2.21 | 0.59 |
| 1:H:1710:LEU:HD22 | 1:H:1750:PHE:HE1 | 1.66 | 0.59 |
| 1:H:2745:GLU:OE1 | 1:H:2749:TRP:NE1 | 2.36 | 0.59 |
| 1:I:2000:VAL:HG12 | 1:I:2051:VAL:HG22 | 1.83 | 0.59 |
| 1:J:737:PHE:CG | 1:J:786:LYS:HB3 | 2.38 | 0.59 |
| 1:J:1541:PRO:O | 1:J:1544:GLU:HG3 | 2.01 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:J:2666:ASP:OD1 | 1:J:2667:TYR:N | 2.35 | 0.59 |
| 1:K:1352:THR:HG21 | 1:K:1535:PHE:HE2 | 1.66 | 0.59 |
| 1:N:238:ASP:OD1 | 1:N:239:HIS:ND1 | 2.36 | 0.59 |
| 1:O:1067:GLN:NE2 | 1:O:1072:LEU:HB2 | 2.17 | 0.59 |
| 1:O:1201:GLU:OE2 | 1:O:1202:ILE:N | 2.35 | 0.59 |
| 1:O:2409:ARG:O | 1:O:2471:TYR:HA | 2.02 | 0.59 |
| 1:P:3266:VAL:HG21 | 1:P:3283:PHE:HE2 | 1.67 | 0.59 |
| 1:Q:1715:ALA:HB1 | 1:Q:1873:HIS:HA | 1.84 | 0.59 |
| 1:Q:2345:ASN:HD21 | 1:Q:2347:PHE:HB3 | 1.67 | 0.59 |
| 1:Q:2648:ARG:HD2 | 1:Q:2656:ARG:HE | 1.68 | 0.59 |
| 1:T:3213:VAL:O | 1:T:3267:THR:OG1 | 2.19 | 0.59 |
| 1:A:259:ASN:ND2 | 1:A:264:THR:OG1 | 2.36 | 0.59 |
| 1:A:1316:VAL:HG11 | 1:A:1321:VAL:HG13 | 1.85 | 0.59 |
| 1:A:2409:ARG:HG3 | 1:A:2424:ALA:HB2 | 1.83 | 0.59 |
| 1:B:238:ASP:OD1 | 1:B:239:HIS:ND1 | 2.35 | 0.59 |
| 1:B:934:LEU:HD12 | 1:B:935:PRO:HD2 | 1.83 | 0.59 |
| 1:C:230:GLN:NE2 | 1:C:235:LYS:HB2 | 2.18 | 0.59 |
| 1:C:2509:SER:O | 1:C:3138:ARG:NH1 | 2.36 | 0.59 |
| 1:D:248:ARG:NH1 | 1:D:802:ASP:O | 2.36 | 0.59 |
| 1:E:613:PRO:HB2 | 1:E:640:HIS:HE1 | 1.68 | 0.59 |
| 1:E:2056:ARG:NH1 | 1:E:2061:SER:O | 2.36 | 0.59 |
| 1:E:2778:ASP:OD1 | 1:E:2779:LEU:N | 2.36 | 0.59 |
| 1:E:3260:ARG:HE | 1:E:3261:VAL:H | 1.48 | 0.59 |
| 1:F:1433:LEU:HD21 | 1:F:1460:HIS:NE2 | 2.18 | 0.59 |
| 1:F:1785:ARG:NH1 | 1:F:1786:ASP:O | 2.36 | 0.59 |
| 1:G:2345:ASN:HD21 | 1:G:2347:PHE:HB3 | 1.68 | 0.59 |
| 1:H:571:GLN:NE2 | 1:H:616:LEU:O | 2.32 | 0.59 |
| 1:H:1319:SER:OG | 1:H:1320:ALA:N | 2.32 | 0.59 |
| 1:H:1427:GLU:O | 1:H:1431:ASN:ND2 | 2.36 | 0.59 |
| 1:H:1722:TYR:HD2 | 1:H:1725:ALA:HB2 | 1.68 | 0.59 |
| 1:L:1541:PRO:O | 1:L:1544:GLU:HG3 | 2.03 | 0.59 |
| 1:M:711:ASP:OD1 | 1:M:712:ASN:N | 2.36 | 0.59 |
| 1:M:2960:HIS:HE1 | 1:M:3119:HIS:HE1 | 1.51 | 0.59 |
| 1:O:276:TYR:HA | 1:O:279:LEU:HD23 | 1.85 | 0.59 |
| 1:O:1307:HIS:CG | 1:O:1602:MET:HE1 | 2.38 | 0.59 |
| 1:O:1814:LYS:HE2 | 1:O:1860:TRP:CZ3 | 2.38 | 0.59 |
| 1:O:2025:SER:O | 1:P:1651:ARG:NH2 | 2.35 | 0.59 |
| 1:P:190:TYR:HD2 | 1:P:349:PHE:HD2 | 1.51 | 0.59 |
| 1:P:297:TYR:O | 1:P:300:LEU:HG | 2.03 | 0.59 |
| 1:Q:1067:GLN:HE21 | 1:Q:1072:LEU:HB2 | 1.67 | 0.59 |
| 1:Q:2398:LEU:HB2 | 1:Q:2441:LEU:HD22 | 1.85 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:R:2666:ASP:OD1 | 1:R:2667:TYR:N | 2.36 | 0.59 |
| 1:S:2001:CYS:HA | 1:S:2007:CYS:HB3 | 1.84 | 0.59 |
| 1:T:960:THR:OG1 | 1:T:964:GLU:OE2 | 2.20 | 0.59 |
| 1:A:2:SER:N | 1:M:838:GLU:OE1 | 2.35 | 0.58 |
| 1:A:460:SER:O | 1:A:1371:ARG:NH1 | 2.36 | 0.58 |
| 1:A:1328:LEU:HD21 | 1:A:1519:VAL:HG22 | 1.84 | 0.58 |
| 1:A:1557:PHE:CG | 1:A:1611:LYS:HD2 | 2.38 | 0.58 |
| 1:A:1574:PHE:HB2 | 1:A:1634:GLU:HB3 | 1.83 | 0.58 |
| 1:A:2025:SER:O | 1:B:1651:ARG:NH2 | 2.36 | 0.58 |
| 1:A:2248:VAL:HG13 | 1:A:2249:LEU:HD12 | 1.84 | 0.58 |
| 1:B:481:ASP:HB3 | 1:I:1644:TYR:HB2 | 1.84 | 0.58 |
| 1:B:501:ARG:NE | 1:B:645:ASP:OD2 | 2.31 | 0.58 |
| 1:B:1676:ILE:HG13 | 1:B:1761:VAL:HG23 | 1.85 | 0.58 |
| 1:B:2923:ARG:NH1 | 1:B:3007:GLY:O | 2.36 | 0.58 |
| 1:C:1684:THR:N | 1:C:1687:GLU:OE2 | 2.31 | 0.58 |
| 1:E:2713:ASP:OD2 | 1:E:2776:TYR:OH | 2.20 | 0.58 |
| 1:F:1254:ILE:HG23 | 1:F:1256:LYS:H | 1.67 | 0.58 |
| 1:H:461:VAL:HG12 | 1:H:1371:ARG:HB2 | 1.85 | 0.58 |
| 1:H:1579:THR:HG21 | 1:H:1585:ASN:HB3 | 1.84 | 0.58 |
| 1:I:248:ARG:HH22 | 1:I:803:GLU:HG2 | 1.66 | 0.58 |
| 1:I:2387:HIS:O | 1:I:2392:ARG:NH1 | 2.36 | 0.58 |
| 1:J:2652:SER:O | 1:J:2656:ARG:NH1 | 2.35 | 0.58 |
| 1:J:3008:ILE:HG21 | 1:J:3116:MET:HB3 | 1.85 | 0.58 |
| 1:K:1708:GLN:HE21 | 1:K:1803:ALA:HB2 | 1.67 | 0.58 |
| 1:L:1026:HIS:HB3 | 1:L:1037:MET:HE1 | 1.85 | 0.58 |
| 1:N:881:ILE:HD12 | 1:N:920:GLN:HE22 | 1.67 | 0.58 |
| 1:N:2671:GLU:O | 1:N:2675:GLU:HG2 | 2.03 | 0.58 |
| 1:N:3334:ARG:HE | 1:N:3335:GLY:H | 1.51 | 0.58 |
| 1:O:1149:VAL:HG11 | 1:O:1206:LEU:HD13 | 1.85 | 0.58 |
| 1:O:1489:LEU:HA | 1:O:1492:MET:HG2 | 1.84 | 0.58 |
| 1:O:2567:CYS:O | 1:O:2569:HIS:ND1 | 2.36 | 0.58 |
| 1:O:2587:ARG:HH12 | 1:O:2753:PRO:HG2 | 1.68 | 0.58 |
| 1:P:1750:PHE:HD2 | 1:P:1882:LEU:HD11 | 1.68 | 0.58 |
| 1:P:2579:ARG:NH1 | 1:P:2766:ALA:O | 2.35 | 0.58 |
| 1:P:3144:ARG:HA | 1:P:3147:LEU:HG | 1.84 | 0.58 |
| 1:Q:1322:PHE:HB3 | 1:Q:1323:PRO:HD3 | 1.85 | 0.58 |
| 1:Q:3300:ALA:HA | 1:Q:3325:LYS:HE3 | 1.85 | 0.58 |
| 1:R:2657:GLN:OE1 | 1:R:2657:GLN:N | 2.34 | 0.58 |
| 1:S:323:ASN:OD1 | 1:S:324:VAL:N | 2.36 | 0.58 |
| 1:S:749:ALA:HA | 1:S:812:ASP:HA | 1.85 | 0.58 |
| 1:A:2249:LEU:HD23 | 1:A:2383:GLU:CD | 2.28 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:2733:ALA:HB3 | 1:A:2740:LEU:HD11 | 1.85 | 0.58 |
| 1:B:1827:ASP:O | 1:B:1832:LYS:NZ | 2.36 | 0.58 |
| 1:B:1828:ASN:OD1 | 1:B:1831:TRP:N | 2.37 | 0.58 |
| 1:C:31:THR:OG1 | 1:C:32:VAL:N | 2.34 | 0.58 |
| 1:C:183:VAL:HG21 | 1:C:365:TYR:CE1 | 2.38 | 0.58 |
| 1:C:1626:ASP:OD1 | 1:C:1627:SER:N | 2.36 | 0.58 |
| 1:C:2580:LEU:HA | 1:C:2583:VAL:HG12 | 1.85 | 0.58 |
| 1:D:244:VAL:HG23 | 1:D:248:ARG:HE | 1.68 | 0.58 |
| 1:D:1992:THR:CA | 1:D:2017:GLY:O | 2.51 | 0.58 |
| 1:D:3038:LYS:O | 1:D:3041:GLN:NE2 | 2.37 | 0.58 |
| 1:E:3037:ILE:HG12 | 1:E:3040:ALA:H | 1.68 | 0.58 |
| 1:G:330:ASP:OD1 | 1:G:331:HIS:N | 2.37 | 0.58 |
| 1:H:980:ARG:NH2 | 1:H:1046:ASP:OD1 | 2.36 | 0.58 |
| 1:H:3131:THR:HA | 1:H:3134:LYS:HE3 | 1.85 | 0.58 |
| 1:I:221:ARG:NH2 | 1:I:287:SER:O | 2.37 | 0.58 |
| 1:I:3113:PRO:HA | 1:I:3116:MET:HG3 | 1.85 | 0.58 |
| 1:J:1012:CYS:O | 1:J:1196:ARG:NH1 | 2.35 | 0.58 |
| 1:K:183:VAL:HG21 | 1:K:365:TYR:CE1 | 2.38 | 0.58 |
| 1:L:497:PRO:HG3 | 1:L:606:PHE:CE2 | 2.38 | 0.58 |
| 1:L:2393:VAL:HG11 | 1:L:2450:LEU:HD12 | 1.85 | 0.58 |
| 1:L:3260:ARG:NH2 | 1:L:3407:ASP:OD2 | 2.36 | 0.58 |
| 1:M:13:ASP:OD1 | 1:M:14:GLN:N | 2.37 | 0.58 |
| 1:M:2279:GLN:HG2 | 1:M:2281:TYR:H | 1.68 | 0.58 |
| 1:N:597:ARG:HD3 | 1:N:658:ARG:HH11 | 1.68 | 0.58 |
| 1:N:1322:PHE:HB3 | 1:N:1323:PRO:HD3 | 1.84 | 0.58 |
| 1:N:2338:ASN:OD1 | 1:N:2339:SER:N | 2.36 | 0.58 |
| 1:P:1728:ARG:NH2 | 4:R:3501:NAG:O7 | 2.36 | 0.58 |
| 1:Q:1730:ALA:N | 1:Q:2020:ALA:O | 2.35 | 0.58 |
| 1:Q:2669:ASN:HA | 1:Q:2672:VAL:HG12 | 1.84 | 0.58 |
| 1:R:613:PRO:HA | 1:R:616:LEU:HB2 | 1.85 | 0.58 |
| 1:R:1919:PRO:HB2 | 1:R:1924:SER:HB2 | 1.83 | 0.58 |
| 1:R:2636:ARG:HH21 | 1:R:2702:ASP:CG | 2.10 | 0.58 |
| 1:S:559:VAL:N | 1:S:564:GLU:O | 2.34 | 0.58 |
| 1:S:3036:GLN:HB2 | 1:S:3043:GLN:HE22 | 1.67 | 0.58 |
| 1:T:1828:ASN:OD1 | 1:T:1831:TRP:N | 2.36 | 0.58 |
| 1:T:2232:LEU:HD12 | 1:T:2274:LEU:HB3 | 1.84 | 0.58 |
| 1:T:2251:VAL:HG21 | 1:T:2267:THR:HG21 | 1.86 | 0.58 |
| 1:A:2456:ARG:N | 1:A:2459:ASP:OD2 | 2.36 | 0.58 |
| 1:C:1148:ARG:HG3 | 1:C:1244:ARG:HB3 | 1.85 | 0.58 |
| 1:C:3173:ARG:HB2 | 1:C:3176:GLN:HG3 | 1.85 | 0.58 |
| 1:D:1992:THR:C | 1:D:2017:GLY:O | 2.46 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:E:1284:ARG:NH2 | 1:E:1377:SER:O | 2.37 | 0.58 |
| 1:E:1576:CYS:HB3 | 1:E:1584:ARG:HD3 | 1.84 | 0.58 |
| 1:F:2264:PHE:HZ | 1:F:2302:VAL:HG13 | 1.68 | 0.58 |
| 1:F:2551:HIS:HB2 | 1:F:2700:ALA:HB2 | 1.84 | 0.58 |
| 1:G:711:ASP:OD1 | 1:G:712:ASN:N | 2.37 | 0.58 |
| 1:H:182:GLU:O | 1:H:186:ASN:ND2 | 2.36 | 0.58 |
| 1:I:1752:ASP:OD1 | 1:I:1753:ALA:N | 2.35 | 0.58 |
| 1:J:2078:LYS:HE3 | 1:J:2078:LYS:HA | 1.84 | 0.58 |
| 1:K:1328:LEU:HB3 | 1:K:1499:PHE:CE2 | 2.38 | 0.58 |
| 1:N:1769:VAL:O | 1:N:1828:ASN:ND2 | 2.36 | 0.58 |
| 1:N:3077:TYR:HE1 | 1:N:3126:TRP:HE1 | 1.50 | 0.58 |
| 1:O:756:LYS:NZ | 1:O:760:GLY:O | 2.35 | 0.58 |
| 1:O:953:GLU:O | 1:O:966:ASN:N | 2.29 | 0.58 |
| 1:P:3082:VAL:O | 1:P:3086:MET:HG2 | 2.03 | 0.58 |
| 1:Q:3260:ARG:HE | 1:Q:3261:VAL:H | 1.50 | 0.58 |
| 1:Q:3395:ARG:NE | 1:Q:3398:GLN:OE1 | 2.33 | 0.58 |
| 1:R:614:HIS:HA | 1:R:625:LEU:HG | 1.85 | 0.58 |
| 1:R:905:HIS:HA | 1:R:910:PHE:HD2 | 1.68 | 0.58 |
| 1:R:2194:PHE:HD1 | 1:R:2212:PHE:HB3 | 1.66 | 0.58 |
| 1:S:520:ILE:HD12 | 1:S:521:PRO:HD2 | 1.85 | 0.58 |
| 1:S:1417:THR:O | 1:S:1475:GLN:NE2 | 2.37 | 0.58 |
| 1:S:2056:ARG:NH1 | 1:S:2061:SER:O | 2.35 | 0.58 |
| 1:S:2997:MET:SD | 1:S:3000:ARG:NH1 | 2.76 | 0.58 |
| 1:T:458:ASP:HB2 | 1:T:1341:GLY:HA3 | 1.84 | 0.58 |
| 1:T:2044:SER:N | 1:T:2047:ASP:OD2 | 2.37 | 0.58 |
| 1:T:2055:LEU:HB2 | 1:T:2063:LEU:HB2 | 1.86 | 0.58 |
| 1:T:2339:SER:O | 1:T:2349:ARG:NH1 | 2.35 | 0.58 |
| 1:A:1144:GLN:OE1 | 1:A:1148:ARG:NH1 | 2.32 | 0.58 |
| 1:A:2085:GLN:HE21 | 1:A:2366:ARG:HH12 | 1.51 | 0.58 |
| 1:B:248:ARG:NH1 | 1:B:802:ASP:O | 2.35 | 0.58 |
| 1:B:869:LEU:HD23 | 1:B:925:LEU:HD11 | 1.85 | 0.58 |
| 1:D:1932:ASP:OD2 | 1:D:1935:THR:N | 2.28 | 0.58 |
| 1:D:2336:PRO:HB2 | 1:D:2342:LEU:HD12 | 1.85 | 0.58 |
| 1:D:2394:PHE:HB2 | 1:D:2492:ILE:HB | 1.86 | 0.58 |
| 1:D:2745:GLU:OE1 | 1:D:2749:TRP:NE1 | 2.36 | 0.58 |
| 1:E:711:ASP:OD1 | 1:E:712:ASN:N | 2.36 | 0.58 |
| 1:F:331:HIS:CE1 | 1:F:672:HIS:HB3 | 2.39 | 0.58 |
| 1:F:1086:LYS:NZ | 1:F:1087:PRO:O | 2.34 | 0.58 |
| 1:F:1332:GLN:OE1 | 1:F:1505:ASN:ND2 | 2.35 | 0.58 |
| 1:F:2738:GLN:HA | 1:F:2741:ARG:HH21 | 1.67 | 0.58 |
| 1:G:854:LEU:HD12 | 1:G:858:GLN:HE21 | 1.68 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:G:1225:ASP:OD1 | 1:G:1229:LYS:N | 2.36 | 0.58 |
| 1:H:757:PRO:HB2 | 1:H:760:GLY:H | 1.69 | 0.58 |
| 1:H:2264:PHE:HZ | 1:H:2302:VAL:HG13 | 1.66 | 0.58 |
| 1:I:836:HIS:HE1 | 1:O:277:ARG:HE | 1.52 | 0.58 |
| 1:I:2409:ARG:O | 1:I:2471:TYR:HA | 2.02 | 0.58 |
| 1:I:3096:GLY:HA3 | 1:I:3104:SER:HB3 | 1.86 | 0.58 |
| 1:I:3358:THR:H | 1:J:3329:LYS:HE3 | 1.69 | 0.58 |
| 1:K:38:LEU:O | 1:K:73:TYR:OH | 2.16 | 0.58 |
| 1:L:1319:SER:OG | 1:L:1320:ALA:N | 2.35 | 0.58 |
| 1:M:866:LEU:HD23 | 1:M:967:PRO:HB2 | 1.86 | 0.58 |
| 1:M:971:GLY:H | 1:M:978:THR:HG1 | 1.49 | 0.58 |
| 1:N:848:ARG:HH12 | 1:N:1121:TYR:HB2 | 1.68 | 0.58 |
| 1:O:3160:GLU:HG2 | 1:O:3169:ARG:HH22 | 1.69 | 0.58 |
| 1:Q:1195:ASP:HB2 | 1:R:2441:LEU:HD21 | 1.85 | 0.58 |
| 1:R:60:VAL:HG23 | 1:R:63:MET:HE2 | 1.84 | 0.58 |
| 1:R:934:LEU:HD12 | 1:R:935:PRO:HD2 | 1.84 | 0.58 |
| 1:R:2712:VAL:HA | 1:R:2715:GLN:NE2 | 2.18 | 0.58 |
| 1:A:2088:PRO:O | 1:A:2090:ASN:N | 2.36 | 0.58 |
| 1:B:1019:GLU:HA | 1:B:1022:HIS:NE2 | 2.17 | 0.58 |
| 1:B:1169:CYS:HA | 1:B:1175:CYS:HA | 1.85 | 0.58 |
| 1:B:2919:LYS:NZ | 1:B:3183:PHE:O | 2.27 | 0.58 |
| 1:B:3076:ASN:ND2 | 1:B:3079:ASP:OD2 | 2.30 | 0.58 |
| 1:C:111:ILE:HD13 | 1:C:122:LYS:HA | 1.86 | 0.58 |
| 1:C:490:VAL:HG13 | 1:C:493:MET:HB3 | 1.85 | 0.58 |
| 1:C:719:THR:HG21 | 1:C:847:VAL:HG21 | 1.85 | 0.58 |
| 1:C:1351:TRP:HE1 | 1:C:1460:HIS:HD2 | 1.51 | 0.58 |
| 1:C:2126:LEU:O | 1:C:2161:TYR:OH | 2.21 | 0.58 |
| 1:C:3213:VAL:HG23 | 1:C:3306:SER:HB2 | 1.86 | 0.58 |
| 1:D:1433:LEU:HA | 1:D:1436:LEU:HB2 | 1.85 | 0.58 |
| 1:E:307:GLU:O | 1:E:308:ARG:NE | 2.36 | 0.58 |
| 1:E:953:GLU:HG3 | 1:E:954:THR:HG23 | 1.85 | 0.58 |
| 1:F:727:ILE:HG22 | 1:F:730:ARG:HH21 | 1.66 | 0.58 |
| 1:F:846:HIS:HB3 | 1:F:1121:TYR:HA | 1.85 | 0.58 |
| 1:F:1913:LEU:HA | 1:F:1916:MET:HG3 | 1.84 | 0.58 |
| 1:G:2420:THR:HG21 | 1:G:2453:LEU:HD21 | 1.86 | 0.58 |
| 1:G:3043:GLN:HG3 | 1:G:3044:VAL:H | 1.68 | 0.58 |
| 1:H:1743:HIS:HD2 | 1:H:1885:HIS:CD2 | 2.22 | 0.58 |
| 1:H:2112:ARG:HE | 1:H:2116:LYS:HZ1 | 1.52 | 0.58 |
| 1:H:3103:MET:HA | 1:H:3109:SER:HA | 1.84 | 0.58 |
| 1:I:1145:HIS:ND1 | 1:I:1146:ASP:OD1 | 2.37 | 0.58 |
| 1:J:1004:LEU:O | 1:J:1008:GLN:NE2 | 2.31 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:K:939:TRP:HZ3 | 1:K:1055:ASN:HB3 | 1.68 | 0.58 |
| 1:K:1539:THR:HG23 | 1:K:1541:PRO:HD2 | 1.85 | 0.58 |
| 1:K:2585:LEU:HD23 | 1:K:2589:LEU:HD23 | 1.86 | 0.58 |
| 1:L:130:ILE:O | 1:L:138:HIS:HA | 2.03 | 0.58 |
| 1:L:245:GLU:HA | 1:L:248:ARG:HD2 | 1.86 | 0.58 |
| 1:L:248:ARG:NH1 | 1:L:802:ASP:O | 2.36 | 0.58 |
| 1:L:1232:SER:OG | 1:L:1234:GLU:OE1 | 2.21 | 0.58 |
| 1:L:2214:ARG:HH21 | 1:S:111:ILE:HG13 | 1.67 | 0.58 |
| 1:L:3077:TYR:HE1 | 1:L:3126:TRP:HE1 | 1.52 | 0.58 |
| 1:M:1294:LYS:O | 1:M:1297:SER:OG | 2.21 | 0.58 |
| 1:O:1557:PHE:CG | 1:O:1611:LYS:HD2 | 2.38 | 0.58 |
| 1:P:229:LEU:HB3 | 1:P:233:ARG:HH21 | 1.69 | 0.58 |
| 1:P:540:THR:HG22 | 1:P:551:HIS:HA | 1.85 | 0.58 |
| 1:P:1545:GLU:HG3 | 1:P:1549:ARG:HH12 | 1.68 | 0.58 |
| 1:P:2552:GLY:HA3 | 1:P:2697:GLU:HA | 1.84 | 0.58 |
| 1:Q:595:GLU:O | 1:Q:597:ARG:NH1 | 2.36 | 0.58 |
| 1:Q:599:PHE:HE2 | 1:Q:648:TRP:HE1 | 1.49 | 0.58 |
| 1:R:591:LEU:HB3 | 1:R:730:ARG:HH22 | 1.69 | 0.58 |
| 1:R:1541:PRO:O | 1:R:1544:GLU:HG3 | 2.03 | 0.58 |
| 1:R:2616:ASP:OD1 | 1:R:2617:LYS:N | 2.36 | 0.58 |
| 1:R:3088:HIS:CE1 | 1:R:3092:HIS:HE2 | 2.21 | 0.58 |
| 1:S:1978:LYS:NZ | 1:S:1979:SER:O | 2.35 | 0.58 |
| 1:S:2383:GLU:O | 1:S:2387:HIS:ND1 | 2.37 | 0.58 |
| 1:S:2926:VAL:HB | 1:S:3023:LEU:HD21 | 1.86 | 0.58 |
| 1:T:569:GLN:HB3 | 1:T:619:GLY:HA3 | 1.84 | 0.58 |
| 1:T:2824:ALA:HB2 | 1:T:2869:VAL:HG23 | 1.85 | 0.58 |
| 1:B:2337:PHE:O | 1:B:2349:ARG:NH2 | 2.33 | 0.58 |
| 1:C:1977:GLU:O | 1:C:2078:LYS:NZ | 2.28 | 0.58 |
| 1:C:2778:ASP:OD1 | 1:C:2779:LEU:N | 2.35 | 0.58 |
| 1:C:2962:ALA:HB2 | 1:C:3107:GLU:HG2 | 1.85 | 0.58 |
| 1:D:650:ILE:HD13 | 1:D:713:LEU:HB3 | 1.85 | 0.58 |
| 1:D:1743:HIS:HD2 | 1:D:1885:HIS:CD2 | 2.21 | 0.58 |
| 1:E:1506:GLU:CD | 1:E:1507:PHE:H | 2.10 | 0.58 |
| 1:E:1689:ARG:NE | 1:E:1786:ASP:OD1 | 2.28 | 0.58 |
| 1:E:2882:THR:HG21 | 4:E:3501:NAG:H3 | 1.85 | 0.58 |
| 1:G:1320:ALA:HA | 1:G:1423:GLU:HG3 | 1.84 | 0.58 |
| 1:H:2865:ARG:HD3 | 1:H:2867:ASP:H | 1.67 | 0.58 |
| 1:J:1271:LEU:HB2 | 1:J:1275:GLU:HG3 | 1.84 | 0.58 |
| 1:J:1828:ASN:OD1 | 1:J:1831:TRP:N | 2.36 | 0.58 |
| 1:J:2416:ASN:ND2 | 1:J:2418:LYS:O | 2.35 | 0.58 |
| 1:K:611:ASN:HD22 | 1:K:771:LEU:H | 1.50 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:K:1531:ASP:OD1 | 1:K:1532:THR:N | 2.36 | 0.58 |
| 1:K:2064:SER:HB3 | 1:K:2067:LEU:HG | 1.84 | 0.58 |
| 1:K:2926:VAL:HB | 1:K:3023:LEU:HD21 | 1.85 | 0.58 |
| 1:K:3301:THR:HB | 1:K:3325:LYS:HB3 | 1.85 | 0.58 |
| 1:L:1116:GLU:HA | 1:L:1120:GLN:HA | 1.85 | 0.58 |
| 1:L:2709:HIS:HA | 1:L:2712:VAL:HG22 | 1.84 | 0.58 |
| 1:M:1572:GLN:HB2 | 1:M:1636:LYS:HB2 | 1.86 | 0.58 |
| 1:M:1741:GLN:N | 1:M:1741:GLN:OE1 | 2.35 | 0.58 |
| 1:N:2639:ARG:HD3 | 1:N:2641:GLN:HE22 | 1.68 | 0.58 |
| 1:O:520:ILE:HD12 | 1:O:521:PRO:HD2 | 1.85 | 0.58 |
| 1:P:1232:SER:OG | 1:P:1234:GLU:OE1 | 2.21 | 0.58 |
| 1:Q:3317:ILE:HG12 | 1:Q:3339:ARG:HB3 | 1.85 | 0.58 |
| 1:R:662:TYR:HE2 | 1:R:700:TYR:HB3 | 1.69 | 0.58 |
| 1:S:109:GLU:O | 1:S:123:ASN:ND2 | 2.27 | 0.58 |
| 1:S:525:TRP:CD1 | 1:S:643:ASN:HD22 | 2.22 | 0.58 |
| 1:S:2456:ARG:N | 1:S:2459:ASP:OD2 | 2.37 | 0.58 |
| 1:A:613:PRO:HB2 | 1:A:640:HIS:CE1 | 2.39 | 0.58 |
| 1:A:2542:ARG:HH22 | 1:A:2591:LEU:HB2 | 1.68 | 0.58 |
| 1:B:81:LEU:HD12 | 1:B:86:LEU:HD13 | 1.86 | 0.58 |
| 1:B:524:ASP:OD2 | 1:B:527:ARG:NH1 | 2.37 | 0.58 |
| 1:B:3133:GLN:HB3 | 1:B:3138:ARG:HB2 | 1.85 | 0.58 |
| 1:C:799:LYS:N | 1:C:802:ASP:OD2 | 2.37 | 0.58 |
| 1:C:1872:LEU:HD21 | 1:C:2016:LEU:HD13 | 1.85 | 0.58 |
| 1:C:2046:ASP:C | 1:D:1493:ARG:HH22 | 2.12 | 0.58 |
| 1:C:2376:ASN:N | 1:C:2379:GLU:OE2 | 2.37 | 0.58 |
| 1:C:2570:GLY:HA3 | 1:C:2845:TRP:HB2 | 1.86 | 0.58 |
| 1:D:735:ARG:HH22 | 1:D:790:THR:H | 1.51 | 0.58 |
| 1:D:2191:PRO:HG2 | 1:D:2194:PHE:CD2 | 2.37 | 0.58 |
| 1:D:2287:HIS:HE2 | 1:D:2431:SER:H | 1.51 | 0.58 |
| 1:D:3124:ARG:O | 1:D:3127:GLN:HG3 | 2.04 | 0.58 |
| 1:D:3218:VAL:HG23 | 1:D:3258:TYR:HB2 | 1.86 | 0.58 |
| 1:D:3395:ARG:NE | 1:D:3398:GLN:OE1 | 2.37 | 0.58 |
| 1:E:1872:LEU:HD21 | 1:E:2016:LEU:HD13 | 1.85 | 0.58 |
| 1:F:130:ILE:O | 1:F:138:HIS:HA | 2.04 | 0.58 |
| 1:F:1321:VAL:HG11 | 1:F:1491:ILE:HG21 | 1.86 | 0.58 |
| 1:F:1480:LEU:HD12 | 1:F:1481:PRO:HD2 | 1.85 | 0.58 |
| 1:G:5:ARG:HD2 | 1:G:283:TYR:HE1 | 1.67 | 0.58 |
| 1:G:259:ASN:ND2 | 1:G:264:THR:OG1 | 2.36 | 0.58 |
| 1:G:1161:SER:OG | 1:G:1185:GLY:N | 2.30 | 0.58 |
| 1:H:918:THR:HA | 1:H:1050:PHE:HE2 | 1.67 | 0.58 |
| 1:I:363:LEU:HD12 | 1:I:364:PRO:HD2 | 1.85 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:I:574:LEU:HD23 | 1:I:616:LEU:HG | 1.86 | 0.58 |
| 1:I:613:PRO:HB2 | 1:I:640:HIS:NE2 | 2.18 | 0.58 |
| 1:I:1359:PRO:HB2 | 1:I:1362:ILE:HG12 | 1.85 | 0.58 |
| 1:I:2027:ASP:OD2 | 1:I:2028:ARG:NH1 | 2.36 | 0.58 |
| 1:I:3174:PRO:HA | 1:I:3177:ILE:HD12 | 1.85 | 0.58 |
| 1:K:2695:THR:OG1 | 1:K:2697:GLU:OE1 | 2.20 | 0.58 |
| 1:K:2893:SER:HA | 1:T:2738:GLN:HE22 | 1.68 | 0.58 |
| 1:L:230:GLN:NE2 | 1:L:236:THR:O | 2.36 | 0.58 |
| 1:L:465:GLN:NE2 | 1:L:558:PRO:O | 2.26 | 0.58 |
| 1:L:2729:ASP:OD2 | 1:L:2732:SER:OG | 2.20 | 0.58 |
| 1:N:1763:ILE:HG12 | 1:N:1882:LEU:HB3 | 1.85 | 0.58 |
| 1:N:3156:PRO:HB2 | 1:N:3162:LYS:HG3 | 1.86 | 0.58 |
| 1:P:1088:LEU:HD22 | 1:P:1109:PRO:HG3 | 1.83 | 0.58 |
| 1:P:2806:PHE:CE2 | 1:P:2892:PRO:HB3 | 2.38 | 0.58 |
| 1:Q:2249:LEU:O | 1:Q:2252:LEU:N | 2.36 | 0.58 |
| 1:R:1098:ASN:HB2 | 1:R:1104:ARG:HD3 | 1.85 | 0.58 |
| 1:R:3080:PHE:HA | 1:R:3083:GLN:HE22 | 1.68 | 0.58 |
| 1:S:309:ALA:H | 1:S:370:SER:HG | 1.52 | 0.58 |
| 1:S:1752:ASP:OD1 | 1:S:1753:ALA:N | 2.36 | 0.58 |
| 1:T:1466:ARG:O | 1:T:1470:ILE:HG12 | 2.03 | 0.58 |
| 1:T:1785:ARG:NH1 | 1:T:1786:ASP:O | 2.37 | 0.58 |
| 1:A:2820:ASP:OD1 | 1:A:2831:ALA:N | 2.34 | 0.58 |
| 1:A:3157:PHE:O | 1:A:3163:ASN:ND2 | 2.37 | 0.58 |
| 1:B:3398:GLN:OE1 | 1:B:3400:THR:OG1 | 2.21 | 0.58 |
| 1:C:3076:ASN:ND2 | 1:C:3079:ASP:OD2 | 2.37 | 0.58 |
| 1:D:1100:ASP:O | 1:D:1104:ARG:NH1 | 2.36 | 0.58 |
| 1:D:1907:ASN:HD22 | 1:D:1945:PHE:HB3 | 1.69 | 0.58 |
| 1:E:1240:THR:HA | 1:F:2328:ASN:HD21 | 1.69 | 0.58 |
| 1:F:1743:HIS:O | 1:F:1747:THR:HG23 | 2.03 | 0.58 |
| 1:G:3160:GLU:HG2 | 1:G:3169:ARG:HH22 | 1.67 | 0.58 |
| 1:H:1827:ASP:HA | 1:H:1831:TRP:CD1 | 2.39 | 0.58 |
| 1:I:2047:ASP:O | 1:J:1493:ARG:NH2 | 2.36 | 0.58 |
| 1:I:2778:ASP:OD1 | 1:I:2779:LEU:N | 2.36 | 0.58 |
| 1:J:190:TYR:HA | 1:J:201:SER:HA | 1.85 | 0.58 |
| 1:J:1086:LYS:NZ | 1:J:1087:PRO:O | 2.34 | 0.58 |
| 1:J:1568:SER:N | 1:J:1597:GLY:O | 2.37 | 0.58 |
| 1:J:1676:ILE:HG13 | 1:J:1761:VAL:HG23 | 1.86 | 0.58 |
| 1:J:3225:SER:O | 1:J:3290:TYR:N | 2.37 | 0.58 |
| 1:L:2112:ARG:HH11 | 1:L:2208:LEU:HD22 | 1.69 | 0.58 |
| 1:M:2056:ARG:HH22 | 1:M:2060:GLY:HA2 | 1.67 | 0.58 |
| 1:M:2234:LYS:HG3 | 1:M:2243:VAL:HG11 | 1.86 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:M:2331:SER:HA | 1:M:2355:LYS:HZ1 | 1.69 | 0.58 |
| 1:N:325:ARG:HE | 1:N:391:TYR:HE2 | 1.51 | 0.58 |
| 1:N:474:PRO:HB2 | 1:N:476:ARG:HH12 | 1.68 | 0.58 |
| 1:N:2251:VAL:HG22 | 1:N:2263:GLN:HG3 | 1.85 | 0.58 |
| 1:N:2286:LEU:HB3 | 1:N:2428:LEU:HD21 | 1.84 | 0.58 |
| 1:O:957:ASN:HD21 | 1:O:959:GLU:HB3 | 1.68 | 0.58 |
| 1:P:81:LEU:HD12 | 1:P:86:LEU:HD13 | 1.85 | 0.58 |
| 1:P:1785:ARG:NH1 | 1:P:1786:ASP:O | 2.37 | 0.58 |
| 1:Q:1186:ASP:N | 1:Q:1189:GLU:OE2 | 2.30 | 0.58 |
| 1:Q:1489:LEU:HA | 1:Q:1492:MET:HG2 | 1.86 | 0.58 |
| 1:Q:1687:GLU:HB2 | 1:Q:1760:LEU:HD21 | 1.86 | 0.58 |
| 1:Q:2580:LEU:HA | 1:Q:2583:VAL:HG12 | 1.85 | 0.58 |
| 1:R:597:ARG:NH2 | 1:R:655:GLN:OE1 | 2.37 | 0.58 |
| 1:R:3332:VAL:HG21 | 1:R:3406:ILE:HD13 | 1.85 | 0.58 |
| 1:S:603:GLU:O | 1:S:607:GLU:HG2 | 2.04 | 0.58 |
| 1:T:913:TRP:CD1 | 1:T:1088:LEU:HD12 | 2.38 | 0.58 |
| 1:T:1143:ARG:O | 1:T:1148:ARG:NH1 | 2.33 | 0.58 |
| 1:A:2345:ASN:HD22 | 1:A:2348:THR:HG23 | 1.69 | 0.58 |
| 1:A:2786:ILE:HD13 | 1:A:2789:LEU:HD21 | 1.85 | 0.58 |
| 1:B:245:GLU:HA | 1:B:248:ARG:HD2 | 1.84 | 0.58 |
| 1:B:1932:ASP:OD2 | 1:B:1935:THR:N | 2.30 | 0.58 |
| 1:C:2456:ARG:N | 1:C:2459:ASP:OD2 | 2.37 | 0.58 |
| 1:C:2917:LYS:H | 1:C:2917:LYS:HD2 | 1.69 | 0.58 |
| 1:D:1816:ASN:OD1 | 1:D:1817:ARG:N | 2.37 | 0.58 |
| 1:D:2345:ASN:ND2 | 1:D:2348:THR:OG1 | 2.37 | 0.58 |
| 1:D:2488:LYS:NZ | 1:D:2489:PRO:O | 2.37 | 0.58 |
| 1:E:390:LEU:HD22 | 1:E:398:LEU:HB3 | 1.85 | 0.58 |
| 1:E:2330:MET:HE1 | 1:E:2354:PRO:HG2 | 1.86 | 0.58 |
| 1:E:2409:ARG:O | 1:E:2471:TYR:HA | 2.03 | 0.58 |
| 1:F:378:LYS:NZ | 1:F:383:ASP:O | 2.36 | 0.58 |
| 1:G:1153:PHE:HE1 | 1:G:1166:LEU:HD21 | 1.68 | 0.58 |
| 1:G:3359:SER:HA | 1:G:3362:LEU:HB2 | 1.86 | 0.58 |
| 1:H:788:GLU:OE2 | 1:H:791:ASP:N | 2.33 | 0.58 |
| 1:H:1372:SER:O | 1:H:1374:THR:OG1 | 2.21 | 0.58 |
| 1:H:1726:ASN:OD1 | 1:H:1727:GLN:N | 2.37 | 0.58 |
| 1:H:1828:ASN:OD1 | 1:H:1831:TRP:N | 2.37 | 0.58 |
| 1:H:2112:ARG:HH11 | 1:H:2208:LEU:HD22 | 1.68 | 0.58 |
| 1:H:2253:GLU:OE2 | 1:H:2388:GLN:NE2 | 2.36 | 0.58 |
| 1:K:3200:ILE:HA | 1:K:3203:ILE:HG22 | 1.86 | 0.58 |
| 1:L:675:LEU:H | 1:L:695:ARG:HH21 | 1.51 | 0.58 |
| 1:L:1827:ASP:HA | 1:L:1831:TRP:CD1 | 2.39 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:M:1865:LYS:HZ2 | 1:M:1867:HIS:HB2 | 1.68 | 0.58 |
| 1:M:2215:GLY:N | 1:M:2224:THR:OG1 | 2.34 | 0.58 |
| 1:M:3304:VAL:HG23 | 1:M:3317:ILE:HB | 1.84 | 0.58 |
| 1:N:248:ARG:NH1 | 1:N:802:ASP:O | 2.36 | 0.58 |
| 1:N:954:THR:HG22 | 1:N:965:PRO:HA | 1.85 | 0.58 |
| 1:N:2488:LYS:NZ | 1:N:2489:PRO:O | 2.37 | 0.58 |
| 1:O:1626:ASP:OD1 | 1:O:1627:SER:N | 2.37 | 0.58 |
| 1:O:3200:ILE:HA | 1:O:3203:ILE:HG22 | 1.84 | 0.58 |
| 1:P:613:PRO:HA | 1:P:616:LEU:HB2 | 1.86 | 0.58 |
| 1:P:1676:ILE:HG13 | 1:P:1761:VAL:HG23 | 1.84 | 0.58 |
| 1:Q:183:VAL:HG21 | 1:Q:365:TYR:CE1 | 2.38 | 0.58 |
| 1:Q:437:VAL:HG12 | 1:Q:521:PRO:HB2 | 1.85 | 0.58 |
| 1:Q:1148:ARG:HG3 | 1:Q:1244:ARG:HB3 | 1.85 | 0.58 |
| 1:Q:1571:VAL:O | 1:Q:1592:SER:OG | 2.17 | 0.58 |
| 1:R:325:ARG:HH21 | 1:R:391:TYR:HE1 | 1.50 | 0.58 |
| 1:R:2126:LEU:HD21 | 1:R:2165:VAL:HG12 | 1.86 | 0.58 |
| 1:S:2462:ASN:O | 1:T:1085:ARG:NH1 | 2.36 | 0.58 |
| 1:T:937:TRP:H | 1:T:1051:LEU:HB2 | 1.69 | 0.58 |
| 1:T:1149:VAL:HG11 | 1:T:1206:LEU:HD23 | 1.86 | 0.58 |
| 1:T:3038:LYS:O | 1:T:3041:GLN:NE2 | 2.36 | 0.58 |
| 1:T:3211:ASP:OD1 | 1:T:3309:ALA:N | 2.37 | 0.58 |
| 1:A:937:TRP:O | 1:A:1055:ASN:ND2 | 2.37 | 0.58 |
| 1:A:2462:ASN:O | 1:B:1085:ARG:NH1 | 2.34 | 0.58 |
| 1:A:2777:ASP:O | 1:A:3137:HIS:NE2 | 2.36 | 0.58 |
| 1:A:3133:GLN:NE2 | 1:A:3138:ARG:O | 2.36 | 0.58 |
| 1:B:2087:LEU:H | 1:B:2366:ARG:NH1 | 2.02 | 0.58 |
| 1:B:2343:ASN:HB3 | 1:B:2349:ARG:HH22 | 1.68 | 0.58 |
| 1:B:2657:GLN:N | 1:B:2657:GLN:OE1 | 2.37 | 0.58 |
| 1:C:1067:GLN:HE21 | 1:C:1072:LEU:HB2 | 1.68 | 0.58 |
| 1:C:2152:PRO:O | 1:C:2257:TYR:OH | 2.22 | 0.58 |
| 1:D:1088:LEU:HD22 | 1:D:1109:PRO:HG3 | 1.86 | 0.58 |
| 1:D:1286:MET:O | 1:D:1291:THR:OG1 | 2.22 | 0.58 |
| 1:D:3122:ILE:HA | 1:D:3125:ILE:HG12 | 1.86 | 0.58 |
| 1:E:1913:LEU:HD21 | 1:F:1629:GLY:HA2 | 1.85 | 0.58 |
| 1:E:2087:LEU:HD11 | 1:E:2366:ARG:HB2 | 1.85 | 0.58 |
| 1:F:613:PRO:HA | 1:F:616:LEU:HB2 | 1.85 | 0.58 |
| 1:F:1285:ARG:O | 1:F:1340:ARG:NH1 | 2.37 | 0.58 |
| 1:G:307:GLU:O | 1:G:308:ARG:NE | 2.37 | 0.58 |
| 1:G:2529:LYS:HD3 | 1:G:2613:LEU:HD11 | 1.85 | 0.58 |
| 1:H:845:LEU:HD22 | 1:H:926:ARG:HD3 | 1.84 | 0.58 |
| 1:H:2923:ARG:HH22 | 1:H:2929:LEU:HD12 | 1.69 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:I:508:GLU:OE2 | 1:I:520:ILE:N | 2.37 | 0.58 |
| 1:I:1671:THR:O | 1:I:1673:ARG:NH2 | 2.36 | 0.58 |
| 1:I:1821:ASP:OD1 | 1:I:1822:GLY:N | 2.36 | 0.58 |
| 1:I:3142:TYR:HE2 | 1:I:3144:ARG:HD3 | 1.68 | 0.58 |
| 1:I:3310:ASN:OD1 | 1:J:1117:ARG:NE | 2.37 | 0.58 |
| 1:J:526:THR:OG1 | 1:J:527:ARG:NH1 | 2.37 | 0.58 |
| 1:K:3267:THR:OG1 | 1:K:3271:GLU:OE1 | 2.17 | 0.58 |
| 1:L:905:HIS:HA | 1:L:910:PHE:HD2 | 1.69 | 0.58 |
| 1:L:1143:ARG:O | 1:L:1148:ARG:NH1 | 2.32 | 0.58 |
| 1:L:1809:VAL:HG22 | 1:L:1811:ARG:HH12 | 1.68 | 0.58 |
| 1:M:1081:ILE:HD13 | 1:N:2460:VAL:HG12 | 1.85 | 0.58 |
| 1:M:2669:ASN:OD1 | 1:M:2849:ARG:NE | 2.35 | 0.58 |
| 1:N:580:TYR:HE2 | 1:N:959:GLU:HB3 | 1.68 | 0.58 |
| 1:N:1795:ASN:HD21 | 1:N:1797:TRP:HB2 | 1.69 | 0.58 |
| 1:O:1773:ASN:OD1 | 1:O:1774:SER:N | 2.36 | 0.58 |
| 1:P:569:GLN:HB3 | 1:P:619:GLY:HA3 | 1.85 | 0.58 |
| 1:P:743:GLN:H | 1:P:823:PHE:HE1 | 1.52 | 0.58 |
| 1:P:2567:CYS:O | 1:P:2569:HIS:ND1 | 2.37 | 0.58 |
| 1:Q:64:ALA:O | 1:Q:174:TYR:OH | 2.22 | 0.58 |
| 1:S:306:ARG:O | 1:S:411:ARG:NH2 | 2.37 | 0.58 |
| 1:S:527:ARG:NH1 | 1:S:528:PRO:O | 2.35 | 0.58 |
| 1:A:363:LEU:HD12 | 1:A:364:PRO:HD2 | 1.85 | 0.57 |
| 1:A:1773:ASN:OD1 | 1:A:1774:SER:N | 2.37 | 0.57 |
| 1:C:259:ASN:ND2 | 1:C:264:THR:OG1 | 2.37 | 0.57 |
| 1:C:2623:GLU:OE1 | 1:C:2623:GLU:N | 2.32 | 0.57 |
| 1:E:915:ARG:HH21 | 1:E:1115:TYR:HB3 | 1.68 | 0.57 |
| 1:E:1163:LEU:HG | 1:E:1182:TYR:HD1 | 1.69 | 0.57 |
| 1:E:1912:ALA:HB3 | 1:E:1916:MET:HE1 | 1.85 | 0.57 |
| 1:E:2267:THR:O | 1:E:2271:ILE:HG12 | 2.05 | 0.57 |
| 1:F:434:ARG:NH1 | 1:F:508:GLU:OE2 | 2.37 | 0.57 |
| 1:F:1286:MET:HE1 | 1:F:1292:PHE:HB2 | 1.86 | 0.57 |
| 1:F:1773:ASN:OD1 | 1:F:1774:SER:N | 2.37 | 0.57 |
| 1:F:3122:ILE:HA | 1:F:3125:ILE:HG12 | 1.84 | 0.57 |
| 1:G:501:ARG:NH1 | 1:G:702:TYR:HB3 | 2.19 | 0.57 |
| 1:G:735:ARG:HE | 1:G:737:PHE:HZ | 1.50 | 0.57 |
| 1:G:2130:HIS:O | 1:G:2130:HIS:ND1 | 2.37 | 0.57 |
| 1:G:2878:ALA:N | 1:G:2882:THR:O | 2.36 | 0.57 |
| 1:H:846:HIS:HB3 | 1:H:1121:TYR:HA | 1.86 | 0.57 |
| 1:H:1965:ALA:HA | 1:H:1968:LEU:HG | 1.86 | 0.57 |
| 1:H:2675:GLU:O | 1:H:2679:ASN:ND2 | 2.36 | 0.57 |
| 1:I:259:ASN:ND2 | 1:I:264:THR:OG1 | 2.37 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:I:2078:LYS:HB3 | 1:I:2080:ARG:HH22 | 1.68 | 0.57 |
| 1:J:3103:MET:HA | 1:J:3109:SER:HA | 1.85 | 0.57 |
| 1:K:757:PRO:HB3 | 1:K:798:LEU:HD11 | 1.85 | 0.57 |
| 1:K:1078:ASN:HB3 | 1:L:2493:PHE:HB3 | 1.86 | 0.57 |
| 1:K:1249:THR:O | 1:K:1251:LYS:NZ | 2.29 | 0.57 |
| 1:K:2939:ASN:C | 1:K:2943:LYS:HZ2 | 2.12 | 0.57 |
| 1:L:1828:ASN:OD1 | 1:L:1831:TRP:N | 2.37 | 0.57 |
| 1:N:1232:SER:OG | 1:N:1234:GLU:OE1 | 2.22 | 0.57 |
| 1:N:2271:ILE:HD12 | 1:N:2298:HIS:NE2 | 2.18 | 0.57 |
| 1:O:1494:GLN:NE2 | 1:O:1500:ASN:OD1 | 2.37 | 0.57 |
| 1:P:259:ASN:O | 1:P:265:ARG:NH2 | 2.37 | 0.57 |
| 1:Q:3385:ASP:O | 1:R:3148:ARG:NH1 | 2.35 | 0.57 |
| 1:R:1087:PRO:HA | 1:R:1109:PRO:HD3 | 1.85 | 0.57 |
| 1:R:2812:LYS:HG2 | 1:R:2840:PRO:HA | 1.86 | 0.57 |
| 1:R:3035:TYR:H | 1:R:3044:VAL:HG22 | 1.68 | 0.57 |
| 1:T:230:GLN:NE2 | 1:T:236:THR:O | 2.35 | 0.57 |
| 1:T:1286:MET:HE1 | 1:T:1292:PHE:HB2 | 1.86 | 0.57 |
| 1:T:1546:VAL:HA | 1:T:1549:ARG:HG2 | 1.85 | 0.57 |
| 1:T:2343:ASN:HD21 | 1:T:2345:ASN:HB3 | 1.69 | 0.57 |
| 1:A:1008:GLN:OE1 | 1:A:1008:GLN:N | 2.36 | 0.57 |
| 1:C:914:HIS:CE1 | 1:C:1053:HIS:CE1 | 2.91 | 0.57 |
| 1:C:1316:VAL:HG11 | 1:C:1321:VAL:HG23 | 1.85 | 0.57 |
| 1:D:1111:GLU:N | 1:D:1111:GLU:OE1 | 2.37 | 0.57 |
| 1:D:2164:GLN:O | 1:D:2164:GLN:NE2 | 2.36 | 0.57 |
| 1:F:2408:VAL:HG22 | 1:F:2473:ILE:HG22 | 1.85 | 0.57 |
| 1:G:1773:ASN:OD1 | 1:G:1774:SER:N | 2.36 | 0.57 |
| 1:G:1977:GLU:O | 1:G:2078:LYS:NZ | 2.34 | 0.57 |
| 1:H:2462:ASN:OD1 | 1:H:2463:ALA:N | 2.38 | 0.57 |
| 1:J:5:ARG:HB3 | 1:J:93:TYR:HD2 | 1.68 | 0.57 |
| 1:J:913:TRP:NE1 | 1:J:1089:GLN:O | 2.38 | 0.57 |
| 1:J:2297:THR:O | 1:J:2300:THR:OG1 | 2.22 | 0.57 |
| 1:K:1026:HIS:HD2 | 1:K:1184:LEU:HD11 | 1.68 | 0.57 |
| 1:K:1715:ALA:HB1 | 1:K:1873:HIS:HA | 1.86 | 0.57 |
| 1:K:3174:PRO:HA | 1:K:3177:ILE:HD12 | 1.86 | 0.57 |
| 1:K:3179:ASP:OD1 | 1:K:3180:ALA:N | 2.37 | 0.57 |
| 1:L:636:ILE:O | 1:L:640:HIS:ND1 | 2.31 | 0.57 |
| 1:L:2970:ALA:O | 1:L:2973:ARG:NE | 2.33 | 0.57 |
| 1:L:3103:MET:HA | 1:L:3109:SER:HA | 1.86 | 0.57 |
| 1:M:494:ALA:HB3 | 1:M:670:MET:HG2 | 1.86 | 0.57 |
| 1:M:3036:GLN:HB2 | 1:M:3043:GLN:HE22 | 1.69 | 0.57 |
| 1:N:1746:TYR:HH | 1:N:1876:SER:HG | 1.38 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:O:20:GLU:O | 1:O:24:ARG:HD3 | 2.04 | 0.57 |
| 1:O:854:LEU:HD12 | 1:O:858:GLN:HG3 | 1.85 | 0.57 |
| 1:O:2456:ARG:N | 1:O:2459:ASP:OD2 | 2.36 | 0.57 |
| 1:P:913:TRP:CD1 | 1:P:1088:LEU:HD12 | 2.39 | 0.57 |
| 1:P:1827:ASP:HA | 1:P:1831:TRP:HD1 | 1.69 | 0.57 |
| 1:Q:1587:ASN:OD1 | 1:Q:1588:HIS:N | 2.37 | 0.57 |
| 1:Q:1812:ASP:HB3 | 1:Q:1863:GLY:HA3 | 1.86 | 0.57 |
| 1:Q:1980:ARG:HE | 1:Q:1982:PHE:HZ | 1.52 | 0.57 |
| 1:S:5:ARG:NH2 | 1:S:78:GLU:HG3 | 2.18 | 0.57 |
| 1:S:1307:HIS:CG | 1:S:1602:MET:HE1 | 2.39 | 0.57 |
| 1:S:1531:ASP:OD1 | 1:S:1532:THR:N | 2.36 | 0.57 |
| 1:S:2566:CYS:O | 1:S:2577:TRP:NE1 | 2.37 | 0.57 |
| 1:T:737:PHE:N | 1:T:829:ILE:O | 2.31 | 0.57 |
| 1:A:2256:ASP:OD2 | 1:A:2440:ARG:NH2 | 2.37 | 0.57 |
| 1:C:678:PHE:O | 1:C:685:ASN:ND2 | 2.37 | 0.57 |
| 1:C:2569:HIS:HA | 1:C:2574:PHE:CE2 | 2.39 | 0.57 |
| 1:C:2585:LEU:HD23 | 1:C:2589:LEU:HD23 | 1.86 | 0.57 |
| 1:D:1086:LYS:NZ | 1:D:1087:PRO:O | 2.33 | 0.57 |
| 1:D:1785:ARG:NH1 | 1:D:1786:ASP:O | 2.38 | 0.57 |
| 1:D:2328:ASN:OD1 | 1:D:2329:TYR:N | 2.37 | 0.57 |
| 1:D:2951:ASN:ND2 | 1:D:3001:ASP:OD2 | 2.37 | 0.57 |
| 1:D:3351:VAL:HG23 | 1:D:3390:SER:HA | 1.86 | 0.57 |
| 1:E:2130:HIS:NE2 | 1:E:2147:CYS:SG | 2.78 | 0.57 |
| 1:E:2709:HIS:HA | 1:E:2712:VAL:HG12 | 1.86 | 0.57 |
| 1:G:1338:LEU:HD21 | 1:G:1345:SER:HA | 1.86 | 0.57 |
| 1:G:1770:ASN:OD1 | 1:G:1772:GLN:NE2 | 2.37 | 0.57 |
| 1:G:2018:GLY:N | 1:G:2021:GLU:OE2 | 2.25 | 0.57 |
| 1:G:2376:ASN:N | 1:G:2379:GLU:OE2 | 2.33 | 0.57 |
| 1:G:2585:LEU:HD23 | 1:G:2589:LEU:HD23 | 1.86 | 0.57 |
| 1:H:958:PRO:HA | 1:H:961:ASN:HA | 1.86 | 0.57 |
| 1:H:2595:ARG:HG3 | 1:H:2596:VAL:HG13 | 1.86 | 0.57 |
| 1:H:3085:GLU:O | 1:H:3089:ASN:ND2 | 2.37 | 0.57 |
| 1:I:524:ASP:OD1 | 1:I:526:THR:OG1 | 2.19 | 0.57 |
| 1:I:2330:MET:HE1 | 1:I:2354:PRO:HG2 | 1.85 | 0.57 |
| 1:J:588:ASP:HA | 1:J:591:LEU:HD12 | 1.87 | 0.57 |
| 1:J:3340:PHE:O | 1:J:3376:ASP:N | 2.26 | 0.57 |
| 1:K:613:PRO:HB2 | 1:K:640:HIS:CE1 | 2.39 | 0.57 |
| 1:K:1773:ASN:OD1 | 1:K:1774:SER:N | 2.37 | 0.57 |
| 1:K:3008:ILE:HD12 | 1:K:3009:PRO:HD2 | 1.85 | 0.57 |
| 1:K:3260:ARG:HH21 | 1:K:3261:VAL:HG12 | 1.69 | 0.57 |
| 1:L:23:LEU:HD21 | 1:L:124:SER:HB2 | 1.85 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:L:3010:TYR:OH | 1:L:3189:ASN:OD1 | 2.19 | 0.57 |
| 1:M:2152:PRO:O | 1:M:2257:TYR:OH | 2.21 | 0.57 |
| 1:N:737:PHE:CG | 1:N:786:LYS:HB3 | 2.39 | 0.57 |
| 1:N:937:TRP:H | 1:N:1051:LEU:HB2 | 1.70 | 0.57 |
| 1:N:2567:CYS:O | 1:N:2569:HIS:ND1 | 2.37 | 0.57 |
| 1:O:484:VAL:O | 1:O:485:ARG:NH1 | 2.37 | 0.57 |
| 1:O:1294:LYS:O | 1:O:1297:SER:OG | 2.21 | 0.57 |
| 1:O:3358:THR:H | 1:P:3329:LYS:HE3 | 1.68 | 0.57 |
| 1:P:598:ASP:HB3 | 1:P:601:ASP:HB3 | 1.86 | 0.57 |
| 1:P:954:THR:HG22 | 1:P:965:PRO:HA | 1.84 | 0.57 |
| 1:Q:1646:GLU:OE1 | 1:T:483:ARG:NH1 | 2.37 | 0.57 |
| 1:R:309:ALA:HB2 | 1:R:380:LEU:HD11 | 1.86 | 0.57 |
| 1:R:1015:GLU:N | 1:R:1015:GLU:OE1 | 2.37 | 0.57 |
| 1:R:1970:SER:HB2 | 1:R:2085:GLN:HE22 | 1.68 | 0.57 |
| 1:R:3122:ILE:HA | 1:R:3125:ILE:HG12 | 1.87 | 0.57 |
| 1:S:657:LYS:NZ | 1:S:720:ILE:O | 2.37 | 0.57 |
| 1:S:851:VAL:HG12 | 1:S:935:PRO:HB2 | 1.87 | 0.57 |
| 1:S:1919:PRO:HB2 | 1:S:1924:SER:HB2 | 1.85 | 0.57 |
| 1:S:2090:ASN:ND2 | 1:S:2175:THR:O | 2.38 | 0.57 |
| 1:T:188:ILE:HA | 1:T:191:LEU:HD12 | 1.84 | 0.57 |
| 1:T:3119:HIS:HA | 1:T:3122:ILE:HG22 | 1.85 | 0.57 |
| 1:A:1249:THR:O | 1:A:1251:LYS:NZ | 2.30 | 0.57 |
| 1:A:1974:LYS:NZ | 1:A:2361:GLN:O | 2.30 | 0.57 |
| 1:B:2113:ASP:HA | 1:B:2116:LYS:HE2 | 1.86 | 0.57 |
| 1:C:2353:LEU:HD13 | 1:C:2355:LYS:HD3 | 1.86 | 0.57 |
| 1:D:259:ASN:O | 1:D:265:ARG:NH2 | 2.38 | 0.57 |
| 1:D:658:ARG:HH12 | 1:D:727:ILE:HD11 | 1.69 | 0.57 |
| 1:E:1312:VAL:HG22 | 1:E:1313:ALA:H | 1.69 | 0.57 |
| 1:E:2286:LEU:HD12 | 1:E:2429:GLY:HA2 | 1.84 | 0.57 |
| 1:E:2462:ASN:O | 1:F:1085:ARG:NH1 | 2.36 | 0.57 |
| 1:E:2977:CYS:HA | 1:E:2987:TRP:CZ3 | 2.40 | 0.57 |
| 1:F:172:ASP:OD1 | 1:F:173:ASP:N | 2.37 | 0.57 |
| 1:F:705:GLU:N | 1:F:705:GLU:OE1 | 2.38 | 0.57 |
| 1:F:1012:CYS:O | 1:F:1196:ARG:NH1 | 2.38 | 0.57 |
| 1:G:957:ASN:HD21 | 1:G:959:GLU:HB3 | 1.70 | 0.57 |
| 1:G:1322:PHE:HB3 | 1:G:1323:PRO:HD3 | 1.86 | 0.57 |
| 1:G:2114:LEU:HG | 1:G:2123:TRP:HB2 | 1.86 | 0.57 |
| 1:H:1272:SER:N | 1:H:1275:GLU:OE2 | 2.33 | 0.57 |
| 1:I:738:VAL:HG23 | 1:I:789:ILE:HD13 | 1.85 | 0.57 |
| 1:I:1294:LYS:O | 1:I:1297:SER:OG | 2.22 | 0.57 |
| 1:I:2348:THR:OG1 | 1:I:2349:ARG:NH1 | 2.38 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:J:913:TRP:CD1 | 1:J:1088:LEU:HD12 | 2.39 | 0.57 |
| 1:J:2251:VAL:HG22 | 1:J:2263:GLN:HG3 | 1.85 | 0.57 |
| 1:J:3334:ARG:HE | 1:J:3335:GLY:H | 1.51 | 0.57 |
| 1:K:481:ASP:OD1 | 1:N:1644:TYR:N | 2.32 | 0.57 |
| 1:K:667:ALA:HB1 | 1:K:670:MET:HB3 | 1.86 | 0.57 |
| 1:K:1426:PHE:HZ | 1:K:1464:VAL:HG13 | 1.69 | 0.57 |
| 1:K:1655:LEU:N | 1:L:1914:GLU:OE1 | 2.21 | 0.57 |
| 1:K:2603:TRP:CH2 | 1:K:2681:ILE:HD11 | 2.40 | 0.57 |
| 1:L:113:LYS:NZ | 1:S:2226:ARG:O | 2.36 | 0.57 |
| 1:M:657:LYS:NZ | 1:M:720:ILE:O | 2.37 | 0.57 |
| 1:M:1420:CYS:HB2 | 1:M:1608:ARG:HH21 | 1.69 | 0.57 |
| 1:M:1544:GLU:OE1 | 1:M:1544:GLU:N | 2.36 | 0.57 |
| 1:M:1905:ASP:HB3 | 1:M:1908:GLU:HB2 | 1.87 | 0.57 |
| 1:N:913:TRP:NE1 | 1:N:1089:GLN:O | 2.37 | 0.57 |
| 1:N:958:PRO:HA | 1:N:961:ASN:HA | 1.86 | 0.57 |
| 1:N:996:THR:HG23 | 1:N:999:ALA:H | 1.68 | 0.57 |
| 1:N:2967:PRO:O | 1:N:2973:ARG:NH1 | 2.38 | 0.57 |
| 1:R:719:THR:H | 1:R:722:GLN:NE2 | 2.02 | 0.57 |
| 1:R:744:ASN:HB3 | 1:R:779:TRP:NE1 | 2.19 | 0.57 |
| 1:R:2488:LYS:NZ | 1:R:2489:PRO:O | 2.37 | 0.57 |
| 1:S:1489:LEU:HA | 1:S:1492:MET:HG2 | 1.87 | 0.57 |
| 1:T:1895:TRP:HA | 1:T:1898:LEU:HD12 | 1.86 | 0.57 |
| 1:A:1352:THR:HG21 | 1:A:1535:PHE:HE1 | 1.68 | 0.57 |
| 1:A:2709:HIS:HA | 1:A:2712:VAL:HG12 | 1.86 | 0.57 |
| 1:A:2996:GLU:OE2 | 1:A:3008:ILE:N | 2.31 | 0.57 |
| 1:B:43:GLY:O | 1:B:46:SER:OG | 2.23 | 0.57 |
| 1:C:1773:ASN:OD1 | 1:C:1774:SER:N | 2.36 | 0.57 |
| 1:C:3074:GLU:OE1 | 1:C:3076:ASN:ND2 | 2.38 | 0.57 |
| 1:D:3276:ASN:ND2 | 1:D:3279:SER:OG | 2.38 | 0.57 |
| 1:E:323:ASN:OD1 | 1:E:324:VAL:N | 2.37 | 0.57 |
| 1:E:1684:THR:N | 1:E:1687:GLU:OE2 | 2.30 | 0.57 |
| 1:E:2750:ASP:HA | 1:E:2758:ARG:HD2 | 1.87 | 0.57 |
| 1:F:166:LEU:HA | 1:F:169:LEU:HG | 1.87 | 0.57 |
| 1:F:2251:VAL:HG21 | 1:F:2267:THR:HG21 | 1.87 | 0.57 |
| 1:G:848:ARG:HG2 | 1:G:933:GLY:HA3 | 1.85 | 0.57 |
| 1:G:1883:LEU:O | 1:G:1886:SER:OG | 2.18 | 0.57 |
| 1:H:662:TYR:HE2 | 1:H:700:TYR:HB3 | 1.69 | 0.57 |
| 1:I:1872:LEU:HD21 | 1:I:2016:LEU:HD13 | 1.85 | 0.57 |
| 1:J:958:PRO:HA | 1:J:961:ASN:HA | 1.86 | 0.57 |
| 1:J:996:THR:HG23 | 1:J:999:ALA:H | 1.69 | 0.57 |
| 1:J:1772:GLN:HB2 | 1:J:1818:LEU:HD11 | 1.86 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:K:390:LEU:HD22 | 1:K:398:LEU:HB3 | 1.87 | 0.57 |
| 1:K:711:ASP:OD1 | 1:K:712:ASN:N | 2.38 | 0.57 |
| 1:K:1240:THR:HA | 1:L:2328:ASN:HD21 | 1.69 | 0.57 |
| 1:K:1654:SER:OG | 1:L:1914:GLU:OE1 | 2.11 | 0.57 |
| 1:L:524:ASP:OD2 | 1:L:527:ARG:NH1 | 2.37 | 0.57 |
| 1:L:627:THR:HG21 | 1:L:630:TYR:HD2 | 1.69 | 0.57 |
| 1:L:2210:ASN:HD21 | 1:L:2212:PHE:HB2 | 1.70 | 0.57 |
| 1:L:2806:PHE:HE1 | 1:L:2892:PRO:HB3 | 1.70 | 0.57 |
| 1:N:6:LYS:HD2 | 1:N:11:LEU:HD13 | 1.86 | 0.57 |
| 1:N:379:LYS:HD3 | 1:N:381:ASN:H | 1.69 | 0.57 |
| 1:N:1827:ASP:HA | 1:N:1831:TRP:CD1 | 2.39 | 0.57 |
| 1:N:2616:ASP:OD1 | 1:N:2617:LYS:N | 2.37 | 0.57 |
| 1:O:2802:VAL:H | 1:O:2856:THR:HG22 | 1.69 | 0.57 |
| 1:P:625:LEU:HA | 1:P:631:SER:HB2 | 1.87 | 0.57 |
| 1:P:1599:GLU:OE2 | 1:P:1600:THR:OG1 | 2.22 | 0.57 |
| 1:P:3103:MET:HA | 1:P:3109:SER:HA | 1.86 | 0.57 |
| 1:Q:1448:LEU:HD21 | 1:Q:1596:LEU:HG | 1.85 | 0.57 |
| 1:Q:1710:LEU:HB3 | 1:Q:1750:PHE:HE1 | 1.68 | 0.57 |
| 1:Q:1830:LEU:HG | 1:Q:1834:PHE:HE2 | 1.69 | 0.57 |
| 1:Q:2695:THR:OG1 | 1:Q:2697:GLU:OE1 | 2.22 | 0.57 |
| 1:R:1769:VAL:O | 1:R:1828:ASN:ND2 | 2.38 | 0.57 |
| 1:R:2264:PHE:HZ | 1:R:2302:VAL:HG13 | 1.69 | 0.57 |
| 1:S:1138:ARG:HH21 | 1:S:1259:VAL:HG23 | 1.70 | 0.57 |
| 1:T:297:TYR:O | 1:T:300:LEU:HG | 2.04 | 0.57 |
| 1:A:608:VAL:HG22 | 1:A:768:LEU:HD22 | 1.85 | 0.57 |
| 1:A:1855:ASN:HD21 | 1:A:2015:VAL:HA | 1.69 | 0.57 |
| 1:B:1736:MET:HG2 | 1:B:1738:THR:H | 1.70 | 0.57 |
| 1:B:2695:THR:HG21 | 1:B:2698:TYR:HD2 | 1.70 | 0.57 |
| 1:B:3114:PHE:HA | 1:B:3117:ILE:HG12 | 1.85 | 0.57 |
| 1:C:187:HIS:HA | 1:C:349:PHE:HD2 | 1.69 | 0.57 |
| 1:C:1322:PHE:HD2 | 1:C:1426:PHE:HE2 | 1.51 | 0.57 |
| 1:C:2025:SER:O | 1:D:1651:ARG:NH2 | 2.38 | 0.57 |
| 1:D:229:LEU:HB3 | 1:D:233:ARG:HH21 | 1.69 | 0.57 |
| 1:D:374:GLU:OE1 | 1:D:374:GLU:N | 2.33 | 0.57 |
| 1:D:454:ARG:NH2 | 1:D:1338:LEU:HG | 2.19 | 0.57 |
| 1:D:1415:GLU:HA | 1:D:1547:LEU:HD21 | 1.86 | 0.57 |
| 1:D:3113:PRO:HA | 1:D:3116:MET:HE2 | 1.85 | 0.57 |
| 1:E:1008:GLN:N | 1:E:1008:GLN:OE1 | 2.37 | 0.57 |
| 1:E:2729:ASP:OD1 | 1:E:2916:THR:OG1 | 2.20 | 0.57 |
| 1:E:2796:ARG:NH1 | 1:E:2799:GLU:OE2 | 2.38 | 0.57 |
| 1:E:2986:HIS:HB3 | 1:E:3177:ILE:HD13 | 1.85 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:F:810:ILE:HG23 | 1:F:818:TRP:HE3 | 1.70 | 0.57 |
| 1:F:811:LYS:NZ | 1:F:815:GLY:O | 2.37 | 0.57 |
| 1:G:2059:ASN:OD1 | 1:G:2060:GLY:N | 2.38 | 0.57 |
| 1:G:2393:VAL:H | 1:G:2447:THR:HG22 | 1.69 | 0.57 |
| 1:H:1004:LEU:O | 1:H:1008:GLN:NE2 | 2.33 | 0.57 |
| 1:H:3080:PHE:N | 1:H:3081:GLU:OE1 | 2.38 | 0.57 |
| 1:I:1903:GLY:HA3 | 1:J:1667:GLN:HB2 | 1.87 | 0.57 |
| 1:I:2603:TRP:HD1 | 1:I:2711:ASN:HD22 | 1.52 | 0.57 |
| 1:I:3332:VAL:O | 1:I:3334:ARG:NH2 | 2.38 | 0.57 |
| 1:J:2118:GLY:HA2 | 1:J:2124:GLN:HE22 | 1.70 | 0.57 |
| 1:K:926:ARG:NH2 | 1:K:931:GLN:O | 2.36 | 0.57 |
| 1:K:953:GLU:HG3 | 1:K:954:THR:HG23 | 1.86 | 0.57 |
| 1:K:1222:SER:OG | 1:K:1230:LYS:NZ | 2.30 | 0.57 |
| 1:K:1587:ASN:OD1 | 1:N:337:GLN:N | 2.37 | 0.57 |
| 1:L:595:GLU:N | 1:L:595:GLU:OE1 | 2.38 | 0.57 |
| 1:L:1268:LEU:HD23 | 1:L:1268:LEU:H | 1.70 | 0.57 |
| 1:M:3078:CYS:HA | 1:M:3081:GLU:CD | 2.29 | 0.57 |
| 1:N:613:PRO:HA | 1:N:616:LEU:HB2 | 1.85 | 0.57 |
| 1:N:1907:ASN:HD22 | 1:N:1945:PHE:HB3 | 1.70 | 0.57 |
| 1:N:3122:ILE:HA | 1:N:3125:ILE:HG12 | 1.86 | 0.57 |
| 1:O:844:GLU:O | 1:O:846:HIS:ND1 | 2.37 | 0.57 |
| 1:O:1085:ARG:NH1 | 1:P:2464:ASP:O | 2.38 | 0.57 |
| 1:R:143:ARG:NH2 | 1:R:209:ASP:OD2 | 2.37 | 0.57 |
| 1:R:2876:ILE:HB | 1:R:2884:LEU:HB2 | 1.86 | 0.57 |
| 1:S:2624:HIS:O | 1:S:2633:LYS:NZ | 2.34 | 0.57 |
| 1:T:757:PRO:HB2 | 1:T:760:GLY:H | 1.69 | 0.57 |
| 1:A:1835:LEU:HA | 1:A:1838:LEU:HD12 | 1.86 | 0.57 |
| 1:B:188:ILE:HG21 | 1:B:215:HIS:NE2 | 2.19 | 0.57 |
| 1:B:1541:PRO:O | 1:B:1544:GLU:HG3 | 2.04 | 0.57 |
| 1:B:2896:PHE:O | 1:C:2734:ASN:ND2 | 2.38 | 0.57 |
| 1:C:3086:MET:O | 1:C:3090:THR:HG23 | 2.05 | 0.57 |
| 1:D:2118:GLY:HA2 | 1:D:2124:GLN:HE22 | 1.69 | 0.57 |
| 1:D:2589:LEU:O | 1:D:2592:GLN:NE2 | 2.30 | 0.57 |
| 1:D:2622:PHE:O | 1:D:2636:ARG:NH2 | 2.37 | 0.57 |
| 1:E:527:ARG:NH1 | 1:E:528:PRO:O | 2.35 | 0.57 |
| 1:E:651:TRP:CZ3 | 1:E:655:GLN:HG3 | 2.39 | 0.57 |
| 1:E:1201:GLU:OE2 | 1:E:1202:ILE:N | 2.37 | 0.57 |
| 1:E:2525:THR:O | 1:E:2529:LYS:HG2 | 2.04 | 0.57 |
| 1:F:74:VAL:HA | 1:F:77:LEU:HD23 | 1.86 | 0.57 |
| 1:G:1865:LYS:HB3 | 1:G:1868:SER:HB3 | 1.85 | 0.57 |
| 1:G:2095:GLU:HB3 | 1:G:2098:HIS:HB2 | 1.87 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:G:3179:ASP:OD1 | 1:G:3180:ALA:N | 2.38 | 0.57 |
| 1:H:540:THR:HG22 | 1:H:551:HIS:HA | 1.86 | 0.57 |
| 1:H:1041:ARG:NH2 | 1:H:1188:TYR:OH | 2.35 | 0.57 |
| 1:H:1192:TRP:HZ3 | 1:H:1194:TYR:HB2 | 1.69 | 0.57 |
| 1:I:2078:LYS:HB2 | 1:I:2080:ARG:HH12 | 1.67 | 0.57 |
| 1:I:2405:SER:HB3 | 1:I:2426:PHE:HE1 | 1.69 | 0.57 |
| 1:J:297:TYR:O | 1:J:300:LEU:HG | 2.04 | 0.57 |
| 1:J:596:GLN:HE21 | 1:J:602:PHE:HD1 | 1.53 | 0.57 |
| 1:J:2997:MET:HE1 | 1:J:3000:ARG:NH2 | 2.18 | 0.57 |
| 1:J:3232:LEU:HD13 | 1:J:3269:ALA:HB3 | 1.87 | 0.57 |
| 1:K:16:VAL:HG21 | 1:K:105:ARG:HH22 | 1.69 | 0.57 |
| 1:K:111:ILE:HG13 | 1:N:2214:ARG:HH21 | 1.69 | 0.57 |
| 1:K:2878:ALA:N | 1:K:2882:THR:O | 2.35 | 0.57 |
| 1:K:3036:GLN:OE1 | 1:K:3043:GLN:NE2 | 2.37 | 0.57 |
| 1:L:2736:ASN:HB3 | 1:L:2739:GLU:HB3 | 1.85 | 0.57 |
| 1:L:2984:PHE:O | 1:L:2988:HIS:ND1 | 2.36 | 0.57 |
| 1:M:109:GLU:O | 1:M:123:ASN:ND2 | 2.31 | 0.57 |
| 1:M:310:LEU:HD23 | 1:M:366:HIS:HB3 | 1.86 | 0.57 |
| 1:M:454:ARG:HH21 | 1:M:514:ARG:HB3 | 1.70 | 0.57 |
| 1:M:2551:HIS:HB2 | 1:M:2581:PHE:HE1 | 1.68 | 0.57 |
| 1:N:188:ILE:HG21 | 1:N:215:HIS:NE2 | 2.20 | 0.57 |
| 1:N:2979:HIS:HA | 1:N:2984:PHE:HD2 | 1.70 | 0.57 |
| 1:O:111:ILE:HG13 | 1:R:2214:ARG:HH21 | 1.69 | 0.57 |
| 1:P:170:GLU:N | 1:P:170:GLU:OE1 | 2.36 | 0.57 |
| 1:P:2754:ASN:OD1 | 1:P:2755:ASP:N | 2.38 | 0.57 |
| 1:Q:1858:HIS:HA | 1:Q:1869:MET:HE1 | 1.87 | 0.57 |
| 1:R:188:ILE:HG21 | 1:R:215:HIS:NE2 | 2.19 | 0.57 |
| 1:S:1349:TRP:NE1 | 1:S:1359:PRO:HG3 | 2.19 | 0.57 |
| 1:S:1626:ASP:OD1 | 1:S:1627:SER:N | 2.38 | 0.57 |
| 1:T:452:LEU:HD23 | 1:T:554:PHE:HE1 | 1.70 | 0.57 |
| 1:B:527:ARG:O | 1:B:530:THR:OG1 | 2.21 | 0.57 |
| 1:B:1913:LEU:HA | 1:B:1916:MET:HG3 | 1.86 | 0.57 |
| 1:B:2254:GLN:HE21 | 1:B:2260:PHE:HA | 1.70 | 0.57 |
| 1:B:2951:ASN:ND2 | 1:B:3001:ASP:OD2 | 2.38 | 0.57 |
| 1:D:1225:ASP:OD1 | 1:D:1226:LEU:N | 2.34 | 0.57 |
| 1:D:1325:TRP:HE3 | 1:D:1496:LEU:HD21 | 1.69 | 0.57 |
| 1:F:958:PRO:HA | 1:F:961:ASN:HA | 1.87 | 0.57 |
| 1:F:980:ARG:NH2 | 1:F:1046:ASP:OD1 | 2.37 | 0.57 |
| 1:G:915:ARG:HD3 | 1:G:1112:VAL:HG22 | 1.87 | 0.57 |
| 1:G:1494:GLN:NE2 | 1:G:1500:ASN:OD1 | 2.37 | 0.57 |
| 1:G:1574:PHE:N | 1:G:1634:GLU:O | 2.29 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:G:2567:CYS:O | 1:G:2569:HIS:ND1 | 2.37 | 0.57 |
| 1:G:3339:ARG:NH2 | 1:G:3376:ASP:O | 2.37 | 0.57 |
| 1:H:303:ARG:HD3 | 1:H:306:ARG:HD3 | 1.85 | 0.57 |
| 1:H:454:ARG:NH2 | 1:H:1338:LEU:O | 2.38 | 0.57 |
| 1:H:737:PHE:CG | 1:H:786:LYS:HB3 | 2.39 | 0.57 |
| 1:H:3114:PHE:HA | 1:H:3117:ILE:HG12 | 1.87 | 0.57 |
| 1:I:1812:ASP:HB3 | 1:I:1863:GLY:HA3 | 1.85 | 0.57 |
| 1:J:1919:PRO:HB2 | 1:J:1924:SER:HB2 | 1.87 | 0.57 |
| 1:J:1932:ASP:OD2 | 1:J:1935:THR:N | 2.28 | 0.57 |
| 1:J:3350:ASN:ND2 | 1:J:3369:ASP:OD1 | 2.38 | 0.57 |
| 1:K:2567:CYS:O | 1:K:2569:HIS:ND1 | 2.35 | 0.57 |
| 1:L:435:LYS:NZ | 1:L:439:THR:OG1 | 2.36 | 0.57 |
| 1:M:1775:LEU:HD12 | 1:M:1779:PHE:HE1 | 1.70 | 0.57 |
| 1:M:2420:THR:HG21 | 1:M:2453:LEU:HD21 | 1.86 | 0.57 |
| 1:M:3157:PHE:O | 1:M:3163:ASN:ND2 | 2.37 | 0.57 |
| 1:N:1514:SER:OG | 1:N:1515:ARG:NH2 | 2.37 | 0.57 |
| 1:N:1828:ASN:OD1 | 1:N:1831:TRP:N | 2.38 | 0.57 |
| 1:N:2064:SER:HG | 1:N:2066:SER:HG | 1.49 | 0.57 |
| 1:O:1855:ASN:HD21 | 1:O:2015:VAL:HA | 1.70 | 0.57 |
| 1:O:2345:ASN:HD22 | 1:O:2348:THR:HG23 | 1.68 | 0.57 |
| 1:P:2812:LYS:HG2 | 1:P:2840:PRO:HA | 1.87 | 0.57 |
| 1:P:3287:LEU:HB3 | 1:P:3295:LEU:HB3 | 1.87 | 0.57 |
| 1:Q:2147:CYS:O | 1:Q:2149:HIS:ND1 | 2.38 | 0.57 |
| 1:Q:3124:ARG:HH12 | 1:Q:3192:LEU:HD21 | 1.70 | 0.57 |
| 1:R:297:TYR:O | 1:R:300:LEU:HG | 2.04 | 0.57 |
| 1:R:597:ARG:HH22 | 1:R:655:GLN:HA | 1.70 | 0.57 |
| 1:R:1495:PRO:HA | 1:R:1515:ARG:HH21 | 1.69 | 0.57 |
| 1:R:3092:HIS:ND1 | 1:R:3103:MET:HE1 | 2.20 | 0.57 |
| 1:R:3260:ARG:NH2 | 1:R:3407:ASP:OD2 | 2.38 | 0.57 |
| 1:S:2994:GLN:OE1 | 1:S:3165:ASN:ND2 | 2.38 | 0.57 |
| 1:T:1865:LYS:HE3 | 1:T:1867:HIS:H | 1.70 | 0.57 |
| 1:T:2938:ARG:NH2 | 1:T:3029:ASN:OD1 | 2.38 | 0.57 |
| 1:A:1466:ARG:NH2 | 1:A:1534:ASN:O | 2.37 | 0.57 |
| 1:A:1494:GLN:NE2 | 1:A:1500:ASN:OD1 | 2.38 | 0.57 |
| 1:A:2566:CYS:O | 1:A:2577:TRP:NE1 | 2.38 | 0.57 |
| 1:B:743:GLN:H | 1:B:823:PHE:HE1 | 1.53 | 0.57 |
| 1:C:1433:LEU:HD11 | 1:C:1460:HIS:CD2 | 2.40 | 0.57 |
| 1:D:596:GLN:HE21 | 1:D:602:PHE:HD2 | 1.53 | 0.57 |
| 1:D:2970:ALA:O | 1:D:2973:ARG:NE | 2.30 | 0.57 |
| 1:E:597:ARG:HH11 | 1:E:658:ARG:CZ | 2.17 | 0.57 |
| 1:E:1124:ASP:OD1 | 1:E:1125:ASP:N | 2.38 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:E:2962:ALA:HB2 | 1:E:3107:GLU:HG2 | 1.85 | 0.57 |
| 1:F:2771:GLN:HG2 | 1:F:2772:PHE:HD1 | 1.70 | 0.57 |
| 1:F:3260:ARG:NH2 | 1:F:3407:ASP:OD2 | 2.37 | 0.57 |
| 1:G:69:TRP:HD1 | 1:G:251:LEU:HD12 | 1.69 | 0.57 |
| 1:G:667:ALA:HB1 | 1:G:670:MET:HB3 | 1.84 | 0.57 |
| 1:G:1900:ARG:O | 1:G:1900:ARG:NH1 | 2.38 | 0.57 |
| 1:G:1932:ASP:OD2 | 1:G:1934:ILE:HG22 | 2.04 | 0.57 |
| 1:G:3125:ILE:HA | 1:G:3128:ILE:HG12 | 1.86 | 0.57 |
| 1:H:2217:ILE:HG22 | 1:H:2220:SER:H | 1.69 | 0.57 |
| 1:H:2985:PRO:HB2 | 1:H:2989:ARG:HH22 | 1.70 | 0.57 |
| 1:I:171:GLU:OE2 | 1:I:173:ASP:N | 2.38 | 0.57 |
| 1:I:172:ASP:OD2 | 1:I:233:ARG:NH1 | 2.37 | 0.57 |
| 1:I:250:LYS:HD2 | 1:I:268:SER:HB3 | 1.87 | 0.57 |
| 1:I:437:VAL:HG12 | 1:I:521:PRO:HB2 | 1.86 | 0.57 |
| 1:I:1328:LEU:HB3 | 1:I:1499:PHE:CE2 | 2.40 | 0.57 |
| 1:I:1651:ARG:NE | 1:J:2025:SER:OG | 2.28 | 0.57 |
| 1:J:149:LEU:HD21 | 1:J:191:LEU:HB3 | 1.87 | 0.57 |
| 1:J:2876:ILE:HB | 1:J:2884:LEU:HB2 | 1.85 | 0.57 |
| 1:J:3131:THR:HA | 1:J:3134:LYS:NZ | 2.20 | 0.57 |
| 1:K:149:LEU:HD21 | 1:K:191:LEU:HB3 | 1.87 | 0.57 |
| 1:K:913:TRP:HD1 | 1:K:1088:LEU:HD23 | 1.69 | 0.57 |
| 1:K:2114:LEU:HG | 1:K:2123:TRP:HB2 | 1.86 | 0.57 |
| 1:L:514:ARG:HH12 | 1:L:1341:GLY:HA2 | 1.70 | 0.57 |
| 1:L:958:PRO:HA | 1:L:961:ASN:HA | 1.86 | 0.57 |
| 1:L:2671:GLU:OE1 | 1:L:2671:GLU:N | 2.28 | 0.57 |
| 1:L:3147:LEU:HA | 1:L:3150:LEU:HD12 | 1.87 | 0.57 |
| 1:M:2567:CYS:O | 1:M:2569:HIS:ND1 | 2.37 | 0.57 |
| 1:N:705:GLU:HG2 | 1:N:706:LEU:HD22 | 1.87 | 0.57 |
| 1:N:1324:HIS:HB3 | 1:N:1519:VAL:HG21 | 1.87 | 0.57 |
| 1:O:2508:VAL:O | 1:O:2515:LYS:NZ | 2.38 | 0.57 |
| 1:O:2697:GLU:HG2 | 1:O:2841:LEU:HD13 | 1.86 | 0.57 |
| 1:P:1169:CYS:HA | 1:P:1175:CYS:HA | 1.87 | 0.57 |
| 1:Q:559:VAL:N | 1:Q:564:GLU:O | 2.31 | 0.57 |
| 1:Q:2376:ASN:N | 1:Q:2379:GLU:OE2 | 2.25 | 0.57 |
| 1:Q:2872:PHE:HD2 | 1:Q:2892:PRO:HG2 | 1.70 | 0.57 |
| 1:T:920:GLN:HB3 | 1:T:1103:THR:HG21 | 1.87 | 0.57 |
| 1:A:2273:TYR:HB2 | 1:A:2428:LEU:HD21 | 1.86 | 0.57 |
| 1:B:787:VAL:HG23 | 1:B:789:ILE:HD11 | 1.87 | 0.57 |
| 1:B:3000:ARG:CZ | 1:B:3000:ARG:HA | 2.34 | 0.57 |
| 1:C:2533:ARG:NH1 | 1:C:2619:ASP:O | 2.37 | 0.57 |
| 1:D:1167:GLU:HA | 1:D:1177:PRO:HA | 1.86 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:D:2666:ASP:OD1 | 1:D:2667:TYR:N | 2.38 | 0.57 |
| 1:D:3114:PHE:HA | 1:D:3117:ILE:HG12 | 1.87 | 0.57 |
| 1:D:3342:SER:OG | 1:D:3344:VAL:O | 2.23 | 0.57 |
| 1:E:1307:HIS:CG | 1:E:1602:MET:HE1 | 2.40 | 0.57 |
| 1:E:2641:GLN:NE2 | 1:E:2645:ASP:OD1 | 2.38 | 0.57 |
| 1:E:3200:ILE:HA | 1:E:3203:ILE:HG22 | 1.85 | 0.57 |
| 1:F:200:LEU:HD21 | 1:F:209:ASP:HB3 | 1.86 | 0.57 |
| 1:F:3076:ASN:ND2 | 1:F:3333:SER:OG | 2.37 | 0.57 |
| 1:G:38:LEU:O | 1:G:73:TYR:OH | 2.17 | 0.57 |
| 1:G:409:VAL:HG13 | 1:G:666:CYS:HA | 1.86 | 0.57 |
| 1:G:1026:HIS:HD2 | 1:G:1184:LEU:HD11 | 1.70 | 0.57 |
| 1:H:130:ILE:O | 1:H:138:HIS:HA | 2.05 | 0.57 |
| 1:H:231:LYS:HB3 | 1:H:237:TYR:HE2 | 1.70 | 0.57 |
| 1:H:524:ASP:OD2 | 1:H:527:ARG:NH1 | 2.38 | 0.57 |
| 1:H:2964:LYS:NZ | 1:H:2973:ARG:O | 2.35 | 0.57 |
| 1:I:1577:VAL:N | 1:I:1584:ARG:HH22 | 2.03 | 0.57 |
| 1:I:2786:ILE:HD13 | 1:I:2789:LEU:HD21 | 1.85 | 0.57 |
| 1:I:3339:ARG:NH2 | 1:I:3376:ASP:O | 2.38 | 0.57 |
| 1:J:757:PRO:HB2 | 1:J:760:GLY:H | 1.69 | 0.57 |
| 1:J:954:THR:HG22 | 1:J:965:PRO:HA | 1.85 | 0.57 |
| 1:J:1896:GLN:NE2 | 1:J:1906:PRO:O | 2.37 | 0.57 |
| 1:K:672:HIS:O | 1:K:695:ARG:NH1 | 2.35 | 0.57 |
| 1:K:1809:VAL:HG23 | 1:K:1868:SER:HA | 1.87 | 0.57 |
| 1:K:2786:ILE:HD13 | 1:K:2789:LEU:HD21 | 1.85 | 0.57 |
| 1:L:450:GLN:O | 1:L:454:ARG:HG2 | 2.04 | 0.57 |
| 1:L:1063:TRP:NE1 | 1:L:1067:GLN:HE22 | 2.02 | 0.57 |
| 1:L:1372:SER:O | 1:L:1374:THR:OG1 | 2.23 | 0.57 |
| 1:L:2217:ILE:HG22 | 1:L:2220:SER:H | 1.69 | 0.57 |
| 1:L:3035:TYR:H | 1:L:3044:VAL:HG22 | 1.69 | 0.57 |
| 1:M:2226:ARG:O | 1:P:113:LYS:NZ | 2.37 | 0.57 |
| 1:M:2641:GLN:NE2 | 1:M:2645:ASP:OD1 | 2.37 | 0.57 |
| 1:N:105:ARG:HA | 1:N:108:GLN:HE22 | 1.70 | 0.57 |
| 1:N:1978:LYS:HD2 | 1:N:2078:LYS:HZ1 | 1.70 | 0.57 |
| 1:N:2521:THR:HG22 | 1:N:2524:GLU:HG2 | 1.86 | 0.57 |
| 1:O:2117:ASP:OD1 | 1:O:2119:THR:OG1 | 2.22 | 0.57 |
| 1:P:1362:ILE:HD13 | 1:P:1456:LEU:HD11 | 1.86 | 0.57 |
| 1:R:737:PHE:N | 1:R:829:ILE:O | 2.27 | 0.57 |
| 1:R:2387:HIS:HB3 | 1:R:2392:ARG:HH21 | 1.68 | 0.57 |
| 1:S:586:LEU:H | 1:S:586:LEU:HD12 | 1.70 | 0.57 |
| 1:S:598:ASP:OD1 | 1:S:599:PHE:N | 2.37 | 0.57 |
| 1:S:767:LYS:HE2 | 1:S:767:LYS:HA | 1.87 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:811:LYS:HD2 | 1:A:815:GLY:HA2 | 1.87 | 0.56 |
| 1:A:1365:ALA:HA | 1:A:1381:PHE:CZ | 2.40 | 0.56 |
| 1:A:1963:ILE:HG23 | 1:A:1967:LEU:HD23 | 1.87 | 0.56 |
| 1:A:3339:ARG:NH2 | 1:A:3376:ASP:O | 2.38 | 0.56 |
| 1:B:538:LYS:NZ | 1:B:540:THR:O | 2.31 | 0.56 |
| 1:B:1501:ASP:HB3 | 1:B:1504:GLN:HB2 | 1.86 | 0.56 |
| 1:C:1812:ASP:HB3 | 1:C:1863:GLY:HA3 | 1.87 | 0.56 |
| 1:D:2376:ASN:O | 1:D:2379:GLU:HG3 | 2.05 | 0.56 |
| 1:E:1626:ASP:OD1 | 1:E:1627:SER:N | 2.37 | 0.56 |
| 1:E:1742:TRP:HD1 | 1:E:1920:LEU:HD12 | 1.69 | 0.56 |
| 1:E:2345:ASN:HD21 | 1:E:2347:PHE:HB3 | 1.70 | 0.56 |
| 1:F:920:GLN:HB3 | 1:F:1103:THR:HG21 | 1.85 | 0.56 |
| 1:F:1289:ASP:OD2 | 1:F:1340:ARG:NH2 | 2.38 | 0.56 |
| 1:F:1710:LEU:HD13 | 1:F:1750:PHE:CZ | 2.39 | 0.56 |
| 1:F:2137:PRO:HD2 | 1:F:2143:LYS:HE2 | 1.87 | 0.56 |
| 1:F:2488:LYS:HD2 | 1:F:2489:PRO:HD2 | 1.85 | 0.56 |
| 1:F:2587:ARG:HH22 | 1:F:2753:PRO:HG2 | 1.69 | 0.56 |
| 1:G:129:GLU:HA | 1:G:140:SER:HA | 1.87 | 0.56 |
| 1:H:597:ARG:NH2 | 1:H:654:LEU:O | 2.38 | 0.56 |
| 1:H:598:ASP:HB3 | 1:H:601:ASP:HB3 | 1.87 | 0.56 |
| 1:H:2157:TRP:HD1 | 1:H:2334:MET:HE3 | 1.70 | 0.56 |
| 1:H:2247:GLU:OE2 | 1:H:2267:THR:OG1 | 2.19 | 0.56 |
| 1:I:1415:GLU:OE1 | 1:I:1551:ARG:NH1 | 2.38 | 0.56 |
| 1:I:3125:ILE:HA | 1:I:3128:ILE:HG12 | 1.87 | 0.56 |
| 1:I:3191:ASN:OD1 | 1:I:3195:HIS:N | 2.38 | 0.56 |
| 1:K:327:LYS:HD2 | 1:K:344:PHE:HA | 1.87 | 0.56 |
| 1:K:1260:ALA:N | 1:K:1529:HIS:HE1 | 2.02 | 0.56 |
| 1:K:1426:PHE:CZ | 1:K:1464:VAL:HG13 | 2.39 | 0.56 |
| 1:M:1262:SER:OG | 1:M:1263:HIS:N | 2.34 | 0.56 |
| 1:M:1362:ILE:HD13 | 1:M:1456:LEU:HD11 | 1.86 | 0.56 |
| 1:N:149:LEU:HD21 | 1:N:191:LEU:HB3 | 1.87 | 0.56 |
| 1:N:221:ARG:HE | 1:N:283:TYR:HD2 | 1.51 | 0.56 |
| 1:N:950:VAL:HA | 1:N:968:PHE:HB3 | 1.87 | 0.56 |
| 1:O:55:ARG:NH2 | 1:O:56:VAL:O | 2.37 | 0.56 |
| 1:O:259:ASN:O | 1:O:265:ARG:NH2 | 2.38 | 0.56 |
| 1:O:718:MET:HE1 | 1:O:723:LEU:HA | 1.86 | 0.56 |
| 1:O:1680:VAL:HG12 | 1:O:1764:PRO:HB2 | 1.87 | 0.56 |
| 1:P:188:ILE:HG21 | 1:P:215:HIS:NE2 | 2.19 | 0.56 |
| 1:P:244:VAL:HG23 | 1:P:248:ARG:HE | 1.71 | 0.56 |
| 1:P:1272:SER:N | 1:P:1275:GLU:OE2 | 2.35 | 0.56 |
| 1:Q:1100:ASP:O | 1:Q:1104:ARG:NH1 | 2.38 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:R:1322:PHE:HB3 | 1:R:1323:PRO:HD3 | 1.87 | 0.56 |
| 1:R:2777:ASP:OD1 | 1:R:2778:ASP:N | 2.30 | 0.56 |
| 1:R:3085:GLU:O | 1:R:3089:ASN:ND2 | 2.37 | 0.56 |
| 1:R:3319:PRO:HB2 | 1:R:3343:PRO:HD3 | 1.86 | 0.56 |
| 1:S:376:LEU:HB3 | 1:S:378:LYS:NZ | 2.20 | 0.56 |
| 1:S:1710:LEU:HB3 | 1:S:1750:PHE:CE1 | 2.38 | 0.56 |
| 1:A:2330:MET:HE1 | 1:A:2354:PRO:HG2 | 1.86 | 0.56 |
| 1:A:2941:LEU:HD23 | 1:A:3031:PRO:HG2 | 1.86 | 0.56 |
| 1:B:744:ASN:HB3 | 1:B:779:TRP:CE2 | 2.40 | 0.56 |
| 1:B:2754:ASN:OD1 | 1:B:2755:ASP:N | 2.38 | 0.56 |
| 1:C:2786:ILE:HD13 | 1:C:2789:LEU:HD21 | 1.87 | 0.56 |
| 1:C:2796:ARG:O | 1:C:2801:ARG:NH2 | 2.36 | 0.56 |
| 1:D:1828:ASN:OD1 | 1:D:1831:TRP:N | 2.38 | 0.56 |
| 1:D:2044:SER:N | 1:D:2047:ASP:OD2 | 2.38 | 0.56 |
| 1:E:1909:ALA:HB1 | 1:E:1916:MET:HE3 | 1.88 | 0.56 |
| 1:E:2110:ALA:HB1 | 1:E:2172:HIS:HB3 | 1.88 | 0.56 |
| 1:E:2796:ARG:O | 1:E:2801:ARG:NH2 | 2.38 | 0.56 |
| 1:E:3113:PRO:HA | 1:E:3116:MET:HG3 | 1.87 | 0.56 |
| 1:F:312:SER:HA | 1:F:365:TYR:O | 2.05 | 0.56 |
| 1:F:905:HIS:HA | 1:F:910:PHE:HD2 | 1.70 | 0.56 |
| 1:F:1232:SER:OG | 1:F:1234:GLU:OE1 | 2.23 | 0.56 |
| 1:F:3214:TYR:N | 1:F:3305:ILE:O | 2.37 | 0.56 |
| 1:G:1684:THR:OG1 | 1:G:1687:GLU:OE1 | 2.18 | 0.56 |
| 1:G:1752:ASP:OD1 | 1:G:1753:ALA:N | 2.38 | 0.56 |
| 1:G:2623:GLU:OE1 | 1:G:2623:GLU:N | 2.37 | 0.56 |
| 1:G:3284:GLN:HE22 | 1:G:3286:THR:HG23 | 1.69 | 0.56 |
| 1:I:612:LEU:HB2 | 1:I:613:PRO:HD3 | 1.87 | 0.56 |
| 1:I:915:ARG:HH21 | 1:I:1115:TYR:HB3 | 1.71 | 0.56 |
| 1:I:3020:LEU:HB3 | 1:I:3024:LEU:HD11 | 1.87 | 0.56 |
| 1:J:461:VAL:HG12 | 1:J:1371:ARG:HB2 | 1.86 | 0.56 |
| 1:J:674:LEU:HD12 | 1:J:695:ARG:HH12 | 1.70 | 0.56 |
| 1:J:1415:GLU:HA | 1:J:1547:LEU:HD11 | 1.87 | 0.56 |
| 1:K:2994:GLN:OE1 | 1:K:3165:ASN:ND2 | 2.37 | 0.56 |
| 1:L:435:LYS:HG2 | 1:L:436:ASP:H | 1.69 | 0.56 |
| 1:L:1293:GLY:HA3 | 1:L:1386:LEU:HD23 | 1.86 | 0.56 |
| 1:L:1616:ASP:HB3 | 1:L:1620:LYS:NZ | 2.20 | 0.56 |
| 1:M:1715:ALA:HB1 | 1:M:1873:HIS:HA | 1.86 | 0.56 |
| 1:M:2164:GLN:OE1 | 1:M:2167:GLN:NE2 | 2.38 | 0.56 |
| 1:M:2773:ASN:HD21 | 1:M:3142:TYR:HB2 | 1.70 | 0.56 |
| 1:P:744:ASN:HB3 | 1:P:779:TRP:NE1 | 2.19 | 0.56 |
| 1:P:1353:GLN:NE2 | 1:P:1536:ASN:OD1 | 2.37 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:P:2671:GLU:CD | 1:P:2671:GLU:H | 2.12 | 0.56 |
| 1:P:3128:ILE:HD11 | 1:P:3197:VAL:HB | 1.86 | 0.56 |
| 1:Q:454:ARG:HH21 | 1:Q:514:ARG:HB3 | 1.70 | 0.56 |
| 1:R:1126:LEU:H | 1:R:1126:LEU:HD23 | 1.71 | 0.56 |
| 1:R:1299:HIS:ND1 | 1:R:1299:HIS:O | 2.38 | 0.56 |
| 1:R:1372:SER:O | 1:R:1374:THR:OG1 | 2.23 | 0.56 |
| 1:R:1960:LEU:N | 1:R:1963:ILE:O | 2.38 | 0.56 |
| 1:S:1899:GLN:HE22 | 1:S:1906:PRO:HA | 1.70 | 0.56 |
| 1:S:2570:GLY:HA2 | 1:S:2847:PHE:HE2 | 1.68 | 0.56 |
| 1:S:2861:GLN:NE2 | 1:T:1538:TRP:HE1 | 2.03 | 0.56 |
| 1:T:2137:PRO:HD2 | 1:T:2143:LYS:HE2 | 1.87 | 0.56 |
| 1:A:512:LYS:HA | 1:A:516:LEU:HB2 | 1.85 | 0.56 |
| 1:A:939:TRP:CD1 | 1:A:998:ILE:HG21 | 2.41 | 0.56 |
| 1:A:1124:ASP:OD1 | 1:A:1125:ASP:N | 2.38 | 0.56 |
| 1:A:1362:ILE:HD12 | 1:A:1380:PHE:HB3 | 1.86 | 0.56 |
| 1:A:1506:GLU:O | 1:A:1507:PHE:HD1 | 1.87 | 0.56 |
| 1:A:1900:ARG:HD3 | 1:A:1906:PRO:HB3 | 1.86 | 0.56 |
| 1:A:2585:LEU:HD22 | 1:A:2706:PHE:CE2 | 2.39 | 0.56 |
| 1:B:253:PRO:HB2 | 1:B:256:ARG:HH12 | 1.70 | 0.56 |
| 1:B:913:TRP:CD1 | 1:B:1088:LEU:HD12 | 2.40 | 0.56 |
| 1:B:1672:GLU:HG3 | 1:B:1673:ARG:HG2 | 1.88 | 0.56 |
| 1:B:2757:ILE:O | 1:B:2761:ALA:HB2 | 2.06 | 0.56 |
| 1:B:3088:HIS:CE1 | 1:B:3119:HIS:HE1 | 2.23 | 0.56 |
| 1:C:592:LEU:HD11 | 1:C:788:GLU:HB2 | 1.88 | 0.56 |
| 1:C:1294:LYS:O | 1:C:1297:SER:OG | 2.23 | 0.56 |
| 1:C:1588:HIS:NE2 | 1:F:337:GLN:HB2 | 2.21 | 0.56 |
| 1:C:2328:ASN:HB3 | 1:D:1241:VAL:HB | 1.87 | 0.56 |
| 1:C:3072:LEU:HA | 1:C:3080:PHE:HE1 | 1.70 | 0.56 |
| 1:D:662:TYR:HE2 | 1:D:700:TYR:HB3 | 1.69 | 0.56 |
| 1:D:2254:GLN:HE21 | 1:D:2260:PHE:HA | 1.70 | 0.56 |
| 1:E:327:LYS:HE2 | 1:E:342:CYS:SG | 2.45 | 0.56 |
| 1:E:484:VAL:O | 1:E:485:ARG:NH1 | 2.38 | 0.56 |
| 1:E:2939:ASN:HB3 | 1:E:2943:LYS:NZ | 2.20 | 0.56 |
| 1:F:413:ALA:HB3 | 1:F:416:PHE:HB2 | 1.87 | 0.56 |
| 1:F:738:VAL:HG23 | 1:F:789:ILE:HG13 | 1.87 | 0.56 |
| 1:F:1238:LYS:NZ | 1:F:1239:VAL:O | 2.39 | 0.56 |
| 1:F:2313:GLN:NE2 | 1:F:2318:LEU:HB3 | 2.20 | 0.56 |
| 1:F:3113:PRO:HA | 1:F:3116:MET:HE2 | 1.88 | 0.56 |
| 1:G:483:ARG:HD2 | 1:G:484:VAL:N | 2.20 | 0.56 |
| 1:G:799:LYS:N | 1:G:802:ASP:OD2 | 2.38 | 0.56 |
| 1:G:2648:ARG:HD2 | 1:G:2656:ARG:NH2 | 2.20 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:G:2820:ASP:OD1 | 1:G:2831:ALA:N | 2.37 | 0.56 |
| 1:H:509:ASP:OD1 | 1:H:510:ALA:N | 2.38 | 0.56 |
| 1:H:2407:GLU:O | 1:H:2473:ILE:HA | 2.06 | 0.56 |
| 1:I:971:GLY:H | 1:I:978:THR:HG1 | 1.53 | 0.56 |
| 1:I:2164:GLN:OE1 | 1:I:2167:GLN:NE2 | 2.38 | 0.56 |
| 1:I:2882:THR:OG1 | 4:I:3501:NAG:N2 | 2.39 | 0.56 |
| 1:I:3144:ARG:HE | 1:I:3147:LEU:HD11 | 1.69 | 0.56 |
| 1:J:2668:CYS:SG | 1:J:2849:ARG:NH2 | 2.78 | 0.56 |
| 1:J:2738:GLN:O | 1:J:2742:GLN:NE2 | 2.38 | 0.56 |
| 1:K:221:ARG:NH2 | 1:K:287:SER:O | 2.38 | 0.56 |
| 1:K:1058:ARG:NH1 | 1:K:1125:ASP:O | 2.39 | 0.56 |
| 1:K:1460:HIS:HA | 1:K:1463:ASN:HD21 | 1.69 | 0.56 |
| 1:K:1560:PHE:HZ | 1:K:1573:LEU:HD21 | 1.71 | 0.56 |
| 1:K:2130:HIS:ND1 | 1:K:2130:HIS:O | 2.39 | 0.56 |
| 1:K:2464:ASP:O | 1:L:1085:ARG:NH1 | 2.38 | 0.56 |
| 1:K:3118:HIS:O | 1:K:3122:ILE:HG12 | 2.05 | 0.56 |
| 1:L:238:ASP:OD1 | 1:L:239:HIS:ND1 | 2.38 | 0.56 |
| 1:L:501:ARG:HE | 1:L:645:ASP:CG | 2.14 | 0.56 |
| 1:L:1041:ARG:NH2 | 1:L:1188:TYR:OH | 2.34 | 0.56 |
| 1:L:1795:ASN:HD21 | 1:L:1797:TRP:HB2 | 1.69 | 0.56 |
| 1:L:2191:PRO:HG2 | 1:L:2194:PHE:CD2 | 2.40 | 0.56 |
| 1:L:2741:ARG:HH22 | 1:M:2870:TYR:H | 1.51 | 0.56 |
| 1:L:3062:ASP:OD2 | 1:L:3065:PHE:N | 2.34 | 0.56 |
| 1:M:854:LEU:HD12 | 1:M:858:GLN:HG3 | 1.86 | 0.56 |
| 1:M:2439:ASP:OD2 | 1:M:2440:ARG:NH1 | 2.39 | 0.56 |
| 1:M:2529:LYS:HE2 | 1:M:2533:ARG:HH21 | 1.70 | 0.56 |
| 1:M:2929:LEU:HD22 | 1:M:2933:GLN:HG3 | 1.87 | 0.56 |
| 1:N:580:TYR:CG | 1:N:958:PRO:HG2 | 2.40 | 0.56 |
| 1:N:2715:GLN:HA | 1:N:2718:ILE:HG12 | 1.86 | 0.56 |
| 1:N:3010:TYR:OH | 1:N:3189:ASN:OD1 | 2.17 | 0.56 |
| 1:O:493:MET:HE1 | 1:O:777:MET:HE1 | 1.87 | 0.56 |
| 1:O:1312:VAL:HG22 | 1:O:1313:ALA:H | 1.70 | 0.56 |
| 1:O:1531:ASP:OD1 | 1:O:1532:THR:N | 2.37 | 0.56 |
| 1:O:1574:PHE:HB2 | 1:O:1634:GLU:HB3 | 1.88 | 0.56 |
| 1:O:2056:ARG:NH1 | 1:O:2057:ALA:O | 2.39 | 0.56 |
| 1:O:2508:VAL:HB | 1:O:3138:ARG:HH11 | 1.70 | 0.56 |
| 1:O:2778:ASP:OD1 | 1:O:2779:LEU:N | 2.37 | 0.56 |
| 1:O:3263:LYS:HD2 | 1:O:3305:ILE:HD11 | 1.86 | 0.56 |
| 1:P:920:GLN:HB3 | 1:P:1103:THR:HG21 | 1.86 | 0.56 |
| 1:P:934:LEU:HD12 | 1:P:935:PRO:HD2 | 1.87 | 0.56 |
| 1:P:1710:LEU:HD22 | 1:P:1750:PHE:HE1 | 1.69 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:P:1763:ILE:HD12 | 1:P:1764:PRO:HD2 | 1.86 | 0.56 |
| 1:P:1828:ASN:OD1 | 1:P:1831:TRP:N | 2.38 | 0.56 |
| 1:P:3000:ARG:CZ | 1:P:3000:ARG:HA | 2.35 | 0.56 |
| 1:Q:1786:ASP:OD2 | 1:Q:1789:LEU:N | 2.29 | 0.56 |
| 1:Q:2802:VAL:H | 1:Q:2856:THR:HG22 | 1.71 | 0.56 |
| 1:Q:3205:GLU:HA | 1:Q:3208:ARG:HB2 | 1.87 | 0.56 |
| 1:R:24:ARG:HD3 | 1:R:123:ASN:HA | 1.87 | 0.56 |
| 1:R:32:VAL:HA | 1:R:37:ASN:HD21 | 1.69 | 0.56 |
| 1:R:248:ARG:NH1 | 1:R:802:ASP:O | 2.38 | 0.56 |
| 1:R:735:ARG:NH2 | 1:R:790:THR:H | 2.03 | 0.56 |
| 1:R:1150:PHE:HB3 | 1:R:1199:GLN:OE1 | 2.06 | 0.56 |
| 1:R:1465:ASP:OD2 | 1:R:1528:TYR:OH | 2.22 | 0.56 |
| 1:R:1649:VAL:HG23 | 1:R:1650:LEU:HD12 | 1.88 | 0.56 |
| 1:R:2376:ASN:HD21 | 1:R:2378:ASP:HB2 | 1.70 | 0.56 |
| 1:R:3103:MET:HE3 | 1:R:3114:PHE:HD2 | 1.71 | 0.56 |
| 1:S:221:ARG:NH2 | 1:S:287:SER:O | 2.38 | 0.56 |
| 1:S:731:ARG:HB3 | 1:S:836:HIS:HE1 | 1.70 | 0.56 |
| 1:S:957:ASN:HD21 | 1:S:959:GLU:HB3 | 1.70 | 0.56 |
| 1:S:2308:VAL:O | 1:S:2311:GLU:HG3 | 2.05 | 0.56 |
| 1:S:3037:ILE:HG12 | 1:S:3040:ALA:H | 1.70 | 0.56 |
| 1:T:1851:GLU:O | 1:T:1855:ASN:ND2 | 2.39 | 0.56 |
| 1:T:2264:PHE:HZ | 1:T:2302:VAL:HG13 | 1.70 | 0.56 |
| 1:T:3142:TYR:O | 1:T:3144:ARG:NH2 | 2.37 | 0.56 |
| 1:A:259:ASN:O | 1:A:265:ARG:NH2 | 2.38 | 0.56 |
| 1:A:2622:PHE:HA | 1:A:2703:PRO:HG2 | 1.86 | 0.56 |
| 1:B:105:ARG:HA | 1:B:108:GLN:HE22 | 1.70 | 0.56 |
| 1:B:595:GLU:OE2 | 1:B:595:GLU:N | 2.35 | 0.56 |
| 1:B:1679:SER:OG | 1:B:1680:VAL:N | 2.37 | 0.56 |
| 1:C:1654:SER:OG | 1:C:1655:LEU:N | 2.39 | 0.56 |
| 1:D:245:GLU:HA | 1:D:248:ARG:HD2 | 1.86 | 0.56 |
| 1:E:678:PHE:O | 1:E:685:ASN:ND2 | 2.39 | 0.56 |
| 1:E:1919:PRO:O | 1:E:1921:LYS:NZ | 2.37 | 0.56 |
| 1:F:848:ARG:HH21 | 1:F:934:LEU:HB3 | 1.70 | 0.56 |
| 1:F:3319:PRO:HB2 | 1:F:3343:PRO:HD3 | 1.86 | 0.56 |
| 1:G:1085:ARG:NH2 | 1:H:2463:ALA:O | 2.37 | 0.56 |
| 1:G:1400:LEU:HD21 | 1:G:1436:LEU:HB3 | 1.86 | 0.56 |
| 1:H:5:ARG:HB3 | 1:H:93:TYR:HD2 | 1.70 | 0.56 |
| 1:I:2579:ARG:HE | 1:I:2774:TYR:HH | 1.50 | 0.56 |
| 1:J:493:MET:SD | 1:J:494:ALA:N | 2.78 | 0.56 |
| 1:J:1232:SER:OG | 1:J:1234:GLU:OE1 | 2.24 | 0.56 |
| 1:J:2271:ILE:HD12 | 1:J:2298:HIS:NE2 | 2.21 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:J:2313:GLN:NE2 | 1:J:2318:LEU:O | 2.39 | 0.56 |
| 1:L:253:PRO:HB2 | 1:L:256:ARG:HH12 | 1.71 | 0.56 |
| 1:L:1282:ALA:O | 1:L:1286:MET:HG3 | 2.05 | 0.56 |
| 1:M:3217:PHE:HE1 | 1:M:3302:PRO:HB3 | 1.70 | 0.56 |
| 1:N:1415:GLU:HA | 1:N:1547:LEU:HD21 | 1.87 | 0.56 |
| 1:N:2944:LEU:HA | 1:N:3002:LYS:HE2 | 1.87 | 0.56 |
| 1:O:937:TRP:O | 1:O:1055:ASN:ND2 | 2.39 | 0.56 |
| 1:O:2961:GLY:HA2 | 1:O:3106:LEU:HD23 | 1.87 | 0.56 |
| 1:P:1047:PRO:HA | 1:P:1050:PHE:CD2 | 2.41 | 0.56 |
| 1:P:1349:TRP:O | 1:P:1463:ASN:ND2 | 2.37 | 0.56 |
| 1:Q:792:ALA:HA | 1:Q:795:LYS:HG2 | 1.87 | 0.56 |
| 1:Q:911:PRO:O | 1:Q:915:ARG:HG2 | 2.06 | 0.56 |
| 1:Q:2056:ARG:HH22 | 1:Q:2060:GLY:HA2 | 1.71 | 0.56 |
| 1:Q:2126:LEU:O | 1:Q:2161:TYR:OH | 2.23 | 0.56 |
| 1:R:245:GLU:HA | 1:R:248:ARG:HD2 | 1.86 | 0.56 |
| 1:R:1919:PRO:HA | 1:R:1941:PRO:HD3 | 1.87 | 0.56 |
| 1:S:3036:GLN:OE1 | 1:S:3043:GLN:NE2 | 2.38 | 0.56 |
| 1:T:1415:GLU:OE2 | 1:T:1555:ARG:NH2 | 2.38 | 0.56 |
| 1:A:1085:ARG:NH1 | 1:B:2464:ASP:O | 2.38 | 0.56 |
| 1:A:1223:VAL:HG13 | 1:A:1231:ILE:HB | 1.88 | 0.56 |
| 1:A:1397:GLN:NE2 | 1:A:1399:GLU:OE1 | 2.39 | 0.56 |
| 1:A:3012:ASP:OD1 | 1:A:3014:THR:OG1 | 2.17 | 0.56 |
| 1:A:3211:ASP:OD1 | 1:A:3212:ARG:N | 2.39 | 0.56 |
| 1:B:1946:ASP:HB3 | 1:B:1950:HIS:HD2 | 1.70 | 0.56 |
| 1:B:3015:ARG:HD3 | 1:B:3016:PRO:HD2 | 1.86 | 0.56 |
| 1:C:164:MET:HE1 | 1:C:187:HIS:CE1 | 2.40 | 0.56 |
| 1:C:525:TRP:CD1 | 1:C:643:ASN:HD22 | 2.23 | 0.56 |
| 1:C:611:ASN:HD22 | 1:C:771:LEU:H | 1.52 | 0.56 |
| 1:D:922:GLU:HG3 | 1:D:934:LEU:HB2 | 1.88 | 0.56 |
| 1:E:1362:ILE:HG22 | 1:E:1380:PHE:HD2 | 1.70 | 0.56 |
| 1:E:2555:GLY:HA3 | 1:E:2841:LEU:HD11 | 1.88 | 0.56 |
| 1:E:3096:GLY:HA3 | 1:E:3104:SER:HB3 | 1.87 | 0.56 |
| 1:F:860:GLN:HE21 | 1:F:864:GLU:HG2 | 1.70 | 0.56 |
| 1:F:1158:ILE:O | 1:F:1160:LYS:NZ | 2.35 | 0.56 |
| 1:F:1452:ALA:HA | 1:F:1457:PHE:CG | 2.40 | 0.56 |
| 1:G:1551:ARG:HB3 | 1:G:1661:GLU:HG3 | 1.88 | 0.56 |
| 1:H:1415:GLU:HA | 1:H:1547:LEU:HD21 | 1.86 | 0.56 |
| 1:I:1380:PHE:O | 1:I:1394:ARG:NH1 | 2.39 | 0.56 |
| 1:J:228:GLU:HA | 1:J:231:LYS:HG3 | 1.88 | 0.56 |
| 1:J:1979:SER:H | 1:J:2078:LYS:HZ1 | 1.54 | 0.56 |
| 1:J:3103:MET:HE3 | 1:J:3114:PHE:HD2 | 1.71 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:K:1322:PHE:HB3 | 1:K:1323:PRO:HD3 | 1.87 | 0.56 |
| 1:K:2392:ARG:HE | 1:K:2447:THR:HG21 | 1.71 | 0.56 |
| 1:L:938:ASP:OD1 | 1:L:1055:ASN:ND2 | 2.38 | 0.56 |
| 1:M:539:GLU:N | 1:M:539:GLU:OE1 | 2.39 | 0.56 |
| 1:M:738:VAL:HG23 | 1:M:789:ILE:HD13 | 1.88 | 0.56 |
| 1:M:782:ASP:OD1 | 1:M:783:ARG:N | 2.38 | 0.56 |
| 1:N:1775:LEU:HD12 | 1:N:1776:PRO:HD2 | 1.87 | 0.56 |
| 1:N:1896:GLN:NE2 | 1:N:1906:PRO:O | 2.39 | 0.56 |
| 1:N:2551:HIS:HB2 | 1:N:2700:ALA:HB2 | 1.87 | 0.56 |
| 1:O:44:GLU:HG3 | 1:O:135:MET:HE1 | 1.88 | 0.56 |
| 1:O:2112:ARG:NH2 | 1:O:2208:LEU:HD21 | 2.21 | 0.56 |
| 1:O:2328:ASN:HD21 | 1:P:1240:THR:HA | 1.71 | 0.56 |
| 1:O:2773:ASN:HD21 | 1:O:3142:TYR:HB2 | 1.70 | 0.56 |
| 1:Q:1124:ASP:OD1 | 1:Q:1125:ASP:N | 2.39 | 0.56 |
| 1:Q:1262:SER:OG | 1:Q:1263:HIS:N | 2.29 | 0.56 |
| 1:Q:1626:ASP:OD1 | 1:Q:1627:SER:N | 2.38 | 0.56 |
| 1:R:2371:LYS:HZ3 | 1:R:2377:LEU:H | 1.52 | 0.56 |
| 1:S:569:GLN:HB3 | 1:S:619:GLY:HA3 | 1.87 | 0.56 |
| 1:S:1124:ASP:OD1 | 1:S:1125:ASP:N | 2.36 | 0.56 |
| 1:S:1721:PRO:HD3 | 1:S:1729:TYR:CZ | 2.41 | 0.56 |
| 1:S:2325:CYS:HA | 1:T:1242:VAL:HG13 | 1.87 | 0.56 |
| 1:S:2399:LEU:HB3 | 1:S:2436:TRP:HH2 | 1.71 | 0.56 |
| 1:T:1722:TYR:CE2 | 1:T:1724:GLU:HG2 | 2.41 | 0.56 |
| 1:T:2340:VAL:HA | 1:T:2349:ARG:HH11 | 1.71 | 0.56 |
| 1:A:680:PHE:HB2 | 1:A:684:LEU:HD22 | 1.87 | 0.56 |
| 1:A:1814:LYS:HE2 | 1:A:1860:TRP:HZ3 | 1.70 | 0.56 |
| 1:A:2056:ARG:HH22 | 1:A:2060:GLY:HA2 | 1.69 | 0.56 |
| 1:B:1047:PRO:HA | 1:B:1050:PHE:CD2 | 2.41 | 0.56 |
| 1:B:1728:ARG:NH2 | 4:D:3501:NAG:O7 | 2.38 | 0.56 |
| 1:B:2552:GLY:HA3 | 1:B:2697:GLU:HA | 1.87 | 0.56 |
| 1:C:2542:ARG:NH1 | 1:C:2588:ALA:O | 2.38 | 0.56 |
| 1:D:1769:VAL:O | 1:D:1828:ASN:ND2 | 2.39 | 0.56 |
| 1:E:1531:ASP:OD1 | 1:E:1532:THR:N | 2.39 | 0.56 |
| 1:E:2989:ARG:NH1 | 1:E:3178:PHE:O | 2.39 | 0.56 |
| 1:G:1312:VAL:HG22 | 1:G:1313:ALA:H | 1.68 | 0.56 |
| 1:G:1316:VAL:HG11 | 1:G:1321:VAL:HG13 | 1.88 | 0.56 |
| 1:H:597:ARG:HE | 1:H:658:ARG:HD2 | 1.70 | 0.56 |
| 1:H:960:THR:OG1 | 1:H:964:GLU:OE2 | 2.23 | 0.56 |
| 1:H:1147:GLU:OE1 | 1:H:1245:PRO:HA | 2.04 | 0.56 |
| 1:H:1247:SER:O | 1:H:1250:LYS:NZ | 2.38 | 0.56 |
| 1:I:143:ARG:NH2 | 1:I:209:ASP:OD2 | 2.38 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:I:148:ARG:HH22 | 1:I:349:PHE:HZ | 1.54 | 0.56 |
| 1:I:1814:LYS:HD2 | 1:I:1860:TRP:CZ3 | 2.40 | 0.56 |
| 1:I:2201:ASP:OD1 | 1:I:2203:TRP:N | 2.36 | 0.56 |
| 1:I:3165:ASN:ND2 | 1:I:3168:THR:H | 2.04 | 0.56 |
| 1:J:1015:GLU:OE1 | 1:J:1015:GLU:N | 2.37 | 0.56 |
| 1:K:363:LEU:HD12 | 1:K:364:PRO:HD2 | 1.85 | 0.56 |
| 1:K:1153:PHE:HE1 | 1:K:1166:LEU:HD21 | 1.70 | 0.56 |
| 1:K:1294:LYS:O | 1:K:1297:SER:OG | 2.23 | 0.56 |
| 1:K:2345:ASN:HD21 | 1:K:2347:PHE:HB3 | 1.71 | 0.56 |
| 1:K:3083:GLN:HA | 1:K:3262:TYR:HE1 | 1.70 | 0.56 |
| 1:L:613:PRO:HA | 1:L:616:LEU:HB2 | 1.86 | 0.56 |
| 1:L:3084:PHE:HD2 | 1:L:3122:ILE:HD11 | 1.71 | 0.56 |
| 1:M:114:ASP:OD2 | 1:M:117:GLY:N | 2.38 | 0.56 |
| 1:M:2981:MET:HE2 | 1:M:3149:ASN:HB2 | 1.86 | 0.56 |
| 1:N:1427:GLU:O | 1:N:1431:ASN:ND2 | 2.38 | 0.56 |
| 1:N:1663:ASN:OD1 | 1:N:1665:GLN:NE2 | 2.30 | 0.56 |
| 1:N:1963:ILE:HD11 | 1:N:1967:LEU:HD11 | 1.88 | 0.56 |
| 1:N:2657:GLN:OE1 | 1:N:2657:GLN:N | 2.34 | 0.56 |
| 1:O:2027:ASP:OD2 | 1:O:2028:ARG:NH1 | 2.39 | 0.56 |
| 1:P:737:PHE:N | 1:P:829:ILE:O | 2.31 | 0.56 |
| 1:P:1742:TRP:HD1 | 1:P:1920:LEU:HD12 | 1.71 | 0.56 |
| 1:P:1788:VAL:HG12 | 1:P:1789:LEU:HD22 | 1.87 | 0.56 |
| 1:P:3351:VAL:HG23 | 1:P:3390:SER:HA | 1.87 | 0.56 |
| 1:Q:203:LEU:HD21 | 1:Q:351:LEU:HB3 | 1.87 | 0.56 |
| 1:Q:1723:PRO:O | 1:Q:1728:ARG:NH1 | 2.38 | 0.56 |
| 1:Q:1883:LEU:O | 1:Q:1886:SER:OG | 2.22 | 0.56 |
| 1:R:188:ILE:HG21 | 1:R:215:HIS:CE1 | 2.41 | 0.56 |
| 1:R:259:ASN:O | 1:R:265:ARG:NH2 | 2.38 | 0.56 |
| 1:R:1012:CYS:O | 1:R:1196:ARG:NH1 | 2.39 | 0.56 |
| 1:R:1828:ASN:OD1 | 1:R:1831:TRP:N | 2.37 | 0.56 |
| 1:R:2264:PHE:O | 1:R:2267:THR:OG1 | 2.19 | 0.56 |
| 1:R:3038:LYS:O | 1:R:3041:GLN:NE2 | 2.38 | 0.56 |
| 1:S:16:VAL:HG21 | 1:S:105:ARG:HH22 | 1.70 | 0.56 |
| 1:S:3263:LYS:HG3 | 1:S:3305:ILE:HD11 | 1.88 | 0.56 |
| 1:T:938:ASP:OD2 | 1:T:940:THR:OG1 | 2.22 | 0.56 |
| 1:T:1626:ASP:OD1 | 1:T:1627:SER:N | 2.38 | 0.56 |
| 1:T:3133:GLN:HB3 | 1:T:3138:ARG:HB2 | 1.87 | 0.56 |
| 1:A:1680:VAL:HG12 | 1:A:1764:PRO:HB2 | 1.86 | 0.56 |
| 1:A:2112:ARG:NH2 | 1:A:2208:LEU:HD21 | 2.21 | 0.56 |
| 1:B:996:THR:HG23 | 1:B:999:ALA:H | 1.71 | 0.56 |
| 1:B:1772:GLN:HB2 | 1:B:1818:LEU:HD11 | 1.86 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:1914:GLU:OE1 | 1:B:1914:GLU:N | 2.32 | 0.56 |
| 1:B:2521:THR:N | 1:B:2524:GLU:OE2 | 2.25 | 0.56 |
| 1:C:1855:ASN:HD21 | 1:C:2015:VAL:HA | 1.70 | 0.56 |
| 1:C:3339:ARG:NH2 | 1:C:3376:ASP:O | 2.39 | 0.56 |
| 1:D:143:ARG:NH2 | 1:D:209:ASP:OD2 | 2.39 | 0.56 |
| 1:D:508:GLU:HA | 1:D:511:LEU:HD12 | 1.88 | 0.56 |
| 1:D:744:ASN:HB3 | 1:D:779:TRP:NE1 | 2.20 | 0.56 |
| 1:D:1063:TRP:NE1 | 1:D:1067:GLN:HE22 | 2.04 | 0.56 |
| 1:E:1085:ARG:NH1 | 1:F:2462:ASN:O | 2.37 | 0.56 |
| 1:E:2768:ASP:HB3 | 1:E:2771:GLN:HE22 | 1.70 | 0.56 |
| 1:F:705:GLU:HG2 | 1:F:706:LEU:HD22 | 1.88 | 0.56 |
| 1:F:1437:VAL:HG23 | 1:F:1445:LEU:HD12 | 1.88 | 0.56 |
| 1:G:1294:LYS:O | 1:G:1297:SER:OG | 2.24 | 0.56 |
| 1:G:1380:PHE:O | 1:G:1394:ARG:NH2 | 2.31 | 0.56 |
| 1:H:110:PRO:HG2 | 1:H:111:ILE:HD12 | 1.87 | 0.56 |
| 1:H:1143:ARG:O | 1:H:1148:ARG:NH1 | 2.33 | 0.56 |
| 1:H:1145:HIS:ND1 | 1:H:1524:ASN:OD1 | 2.39 | 0.56 |
| 1:I:1420:CYS:HB2 | 1:I:1608:ARG:HH21 | 1.70 | 0.56 |
| 1:J:1427:GLU:O | 1:J:1431:ASN:ND2 | 2.39 | 0.56 |
| 1:K:436:ASP:HB3 | 1:K:522:TYR:CZ | 2.40 | 0.56 |
| 1:K:1883:LEU:O | 1:K:1886:SER:OG | 2.20 | 0.56 |
| 1:K:3312:ASP:OD1 | 1:K:3313:TYR:N | 2.39 | 0.56 |
| 1:L:3392:ASN:HB3 | 1:L:3395:ARG:HG2 | 1.88 | 0.56 |
| 1:N:244:VAL:HG23 | 1:N:248:ARG:HE | 1.70 | 0.56 |
| 1:O:64:ALA:HA | 1:O:178:GLU:HG3 | 1.87 | 0.56 |
| 1:O:926:ARG:NH1 | 1:O:931:GLN:O | 2.38 | 0.56 |
| 1:O:1122:HIS:ND1 | 1:O:1123:TYR:O | 2.38 | 0.56 |
| 1:O:1352:THR:HG21 | 1:O:1535:PHE:HE1 | 1.71 | 0.56 |
| 1:O:1494:GLN:NE2 | 1:O:1495:PRO:O | 2.38 | 0.56 |
| 1:O:2864:LEU:HG | 1:O:2868:SER:HB2 | 1.88 | 0.56 |
| 1:O:2960:HIS:HE1 | 1:O:3119:HIS:HE1 | 1.54 | 0.56 |
| 1:O:3333:SER:OG | 1:O:3336:THR:OG1 | 2.23 | 0.56 |
| 1:P:188:ILE:HG21 | 1:P:215:HIS:CE1 | 2.41 | 0.56 |
| 1:P:1411:LEU:HD12 | 1:P:1412:LEU:HD22 | 1.86 | 0.56 |
| 1:P:2602:ASP:OD2 | 1:P:2604:THR:OG1 | 2.22 | 0.56 |
| 1:Q:111:ILE:HD13 | 1:Q:122:LYS:HA | 1.87 | 0.56 |
| 1:Q:651:TRP:CZ3 | 1:Q:655:GLN:HG3 | 2.41 | 0.56 |
| 1:Q:2044:SER:OG | 1:Q:2046:ASP:OD1 | 2.23 | 0.56 |
| 1:R:2757:ILE:O | 1:R:2761:ALA:HB2 | 2.06 | 0.56 |
| 1:S:2345:ASN:HD21 | 1:S:2347:PHE:HB3 | 1.71 | 0.56 |
| 1:S:3334:ARG:HH21 | 1:S:3406:ILE:HG23 | 1.69 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:T:374:GLU:OE1 | 1:T:374:GLU:N | 2.35 | 0.56 |
| 1:T:925:LEU:HD22 | 1:T:928:LYS:HZ3 | 1.69 | 0.56 |
| 1:T:1232:SER:OG | 1:T:1234:GLU:OE1 | 2.23 | 0.56 |
| 1:T:2264:PHE:O | 1:T:2267:THR:OG1 | 2.19 | 0.56 |
| 1:A:183:VAL:HG21 | 1:A:365:TYR:CE1 | 2.41 | 0.56 |
| 1:B:418:ASP:OD2 | 1:B:662:TYR:N | 2.37 | 0.56 |
| 1:B:597:ARG:HD3 | 1:B:658:ARG:HH11 | 1.70 | 0.56 |
| 1:B:3124:ARG:O | 1:B:3127:GLN:HG3 | 2.06 | 0.56 |
| 1:C:2917:LYS:HD2 | 1:C:2917:LYS:N | 2.21 | 0.56 |
| 1:D:1713:PHE:HE1 | 1:D:1929:TYR:HB3 | 1.70 | 0.56 |
| 1:E:3173:ARG:HB2 | 1:E:3176:GLN:HG3 | 1.87 | 0.56 |
| 1:F:662:TYR:HE2 | 1:F:700:TYR:HB3 | 1.71 | 0.56 |
| 1:F:3010:TYR:OH | 1:F:3189:ASN:OD1 | 2.24 | 0.56 |
| 1:G:203:LEU:HD21 | 1:G:351:LEU:HB3 | 1.88 | 0.56 |
| 1:G:1588:HIS:ND1 | 1:J:337:GLN:OE1 | 2.36 | 0.56 |
| 1:G:2508:VAL:O | 1:G:2515:LYS:NZ | 2.38 | 0.56 |
| 1:I:782:ASP:OD1 | 1:I:783:ARG:N | 2.39 | 0.56 |
| 1:I:1153:PHE:HE1 | 1:I:1166:LEU:HD21 | 1.71 | 0.56 |
| 1:I:3213:VAL:HG23 | 1:I:3306:SER:HB2 | 1.87 | 0.56 |
| 1:J:256:ARG:O | 1:J:265:ARG:NH1 | 2.33 | 0.56 |
| 1:J:2984:PHE:O | 1:J:2988:HIS:ND1 | 2.33 | 0.56 |
| 1:K:1684:THR:N | 1:K:1687:GLU:OE2 | 2.34 | 0.56 |
| 1:K:2046:ASP:O | 1:L:1493:ARG:HD3 | 2.06 | 0.56 |
| 1:K:2974:TYR:HB3 | 1:L:3367:PRO:HB2 | 1.86 | 0.56 |
| 1:L:739:GLY:HA3 | 1:L:784:LEU:HB3 | 1.87 | 0.56 |
| 1:L:788:GLU:OE2 | 1:L:791:ASP:N | 2.34 | 0.56 |
| 1:L:1488:ALA:HB1 | 1:L:1491:ILE:HD13 | 1.87 | 0.56 |
| 1:M:1083:SER:O | 1:M:1086:LYS:NZ | 2.37 | 0.56 |
| 1:M:1144:GLN:OE1 | 1:M:1148:ARG:NH1 | 2.37 | 0.56 |
| 1:O:3144:ARG:HA | 1:O:3147:LEU:HG | 1.87 | 0.56 |
| 1:P:1448:LEU:HD21 | 1:P:1596:LEU:HG | 1.88 | 0.56 |
| 1:P:1568:SER:N | 1:P:1597:GLY:O | 2.39 | 0.56 |
| 1:P:1773:ASN:OD1 | 1:P:1774:SER:N | 2.39 | 0.56 |
| 1:Q:3212:ARG:HG3 | 1:Q:3214:TYR:CZ | 2.41 | 0.56 |
| 1:R:449:ARG:HH21 | 1:R:535:ILE:HA | 1.71 | 0.56 |
| 1:R:1501:ASP:HB3 | 1:R:1504:GLN:HB2 | 1.87 | 0.56 |
| 1:R:2191:PRO:HG2 | 1:R:2194:PHE:CD2 | 2.38 | 0.56 |
| 1:R:2271:ILE:HD12 | 1:R:2298:HIS:NE2 | 2.21 | 0.56 |
| 1:S:2580:LEU:HA | 1:S:2583:VAL:HG12 | 1.87 | 0.56 |
| 1:T:256:ARG:O | 1:T:265:ARG:NH1 | 2.36 | 0.56 |
| 1:T:596:GLN:HE21 | 1:T:602:PHE:HD1 | 1.51 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:T:1501:ASP:HB3 | 1:T:1504:GLN:HB2 | 1.87 | 0.56 |
| 1:T:2283:LEU:HD21 | 1:T:2292:ASP:HB3 | 1.88 | 0.56 |
| 1:A:1312:VAL:HG22 | 1:A:1313:ALA:H | 1.70 | 0.56 |
| 1:A:2780:ASN:OD1 | 1:A:2781:PHE:N | 2.39 | 0.56 |
| 1:A:3114:PHE:HA | 1:A:3117:ILE:HG12 | 1.88 | 0.56 |
| 1:B:1238:LYS:NZ | 1:B:1239:VAL:O | 2.38 | 0.56 |
| 1:B:1898:LEU:HD21 | 1:B:1965:ALA:HB1 | 1.87 | 0.56 |
| 1:C:164:MET:HE1 | 1:C:187:HIS:HE1 | 1.71 | 0.56 |
| 1:C:2488:LYS:HD3 | 1:C:2489:PRO:HD2 | 1.88 | 0.56 |
| 1:D:435:LYS:HG2 | 1:D:436:ASP:H | 1.70 | 0.56 |
| 1:D:1019:GLU:HA | 1:D:1022:HIS:NE2 | 2.21 | 0.56 |
| 1:D:3085:GLU:O | 1:D:3089:ASN:ND2 | 2.38 | 0.56 |
| 1:E:1551:ARG:HG2 | 1:E:1661:GLU:HG3 | 1.87 | 0.56 |
| 1:E:2587:ARG:HH12 | 1:E:2753:PRO:HG2 | 1.71 | 0.56 |
| 1:F:170:GLU:HG3 | 1:F:304:ARG:HH22 | 1.69 | 0.56 |
| 1:F:313:PHE:HE2 | 1:F:406:PRO:HB3 | 1.70 | 0.56 |
| 1:F:1372:SER:O | 1:F:1374:THR:OG1 | 2.24 | 0.56 |
| 1:F:1895:TRP:HA | 1:F:1898:LEU:HB2 | 1.88 | 0.56 |
| 1:F:2866:PRO:O | 1:G:2741:ARG:NE | 2.39 | 0.56 |
| 1:G:159:THR:HG23 | 1:G:162:PHE:H | 1.71 | 0.56 |
| 1:G:323:ASN:OD1 | 1:G:324:VAL:N | 2.39 | 0.56 |
| 1:G:1488:ALA:O | 1:G:1492:MET:HG2 | 2.06 | 0.56 |
| 1:G:2509:SER:O | 1:G:3138:ARG:NH1 | 2.39 | 0.56 |
| 1:G:2929:LEU:HD22 | 1:G:2933:GLN:HG3 | 1.88 | 0.56 |
| 1:H:1541:PRO:O | 1:H:1544:GLU:HG3 | 2.05 | 0.56 |
| 1:J:270:ALA:HA | 1:J:273:LEU:HD12 | 1.86 | 0.56 |
| 1:J:3122:ILE:HA | 1:J:3125:ILE:HG12 | 1.88 | 0.56 |
| 1:K:540:THR:HG22 | 1:K:551:HIS:HA | 1.88 | 0.56 |
| 1:K:718:MET:SD | 1:K:722:GLN:HG2 | 2.46 | 0.56 |
| 1:M:1049:PHE:HE1 | 1:M:1053:HIS:CE1 | 2.24 | 0.56 |
| 1:M:2328:ASN:HB3 | 1:N:1241:VAL:HB | 1.88 | 0.56 |
| 1:N:230:GLN:NE2 | 1:N:236:THR:O | 2.35 | 0.56 |
| 1:N:2487:SER:OG | 1:N:2488:LYS:N | 2.39 | 0.56 |
| 1:O:811:LYS:HD2 | 1:O:815:GLY:HA2 | 1.88 | 0.56 |
| 1:O:1576:CYS:HB2 | 1:O:1632:ASP:HB3 | 1.87 | 0.56 |
| 1:O:2109:ALA:HA | 1:O:2112:ARG:NH2 | 2.21 | 0.56 |
| 1:O:2155:PRO:HB2 | 1:O:2306:TRP:CZ3 | 2.41 | 0.56 |
| 1:O:2797:ARG:HA | 1:O:2801:ARG:HH22 | 1.71 | 0.56 |
| 1:P:492:GLY:HA2 | 1:P:607:GLU:HG2 | 1.87 | 0.56 |
| 1:P:735:ARG:HH22 | 1:P:790:THR:H | 1.53 | 0.56 |
| 1:P:1365:ALA:HA | 1:P:1378:ASN:HB3 | 1.88 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:P:1488:ALA:HB1 | 1:P:1491:ILE:HD12 | 1.87 | 0.56 |
| 1:P:3085:GLU:O | 1:P:3089:ASN:ND2 | 2.39 | 0.56 |
| 1:Q:539:GLU:N | 1:Q:539:GLU:OE1 | 2.39 | 0.56 |
| 1:Q:2570:GLY:HA3 | 1:Q:2845:TRP:HB2 | 1.86 | 0.56 |
| 1:R:501:ARG:HH22 | 1:R:702:TYR:HB3 | 1.69 | 0.56 |
| 1:R:3287:LEU:HB3 | 1:R:3295:LEU:HB3 | 1.87 | 0.56 |
| 1:S:2567:CYS:O | 1:S:2569:HIS:ND1 | 2.37 | 0.56 |
| 1:S:2614:LEU:HB3 | 1:S:2636:ARG:HH12 | 1.69 | 0.56 |
| 1:T:38:LEU:O | 1:T:73:TYR:OH | 2.24 | 0.56 |
| 1:T:1556:LEU:HB2 | 1:T:1625:LEU:HD21 | 1.88 | 0.56 |
| 1:A:866:LEU:HD23 | 1:A:967:PRO:HB2 | 1.88 | 0.56 |
| 1:A:903:CYS:O | 1:A:905:HIS:ND1 | 2.39 | 0.56 |
| 1:A:913:TRP:HE3 | 1:A:914:HIS:HD2 | 1.52 | 0.56 |
| 1:A:1381:PHE:O | 1:A:1394:ARG:NH2 | 2.39 | 0.56 |
| 1:B:613:PRO:HA | 1:B:616:LEU:HB2 | 1.87 | 0.56 |
| 1:B:2408:VAL:HG22 | 1:B:2473:ILE:HG22 | 1.86 | 0.56 |
| 1:B:2741:ARG:HH22 | 1:C:2869:VAL:HG23 | 1.70 | 0.56 |
| 1:C:2974:TYR:HB3 | 1:D:3367:PRO:HB2 | 1.87 | 0.56 |
| 1:E:559:VAL:N | 1:E:564:GLU:O | 2.34 | 0.56 |
| 1:F:1067:GLN:HA | 1:F:1070:ARG:HG2 | 1.88 | 0.56 |
| 1:F:3132:LEU:HG | 1:F:3136:ARG:NH1 | 2.21 | 0.56 |
| 1:G:2001:CYS:HA | 1:G:2007:CYS:HB3 | 1.87 | 0.56 |
| 1:H:374:GLU:OE1 | 1:H:374:GLU:N | 2.35 | 0.56 |
| 1:H:3080:PHE:HE2 | 1:H:3126:TRP:HD1 | 1.54 | 0.56 |
| 1:I:2585:LEU:HD23 | 1:I:2589:LEU:HD23 | 1.88 | 0.56 |
| 1:J:1599:GLU:OE2 | 1:J:1600:THR:OG1 | 2.24 | 0.56 |
| 1:J:3320:LEU:N | 1:J:3341:HIS:O | 2.38 | 0.56 |
| 1:K:2622:PHE:HA | 1:K:2703:PRO:HG2 | 1.88 | 0.56 |
| 1:K:3160:GLU:HG2 | 1:K:3169:ARG:HH22 | 1.71 | 0.56 |
| 1:L:2602:ASP:OD1 | 1:L:2603:TRP:N | 2.39 | 0.56 |
| 1:L:2771:GLN:HG2 | 1:L:2772:PHE:HD1 | 1.71 | 0.56 |
| 1:M:1834:PHE:HE2 | 1:M:1891:ILE:HG13 | 1.71 | 0.56 |
| 1:N:2287:HIS:CE1 | 1:N:2432:LEU:HB2 | 2.41 | 0.56 |
| 1:N:3395:ARG:NE | 1:N:3398:GLN:OE1 | 2.39 | 0.56 |
| 1:O:471:HIS:NE2 | 1:O:489:CYS:SG | 2.79 | 0.56 |
| 1:O:1338:LEU:HD21 | 1:O:1345:SER:HA | 1.87 | 0.56 |
| 1:O:2156:HIS:HB3 | 1:O:2357:VAL:HG21 | 1.86 | 0.56 |
| 1:O:2941:LEU:HD23 | 1:O:3031:PRO:HG2 | 1.88 | 0.56 |
| 1:O:3385:ASP:OD1 | 1:O:3403:GLN:NE2 | 2.38 | 0.56 |
| 1:P:2639:ARG:HD3 | 1:P:2641:GLN:HE22 | 1.70 | 0.56 |
| 1:P:3132:LEU:HG | 1:P:3136:ARG:NH1 | 2.20 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:Q:1328:LEU:HB3 | 1:Q:1499:PHE:CE2 | 2.40 | 0.56 |
| 1:S:1557:PHE:CG | 1:S:1611:LYS:HD2 | 2.41 | 0.56 |
| 1:S:1756:ARG:HH22 | 1:T:2102:ARG:CZ | 2.19 | 0.56 |
| 1:T:1763:ILE:HD12 | 1:T:1764:PRO:HD2 | 1.88 | 0.56 |
| 1:T:2630:LEU:HD11 | 1:T:2698:TYR:HE1 | 1.71 | 0.56 |
| 1:A:2587:ARG:HH12 | 1:A:2753:PRO:HB2 | 1.70 | 0.55 |
| 1:B:374:GLU:OE1 | 1:B:374:GLU:N | 2.31 | 0.55 |
| 1:B:885:HIS:HD1 | 1:B:1044:ALA:HB2 | 1.70 | 0.55 |
| 1:B:2454:HIS:HA | 1:B:2456:ARG:HH22 | 1.70 | 0.55 |
| 1:B:2626:GLU:HB2 | 1:B:2633:LYS:HD3 | 1.88 | 0.55 |
| 1:B:3124:ARG:O | 1:B:3128:ILE:HG12 | 2.06 | 0.55 |
| 1:C:277:ARG:NH2 | 1:K:834:THR:O | 2.36 | 0.55 |
| 1:D:595:GLU:OE1 | 1:D:730:ARG:NH1 | 2.38 | 0.55 |
| 1:D:1299:HIS:ND1 | 1:D:1299:HIS:O | 2.38 | 0.55 |
| 1:D:3088:HIS:HE1 | 1:D:3119:HIS:CE1 | 2.24 | 0.55 |
| 1:E:835:THR:OG1 | 1:S:277:ARG:NH2 | 2.38 | 0.55 |
| 1:E:2696:LEU:O | 1:E:2699:SER:OG | 2.22 | 0.55 |
| 1:E:3087:LEU:O | 1:E:3090:THR:OG1 | 2.21 | 0.55 |
| 1:F:714:GLN:HE22 | 1:F:719:THR:HB | 1.71 | 0.55 |
| 1:F:1431:ASN:OD1 | 1:F:1594:SER:OG | 2.24 | 0.55 |
| 1:G:1154:MET:HE3 | 1:G:1155:LEU:H | 1.71 | 0.55 |
| 1:G:1474:LEU:HD11 | 1:G:1543:LEU:HD11 | 1.86 | 0.55 |
| 1:G:1899:GLN:NE2 | 1:G:1905:ASP:O | 2.39 | 0.55 |
| 1:H:1895:TRP:HA | 1:H:1898:LEU:HD12 | 1.89 | 0.55 |
| 1:H:2820:ASP:OD1 | 1:H:2821:LEU:N | 2.39 | 0.55 |
| 1:J:309:ALA:H | 1:J:370:SER:HG | 1.51 | 0.55 |
| 1:J:1416:GLN:HE21 | 1:J:1422:PHE:HA | 1.70 | 0.55 |
| 1:J:1542:GLN:HA | 1:J:1545:GLU:CD | 2.31 | 0.55 |
| 1:J:3124:ARG:O | 1:J:3127:GLN:HG3 | 2.06 | 0.55 |
| 1:K:126:PHE:HA | 1:K:143:ARG:HH22 | 1.71 | 0.55 |
| 1:K:650:ILE:HG22 | 1:K:713:LEU:HD12 | 1.87 | 0.55 |
| 1:K:2049:PHE:O | 1:L:1490:ASN:ND2 | 2.39 | 0.55 |
| 1:K:2508:VAL:O | 1:K:2515:LYS:NZ | 2.39 | 0.55 |
| 1:K:2553:TYR:CD2 | 1:K:2554:PRO:HA | 2.41 | 0.55 |
| 1:K:2585:LEU:HD13 | 1:K:2706:PHE:CZ | 2.41 | 0.55 |
| 1:L:3008:ILE:HG21 | 1:L:3116:MET:HB3 | 1.88 | 0.55 |
| 1:M:323:ASN:OD1 | 1:M:324:VAL:N | 2.40 | 0.55 |
| 1:N:595:GLU:OE1 | 1:N:730:ARG:NH1 | 2.38 | 0.55 |
| 1:N:913:TRP:CD1 | 1:N:1088:LEU:HD12 | 2.41 | 0.55 |
| 1:N:2088:PRO:O | 1:N:2090:ASN:N | 2.37 | 0.55 |
| 1:O:1144:GLN:HA | 1:O:1148:ARG:HH22 | 1.70 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:O:1350:ASP:OD1 | 1:O:1352:THR:OG1 | 2.19 | 0.55 |
| 1:O:1919:PRO:O | 1:O:1921:LYS:NZ | 2.39 | 0.55 |
| 1:P:2652:SER:O | 1:P:2656:ARG:NH1 | 2.38 | 0.55 |
| 1:P:3015:ARG:HD3 | 1:P:3016:PRO:HD2 | 1.88 | 0.55 |
| 1:P:3062:ASP:HB3 | 1:P:3065:PHE:HB3 | 1.89 | 0.55 |
| 1:P:3077:TYR:HE1 | 1:P:3126:TRP:HE1 | 1.53 | 0.55 |
| 1:Q:938:ASP:HA | 1:Q:1055:ASN:HD21 | 1.71 | 0.55 |
| 1:Q:3173:ARG:HB2 | 1:Q:3176:GLN:HG3 | 1.87 | 0.55 |
| 1:R:312:SER:HA | 1:R:365:TYR:O | 2.06 | 0.55 |
| 1:R:329:CYS:HA | 1:R:342:CYS:HB2 | 1.87 | 0.55 |
| 1:R:1492:MET:HA | 1:R:1516:PRO:HG2 | 1.87 | 0.55 |
| 1:S:651:TRP:CZ3 | 1:S:655:GLN:HG3 | 2.41 | 0.55 |
| 1:S:2802:VAL:H | 1:S:2856:THR:HG22 | 1.71 | 0.55 |
| 1:T:705:GLU:HG2 | 1:T:706:LEU:HD22 | 1.89 | 0.55 |
| 1:A:1294:LYS:O | 1:A:1297:SER:OG | 2.24 | 0.55 |
| 1:A:3125:ILE:HA | 1:A:3128:ILE:HG12 | 1.87 | 0.55 |
| 1:B:259:ASN:O | 1:B:265:ARG:NH2 | 2.40 | 0.55 |
| 1:B:1362:ILE:HD13 | 1:B:1456:LEU:HD11 | 1.88 | 0.55 |
| 1:B:2488:LYS:NZ | 1:B:2489:PRO:O | 2.38 | 0.55 |
| 1:B:2579:ARG:HH21 | 1:B:2769:TYR:HB3 | 1.71 | 0.55 |
| 1:B:2602:ASP:OD2 | 1:B:2604:THR:OG1 | 2.23 | 0.55 |
| 1:C:2096:ILE:HD13 | 1:C:2179:PRO:HG2 | 1.89 | 0.55 |
| 1:C:2108:LYS:O | 1:C:2112:ARG:NH1 | 2.39 | 0.55 |
| 1:C:2117:ASP:OD1 | 1:C:2119:THR:OG1 | 2.20 | 0.55 |
| 1:D:105:ARG:HA | 1:D:108:GLN:HE22 | 1.71 | 0.55 |
| 1:D:887:GLN:HE22 | 1:D:889:ASN:HB2 | 1.71 | 0.55 |
| 1:E:1919:PRO:HG3 | 1:E:1940:LYS:NZ | 2.22 | 0.55 |
| 1:F:473:LEU:H | 1:F:629:HIS:HB3 | 1.71 | 0.55 |
| 1:F:597:ARG:NH2 | 1:F:655:GLN:OE1 | 2.38 | 0.55 |
| 1:F:1539:THR:HG22 | 1:F:1542:GLN:NE2 | 2.21 | 0.55 |
| 1:G:1539:THR:HG23 | 1:G:1541:PRO:HD2 | 1.88 | 0.55 |
| 1:G:2421:ARG:HH22 | 1:G:2424:ALA:HB2 | 1.71 | 0.55 |
| 1:G:3153:PRO:HB2 | 1:G:3158:ASN:HD22 | 1.70 | 0.55 |
| 1:H:1143:ARG:HB3 | 1:H:1148:ARG:HH22 | 1.71 | 0.55 |
| 1:H:1932:ASP:OD2 | 1:H:1935:THR:N | 2.28 | 0.55 |
| 1:I:2623:GLU:OE1 | 1:I:2623:GLU:N | 2.33 | 0.55 |
| 1:I:2669:ASN:OD1 | 1:I:2849:ARG:NE | 2.38 | 0.55 |
| 1:J:527:ARG:O | 1:J:530:THR:OG1 | 2.23 | 0.55 |
| 1:J:737:PHE:N | 1:J:829:ILE:O | 2.34 | 0.55 |
| 1:J:756:LYS:HD3 | 1:J:762:SER:HB2 | 1.88 | 0.55 |
| 1:J:851:VAL:HG12 | 1:J:935:PRO:HB2 | 1.89 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:J:2088:PRO:O | 1:J:2090:ASN:N | 2.33 | 0.55 |
| 1:K:2961:GLY:HA2 | 1:K:3106:LEU:HD23 | 1.88 | 0.55 |
| 1:L:780:ASN:OD1 | 1:L:781:PHE:N | 2.39 | 0.55 |
| 1:L:1568:SER:N | 1:L:1597:GLY:O | 2.39 | 0.55 |
| 1:M:1623:LEU:HD23 | 1:N:2785:THR:HG21 | 1.88 | 0.55 |
| 1:M:2802:VAL:H | 1:M:2856:THR:HG22 | 1.69 | 0.55 |
| 1:O:460:SER:O | 1:O:1371:ARG:NH1 | 2.38 | 0.55 |
| 1:O:981:SER:HB2 | 1:O:1031:GLY:HA3 | 1.89 | 0.55 |
| 1:O:1775:LEU:HD11 | 1:O:1780:ASN:HD21 | 1.71 | 0.55 |
| 1:P:421:PRO:HG3 | 1:P:662:TYR:HE1 | 1.70 | 0.55 |
| 1:P:1116:GLU:HA | 1:P:1120:GLN:HA | 1.88 | 0.55 |
| 1:P:2343:ASN:HB3 | 1:P:2349:ARG:HH22 | 1.71 | 0.55 |
| 1:P:2469:LEU:HD11 | 1:P:2489:PRO:HB2 | 1.88 | 0.55 |
| 1:Q:159:THR:HG23 | 1:Q:162:PHE:H | 1.70 | 0.55 |
| 1:Q:2025:SER:O | 1:R:1651:ARG:NH2 | 2.39 | 0.55 |
| 1:R:465:GLN:NE2 | 1:R:558:PRO:O | 2.34 | 0.55 |
| 1:R:703:GLU:N | 1:R:703:GLU:OE1 | 2.40 | 0.55 |
| 1:R:919:VAL:O | 1:R:923:ASN:ND2 | 2.39 | 0.55 |
| 1:R:2138:SER:OG | 1:R:2143:LYS:NZ | 2.37 | 0.55 |
| 1:S:2509:SER:H | 1:S:3138:ARG:HH12 | 1.54 | 0.55 |
| 1:S:3385:ASP:O | 1:T:3148:ARG:NH1 | 2.35 | 0.55 |
| 1:T:493:MET:HE2 | 1:T:493:MET:HA | 1.89 | 0.55 |
| 1:T:2657:GLN:N | 1:T:2657:GLN:OE1 | 2.38 | 0.55 |
| 1:T:3085:GLU:O | 1:T:3089:ASN:ND2 | 2.39 | 0.55 |
| 1:A:1338:LEU:HD21 | 1:A:1345:SER:HA | 1.89 | 0.55 |
| 1:A:2674:TYR:OH | 1:A:2712:VAL:HG22 | 2.05 | 0.55 |
| 1:B:160:GLN:NE2 | 1:B:161:LEU:HG | 2.20 | 0.55 |
| 1:B:1919:PRO:HB2 | 1:B:1924:SER:HB2 | 1.87 | 0.55 |
| 1:C:3200:ILE:HA | 1:C:3203:ILE:HG22 | 1.89 | 0.55 |
| 1:C:3301:THR:HG22 | 1:C:3326:LEU:HA | 1.88 | 0.55 |
| 1:D:1268:LEU:HD23 | 1:D:1268:LEU:H | 1.72 | 0.55 |
| 1:E:2664:GLN:HE21 | 1:E:2670:PHE:HA | 1.70 | 0.55 |
| 1:E:3213:VAL:HG23 | 1:E:3306:SER:HB2 | 1.88 | 0.55 |
| 1:F:812:ASP:HB3 | 1:F:818:TRP:HH2 | 1.72 | 0.55 |
| 1:F:1015:GLU:N | 1:F:1015:GLU:OE1 | 2.39 | 0.55 |
| 1:F:2326:ALA:HB3 | 1:F:2330:MET:HE3 | 1.88 | 0.55 |
| 1:F:2552:GLY:HA3 | 1:F:2697:GLU:HA | 1.89 | 0.55 |
| 1:G:143:ARG:NH2 | 1:G:209:ASP:OD2 | 2.31 | 0.55 |
| 1:G:596:GLN:C | 1:G:597:ARG:HE | 2.15 | 0.55 |
| 1:G:3358:THR:H | 1:H:3329:LYS:HE3 | 1.71 | 0.55 |
| 1:H:276:TYR:O | 1:H:280:GLY:N | 2.39 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:I:851:VAL:HG12 | 1:I:935:PRO:HB2 | 1.88 | 0.55 |
| 1:I:937:TRP:CD1 | 1:I:938:ASP:H | 2.24 | 0.55 |
| 1:I:953:GLU:O | 1:I:966:ASN:N | 2.28 | 0.55 |
| 1:I:2872:PHE:HD2 | 1:I:2892:PRO:HG2 | 1.71 | 0.55 |
| 1:J:2574:PHE:HE1 | 1:J:2578:HIS:CE1 | 2.25 | 0.55 |
| 1:J:3234:PRO:HG2 | 1:J:3237:GLY:HA3 | 1.88 | 0.55 |
| 1:J:3392:ASN:HB3 | 1:J:3395:ARG:HG2 | 1.88 | 0.55 |
| 1:K:1316:VAL:HG11 | 1:K:1321:VAL:HG13 | 1.89 | 0.55 |
| 1:K:2156:HIS:HB3 | 1:K:2357:VAL:HG21 | 1.88 | 0.55 |
| 1:L:374:GLU:OE1 | 1:L:374:GLU:N | 2.35 | 0.55 |
| 1:L:934:LEU:HD12 | 1:L:935:PRO:HD2 | 1.88 | 0.55 |
| 1:L:2865:ARG:HG2 | 1:L:2866:PRO:HD2 | 1.88 | 0.55 |
| 1:L:3157:PHE:O | 1:L:3169:ARG:NH1 | 2.40 | 0.55 |
| 1:M:580:TYR:HE2 | 1:M:959:GLU:HB2 | 1.71 | 0.55 |
| 1:M:2812:LYS:HG3 | 1:M:2840:PRO:HA | 1.87 | 0.55 |
| 1:M:3125:ILE:HA | 1:M:3128:ILE:HG12 | 1.88 | 0.55 |
| 1:N:1677:ARG:NH1 | 1:N:1763:ILE:O | 2.34 | 0.55 |
| 1:N:2481:LEU:HD21 | 3:aA:1:NAG:H62 | 1.87 | 0.55 |
| 1:P:845:LEU:HD22 | 1:P:926:ARG:HD3 | 1.88 | 0.55 |
| 1:P:1898:LEU:HD21 | 1:P:1965:ALA:HB1 | 1.88 | 0.55 |
| 1:P:2191:PRO:HG2 | 1:P:2194:PHE:HD2 | 1.70 | 0.55 |
| 1:P:3234:PRO:HG2 | 1:P:3237:GLY:HA3 | 1.88 | 0.55 |
| 1:Q:1420:CYS:HB2 | 1:Q:1608:ARG:HH21 | 1.71 | 0.55 |
| 1:R:1742:TRP:HD1 | 1:R:1920:LEU:HD12 | 1.70 | 0.55 |
| 1:R:2614:LEU:HD11 | 1:R:2636:ARG:HH12 | 1.71 | 0.55 |
| 1:R:2896:PHE:O | 1:S:2734:ASN:ND2 | 2.39 | 0.55 |
| 1:S:539:GLU:HA | 1:S:555:PHE:HB2 | 1.89 | 0.55 |
| 1:S:2409:ARG:O | 1:S:2471:TYR:HA | 2.06 | 0.55 |
| 1:S:2532:LEU:HG | 1:S:2536:GLN:NE2 | 2.21 | 0.55 |
| 1:S:3203:ILE:HA | 1:S:3206:ASN:HB2 | 1.89 | 0.55 |
| 1:S:3228:ALA:O | 1:S:3245:PHE:N | 2.39 | 0.55 |
| 1:T:244:VAL:HG22 | 1:T:828:ILE:HG21 | 1.88 | 0.55 |
| 1:T:1262:SER:OG | 1:T:1263:HIS:N | 2.33 | 0.55 |
| 1:T:1433:LEU:HD21 | 1:T:1460:HIS:NE2 | 2.20 | 0.55 |
| 1:A:1494:GLN:NE2 | 1:A:1495:PRO:O | 2.39 | 0.55 |
| 1:A:2517:ILE:HD13 | 1:A:2601:TRP:HB2 | 1.89 | 0.55 |
| 1:B:2771:GLN:HG2 | 1:B:2772:PHE:HD1 | 1.71 | 0.55 |
| 1:D:725:HIS:O | 1:D:729:GLU:HG2 | 2.05 | 0.55 |
| 1:E:1905:ASP:HB3 | 1:E:1908:GLU:HB2 | 1.87 | 0.55 |
| 1:E:2027:ASP:OD1 | 1:E:2028:ARG:N | 2.39 | 0.55 |
| 1:F:182:GLU:O | 1:F:186:ASN:ND2 | 2.39 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:F:954:THR:HG22 | 1:F:965:PRO:HA | 1.87 | 0.55 |
| 1:F:1088:LEU:O | 1:F:1089:GLN:NE2 | 2.40 | 0.55 |
| 1:F:1142:HIS:HE1 | 1:F:1524:ASN:HA | 1.71 | 0.55 |
| 1:F:2231:GLU:CD | 1:F:2231:GLU:H | 2.14 | 0.55 |
| 1:F:2568:HIS:C | 1:F:2569:HIS:HD1 | 2.14 | 0.55 |
| 1:G:632:ALA:HA | 1:G:637:PHE:HD2 | 1.71 | 0.55 |
| 1:G:2234:LYS:HG3 | 1:G:2243:VAL:HG11 | 1.89 | 0.55 |
| 1:G:3229:ASN:OD1 | 1:G:3231:LYS:NZ | 2.28 | 0.55 |
| 1:H:532:VAL:HG13 | 1:H:537:SER:HB3 | 1.88 | 0.55 |
| 1:H:848:ARG:HE | 1:H:934:LEU:HG | 1.71 | 0.55 |
| 1:H:2238:ASP:O | 1:H:2240:LYS:NZ | 2.34 | 0.55 |
| 1:I:408:GLY:N | 1:I:669:THR:OG1 | 2.35 | 0.55 |
| 1:I:1572:GLN:HB2 | 1:I:1636:LYS:HB2 | 1.87 | 0.55 |
| 1:I:2234:LYS:HG3 | 1:I:2243:VAL:HG11 | 1.87 | 0.55 |
| 1:J:198:HIS:HD1 | 1:J:205:TRP:CD1 | 2.25 | 0.55 |
| 1:J:374:GLU:OE1 | 1:J:374:GLU:N | 2.35 | 0.55 |
| 1:J:1088:LEU:HD22 | 1:J:1109:PRO:HG3 | 1.88 | 0.55 |
| 1:J:1205:ILE:HD12 | 1:J:1208:LYS:HE3 | 1.88 | 0.55 |
| 1:J:1238:LYS:NZ | 1:J:1239:VAL:O | 2.39 | 0.55 |
| 1:J:1415:GLU:OE1 | 1:J:1555:ARG:NH2 | 2.40 | 0.55 |
| 1:K:454:ARG:HH21 | 1:K:514:ARG:HB3 | 1.71 | 0.55 |
| 1:K:1124:ASP:OD1 | 1:K:1125:ASP:N | 2.40 | 0.55 |
| 1:M:1070:ARG:HH12 | 1:M:1137:GLN:HE22 | 1.55 | 0.55 |
| 1:M:1932:ASP:OD2 | 1:M:1934:ILE:HG22 | 2.06 | 0.55 |
| 1:N:2738:GLN:O | 1:N:2742:GLN:NE2 | 2.38 | 0.55 |
| 1:O:1124:ASP:OD1 | 1:O:1125:ASP:N | 2.39 | 0.55 |
| 1:O:1144:GLN:OE1 | 1:O:1148:ARG:NH1 | 2.32 | 0.55 |
| 1:O:2085:GLN:HE21 | 1:O:2366:ARG:HH12 | 1.55 | 0.55 |
| 1:P:1809:VAL:HG22 | 1:P:1811:ARG:HH12 | 1.71 | 0.55 |
| 1:P:2093:ARG:HD2 | 1:P:2367:TYR:HE1 | 1.71 | 0.55 |
| 1:Q:1048:ILE:HA | 1:Q:1051:LEU:HD12 | 1.87 | 0.55 |
| 1:R:2044:SER:N | 1:R:2047:ASP:OD2 | 2.40 | 0.55 |
| 1:R:3350:ASN:OD1 | 1:R:3351:VAL:N | 2.40 | 0.55 |
| 1:S:1865:LYS:HB3 | 1:S:1868:SER:HB3 | 1.88 | 0.55 |
| 1:T:848:ARG:HD2 | 1:T:1123:TYR:CE2 | 2.42 | 0.55 |
| 1:A:126:PHE:O | 1:A:143:ARG:NH2 | 2.40 | 0.55 |
| 1:A:1058:ARG:NH1 | 1:A:1125:ASP:O | 2.39 | 0.55 |
| 1:A:1852:ILE:HD13 | 1:A:2030:TYR:CZ | 2.42 | 0.55 |
| 1:A:2626:GLU:HG3 | 1:A:2633:LYS:HD2 | 1.88 | 0.55 |
| 1:A:2961:GLY:HA2 | 1:A:3106:LEU:HD23 | 1.86 | 0.55 |
| 1:B:569:GLN:HB3 | 1:B:619:GLY:HA3 | 1.88 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:1568:SER:N | 1:B:1597:GLY:O | 2.40 | 0.55 |
| 1:B:1837:ALA:HA | 1:B:1849:GLN:HE21 | 1.72 | 0.55 |
| 1:B:2930:SER:HA | 1:C:2943:LYS:HZ2 | 1.71 | 0.55 |
| 1:B:3132:LEU:HG | 1:B:3136:ARG:NH1 | 2.22 | 0.55 |
| 1:B:3234:PRO:HG2 | 1:B:3237:GLY:HA3 | 1.88 | 0.55 |
| 1:C:1070:ARG:HH12 | 1:C:1137:GLN:HE22 | 1.54 | 0.55 |
| 1:C:3157:PHE:O | 1:C:3163:ASN:ND2 | 2.40 | 0.55 |
| 1:D:465:GLN:NE2 | 1:D:558:PRO:O | 2.33 | 0.55 |
| 1:D:2812:LYS:HG2 | 1:D:2840:PRO:HA | 1.88 | 0.55 |
| 1:E:111:ILE:HD13 | 1:E:122:LYS:HA | 1.88 | 0.55 |
| 1:E:602:PHE:HA | 1:E:605:GLN:NE2 | 2.22 | 0.55 |
| 1:E:2508:VAL:O | 1:E:2515:LYS:NZ | 2.39 | 0.55 |
| 1:E:2626:GLU:OE2 | 1:E:2633:LYS:NZ | 2.39 | 0.55 |
| 1:F:757:PRO:HB2 | 1:F:760:GLY:H | 1.72 | 0.55 |
| 1:F:2313:GLN:HE22 | 1:F:2318:LEU:HB3 | 1.72 | 0.55 |
| 1:G:608:VAL:HG22 | 1:G:768:LEU:HD22 | 1.89 | 0.55 |
| 1:G:2641:GLN:NE2 | 1:G:2645:ASP:OD1 | 2.36 | 0.55 |
| 1:G:3205:GLU:HG3 | 1:H:1117:ARG:HH12 | 1.70 | 0.55 |
| 1:H:473:LEU:H | 1:H:629:HIS:HB3 | 1.71 | 0.55 |
| 1:H:1086:LYS:HZ3 | 1:H:1087:PRO:HD2 | 1.72 | 0.55 |
| 1:I:50:LYS:HG3 | 1:I:52:ASP:H | 1.72 | 0.55 |
| 1:I:1262:SER:OG | 1:I:1263:HIS:N | 2.28 | 0.55 |
| 1:I:2328:ASN:HB3 | 1:J:1241:VAL:HB | 1.88 | 0.55 |
| 1:J:1324:HIS:HA | 1:J:1519:VAL:HG11 | 1.89 | 0.55 |
| 1:J:1431:ASN:OD1 | 1:J:1594:SER:OG | 2.24 | 0.55 |
| 1:L:24:ARG:HD3 | 1:L:123:ASN:HA | 1.87 | 0.55 |
| 1:L:418:ASP:OD2 | 1:L:662:TYR:N | 2.35 | 0.55 |
| 1:L:1100:ASP:O | 1:L:1104:ARG:NH1 | 2.40 | 0.55 |
| 1:L:1466:ARG:O | 1:L:1470:ILE:HG12 | 2.05 | 0.55 |
| 1:M:612:LEU:HB2 | 1:M:613:PRO:HD3 | 1.88 | 0.55 |
| 1:N:1847:GLU:HA | 1:N:1850:PHE:HB3 | 1.89 | 0.55 |
| 1:O:1223:VAL:HG13 | 1:O:1231:ILE:HB | 1.87 | 0.55 |
| 1:O:1365:ALA:HA | 1:O:1381:PHE:CZ | 2.41 | 0.55 |
| 1:O:3395:ARG:HH21 | 1:O:3398:GLN:HE22 | 1.54 | 0.55 |
| 1:P:1564:ASN:HB3 | 1:P:1604:PHE:CE1 | 2.42 | 0.55 |
| 1:Q:1815:ARG:HA | 1:Q:1818:LEU:HG | 1.88 | 0.55 |
| 1:Q:2648:ARG:HB2 | 1:Q:2656:ARG:HH21 | 1.72 | 0.55 |
| 1:Q:2964:LYS:HD3 | 1:Q:2974:TYR:HA | 1.89 | 0.55 |
| 1:R:81:LEU:HB3 | 1:R:86:LEU:HB2 | 1.87 | 0.55 |
| 1:R:950:VAL:HA | 1:R:968:PHE:HB3 | 1.87 | 0.55 |
| 1:R:1267:ASN:HB3 | 1:R:1348:TYR:CZ | 2.41 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:R:1773:ASN:OD1 | 1:R:1774:SER:N | 2.40 | 0.55 |
| 1:R:2675:GLU:O | 1:R:2679:ASN:ND2 | 2.39 | 0.55 |
| 1:R:3229:ASN:H | 1:R:3286:THR:HG22 | 1.70 | 0.55 |
| 1:S:1773:ASN:OD1 | 1:S:1774:SER:N | 2.38 | 0.55 |
| 1:S:2576:GLN:HE21 | 1:S:2766:ALA:HB1 | 1.72 | 0.55 |
| 1:T:613:PRO:HA | 1:T:616:LEU:HB2 | 1.87 | 0.55 |
| 1:T:1743:HIS:O | 1:T:1747:THR:HG23 | 2.05 | 0.55 |
| 1:A:957:ASN:HD21 | 1:A:959:GLU:HB3 | 1.70 | 0.55 |
| 1:A:1737:ALA:O | 1:A:1843:TYR:OH | 2.24 | 0.55 |
| 1:B:3085:GLU:O | 1:B:3089:ASN:ND2 | 2.39 | 0.55 |
| 1:C:41:PHE:HA | 1:C:47:MET:HE1 | 1.89 | 0.55 |
| 1:C:866:LEU:HD23 | 1:C:967:PRO:HB2 | 1.89 | 0.55 |
| 1:C:2232:LEU:HB2 | 1:C:2274:LEU:HD21 | 1.88 | 0.55 |
| 1:C:2454:HIS:O | 1:C:2456:ARG:NH1 | 2.39 | 0.55 |
| 1:D:2752:ASN:HD21 | 1:D:2757:ILE:HG13 | 1.71 | 0.55 |
| 1:E:1084:LEU:HB3 | 1:E:1110:PHE:HE1 | 1.70 | 0.55 |
| 1:E:3312:ASP:OD1 | 1:E:3313:TYR:N | 2.39 | 0.55 |
| 1:F:3350:ASN:OD1 | 1:F:3351:VAL:N | 2.40 | 0.55 |
| 1:G:1570:ASP:HB2 | 1:G:1638:ARG:HB3 | 1.87 | 0.55 |
| 1:G:1731:CYS:HA | 1:G:2022:MET:HE1 | 1.88 | 0.55 |
| 1:G:2254:GLN:N | 1:G:2254:GLN:OE1 | 2.39 | 0.55 |
| 1:G:2962:ALA:HB2 | 1:G:3107:GLU:HG2 | 1.89 | 0.55 |
| 1:H:435:LYS:HG2 | 1:H:436:ASP:H | 1.70 | 0.55 |
| 1:H:580:TYR:CG | 1:H:958:PRO:HG2 | 2.40 | 0.55 |
| 1:H:1365:ALA:HA | 1:H:1378:ASN:HB3 | 1.86 | 0.55 |
| 1:I:42:HIS:NE2 | 1:I:59:CYS:SG | 2.80 | 0.55 |
| 1:I:855:THR:HG22 | 1:I:858:GLN:NE2 | 2.22 | 0.55 |
| 1:I:1556:LEU:HD11 | 1:I:1655:LEU:HD21 | 1.87 | 0.55 |
| 1:I:2709:HIS:HA | 1:I:2712:VAL:HG22 | 1.89 | 0.55 |
| 1:J:1286:MET:O | 1:J:1291:THR:OG1 | 2.24 | 0.55 |
| 1:J:1407:LEU:HD23 | 1:J:1411:LEU:HD23 | 1.88 | 0.55 |
| 1:L:1427:GLU:O | 1:L:1431:ASN:ND2 | 2.39 | 0.55 |
| 1:L:2788:GLN:HA | 1:L:2791:GLU:OE2 | 2.07 | 0.55 |
| 1:M:855:THR:HG22 | 1:M:858:GLN:NE2 | 2.21 | 0.55 |
| 1:M:1466:ARG:NH2 | 1:M:1534:ASN:O | 2.39 | 0.55 |
| 1:O:437:VAL:HG12 | 1:O:521:PRO:HB2 | 1.89 | 0.55 |
| 1:O:855:THR:HG22 | 1:O:858:GLN:NE2 | 2.21 | 0.55 |
| 1:O:1266:ARG:NH2 | 1:O:1270:ASP:OD1 | 2.40 | 0.55 |
| 1:O:1466:ARG:NH2 | 1:O:1534:ASN:O | 2.39 | 0.55 |
| 1:O:1887:SER:O | 1:O:1890:ARG:HG2 | 2.07 | 0.55 |
| 1:O:2679:ASN:HD21 | 1:O:2837:LEU:N | 2.04 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:O:3091:ILE:HG22 | 1:O:3094:LEU:HD12 | 1.89 | 0.55 |
| 1:P:454:ARG:NH2 | 1:P:1338:LEU:HG | 2.19 | 0.55 |
| 1:P:597:ARG:HH21 | 1:P:658:ARG:HB2 | 1.70 | 0.55 |
| 1:P:881:ILE:HD12 | 1:P:920:GLN:HE22 | 1.72 | 0.55 |
| 1:P:1716:VAL:HG23 | 1:P:1718:PRO:HD3 | 1.87 | 0.55 |
| 1:P:1839:GLU:HA | 1:P:1902:ARG:HH22 | 1.72 | 0.55 |
| 1:Q:225:ILE:O | 1:Q:228:GLU:HG3 | 2.07 | 0.55 |
| 1:Q:593:ALA:HA | 1:Q:605:GLN:HG3 | 1.88 | 0.55 |
| 1:Q:836:HIS:CE1 | 1:Q:838:GLU:HB3 | 2.42 | 0.55 |
| 1:Q:2393:VAL:H | 1:Q:2447:THR:HG22 | 1.72 | 0.55 |
| 1:Q:3105:THR:O | 1:Q:3109:SER:HB3 | 2.07 | 0.55 |
| 1:R:454:ARG:C | 1:R:514:ARG:HH12 | 2.15 | 0.55 |
| 1:R:1626:ASP:OD1 | 1:R:1627:SER:N | 2.40 | 0.55 |
| 1:S:47:MET:SD | 1:S:47:MET:N | 2.80 | 0.55 |
| 1:S:196:HIS:O | 1:S:199:SER:OG | 2.24 | 0.55 |
| 1:S:2313:GLN:HG2 | 1:S:2320:TYR:HB3 | 1.88 | 0.55 |
| 1:T:1012:CYS:O | 1:T:1196:ARG:NH1 | 2.39 | 0.55 |
| 1:T:1736:MET:HG2 | 1:T:1738:THR:H | 1.72 | 0.55 |
| 1:T:1785:ARG:HH12 | 1:T:1790:ASP:HA | 1.72 | 0.55 |
| 1:A:484:VAL:O | 1:A:485:ARG:NH1 | 2.39 | 0.55 |
| 1:A:1407:LEU:O | 1:A:1411:LEU:HD23 | 2.06 | 0.55 |
| 1:A:2443:LYS:HG3 | 1:A:2492:ILE:HD11 | 1.89 | 0.55 |
| 1:A:2778:ASP:OD1 | 1:A:2779:LEU:N | 2.40 | 0.55 |
| 1:C:1588:HIS:N | 1:F:337:GLN:OE1 | 2.35 | 0.55 |
| 1:C:2118:GLY:HA2 | 1:C:2124:GLN:HE22 | 1.71 | 0.55 |
| 1:C:2249:LEU:HD23 | 1:C:2383:GLU:CD | 2.31 | 0.55 |
| 1:D:846:HIS:HB3 | 1:D:1121:TYR:HA | 1.88 | 0.55 |
| 1:D:1084:LEU:HB3 | 1:D:1110:PHE:HE1 | 1.70 | 0.55 |
| 1:D:1599:GLU:OE2 | 1:D:1600:THR:OG1 | 2.25 | 0.55 |
| 1:E:2580:LEU:HA | 1:E:2583:VAL:HG12 | 1.88 | 0.55 |
| 1:E:3075:THR:O | 1:E:3138:ARG:NH1 | 2.40 | 0.55 |
| 1:F:866:LEU:HD12 | 1:F:869:LEU:HD21 | 1.88 | 0.55 |
| 1:F:3078:CYS:SG | 1:F:3260:ARG:NE | 2.76 | 0.55 |
| 1:F:3287:LEU:HB3 | 1:F:3295:LEU:HB3 | 1.87 | 0.55 |
| 1:G:1144:GLN:HA | 1:G:1148:ARG:HH22 | 1.71 | 0.55 |
| 1:G:2110:ALA:HB1 | 1:G:2172:HIS:HB3 | 1.89 | 0.55 |
| 1:G:2159:ARG:NH1 | 1:G:2303:ASP:OD1 | 2.39 | 0.55 |
| 1:H:1676:ILE:HG13 | 1:H:1761:VAL:HG23 | 1.88 | 0.55 |
| 1:H:3156:PRO:HB2 | 1:H:3162:LYS:HG3 | 1.89 | 0.55 |
| 1:I:1815:ARG:HA | 1:I:1818:LEU:HG | 1.87 | 0.55 |
| 1:I:2821:LEU:HD11 | 1:I:2862:MET:HG3 | 1.87 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:J:2430:GLY:N | 1:J:2433:GLU:OE2 | 2.39 | 0.55 |
| 1:J:2487:SER:OG | 1:J:2488:LYS:N | 2.40 | 0.55 |
| 1:K:1627:SER:O | 1:L:1917:ARG:NH2 | 2.40 | 0.55 |
| 1:K:1756:ARG:HD2 | 1:L:2089:PRO:HB2 | 1.89 | 0.55 |
| 1:K:1760:LEU:HD12 | 1:K:1761:VAL:HB | 1.89 | 0.55 |
| 1:K:1865:LYS:HZ2 | 1:K:1867:HIS:HB2 | 1.70 | 0.55 |
| 1:L:1890:ARG:NH2 | 1:L:1959:GLU:OE2 | 2.36 | 0.55 |
| 1:L:1960:LEU:N | 1:L:1963:ILE:O | 2.38 | 0.55 |
| 1:M:2970:ALA:O | 1:M:2973:ARG:NH1 | 2.40 | 0.55 |
| 1:M:3200:ILE:HA | 1:M:3203:ILE:HG22 | 1.89 | 0.55 |
| 1:N:597:ARG:NH2 | 1:N:658:ARG:HB2 | 2.22 | 0.55 |
| 1:N:787:VAL:HG23 | 1:N:789:ILE:HD11 | 1.89 | 0.55 |
| 1:N:1272:SER:N | 1:N:1275:GLU:OE2 | 2.39 | 0.55 |
| 1:N:2817:VAL:O | 1:N:2833:THR:OG1 | 2.22 | 0.55 |
| 1:O:313:PHE:HZ | 1:O:326:ILE:HD13 | 1.71 | 0.55 |
| 1:O:2130:HIS:ND1 | 1:O:2130:HIS:O | 2.39 | 0.55 |
| 1:O:2724:ARG:NH1 | 1:O:2730:TYR:OH | 2.32 | 0.55 |
| 1:P:950:VAL:HA | 1:P:968:PHE:HB3 | 1.88 | 0.55 |
| 1:Q:605:GLN:HA | 1:Q:608:VAL:HG12 | 1.87 | 0.55 |
| 1:Q:699:ILE:HG13 | 1:Q:706:LEU:HD21 | 1.89 | 0.55 |
| 1:Q:2399:LEU:HB3 | 1:Q:2436:TRP:HH2 | 1.72 | 0.55 |
| 1:Q:3191:ASN:OD1 | 1:Q:3195:HIS:N | 2.39 | 0.55 |
| 1:R:170:GLU:OE1 | 1:R:304:ARG:NH1 | 2.39 | 0.55 |
| 1:R:1270:ASP:OD2 | 1:R:1271:LEU:N | 2.39 | 0.55 |
| 1:R:2741:ARG:HH12 | 1:S:2870:TYR:H | 1.53 | 0.55 |
| 1:R:3156:PRO:HB2 | 1:R:3162:LYS:HG3 | 1.89 | 0.55 |
| 1:S:514:ARG:NH2 | 1:S:1341:GLY:O | 2.40 | 0.55 |
| 1:S:1046:ASP:OD1 | 1:S:1048:ILE:HG12 | 2.07 | 0.55 |
| 1:S:2376:ASN:N | 1:S:2379:GLU:OE2 | 2.36 | 0.55 |
| 1:T:1710:LEU:HD13 | 1:T:1750:PHE:CZ | 2.41 | 0.55 |
| 1:A:914:HIS:CE1 | 1:A:1053:HIS:CE1 | 2.95 | 0.55 |
| 1:B:3026:SER:OG | 1:B:3030:ASN:ND2 | 2.39 | 0.55 |
| 1:C:3211:ASP:HB2 | 1:C:3309:ALA:HB2 | 1.88 | 0.55 |
| 1:D:176:HIS:HA | 1:D:179:VAL:HG12 | 1.89 | 0.55 |
| 1:D:891:CYS:SG | 1:D:899:LYS:NZ | 2.76 | 0.55 |
| 1:D:2652:SER:O | 1:D:2656:ARG:NH1 | 2.39 | 0.55 |
| 1:D:3188:ASP:OD2 | 1:D:3189:ASN:ND2 | 2.37 | 0.55 |
| 1:E:204:GLU:OE2 | 1:E:354:ALA:N | 2.38 | 0.55 |
| 1:E:293:ILE:H | 1:E:293:ILE:HD12 | 1.71 | 0.55 |
| 1:F:403:LEU:O | 1:F:405:ARG:NH1 | 2.40 | 0.55 |
| 1:F:938:ASP:OD1 | 1:F:1055:ASN:ND2 | 2.39 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:G:1915:LEU:C | 1:G:1916:MET:HE2 | 2.32 | 0.55 |
| 1:H:1493:ARG:HH21 | 1:H:1515:ARG:HD2 | 1.72 | 0.55 |
| 1:H:1531:ASP:OD1 | 1:H:1532:THR:N | 2.40 | 0.55 |
| 1:H:1564:ASN:HB3 | 1:H:1604:PHE:CE1 | 2.42 | 0.55 |
| 1:H:3102:SER:HG | 1:H:3104:SER:HG | 1.49 | 0.55 |
| 1:I:203:LEU:HD21 | 1:I:351:LEU:HB3 | 1.89 | 0.55 |
| 1:I:953:GLU:HG3 | 1:I:954:THR:HG23 | 1.88 | 0.55 |
| 1:I:3089:ASN:HD21 | 1:I:3247:ILE:HD12 | 1.71 | 0.55 |
| 1:J:1710:LEU:HB3 | 1:J:1750:PHE:CZ | 2.42 | 0.55 |
| 1:K:473:LEU:HD23 | 1:K:775:LYS:HZ1 | 1.72 | 0.55 |
| 1:K:1262:SER:OG | 1:K:1263:HIS:N | 2.30 | 0.55 |
| 1:L:71:ARG:NH1 | 1:L:273:LEU:O | 2.34 | 0.55 |
| 1:L:662:TYR:HE2 | 1:L:700:TYR:HB3 | 1.71 | 0.55 |
| 1:L:1055:ASN:HA | 1:L:1058:ARG:HG3 | 1.88 | 0.55 |
| 1:L:2112:ARG:HE | 1:L:2116:LYS:NZ | 2.05 | 0.55 |
| 1:M:259:ASN:ND2 | 1:M:264:THR:OG1 | 2.39 | 0.55 |
| 1:M:1539:THR:H | 1:M:1542:GLN:HE22 | 1.54 | 0.55 |
| 1:M:2956:ILE:HD12 | 1:M:2959:PHE:HE2 | 1.71 | 0.55 |
| 1:M:3113:PRO:HA | 1:M:3116:MET:HG3 | 1.88 | 0.55 |
| 1:O:914:HIS:CE1 | 1:O:1053:HIS:HE1 | 2.25 | 0.55 |
| 1:P:254:PHE:HD2 | 1:P:264:THR:HB | 1.71 | 0.55 |
| 1:P:2088:PRO:O | 1:P:2090:ASN:N | 2.32 | 0.55 |
| 1:R:130:ILE:O | 1:R:138:HIS:HA | 2.07 | 0.55 |
| 1:S:922:GLU:O | 1:S:926:ARG:HG2 | 2.07 | 0.55 |
| 1:S:1249:THR:O | 1:S:1251:LYS:NZ | 2.28 | 0.55 |
| 1:S:2551:HIS:HB2 | 1:S:2581:PHE:CZ | 2.42 | 0.55 |
| 1:A:3301:THR:HB | 1:A:3325:LYS:HB3 | 1.89 | 0.55 |
| 1:B:97:THR:HG22 | 1:B:165:VAL:HG21 | 1.88 | 0.55 |
| 1:B:914:HIS:O | 1:B:918:THR:HG23 | 2.07 | 0.55 |
| 1:B:1019:GLU:HA | 1:B:1022:HIS:CD2 | 2.42 | 0.55 |
| 1:B:2088:PRO:O | 1:B:2090:ASN:N | 2.34 | 0.55 |
| 1:C:1195:ASP:OD1 | 1:C:1196:ARG:N | 2.40 | 0.55 |
| 1:C:1623:LEU:HD13 | 1:C:1631:ILE:HD11 | 1.89 | 0.55 |
| 1:C:1646:GLU:OE1 | 1:F:483:ARG:NH2 | 2.39 | 0.55 |
| 1:C:1865:LYS:HB3 | 1:C:1868:SER:HB3 | 1.88 | 0.55 |
| 1:C:2088:PRO:O | 1:C:2090:ASN:N | 2.36 | 0.55 |
| 1:C:2620:ASN:HD21 | 1:C:2622:PHE:HB2 | 1.72 | 0.55 |
| 1:D:420:LYS:NZ | 1:D:422:SER:O | 2.31 | 0.55 |
| 1:D:1773:ASN:OD1 | 1:D:1774:SER:N | 2.40 | 0.55 |
| 1:D:2194:PHE:CD1 | 1:D:2212:PHE:HB3 | 2.42 | 0.55 |
| 1:D:3266:VAL:HG21 | 1:D:3283:PHE:CE1 | 2.42 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:E:1294:LYS:O | 1:E:1297:SER:OG | 2.25 | 0.55 |
| 1:E:1494:GLN:NE2 | 1:E:1495:PRO:O | 2.39 | 0.55 |
| 1:E:1568:SER:HB2 | 1:E:1597:GLY:H | 1.70 | 0.55 |
| 1:E:1710:LEU:HB3 | 1:E:1750:PHE:CE1 | 2.41 | 0.55 |
| 1:F:176:HIS:HA | 1:F:179:VAL:HG12 | 1.89 | 0.55 |
| 1:F:1397:GLN:HB2 | 1:F:1400:LEU:HD23 | 1.88 | 0.55 |
| 1:G:1124:ASP:OD1 | 1:G:1125:ASP:N | 2.40 | 0.55 |
| 1:G:1835:LEU:HA | 1:G:1838:LEU:HD12 | 1.89 | 0.55 |
| 1:G:2585:LEU:HD13 | 1:G:2706:PHE:CZ | 2.42 | 0.55 |
| 1:G:2604:THR:HA | 1:G:2654:PHE:CE2 | 2.41 | 0.55 |
| 1:H:869:LEU:HD23 | 1:H:925:LEU:HD11 | 1.89 | 0.55 |
| 1:H:1088:LEU:O | 1:H:1089:GLN:NE2 | 2.40 | 0.55 |
| 1:H:1851:GLU:O | 1:H:1855:ASN:ND2 | 2.40 | 0.55 |
| 1:H:3119:HIS:HA | 1:H:3122:ILE:HG22 | 1.87 | 0.55 |
| 1:I:2254:GLN:N | 1:I:2254:GLN:OE1 | 2.40 | 0.55 |
| 1:I:2271:ILE:HG13 | 1:I:2298:HIS:HE1 | 1.72 | 0.55 |
| 1:J:594:LEU:HA | 1:J:602:PHE:CE1 | 2.42 | 0.55 |
| 1:J:937:TRP:H | 1:J:1051:LEU:HB2 | 1.71 | 0.55 |
| 1:J:1127:GLU:OE2 | 1:J:1131:PHE:N | 2.40 | 0.55 |
| 1:J:2626:GLU:OE1 | 1:J:2633:LYS:NZ | 2.33 | 0.55 |
| 1:K:1730:ALA:N | 1:K:2020:ALA:O | 2.39 | 0.55 |
| 1:L:5:ARG:HD2 | 1:L:283:TYR:CE1 | 2.42 | 0.55 |
| 1:L:2741:ARG:NH1 | 1:M:2868:SER:O | 2.39 | 0.55 |
| 1:M:1111:GLU:N | 1:M:1111:GLU:OE1 | 2.40 | 0.55 |
| 1:M:1153:PHE:HE1 | 1:M:1166:LEU:HD21 | 1.72 | 0.55 |
| 1:M:2095:GLU:CD | 1:M:2097:SER:H | 2.15 | 0.55 |
| 1:N:523:TRP:HB3 | 1:N:639:LEU:HD13 | 1.88 | 0.55 |
| 1:N:1431:ASN:OD1 | 1:N:1594:SER:OG | 2.23 | 0.55 |
| 1:N:3218:VAL:HG23 | 1:N:3258:TYR:HB2 | 1.88 | 0.55 |
| 1:O:1733:VAL:HG23 | 1:O:1736:MET:HE2 | 1.89 | 0.55 |
| 1:O:1802:ILE:HD12 | 1:O:1805:GLU:HB2 | 1.89 | 0.55 |
| 1:O:1865:LYS:HB3 | 1:O:1868:SER:HB3 | 1.87 | 0.55 |
| 1:O:2330:MET:HE1 | 1:O:2354:PRO:HG2 | 1.88 | 0.55 |
| 1:P:1742:TRP:CD1 | 1:P:1920:LEU:HD12 | 2.42 | 0.55 |
| 1:Q:1568:SER:N | 1:Q:1597:GLY:O | 2.40 | 0.55 |
| 1:Q:1865:LYS:HB3 | 1:Q:1868:SER:HB3 | 1.88 | 0.55 |
| 1:Q:1943:ASP:OD1 | 1:Q:1943:ASP:N | 2.40 | 0.55 |
| 1:R:3077:TYR:HE1 | 1:R:3126:TRP:HE1 | 1.54 | 0.55 |
| 1:R:3214:TYR:N | 1:R:3305:ILE:O | 2.35 | 0.55 |
| 1:S:914:HIS:CE1 | 1:S:1053:HIS:HE1 | 2.25 | 0.55 |
| 1:T:63:MET:SD | 1:T:64:ALA:N | 2.80 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:T:1420:CYS:SG | 1:T:1485:SER:OG | 2.63 | 0.55 |
| 1:T:2111:LEU:HD13 | 1:T:2212:PHE:CE1 | 2.42 | 0.55 |
| 1:T:2112:ARG:HH21 | 1:T:2116:LYS:HE3 | 1.71 | 0.55 |
| 1:T:2217:ILE:HG22 | 1:T:2220:SER:H | 1.72 | 0.55 |
| 1:A:1684:THR:OG1 | 1:A:1687:GLU:OE1 | 2.24 | 0.55 |
| 1:A:2862:MET:HG3 | 1:A:2864:LEU:HB2 | 1.88 | 0.55 |
| 1:B:744:ASN:HB3 | 1:B:779:TRP:NE1 | 2.22 | 0.55 |
| 1:B:1086:LYS:HZ3 | 1:B:1087:PRO:HD2 | 1.72 | 0.55 |
| 1:B:1946:ASP:HB3 | 1:B:1950:HIS:CD2 | 2.42 | 0.55 |
| 1:C:1100:ASP:O | 1:C:1104:ARG:NH1 | 2.40 | 0.55 |
| 1:D:130:ILE:O | 1:D:138:HIS:HA | 2.07 | 0.55 |
| 1:D:217:SER:O | 1:D:283:TYR:OH | 2.22 | 0.55 |
| 1:D:497:PRO:O | 1:D:501:ARG:HG2 | 2.07 | 0.55 |
| 1:F:2271:ILE:HD12 | 1:F:2298:HIS:NE2 | 2.21 | 0.55 |
| 1:F:2336:PRO:HB2 | 1:F:2342:LEU:HD12 | 1.89 | 0.55 |
| 1:F:3032:PHE:HA | 1:F:3113:PRO:HG2 | 1.87 | 0.55 |
| 1:H:105:ARG:HD2 | 1:H:106:LEU:HD22 | 1.89 | 0.55 |
| 1:H:197:ASP:OD1 | 1:H:197:ASP:N | 2.40 | 0.55 |
| 1:H:922:GLU:HB2 | 1:H:934:LEU:HD23 | 1.89 | 0.55 |
| 1:H:1888:THR:HA | 1:H:1891:ILE:HD12 | 1.87 | 0.55 |
| 1:H:2970:ALA:O | 1:H:2973:ARG:NE | 2.33 | 0.55 |
| 1:I:186:ASN:HB3 | 1:I:351:LEU:HD13 | 1.89 | 0.55 |
| 1:I:1320:ALA:HA | 1:I:1423:GLU:HG3 | 1.88 | 0.55 |
| 1:I:2096:ILE:HD13 | 1:I:2179:PRO:HG2 | 1.89 | 0.55 |
| 1:J:658:ARG:HH12 | 1:J:727:ILE:HD11 | 1.72 | 0.55 |
| 1:K:1338:LEU:HD21 | 1:K:1345:SER:HA | 1.88 | 0.55 |
| 1:L:597:ARG:HD3 | 1:L:658:ARG:HH11 | 1.71 | 0.55 |
| 1:L:2126:LEU:HD21 | 1:L:2165:VAL:HG12 | 1.89 | 0.55 |
| 1:M:1312:VAL:HG22 | 1:M:1313:ALA:H | 1.72 | 0.55 |
| 1:N:3124:ARG:O | 1:N:3127:GLN:HG3 | 2.06 | 0.55 |
| 1:O:2495:PRO:HB2 | 1:O:2500:ARG:HD2 | 1.89 | 0.55 |
| 1:P:3266:VAL:HG21 | 1:P:3283:PHE:CE2 | 2.42 | 0.55 |
| 1:Q:441:THR:OG1 | 1:Q:443:GLU:OE1 | 2.24 | 0.55 |
| 1:Q:1835:LEU:HA | 1:Q:1838:LEU:HD12 | 1.89 | 0.55 |
| 1:Q:2109:ALA:HA | 1:Q:2112:ARG:NH2 | 2.21 | 0.55 |
| 1:Q:2585:LEU:HD23 | 1:Q:2589:LEU:HD23 | 1.89 | 0.55 |
| 1:Q:2926:VAL:HG12 | 1:Q:3009:PRO:HB2 | 1.89 | 0.55 |
| 1:Q:3385:ASP:OD1 | 1:Q:3403:GLN:NE2 | 2.40 | 0.55 |
| 1:R:200:LEU:HD21 | 1:R:209:ASP:HB3 | 1.89 | 0.55 |
| 1:R:960:THR:OG1 | 1:R:964:GLU:OE2 | 2.22 | 0.55 |
| 1:R:2287:HIS:HE1 | 1:R:2432:LEU:HB2 | 1.72 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:S:1267:ASN:OD1 | 1:S:1268:LEU:N | 2.40 | 0.55 |
| 1:T:3395:ARG:O | 1:T:3401:ARG:NH2 | 2.34 | 0.55 |
| 1:A:731:ARG:CZ | 1:A:735:ARG:HH11 | 2.19 | 0.54 |
| 1:A:1388:THR:O | 1:A:1390:LYS:NZ | 2.41 | 0.54 |
| 1:A:2773:ASN:HD21 | 1:A:3142:TYR:HB2 | 1.72 | 0.54 |
| 1:A:2966:CYS:O | 1:A:2974:TYR:N | 2.33 | 0.54 |
| 1:A:3091:ILE:HA | 1:A:3094:LEU:HD23 | 1.89 | 0.54 |
| 1:B:1294:LYS:O | 1:B:1297:SER:OG | 2.23 | 0.54 |
| 1:C:1651:ARG:NH1 | 1:D:2026:PHE:O | 2.40 | 0.54 |
| 1:C:2586:GLU:HA | 1:C:2589:LEU:HG | 1.89 | 0.54 |
| 1:C:3385:ASP:H | 1:D:3148:ARG:HH21 | 1.54 | 0.54 |
| 1:D:2251:VAL:HG21 | 1:D:2267:THR:HG21 | 1.89 | 0.54 |
| 1:D:3214:TYR:N | 1:D:3305:ILE:O | 2.35 | 0.54 |
| 1:D:3319:PRO:HB2 | 1:D:3343:PRO:HD3 | 1.90 | 0.54 |
| 1:E:183:VAL:HG21 | 1:E:365:TYR:CE1 | 2.43 | 0.54 |
| 1:E:257:ASP:O | 1:E:265:ARG:NH2 | 2.36 | 0.54 |
| 1:E:376:LEU:HB3 | 1:E:378:LYS:NZ | 2.21 | 0.54 |
| 1:F:1420:CYS:SG | 1:F:1485:SER:OG | 2.64 | 0.54 |
| 1:F:2812:LYS:HG2 | 1:F:2840:PRO:HA | 1.88 | 0.54 |
| 1:F:3142:TYR:HA | 1:F:3144:ARG:HH11 | 1.72 | 0.54 |
| 1:G:2517:ILE:HD11 | 1:G:2601:TRP:HD1 | 1.72 | 0.54 |
| 1:H:1015:GLU:N | 1:H:1015:GLU:OE1 | 2.39 | 0.54 |
| 1:J:571:GLN:NE2 | 1:J:616:LEU:O | 2.29 | 0.54 |
| 1:J:1022:HIS:HD2 | 1:J:1026:HIS:CE1 | 2.25 | 0.54 |
| 1:K:1295:ILE:HD12 | 1:K:1333:VAL:HG22 | 1.90 | 0.54 |
| 1:K:2027:ASP:OD1 | 1:K:2028:ARG:N | 2.40 | 0.54 |
| 1:K:3067:GLN:O | 1:K:3071:THR:HG23 | 2.07 | 0.54 |
| 1:K:3227:THR:OG1 | 1:K:3245:PHE:O | 2.16 | 0.54 |
| 1:L:2514:ARG:HH22 | 1:L:2586:GLU:HG2 | 1.72 | 0.54 |
| 1:M:2088:PRO:O | 1:M:2090:ASN:N | 2.38 | 0.54 |
| 1:N:860:GLN:HE21 | 1:N:864:GLU:HG2 | 1.71 | 0.54 |
| 1:O:559:VAL:N | 1:O:564:GLU:O | 2.37 | 0.54 |
| 1:O:711:ASP:OD1 | 1:O:712:ASN:N | 2.39 | 0.54 |
| 1:O:2586:GLU:O | 1:O:2590:THR:OG1 | 2.20 | 0.54 |
| 1:P:180:GLN:OE1 | 1:P:366:HIS:N | 2.28 | 0.54 |
| 1:P:253:PRO:HB2 | 1:P:256:ARG:HH12 | 1.72 | 0.54 |
| 1:Q:5:ARG:HD2 | 1:Q:91:VAL:O | 2.07 | 0.54 |
| 1:Q:1579:THR:HG1 | 1:Q:1584:ARG:HH21 | 1.54 | 0.54 |
| 1:S:1156:HIS:HB3 | 1:S:1193:GLN:HE22 | 1.71 | 0.54 |
| 1:A:2325:CYS:HA | 1:B:1242:VAL:HG13 | 1.89 | 0.54 |
| 1:A:3214:TYR:CD1 | 1:A:3265:ASP:HA | 2.42 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:1546:VAL:HA | 1:B:1549:ARG:HG2 | 1.88 | 0.54 |
| 1:B:3266:VAL:HG21 | 1:B:3283:PHE:HE2 | 1.72 | 0.54 |
| 1:B:3351:VAL:HG23 | 1:B:3390:SER:HA | 1.88 | 0.54 |
| 1:C:2059:ASN:OD1 | 1:C:2061:SER:N | 2.39 | 0.54 |
| 1:D:937:TRP:H | 1:D:1051:LEU:HB2 | 1.71 | 0.54 |
| 1:D:1362:ILE:HD13 | 1:D:1456:LEU:HD11 | 1.89 | 0.54 |
| 1:E:1760:LEU:HD12 | 1:E:1761:VAL:HB | 1.88 | 0.54 |
| 1:E:2090:ASN:C | 1:E:2091:ARG:HD3 | 2.32 | 0.54 |
| 1:E:2470:ARG:NH2 | 1:E:2471:TYR:O | 2.38 | 0.54 |
| 1:F:1149:VAL:HG11 | 1:F:1206:LEU:HD13 | 1.89 | 0.54 |
| 1:F:1579:THR:HG21 | 1:F:1585:ASN:HB3 | 1.87 | 0.54 |
| 1:F:3270:LEU:HD11 | 1:F:3281:PHE:CZ | 2.42 | 0.54 |
| 1:H:501:ARG:HG2 | 1:H:645:ASP:CG | 2.32 | 0.54 |
| 1:H:507:VAL:HG21 | 1:H:638:ILE:HD11 | 1.89 | 0.54 |
| 1:H:925:LEU:HD22 | 1:H:928:LYS:HZ3 | 1.72 | 0.54 |
| 1:H:1960:LEU:N | 1:H:1963:ILE:O | 2.39 | 0.54 |
| 1:I:752:ILE:O | 1:I:808:LEU:HA | 2.07 | 0.54 |
| 1:I:836:HIS:CE1 | 1:O:277:ARG:HE | 2.25 | 0.54 |
| 1:I:885:HIS:ND1 | 1:I:885:HIS:O | 2.41 | 0.54 |
| 1:I:2008:LYS:NZ | 1:I:2037:VAL:O | 2.40 | 0.54 |
| 1:I:2780:ASN:OD1 | 1:I:2784:LEU:N | 2.37 | 0.54 |
| 1:I:3157:PHE:O | 1:I:3163:ASN:ND2 | 2.40 | 0.54 |
| 1:J:597:ARG:HH22 | 1:J:655:GLN:HA | 1.72 | 0.54 |
| 1:K:731:ARG:HA | 1:K:735:ARG:HH21 | 1.72 | 0.54 |
| 1:K:855:THR:HG22 | 1:K:858:GLN:NE2 | 2.21 | 0.54 |
| 1:L:721:ASP:OD1 | 1:L:722:GLN:N | 2.40 | 0.54 |
| 1:M:1756:ARG:NH2 | 1:N:2176:VAL:HG13 | 2.22 | 0.54 |
| 1:N:1299:HIS:ND1 | 1:N:1299:HIS:O | 2.41 | 0.54 |
| 1:O:1168:VAL:N | 1:O:1178:GLU:OE1 | 2.40 | 0.54 |
| 1:O:2567:CYS:SG | 1:O:2578:HIS:NE2 | 2.79 | 0.54 |
| 1:P:105:ARG:HA | 1:P:108:GLN:HE22 | 1.72 | 0.54 |
| 1:P:934:LEU:HD23 | 1:P:1054:SER:HB3 | 1.89 | 0.54 |
| 1:P:1489:LEU:O | 1:P:1493:ARG:NH2 | 2.40 | 0.54 |
| 1:P:1492:MET:HA | 1:P:1516:PRO:HG2 | 1.89 | 0.54 |
| 1:Q:50:LYS:HG3 | 1:Q:52:ASP:H | 1.73 | 0.54 |
| 1:Q:750:LEU:HD11 | 1:Q:767:LYS:HD2 | 1.89 | 0.54 |
| 1:Q:1978:LYS:NZ | 1:Q:1979:SER:O | 2.39 | 0.54 |
| 1:Q:2439:ASP:OD2 | 1:Q:2440:ARG:NE | 2.39 | 0.54 |
| 1:Q:2567:CYS:O | 1:Q:2569:HIS:ND1 | 2.38 | 0.54 |
| 1:S:1881:PHE:O | 1:S:1885:HIS:ND1 | 2.37 | 0.54 |
| 1:S:2375:LEU:HB3 | 1:S:2379:GLU:HG3 | 1.88 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:S:2553:TYR:CD1 | 1:S:2554:PRO:HA | 2.43 | 0.54 |
| 1:S:3012:ASP:OD1 | 1:S:3014:THR:OG1 | 2.25 | 0.54 |
| 1:T:312:SER:HA | 1:T:365:TYR:O | 2.08 | 0.54 |
| 1:T:1827:ASP:HA | 1:T:1831:TRP:HD1 | 1.71 | 0.54 |
| 1:A:1816:ASN:OD1 | 1:A:1817:ARG:N | 2.40 | 0.54 |
| 1:A:2130:HIS:ND1 | 1:A:2130:HIS:O | 2.40 | 0.54 |
| 1:B:954:THR:HG22 | 1:B:965:PRO:HA | 1.90 | 0.54 |
| 1:B:2251:VAL:HG21 | 1:B:2267:THR:HG21 | 1.89 | 0.54 |
| 1:B:2283:LEU:HD21 | 1:B:2292:ASP:HB3 | 1.89 | 0.54 |
| 1:B:3324:ASN:OD1 | 1:B:3395:ARG:NH2 | 2.41 | 0.54 |
| 1:C:425:ASP:OD1 | 1:C:426:VAL:N | 2.38 | 0.54 |
| 1:C:494:ALA:HA | 1:C:603:GLU:OE1 | 2.06 | 0.54 |
| 1:C:855:THR:HG22 | 1:C:858:GLN:NE2 | 2.22 | 0.54 |
| 1:D:486:TYR:HB3 | 1:D:777:MET:HE1 | 1.90 | 0.54 |
| 1:D:735:ARG:NH2 | 1:D:790:THR:H | 2.04 | 0.54 |
| 1:E:525:TRP:CD1 | 1:E:643:ASN:HD22 | 2.25 | 0.54 |
| 1:E:1417:THR:O | 1:E:1475:GLN:NE2 | 2.40 | 0.54 |
| 1:E:1684:THR:OG1 | 1:E:1687:GLU:OE1 | 2.21 | 0.54 |
| 1:E:1815:ARG:HA | 1:E:1818:LEU:HG | 1.88 | 0.54 |
| 1:F:1736:MET:HG2 | 1:F:1738:THR:H | 1.72 | 0.54 |
| 1:F:2659:LEU:HD13 | 1:F:2796:ARG:HG2 | 1.89 | 0.54 |
| 1:F:3142:TYR:HA | 1:F:3144:ARG:NH1 | 2.22 | 0.54 |
| 1:G:501:ARG:CZ | 1:G:648:TRP:HZ3 | 2.21 | 0.54 |
| 1:G:1607:ASP:OD1 | 1:G:1608:ARG:N | 2.37 | 0.54 |
| 1:G:2534:ALA:HA | 1:G:2537:GLN:HE22 | 1.73 | 0.54 |
| 1:H:636:ILE:O | 1:H:640:HIS:ND1 | 2.33 | 0.54 |
| 1:H:2339:SER:O | 1:H:2349:ARG:NH1 | 2.40 | 0.54 |
| 1:I:44:GLU:HG3 | 1:I:135:MET:HE1 | 1.89 | 0.54 |
| 1:I:114:ASP:OD2 | 1:I:117:GLY:N | 2.39 | 0.54 |
| 1:I:1809:VAL:HG23 | 1:I:1868:SER:HA | 1.89 | 0.54 |
| 1:I:2673:GLN:HE22 | 1:I:2852:GLN:H | 1.55 | 0.54 |
| 1:J:313:PHE:HB3 | 1:J:315:LEU:HD23 | 1.90 | 0.54 |
| 1:J:569:GLN:HB3 | 1:J:619:GLY:HA3 | 1.88 | 0.54 |
| 1:J:1713:PHE:HE1 | 1:J:1929:TYR:HB3 | 1.73 | 0.54 |
| 1:J:2623:GLU:HA | 1:J:2636:ARG:HH22 | 1.72 | 0.54 |
| 1:K:1013:THR:HG22 | 1:K:1196:ARG:HD2 | 1.90 | 0.54 |
| 1:K:1835:LEU:HA | 1:K:1838:LEU:HD12 | 1.90 | 0.54 |
| 1:M:50:LYS:HG3 | 1:M:52:ASP:H | 1.71 | 0.54 |
| 1:M:949:ILE:HG23 | 1:M:950:VAL:HG13 | 1.88 | 0.54 |
| 1:N:1785:ARG:NH1 | 1:N:1786:ASP:O | 2.41 | 0.54 |
| 1:O:17:LEU:O | 1:O:20:GLU:HG3 | 2.07 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:O:851:VAL:HG12 | 1:O:935:PRO:HB2 | 1.88 | 0.54 |
| 1:O:2114:LEU:HD13 | 1:O:2172:HIS:HE1 | 1.71 | 0.54 |
| 1:O:2535:VAL:HG22 | 1:O:2592:GLN:HE21 | 1.72 | 0.54 |
| 1:P:1023:ASN:HD21 | 1:P:1184:LEU:HD22 | 1.72 | 0.54 |
| 1:P:2041:LYS:HG3 | 1:P:2043:LEU:HD23 | 1.89 | 0.54 |
| 1:P:2970:ALA:O | 1:P:2973:ARG:NE | 2.34 | 0.54 |
| 1:Q:525:TRP:CD1 | 1:Q:643:ASN:HD22 | 2.25 | 0.54 |
| 1:Q:799:LYS:N | 1:Q:802:ASP:OD2 | 2.37 | 0.54 |
| 1:Q:2420:THR:HG21 | 1:Q:2453:LEU:HD21 | 1.88 | 0.54 |
| 1:Q:2585:LEU:HD13 | 1:Q:2706:PHE:HE2 | 1.73 | 0.54 |
| 1:R:475:ALA:HB3 | 1:R:485:ARG:HB3 | 1.89 | 0.54 |
| 1:S:376:LEU:HB3 | 1:S:378:LYS:HZ1 | 1.72 | 0.54 |
| 1:S:678:PHE:O | 1:S:685:ASN:ND2 | 2.41 | 0.54 |
| 1:S:2152:PRO:HD2 | 1:S:2329:TYR:HD2 | 1.72 | 0.54 |
| 1:T:1142:HIS:HE1 | 1:T:1524:ASN:HA | 1.72 | 0.54 |
| 1:T:1351:TRP:HZ3 | 1:T:1463:ASN:HB3 | 1.72 | 0.54 |
| 1:A:323:ASN:OD1 | 1:A:324:VAL:N | 2.41 | 0.54 |
| 1:A:3067:GLN:HE22 | 1:A:3087:LEU:HG | 1.72 | 0.54 |
| 1:B:270:ALA:HA | 1:B:273:LEU:HD12 | 1.89 | 0.54 |
| 1:C:1328:LEU:HB3 | 1:C:1499:PHE:CE2 | 2.42 | 0.54 |
| 1:C:1587:ASN:N | 1:F:337:GLN:OE1 | 2.36 | 0.54 |
| 1:C:1775:LEU:HD11 | 1:C:1780:ASN:HD21 | 1.72 | 0.54 |
| 1:C:2109:ALA:HA | 1:C:2112:ARG:NH2 | 2.22 | 0.54 |
| 1:C:2587:ARG:HH12 | 1:C:2753:PRO:HB2 | 1.71 | 0.54 |
| 1:D:5:ARG:HH21 | 1:D:90:GLY:HA3 | 1.73 | 0.54 |
| 1:D:1663:ASN:OD1 | 1:D:1665:GLN:NE2 | 2.40 | 0.54 |
| 1:E:1587:ASN:OD1 | 1:E:1588:HIS:ND1 | 2.40 | 0.54 |
| 1:F:1932:ASP:OD2 | 1:F:1935:THR:N | 2.28 | 0.54 |
| 1:F:3266:VAL:HG21 | 1:F:3283:PHE:HE2 | 1.71 | 0.54 |
| 1:G:304:ARG:CZ | 1:G:304:ARG:HA | 2.37 | 0.54 |
| 1:G:1641:ASN:OD1 | 1:G:1642:GLY:N | 2.41 | 0.54 |
| 1:G:1809:VAL:HG23 | 1:G:1868:SER:HA | 1.88 | 0.54 |
| 1:H:1970:SER:HB2 | 1:H:2085:GLN:HE22 | 1.72 | 0.54 |
| 1:I:1775:LEU:HD12 | 1:I:1779:PHE:HE1 | 1.73 | 0.54 |
| 1:K:2155:PRO:HB2 | 1:K:2306:TRP:CZ3 | 2.43 | 0.54 |
| 1:K:2620:ASN:ND2 | 1:K:2623:GLU:OE1 | 2.40 | 0.54 |
| 1:L:860:GLN:O | 1:L:860:GLN:NE2 | 2.40 | 0.54 |
| 1:L:1415:GLU:HA | 1:L:1547:LEU:HD21 | 1.88 | 0.54 |
| 1:L:1769:VAL:O | 1:L:1828:ASN:ND2 | 2.41 | 0.54 |
| 1:M:1249:THR:O | 1:M:1251:LYS:NZ | 2.29 | 0.54 |
| 1:M:2454:HIS:O | 1:M:2456:ARG:NH1 | 2.41 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:M:2553:TYR:HB2 | 1:M:2697:GLU:HB3 | 1.89 | 0.54 |
| 1:N:3360:LEU:HG | 1:N:3401:ARG:HD3 | 1.88 | 0.54 |
| 1:O:292:ASN:H | 1:O:295:GLN:NE2 | 2.04 | 0.54 |
| 1:O:2443:LYS:HG3 | 1:O:2492:ILE:HD11 | 1.90 | 0.54 |
| 1:Q:1067:GLN:NE2 | 1:Q:1072:LEU:HB2 | 2.22 | 0.54 |
| 1:Q:1775:LEU:HD22 | 1:Q:1815:ARG:HH12 | 1.71 | 0.54 |
| 1:Q:2878:ALA:N | 1:Q:2882:THR:O | 2.39 | 0.54 |
| 1:R:597:ARG:HD3 | 1:R:658:ARG:HH11 | 1.72 | 0.54 |
| 1:S:1111:GLU:N | 1:S:1111:GLU:OE1 | 2.40 | 0.54 |
| 1:S:1622:GLY:HA3 | 1:T:2786:ILE:HD13 | 1.90 | 0.54 |
| 1:T:1299:HIS:ND1 | 1:T:1299:HIS:O | 2.41 | 0.54 |
| 1:A:438:ASP:OD1 | 1:A:438:ASP:N | 2.38 | 0.54 |
| 1:A:1889:ASP:OD2 | 1:A:1955:TYR:OH | 2.22 | 0.54 |
| 1:A:2213:ALA:O | 1:A:2226:ARG:NH1 | 2.31 | 0.54 |
| 1:B:2824:ALA:HB2 | 1:B:2869:VAL:HG23 | 1.89 | 0.54 |
| 1:C:438:ASP:OD1 | 1:C:439:THR:N | 2.41 | 0.54 |
| 1:C:1742:TRP:CD1 | 1:C:1920:LEU:HD12 | 2.42 | 0.54 |
| 1:D:735:ARG:HB3 | 1:D:831:GLU:HB3 | 1.89 | 0.54 |
| 1:E:307:GLU:OE2 | 1:E:413:ALA:N | 2.39 | 0.54 |
| 1:E:2078:LYS:HB2 | 1:E:2080:ARG:HH12 | 1.71 | 0.54 |
| 1:E:2939:ASN:HB3 | 1:E:2943:LYS:HZ1 | 1.71 | 0.54 |
| 1:F:259:ASN:O | 1:F:265:ARG:NH2 | 2.41 | 0.54 |
| 1:F:1488:ALA:HB1 | 1:F:1491:ILE:HD13 | 1.88 | 0.54 |
| 1:H:860:GLN:O | 1:H:860:GLN:NE2 | 2.40 | 0.54 |
| 1:H:1008:GLN:N | 1:H:1008:GLN:OE1 | 2.41 | 0.54 |
| 1:H:3038:LYS:O | 1:H:3041:GLN:NE2 | 2.41 | 0.54 |
| 1:I:323:ASN:OD1 | 1:I:324:VAL:N | 2.41 | 0.54 |
| 1:I:482:ALA:O | 1:I:485:ARG:NH2 | 2.40 | 0.54 |
| 1:I:2521:THR:HG23 | 1:I:2524:GLU:H | 1.73 | 0.54 |
| 1:J:705:GLU:N | 1:J:705:GLU:OE1 | 2.40 | 0.54 |
| 1:J:1056:THR:HA | 1:J:1059:ILE:HD12 | 1.88 | 0.54 |
| 1:J:1773:ASN:OD1 | 1:J:1774:SER:N | 2.40 | 0.54 |
| 1:K:2269:ASN:ND2 | 1:K:2428:LEU:H | 2.06 | 0.54 |
| 1:L:597:ARG:HH22 | 1:L:655:GLN:HA | 1.70 | 0.54 |
| 1:L:3395:ARG:O | 1:L:3401:ARG:NH1 | 2.26 | 0.54 |
| 1:M:1752:ASP:OD1 | 1:M:1753:ALA:N | 2.41 | 0.54 |
| 1:N:1163:LEU:N | 1:N:1224:ILE:O | 2.31 | 0.54 |
| 1:O:915:ARG:HD2 | 1:O:1060:TRP:HZ3 | 1.72 | 0.54 |
| 1:O:2941:LEU:HD22 | 1:O:3032:PHE:CD1 | 2.42 | 0.54 |
| 1:P:1542:GLN:HA | 1:P:1545:GLU:HG2 | 1.89 | 0.54 |
| 1:P:3114:PHE:HA | 1:P:3117:ILE:HG12 | 1.88 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:Q:47:MET:C | 1:Q:55:ARG:HH12 | 2.16 | 0.54 |
| 1:Q:635:PRO:O | 1:Q:638:ILE:HG12 | 2.08 | 0.54 |
| 1:Q:1579:THR:OG1 | 1:Q:1583:GLU:O | 2.24 | 0.54 |
| 1:Q:2454:HIS:O | 1:Q:2456:ARG:NH1 | 2.41 | 0.54 |
| 1:Q:2805:ASN:ND2 | 1:Q:2852:GLN:OE1 | 2.40 | 0.54 |
| 1:Q:3088:HIS:ND1 | 1:Q:3122:ILE:HG13 | 2.23 | 0.54 |
| 1:R:2112:ARG:HE | 1:R:2116:LYS:NZ | 2.05 | 0.54 |
| 1:R:2984:PHE:O | 1:R:2988:HIS:ND1 | 2.36 | 0.54 |
| 1:R:3080:PHE:N | 1:R:3081:GLU:OE1 | 2.40 | 0.54 |
| 1:S:230:GLN:NE2 | 1:S:235:LYS:O | 2.40 | 0.54 |
| 1:S:1883:LEU:O | 1:S:1886:SER:OG | 2.24 | 0.54 |
| 1:T:196:HIS:CE1 | 1:T:198:HIS:HB2 | 2.43 | 0.54 |
| 1:T:1225:ASP:OD1 | 1:T:1226:LEU:N | 2.38 | 0.54 |
| 1:T:2439:ASP:OD2 | 1:T:2440:ARG:NH1 | 2.41 | 0.54 |
| 1:T:2567:CYS:SG | 1:T:2569:HIS:HE1 | 2.30 | 0.54 |
| 1:T:2964:LYS:HG2 | 1:T:2973:ARG:HB2 | 1.90 | 0.54 |
| 1:A:1404:ASP:O | 1:A:1408:ASN:ND2 | 2.41 | 0.54 |
| 1:A:1475:GLN:HB3 | 1:A:1482:ASP:HB3 | 1.89 | 0.54 |
| 1:A:1752:ASP:OD1 | 1:A:1753:ALA:N | 2.41 | 0.54 |
| 1:A:1883:LEU:O | 1:A:1886:SER:OG | 2.21 | 0.54 |
| 1:B:111:ILE:HG23 | 1:B:122:LYS:HB2 | 1.89 | 0.54 |
| 1:B:836:HIS:NE2 | 1:B:838:GLU:OE2 | 2.40 | 0.54 |
| 1:B:885:HIS:HE1 | 1:B:1043:THR:HG23 | 1.71 | 0.54 |
| 1:B:3127:GLN:HE22 | 1:B:3190:LEU:HD22 | 1.73 | 0.54 |
| 1:C:60:VAL:HG13 | 1:C:63:MET:HE2 | 1.90 | 0.54 |
| 1:C:399:ASN:HD21 | 1:C:401:ASN:HD21 | 1.56 | 0.54 |
| 1:C:2685:ILE:HG23 | 1:C:2693:MET:HE1 | 1.90 | 0.54 |
| 1:C:3332:VAL:O | 1:C:3334:ARG:NH2 | 2.41 | 0.54 |
| 1:D:2865:ARG:HG2 | 1:D:2868:SER:HB3 | 1.88 | 0.54 |
| 1:E:38:LEU:O | 1:E:73:TYR:OH | 2.20 | 0.54 |
| 1:E:601:ASP:O | 1:E:604:VAL:HG22 | 2.07 | 0.54 |
| 1:E:757:PRO:HB3 | 1:E:798:LEU:HD11 | 1.90 | 0.54 |
| 1:E:981:SER:HB2 | 1:E:1031:GLY:HA3 | 1.89 | 0.54 |
| 1:E:2974:TYR:HB3 | 1:F:3367:PRO:HB2 | 1.89 | 0.54 |
| 1:F:475:ALA:O | 1:F:476:ARG:NH1 | 2.35 | 0.54 |
| 1:F:1842:ASN:OD1 | 1:F:1843:TYR:N | 2.40 | 0.54 |
| 1:G:2509:SER:H | 1:G:3138:ARG:HH22 | 1.55 | 0.54 |
| 1:H:267:TYR:HB3 | 1:H:273:LEU:HD21 | 1.90 | 0.54 |
| 1:H:1353:GLN:NE2 | 1:H:1536:ASN:OD1 | 2.41 | 0.54 |
| 1:H:1492:MET:HB3 | 1:H:1517:ILE:HG23 | 1.88 | 0.54 |
| 1:H:2589:LEU:O | 1:H:2592:GLN:NE2 | 2.29 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:I:2773:ASN:HD21 | 1:I:3142:TYR:HB2 | 1.72 | 0.54 |
| 1:I:2801:ARG:HD3 | 1:I:2803:PHE:CZ | 2.42 | 0.54 |
| 1:J:2530:LYS:HB2 | 1:J:2533:ARG:HH22 | 1.73 | 0.54 |
| 1:K:164:MET:HE1 | 1:K:187:HIS:HE1 | 1.72 | 0.54 |
| 1:K:484:VAL:O | 1:K:485:ARG:NH1 | 2.40 | 0.54 |
| 1:L:725:HIS:O | 1:L:729:GLU:HG2 | 2.08 | 0.54 |
| 1:L:1056:THR:HA | 1:L:1059:ILE:HD12 | 1.90 | 0.54 |
| 1:L:1564:ASN:HB3 | 1:L:1604:PHE:CE1 | 2.43 | 0.54 |
| 1:M:1651:ARG:NH2 | 1:N:2025:SER:O | 2.39 | 0.54 |
| 1:M:2201:ASP:OD1 | 1:M:2203:TRP:N | 2.37 | 0.54 |
| 1:N:739:GLY:HA3 | 1:N:784:LEU:HB3 | 1.89 | 0.54 |
| 1:N:1134:PRO:C | 1:N:1138:ARG:HE | 2.16 | 0.54 |
| 1:N:1845:ASP:HB3 | 1:N:2028:ARG:HD2 | 1.89 | 0.54 |
| 1:O:1404:ASP:O | 1:O:1408:ASN:ND2 | 2.40 | 0.54 |
| 1:O:1407:LEU:O | 1:O:1411:LEU:HD23 | 2.08 | 0.54 |
| 1:O:2532:LEU:HG | 1:O:2536:GLN:NE2 | 2.23 | 0.54 |
| 1:O:3105:THR:O | 1:O:3109:SER:HB3 | 2.07 | 0.54 |
| 1:P:524:ASP:OD2 | 1:P:527:ARG:NH1 | 2.40 | 0.54 |
| 1:Q:438:ASP:OD1 | 1:Q:439:THR:N | 2.41 | 0.54 |
| 1:Q:1654:SER:OG | 1:Q:1655:LEU:N | 2.40 | 0.54 |
| 1:R:1750:PHE:HD2 | 1:R:1882:LEU:HD11 | 1.73 | 0.54 |
| 1:R:2251:VAL:HG21 | 1:R:2267:THR:HG21 | 1.90 | 0.54 |
| 1:S:1067:GLN:NE2 | 1:S:1072:LEU:HB2 | 2.22 | 0.54 |
| 1:S:1715:ALA:HB1 | 1:S:1873:HIS:HA | 1.90 | 0.54 |
| 1:S:1751:GLU:OE2 | 1:S:1763:ILE:N | 2.40 | 0.54 |
| 1:T:378:LYS:NZ | 1:T:383:ASP:O | 2.39 | 0.54 |
| 1:T:1321:VAL:HG11 | 1:T:1491:ILE:HG21 | 1.90 | 0.54 |
| 1:T:1345:SER:OG | 1:T:1346:VAL:N | 2.41 | 0.54 |
| 1:T:1372:SER:O | 1:T:1374:THR:OG1 | 2.25 | 0.54 |
| 1:T:1427:GLU:O | 1:T:1431:ASN:ND2 | 2.40 | 0.54 |
| 1:A:9:ASP:OD1 | 1:A:9:ASP:N | 2.39 | 0.54 |
| 1:A:1081:ILE:HD13 | 1:B:2460:VAL:HG12 | 1.88 | 0.54 |
| 1:B:674:LEU:HA | 1:B:695:ARG:HH22 | 1.72 | 0.54 |
| 1:B:1324:HIS:CE1 | 1:B:1492:MET:HE1 | 2.43 | 0.54 |
| 1:B:1716:VAL:HG23 | 1:B:1718:PRO:HD3 | 1.90 | 0.54 |
| 1:B:2970:ALA:O | 1:B:2973:ARG:NE | 2.34 | 0.54 |
| 1:B:2982:PRO:HA | 1:B:3081:GLU:HG2 | 1.89 | 0.54 |
| 1:B:3287:LEU:HD21 | 1:B:3299:LEU:HD21 | 1.89 | 0.54 |
| 1:C:307:GLU:OE2 | 1:C:413:ALA:N | 2.39 | 0.54 |
| 1:D:1541:PRO:O | 1:D:1544:GLU:HG3 | 2.07 | 0.54 |
| 1:D:1736:MET:HE1 | 1:D:2022:MET:HE1 | 1.90 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:D:3226:ALA:HA | 1:D:3289:LYS:HA | 1.90 | 0.54 |
| 1:E:42:HIS:NE2 | 1:E:59:CYS:SG | 2.81 | 0.54 |
| 1:E:749:ALA:HA | 1:E:812:ASP:HA | 1.90 | 0.54 |
| 1:F:1056:THR:HA | 1:F:1059:ILE:HD12 | 1.89 | 0.54 |
| 1:H:1055:ASN:HA | 1:H:1058:ARG:HG3 | 1.90 | 0.54 |
| 1:H:2541:PRO:HD2 | 1:H:2542:ARG:N | 2.22 | 0.54 |
| 1:I:1756:ARG:HG3 | 1:J:2089:PRO:HB2 | 1.88 | 0.54 |
| 1:J:222:ILE:HA | 1:J:225:ILE:HG12 | 1.88 | 0.54 |
| 1:J:568:ARG:NH1 | 1:J:634:ASP:OD2 | 2.40 | 0.54 |
| 1:K:1365:ALA:HA | 1:K:1381:PHE:CZ | 2.42 | 0.54 |
| 1:K:1474:LEU:HD11 | 1:K:1543:LEU:HD11 | 1.90 | 0.54 |
| 1:K:2393:VAL:H | 1:K:2447:THR:HG22 | 1.71 | 0.54 |
| 1:L:2412:VAL:H | 1:L:2422:ALA:HB2 | 1.73 | 0.54 |
| 1:L:3360:LEU:HD12 | 1:L:3387:PHE:HB3 | 1.88 | 0.54 |
| 1:M:2583:VAL:HG21 | 1:M:2772:PHE:HB3 | 1.88 | 0.54 |
| 1:M:3149:ASN:HA | 1:M:3152:ARG:NH1 | 2.23 | 0.54 |
| 1:M:3211:ASP:HB2 | 1:M:3309:ALA:HB2 | 1.87 | 0.54 |
| 1:N:735:ARG:NH2 | 1:N:790:THR:H | 2.06 | 0.54 |
| 1:N:751:VAL:HG22 | 1:N:810:ILE:HD13 | 1.89 | 0.54 |
| 1:N:1433:LEU:HD21 | 1:N:1460:HIS:NE2 | 2.22 | 0.54 |
| 1:O:606:PHE:CZ | 1:O:644:VAL:HG13 | 2.42 | 0.54 |
| 1:O:2001:CYS:HA | 1:O:2007:CYS:HB3 | 1.89 | 0.54 |
| 1:O:3125:ILE:HA | 1:O:3128:ILE:HG12 | 1.89 | 0.54 |
| 1:P:1356:ARG:NE | 1:P:1356:ARG:HA | 2.21 | 0.54 |
| 1:P:2785:THR:OG1 | 1:P:2788:GLN:OE1 | 2.17 | 0.54 |
| 1:R:176:HIS:HA | 1:R:179:VAL:HG12 | 1.89 | 0.54 |
| 1:R:1427:GLU:O | 1:R:1431:ASN:ND2 | 2.41 | 0.54 |
| 1:R:1743:HIS:CD2 | 1:R:1885:HIS:HD2 | 2.24 | 0.54 |
| 1:S:580:TYR:HE2 | 1:S:959:GLU:HB2 | 1.72 | 0.54 |
| 1:T:42:HIS:HB3 | 1:T:207:ALA:HB1 | 1.89 | 0.54 |
| 1:A:937:TRP:CD1 | 1:A:938:ASP:H | 2.26 | 0.54 |
| 1:A:3333:SER:OG | 1:A:3336:THR:OG1 | 2.26 | 0.54 |
| 1:B:2720:GLN:NE2 | 1:B:2730:TYR:O | 2.34 | 0.54 |
| 1:B:3157:PHE:HA | 1:B:3169:ARG:HH22 | 1.71 | 0.54 |
| 1:C:284:ASP:OD1 | 1:C:285:ASP:N | 2.40 | 0.54 |
| 1:C:704:HIS:ND1 | 1:C:705:GLU:OE2 | 2.41 | 0.54 |
| 1:C:1404:ASP:O | 1:C:1408:ASN:ND2 | 2.41 | 0.54 |
| 1:C:1494:GLN:NE2 | 1:C:1495:PRO:O | 2.40 | 0.54 |
| 1:C:2234:LYS:HG3 | 1:C:2243:VAL:HG11 | 1.89 | 0.54 |
| 1:C:2961:GLY:HA2 | 1:C:3106:LEU:HD23 | 1.89 | 0.54 |
| 1:C:3015:ARG:HG2 | 1:C:3016:PRO:HD2 | 1.89 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:D:43:GLY:O | 1:D:46:SER:OG | 2.25 | 0.54 |
| 1:D:454:ARG:HH22 | 1:D:1338:LEU:HG | 1.72 | 0.54 |
| 1:D:836:HIS:NE2 | 1:D:838:GLU:OE2 | 2.40 | 0.54 |
| 1:D:3018:LYS:HB2 | 1:D:3053:TYR:HA | 1.90 | 0.54 |
| 1:E:428:SER:OG | 1:E:429:ALA:N | 2.40 | 0.54 |
| 1:E:1732:CYS:C | 1:E:1734:HIS:HD1 | 2.15 | 0.54 |
| 1:E:2532:LEU:HG | 1:E:2536:GLN:NE2 | 2.23 | 0.54 |
| 1:E:3226:ALA:HA | 1:E:3289:LYS:HA | 1.88 | 0.54 |
| 1:F:1326:HIS:HD2 | 1:F:1461:HIS:CD2 | 2.25 | 0.54 |
| 1:F:2867:ASP:HA | 1:G:2741:ARG:CZ | 2.37 | 0.54 |
| 1:F:3342:SER:OG | 1:F:3344:VAL:O | 2.26 | 0.54 |
| 1:G:782:ASP:OD1 | 1:G:783:ARG:N | 2.41 | 0.54 |
| 1:H:1701:ASP:OD1 | 1:H:1701:ASP:N | 2.41 | 0.54 |
| 1:H:3332:VAL:HG22 | 1:H:3406:ILE:HA | 1.89 | 0.54 |
| 1:I:1433:LEU:HD21 | 1:I:1460:HIS:HE2 | 1.73 | 0.54 |
| 1:I:2095:GLU:CD | 1:I:2097:SER:H | 2.15 | 0.54 |
| 1:I:2604:THR:HA | 1:I:2654:PHE:CE2 | 2.43 | 0.54 |
| 1:J:284:ASP:OD1 | 1:J:284:ASP:N | 2.38 | 0.54 |
| 1:J:554:PHE:O | 1:J:568:ARG:NH2 | 2.41 | 0.54 |
| 1:K:1674:ARG:HD2 | 1:K:1954:GLU:HG2 | 1.88 | 0.54 |
| 1:K:2439:ASP:OD2 | 1:K:2440:ARG:NE | 2.41 | 0.54 |
| 1:L:811:LYS:NZ | 1:L:815:GLY:O | 2.36 | 0.54 |
| 1:L:1736:MET:HG2 | 1:L:1738:THR:H | 1.73 | 0.54 |
| 1:L:2111:LEU:HD13 | 1:L:2212:PHE:HE1 | 1.72 | 0.54 |
| 1:L:3038:LYS:O | 1:L:3041:GLN:NE2 | 2.40 | 0.54 |
| 1:M:481:ASP:OD1 | 1:P:1644:TYR:N | 2.41 | 0.54 |
| 1:M:885:HIS:ND1 | 1:M:885:HIS:O | 2.41 | 0.54 |
| 1:M:1508:ASP:O | 1:M:1510:THR:N | 2.41 | 0.54 |
| 1:N:524:ASP:HA | 1:N:643:ASN:ND2 | 2.23 | 0.54 |
| 1:N:934:LEU:HD12 | 1:N:935:PRO:HD2 | 1.89 | 0.54 |
| 1:N:1722:TYR:CE2 | 1:N:1724:GLU:HG2 | 2.43 | 0.54 |
| 1:N:2152:PRO:HD2 | 1:N:2329:TYR:HD2 | 1.73 | 0.54 |
| 1:N:3218:VAL:HG11 | 1:N:3327:PRO:HG3 | 1.89 | 0.54 |
| 1:O:2090:ASN:ND2 | 1:O:2175:THR:O | 2.41 | 0.54 |
| 1:O:2991:LEU:HD22 | 1:O:3157:PHE:HZ | 1.71 | 0.54 |
| 1:O:3260:ARG:HE | 1:O:3261:VAL:H | 1.54 | 0.54 |
| 1:P:1126:LEU:HD23 | 1:P:1126:LEU:H | 1.73 | 0.54 |
| 1:P:2790:GLU:HG2 | 1:P:2791:GLU:N | 2.23 | 0.54 |
| 1:Q:183:VAL:HA | 1:Q:186:ASN:HD22 | 1.73 | 0.54 |
| 1:Q:1433:LEU:HD11 | 1:Q:1460:HIS:CD2 | 2.43 | 0.54 |
| 1:Q:3160:GLU:HG2 | 1:Q:3169:ARG:HH22 | 1.71 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:Q:3339:ARG:NH2 | 1:Q:3376:ASP:O | 2.41 | 0.54 |
| 1:R:1049:PHE:O | 1:R:1053:HIS:ND1 | 2.35 | 0.54 |
| 1:R:1225:ASP:OD1 | 1:R:1226:LEU:N | 2.34 | 0.54 |
| 1:R:2709:HIS:HA | 1:R:2712:VAL:HG12 | 1.89 | 0.54 |
| 1:S:436:ASP:OD1 | 1:S:436:ASP:N | 2.40 | 0.54 |
| 1:S:2510:GLY:HA3 | 1:S:2513:VAL:HB | 1.90 | 0.54 |
| 1:T:1307:HIS:HB2 | 1:T:1602:MET:HE1 | 1.89 | 0.54 |
| 1:A:1968:LEU:O | 1:A:1972:ILE:HG12 | 2.08 | 0.54 |
| 1:A:2109:ALA:HA | 1:A:2112:ARG:NH2 | 2.22 | 0.54 |
| 1:B:848:ARG:HD2 | 1:B:1123:TYR:CE2 | 2.43 | 0.54 |
| 1:B:2873:ASP:OD2 | 1:B:2875:HIS:NE2 | 2.40 | 0.54 |
| 1:C:2713:ASP:OD2 | 1:C:2776:TYR:OH | 2.26 | 0.54 |
| 1:D:613:PRO:HA | 1:D:616:LEU:HB2 | 1.88 | 0.54 |
| 1:D:978:THR:HB | 1:D:1036:SER:HA | 1.90 | 0.54 |
| 1:D:1992:THR:HA | 1:D:2017:GLY:O | 2.08 | 0.54 |
| 1:F:74:VAL:HG12 | 1:F:213:PHE:HD1 | 1.73 | 0.54 |
| 1:F:2788:GLN:HA | 1:F:2791:GLU:OE2 | 2.08 | 0.54 |
| 1:F:2967:PRO:O | 1:F:2973:ARG:NH1 | 2.41 | 0.54 |
| 1:G:168:ALA:HA | 1:G:180:GLN:HG3 | 1.90 | 0.54 |
| 1:G:1644:TYR:N | 1:J:481:ASP:OD1 | 2.41 | 0.54 |
| 1:H:1299:HIS:ND1 | 1:H:1299:HIS:O | 2.40 | 0.54 |
| 1:H:2602:ASP:OD1 | 1:H:2603:TRP:N | 2.41 | 0.54 |
| 1:J:1270:ASP:OD1 | 1:J:1271:LEU:N | 2.41 | 0.54 |
| 1:J:1539:THR:H | 1:J:1542:GLN:NE2 | 2.06 | 0.54 |
| 1:J:2376:ASN:O | 1:J:2379:GLU:HG3 | 2.08 | 0.54 |
| 1:K:1404:ASP:O | 1:K:1408:ASN:ND2 | 2.41 | 0.54 |
| 1:K:2330:MET:HE1 | 1:K:2354:PRO:HG2 | 1.89 | 0.54 |
| 1:K:2585:LEU:HD22 | 1:K:2706:PHE:HE2 | 1.72 | 0.54 |
| 1:L:1775:LEU:HD12 | 1:L:1776:PRO:HD2 | 1.90 | 0.54 |
| 1:L:3225:SER:O | 1:L:3290:TYR:N | 2.41 | 0.54 |
| 1:M:524:ASP:OD1 | 1:M:526:THR:OG1 | 2.18 | 0.54 |
| 1:M:593:ALA:HA | 1:M:605:GLN:HG3 | 1.90 | 0.54 |
| 1:M:2558:LYS:HE3 | 1:M:2561:GLY:HA2 | 1.90 | 0.54 |
| 1:M:2601:TRP:CZ2 | 1:M:2603:TRP:HB3 | 2.43 | 0.54 |
| 1:M:2637:SER:HB2 | 1:M:2687:GLY:HA3 | 1.88 | 0.54 |
| 1:N:920:GLN:HB3 | 1:N:1103:THR:HG21 | 1.90 | 0.54 |
| 1:N:2865:ARG:HG2 | 1:N:2866:PRO:HD2 | 1.88 | 0.54 |
| 1:O:323:ASN:OD1 | 1:O:324:VAL:N | 2.40 | 0.54 |
| 1:P:3218:VAL:HG23 | 1:P:3258:TYR:HB2 | 1.90 | 0.54 |
| 1:Q:1278:SER:O | 1:Q:1281:SER:OG | 2.23 | 0.54 |
| 1:Q:1744:ARG:HH21 | 1:Q:1947:TYR:HB3 | 1.71 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:Q:2508:VAL:O | 1:Q:2515:LYS:NZ | 2.41 | 0.54 |
| 1:R:310:LEU:HD13 | 1:R:366:HIS:HB3 | 1.89 | 0.54 |
| 1:R:938:ASP:CG | 1:R:1055:ASN:HD21 | 2.16 | 0.54 |
| 1:R:1722:TYR:HD2 | 1:R:1725:ALA:HB2 | 1.73 | 0.54 |
| 1:S:3212:ARG:HG3 | 1:S:3214:TYR:CE1 | 2.34 | 0.54 |
| 1:A:310:LEU:HD23 | 1:A:366:HIS:HB3 | 1.89 | 0.54 |
| 1:A:851:VAL:HG12 | 1:A:935:PRO:HB2 | 1.90 | 0.54 |
| 1:A:3260:ARG:HE | 1:A:3261:VAL:H | 1.56 | 0.54 |
| 1:B:2741:ARG:HH12 | 1:C:2870:TYR:N | 2.06 | 0.54 |
| 1:C:204:GLU:OE2 | 1:C:354:ALA:N | 2.35 | 0.54 |
| 1:D:6:LYS:HD3 | 1:D:11:LEU:HD13 | 1.90 | 0.54 |
| 1:D:379:LYS:HD3 | 1:D:381:ASN:H | 1.73 | 0.54 |
| 1:D:1716:VAL:HG23 | 1:D:1718:PRO:HD3 | 1.89 | 0.54 |
| 1:F:38:LEU:O | 1:F:73:TYR:OH | 2.25 | 0.54 |
| 1:F:1284:ARG:NH2 | 1:F:1376:GLU:HG3 | 2.23 | 0.54 |
| 1:F:1427:GLU:O | 1:F:1431:ASN:ND2 | 2.41 | 0.54 |
| 1:G:2602:ASP:OD2 | 1:G:2604:THR:HG22 | 2.08 | 0.54 |
| 1:G:2934:VAL:O | 1:G:2938:ARG:HG2 | 2.08 | 0.54 |
| 1:H:313:PHE:CE2 | 1:H:406:PRO:HB3 | 2.43 | 0.54 |
| 1:H:1602:MET:HE3 | 1:H:1603:PRO:HD2 | 1.89 | 0.54 |
| 1:H:1746:TYR:HH | 1:H:1876:SER:HG | 1.56 | 0.54 |
| 1:H:2752:ASN:HD21 | 1:H:2757:ILE:HG13 | 1.72 | 0.54 |
| 1:H:3035:TYR:H | 1:H:3044:VAL:HG22 | 1.73 | 0.54 |
| 1:J:2522:VAL:O | 1:J:2526:GLU:HG2 | 2.07 | 0.54 |
| 1:J:2602:ASP:OD2 | 1:J:2604:THR:OG1 | 2.26 | 0.54 |
| 1:J:3260:ARG:NH2 | 1:J:3407:ASP:OD2 | 2.41 | 0.54 |
| 1:K:603:GLU:N | 1:K:603:GLU:OE1 | 2.41 | 0.54 |
| 1:K:1011:PHE:HA | 1:K:1014:PHE:HB3 | 1.89 | 0.54 |
| 1:K:1168:VAL:N | 1:K:1178:GLU:OE1 | 2.40 | 0.54 |
| 1:L:1560:PHE:HZ | 1:L:1573:LEU:HD11 | 1.73 | 0.54 |
| 1:L:2392:ARG:HH11 | 1:L:2394:PHE:HZ | 1.56 | 0.54 |
| 1:M:363:LEU:HD12 | 1:M:364:PRO:HD2 | 1.90 | 0.54 |
| 1:M:471:HIS:HB3 | 1:M:632:ALA:HB2 | 1.89 | 0.54 |
| 1:M:2096:ILE:HD13 | 1:M:2179:PRO:HG2 | 1.90 | 0.54 |
| 1:N:740:LEU:HB2 | 1:N:785:VAL:HB | 1.90 | 0.54 |
| 1:N:1626:ASP:OD1 | 1:N:1627:SER:N | 2.41 | 0.54 |
| 1:O:939:TRP:HZ3 | 1:O:1055:ASN:HB3 | 1.73 | 0.54 |
| 1:O:1322:PHE:HB3 | 1:O:1323:PRO:HD3 | 1.90 | 0.54 |
| 1:O:2090:ASN:C | 1:O:2091:ARG:HD3 | 2.33 | 0.54 |
| 1:O:2196:GLU:OE2 | 1:O:2210:ASN:ND2 | 2.41 | 0.54 |
| 1:P:374:GLU:OE1 | 1:P:374:GLU:N | 2.31 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:P:608:VAL:HG21 | 1:P:785:VAL:HG21 | 1.89 | 0.54 |
| 1:P:735:ARG:NH2 | 1:P:790:THR:H | 2.06 | 0.54 |
| 1:P:1722:TYR:CE2 | 1:P:1724:GLU:HG2 | 2.43 | 0.54 |
| 1:P:2984:PHE:O | 1:P:2988:HIS:ND1 | 2.35 | 0.54 |
| 1:Q:849:SER:OG | 1:Q:850:ASP:N | 2.41 | 0.54 |
| 1:Q:1684:THR:N | 1:Q:1687:GLU:OE2 | 2.34 | 0.54 |
| 1:Q:2857:SER:O | 1:Q:2861:GLN:HG3 | 2.08 | 0.54 |
| 1:R:744:ASN:HD21 | 1:R:778:PRO:HA | 1.73 | 0.54 |
| 1:R:2376:ASN:O | 1:R:2379:GLU:HG3 | 2.07 | 0.54 |
| 1:S:42:HIS:NE2 | 1:S:59:CYS:SG | 2.81 | 0.54 |
| 1:T:2111:LEU:HD13 | 1:T:2212:PHE:HE1 | 1.72 | 0.54 |
| 1:T:3127:GLN:O | 1:T:3130:GLN:HG3 | 2.07 | 0.54 |
| 1:A:1554:ASP:N | 1:A:1554:ASP:OD1 | 2.40 | 0.53 |
| 1:A:1865:LYS:HB3 | 1:A:1868:SER:HB3 | 1.90 | 0.53 |
| 1:A:2155:PRO:HB2 | 1:A:2306:TRP:CZ3 | 2.43 | 0.53 |
| 1:A:2190:LEU:HD21 | 1:A:2194:PHE:CD2 | 2.43 | 0.53 |
| 1:A:2234:LYS:HG3 | 1:A:2243:VAL:HG11 | 1.90 | 0.53 |
| 1:A:2934:VAL:O | 1:A:2938:ARG:HG3 | 2.08 | 0.53 |
| 1:A:3086:MET:O | 1:A:3090:THR:HG23 | 2.08 | 0.53 |
| 1:A:3374:ASP:O | 1:A:3379:TYR:OH | 2.25 | 0.53 |
| 1:B:540:THR:HG22 | 1:B:551:HIS:HA | 1.90 | 0.53 |
| 1:B:1788:VAL:HG12 | 1:B:1789:LEU:HD22 | 1.90 | 0.53 |
| 1:B:2567:CYS:O | 1:B:2569:HIS:ND1 | 2.41 | 0.53 |
| 1:C:850:ASP:OD1 | 1:C:852:SER:OG | 2.24 | 0.53 |
| 1:C:2420:THR:HG21 | 1:C:2453:LEU:HD21 | 1.89 | 0.53 |
| 1:D:1135:GLN:HA | 1:D:1138:ARG:HE | 1.73 | 0.53 |
| 1:F:2477:ASN:HB3 | 3:w:1:NAG:N2 | 2.22 | 0.53 |
| 1:G:164:MET:HE1 | 1:G:187:HIS:HE1 | 1.72 | 0.53 |
| 1:G:1641:ASN:OD1 | 1:G:1643:SER:N | 2.33 | 0.53 |
| 1:G:3033:SER:O | 1:G:3046:ARG:NH2 | 2.42 | 0.53 |
| 1:H:1220:LYS:NZ | 1:H:1221:TYR:O | 2.33 | 0.53 |
| 1:H:2693:MET:HE1 | 1:H:2702:ASP:HB3 | 1.89 | 0.53 |
| 1:I:1111:GLU:N | 1:I:1111:GLU:OE1 | 2.41 | 0.53 |
| 1:I:1823:GLU:N | 1:I:1827:ASP:OD2 | 2.38 | 0.53 |
| 1:I:2864:LEU:HD21 | 1:I:2870:TYR:CD1 | 2.42 | 0.53 |
| 1:J:845:LEU:O | 1:J:926:ARG:NH1 | 2.41 | 0.53 |
| 1:J:1284:ARG:HH11 | 1:J:1284:ARG:HG2 | 1.73 | 0.53 |
| 1:J:2630:LEU:HD11 | 1:J:2698:TYR:HE1 | 1.72 | 0.53 |
| 1:J:3114:PHE:HA | 1:J:3117:ILE:HG12 | 1.89 | 0.53 |
| 1:K:1752:ASP:OD1 | 1:K:1753:ALA:N | 2.42 | 0.53 |
| 1:K:2383:GLU:O | 1:K:2387:HIS:ND1 | 2.36 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:K:2741:ARG:CZ | 1:T:2867:ASP:HA | 2.38 | 0.53 |
| 1:L:1851:GLU:O | 1:L:1855:ASN:ND2 | 2.41 | 0.53 |
| 1:M:939:TRP:HE1 | 1:M:998:ILE:HG21 | 1.74 | 0.53 |
| 1:M:1809:VAL:HG23 | 1:M:1868:SER:HA | 1.89 | 0.53 |
| 1:M:2603:TRP:NE1 | 1:M:2711:ASN:HD22 | 2.06 | 0.53 |
| 1:N:1086:LYS:HZ3 | 1:N:1087:PRO:HD2 | 1.72 | 0.53 |
| 1:N:1169:CYS:HA | 1:N:1175:CYS:HA | 1.90 | 0.53 |
| 1:O:2714:ARG:NH2 | 1:O:2778:ASP:O | 2.41 | 0.53 |
| 1:O:2786:ILE:HD13 | 1:O:2789:LEU:HD21 | 1.90 | 0.53 |
| 1:O:3339:ARG:NH2 | 1:O:3376:ASP:O | 2.40 | 0.53 |
| 1:P:552:ASN:HD21 | 1:P:554:PHE:HB2 | 1.73 | 0.53 |
| 1:P:1579:THR:HG21 | 1:P:1585:ASN:HB3 | 1.90 | 0.53 |
| 1:P:1827:ASP:HA | 1:P:1831:TRP:CD1 | 2.43 | 0.53 |
| 1:P:2182:ASP:HA | 1:P:2301:PHE:CE2 | 2.43 | 0.53 |
| 1:P:2660:LEU:HD21 | 1:P:2803:PHE:HE1 | 1.73 | 0.53 |
| 1:Q:1240:THR:HA | 1:R:2328:ASN:HD21 | 1.72 | 0.53 |
| 1:Q:1420:CYS:HA | 1:Q:1423:GLU:HG2 | 1.90 | 0.53 |
| 1:Q:1531:ASP:OD1 | 1:Q:1532:THR:N | 2.41 | 0.53 |
| 1:Q:1587:ASN:CG | 1:Q:1588:HIS:HD1 | 2.16 | 0.53 |
| 1:Q:1828:ASN:OD1 | 1:Q:1829:TRP:N | 2.41 | 0.53 |
| 1:Q:2666:ASP:OD1 | 1:Q:2669:ASN:HB2 | 2.08 | 0.53 |
| 1:R:2587:ARG:HH22 | 1:R:2753:PRO:HG2 | 1.73 | 0.53 |
| 1:T:269:THR:HB | 1:T:271:LYS:HZ3 | 1.73 | 0.53 |
| 1:T:810:ILE:HG21 | 1:T:818:TRP:HB2 | 1.89 | 0.53 |
| 1:T:1153:PHE:HB2 | 1:T:1198:PHE:HD2 | 1.71 | 0.53 |
| 1:A:1085:ARG:NH1 | 1:B:2462:ASN:O | 2.41 | 0.53 |
| 1:A:1168:VAL:N | 1:A:1178:GLU:OE1 | 2.41 | 0.53 |
| 1:A:2297:THR:O | 1:A:2300:THR:OG1 | 2.25 | 0.53 |
| 1:A:2495:PRO:HB2 | 1:A:2500:ARG:HD2 | 1.89 | 0.53 |
| 1:B:454:ARG:NH2 | 1:B:1338:LEU:HG | 2.21 | 0.53 |
| 1:B:1262:SER:OG | 1:B:1263:HIS:N | 2.41 | 0.53 |
| 1:B:1978:LYS:HD2 | 1:B:2078:LYS:HZ1 | 1.72 | 0.53 |
| 1:C:782:ASP:OD1 | 1:C:783:ARG:N | 2.42 | 0.53 |
| 1:C:3125:ILE:HA | 1:C:3128:ILE:HG12 | 1.90 | 0.53 |
| 1:C:3289:LYS:HB3 | 1:C:3295:LEU:HD11 | 1.91 | 0.53 |
| 1:D:597:ARG:NH2 | 1:D:655:GLN:OE1 | 2.41 | 0.53 |
| 1:D:1254:ILE:HG23 | 1:D:1256:LYS:H | 1.73 | 0.53 |
| 1:D:1427:GLU:O | 1:D:1431:ASN:ND2 | 2.41 | 0.53 |
| 1:D:2210:ASN:HD21 | 1:D:2212:PHE:HB2 | 1.73 | 0.53 |
| 1:D:2580:LEU:HA | 1:D:2583:VAL:HG12 | 1.90 | 0.53 |
| 1:E:580:TYR:OH | 1:E:860:GLN:OE1 | 2.24 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:F:337:GLN:OE1 | 1:F:337:GLN:N | 2.41 | 0.53 |
| 1:F:435:LYS:HG2 | 1:F:436:ASP:H | 1.73 | 0.53 |
| 1:F:1282:ALA:O | 1:F:1286:MET:HG3 | 2.09 | 0.53 |
| 1:G:2622:PHE:HA | 1:G:2703:PRO:HG2 | 1.90 | 0.53 |
| 1:H:787:VAL:HG23 | 1:H:789:ILE:HD11 | 1.90 | 0.53 |
| 1:H:795:LYS:HD3 | 1:H:796:LYS:HD3 | 1.90 | 0.53 |
| 1:H:1135:GLN:HA | 1:H:1138:ARG:HG2 | 1.91 | 0.53 |
| 1:H:2979:HIS:HA | 1:H:2984:PHE:HD2 | 1.73 | 0.53 |
| 1:H:3211:ASP:OD1 | 1:H:3309:ALA:N | 2.41 | 0.53 |
| 1:I:2249:LEU:HD23 | 1:I:2383:GLU:CD | 2.33 | 0.53 |
| 1:J:6:LYS:HD2 | 1:J:11:LEU:HD13 | 1.90 | 0.53 |
| 1:J:735:ARG:NH2 | 1:J:790:THR:H | 2.06 | 0.53 |
| 1:J:2126:LEU:HD11 | 1:J:2165:VAL:HG12 | 1.91 | 0.53 |
| 1:K:1342:SER:OG | 1:K:1344:VAL:O | 2.24 | 0.53 |
| 1:K:2201:ASP:OD1 | 1:K:2203:TRP:N | 2.35 | 0.53 |
| 1:L:1185:GLY:HA2 | 1:L:1189:GLU:HG3 | 1.91 | 0.53 |
| 1:L:2614:LEU:HD11 | 1:L:2636:ARG:HH22 | 1.72 | 0.53 |
| 1:M:2130:HIS:HB3 | 1:M:2290:SER:HB3 | 1.89 | 0.53 |
| 1:M:2399:LEU:HB3 | 1:M:2436:TRP:HH2 | 1.73 | 0.53 |
| 1:M:3081:GLU:HA | 1:M:3084:PHE:HB3 | 1.89 | 0.53 |
| 1:M:3165:ASN:ND2 | 1:M:3168:THR:H | 2.06 | 0.53 |
| 1:N:2138:SER:OG | 1:N:2143:LYS:NZ | 2.40 | 0.53 |
| 1:N:3142:TYR:HD2 | 1:N:3144:ARG:HD3 | 1.72 | 0.53 |
| 1:O:2994:GLN:OE1 | 1:O:3165:ASN:ND2 | 2.40 | 0.53 |
| 1:P:1284:ARG:HH21 | 1:P:1287:GLN:HG2 | 1.72 | 0.53 |
| 1:P:2055:LEU:HB2 | 1:P:2063:LEU:HB2 | 1.90 | 0.53 |
| 1:Q:202:THR:OG1 | 1:Q:204:GLU:OE1 | 2.25 | 0.53 |
| 1:Q:1166:LEU:HD22 | 1:Q:1200:TYR:HD2 | 1.72 | 0.53 |
| 1:Q:3086:MET:O | 1:Q:3090:THR:HG23 | 2.07 | 0.53 |
| 1:R:1743:HIS:HD2 | 1:R:1885:HIS:CD2 | 2.26 | 0.53 |
| 1:R:2343:ASN:HD21 | 1:R:2345:ASN:HB3 | 1.74 | 0.53 |
| 1:R:2343:ASN:OD1 | 1:R:2344:GLU:N | 2.41 | 0.53 |
| 1:R:3113:PRO:HA | 1:R:3116:MET:HE2 | 1.89 | 0.53 |
| 1:S:44:GLU:HG3 | 1:S:135:MET:HE1 | 1.89 | 0.53 |
| 1:S:734:ASP:OD1 | 1:S:734:ASP:N | 2.40 | 0.53 |
| 1:S:2027:ASP:OD2 | 1:S:2028:ARG:NH1 | 2.41 | 0.53 |
| 1:S:2454:HIS:O | 1:S:2456:ARG:NH1 | 2.41 | 0.53 |
| 1:S:3114:PHE:HA | 1:S:3117:ILE:HG12 | 1.90 | 0.53 |
| 1:T:105:ARG:HA | 1:T:108:GLN:HE22 | 1.71 | 0.53 |
| 1:T:1087:PRO:HA | 1:T:1109:PRO:HD3 | 1.90 | 0.53 |
| 1:T:1742:TRP:HD1 | 1:T:1920:LEU:HD12 | 1.73 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:T:1995:HIS:ND1 | 1:T:2013:PHE:O | 2.40 | 0.53 |
| 1:T:2408:VAL:HG22 | 1:T:2473:ILE:HG22 | 1.89 | 0.53 |
| 1:T:2661:ALA:HA | 1:T:2664:GLN:HE22 | 1.73 | 0.53 |
| 1:T:3342:SER:OG | 1:T:3344:VAL:O | 2.25 | 0.53 |
| 1:A:221:ARG:NH2 | 1:A:287:SER:O | 2.42 | 0.53 |
| 1:A:711:ASP:OD1 | 1:A:712:ASN:N | 2.38 | 0.53 |
| 1:A:1178:GLU:HG3 | 1:A:1205:ILE:HG12 | 1.89 | 0.53 |
| 1:A:1322:PHE:HB3 | 1:A:1323:PRO:HD3 | 1.90 | 0.53 |
| 1:A:2090:ASN:ND2 | 1:A:2175:THR:O | 2.41 | 0.53 |
| 1:A:2309:TRP:HH2 | 1:A:2313:GLN:HE21 | 1.55 | 0.53 |
| 1:A:2989:ARG:NH1 | 1:A:3177:ILE:O | 2.42 | 0.53 |
| 1:B:2338:ASN:OD1 | 1:B:2339:SER:N | 2.42 | 0.53 |
| 1:B:2514:ARG:HE | 1:B:2774:TYR:HD2 | 1.56 | 0.53 |
| 1:C:2105:MET:HA | 1:C:2108:LYS:HG2 | 1.90 | 0.53 |
| 1:D:1626:ASP:OD1 | 1:D:1627:SER:N | 2.42 | 0.53 |
| 1:E:17:LEU:O | 1:E:20:GLU:HG3 | 2.08 | 0.53 |
| 1:E:392:SER:OG | 1:E:393:VAL:N | 2.41 | 0.53 |
| 1:E:885:HIS:ND1 | 1:E:885:HIS:O | 2.41 | 0.53 |
| 1:E:1298:PHE:HZ | 1:E:1504:GLN:HB3 | 1.73 | 0.53 |
| 1:E:1572:GLN:HB2 | 1:E:1636:LYS:HB2 | 1.89 | 0.53 |
| 1:E:2197:GLN:HG3 | 1:H:110:PRO:HD3 | 1.90 | 0.53 |
| 1:F:1353:GLN:NE2 | 1:F:1536:ASN:OD1 | 2.42 | 0.53 |
| 1:G:327:LYS:HD2 | 1:G:344:PHE:HA | 1.89 | 0.53 |
| 1:G:1433:LEU:HD11 | 1:G:1460:HIS:CD2 | 2.43 | 0.53 |
| 1:G:1710:LEU:HB3 | 1:G:1750:PHE:HE1 | 1.73 | 0.53 |
| 1:G:2037:VAL:HA | 1:G:2040:LYS:HG2 | 1.91 | 0.53 |
| 1:G:2090:ASN:O | 1:G:2091:ARG:HG2 | 2.09 | 0.53 |
| 1:G:2989:ARG:NH1 | 1:G:3177:ILE:O | 2.40 | 0.53 |
| 1:H:259:ASN:O | 1:H:265:ARG:NH2 | 2.42 | 0.53 |
| 1:H:1716:VAL:HG23 | 1:H:1718:PRO:HD3 | 1.91 | 0.53 |
| 1:H:3270:LEU:HD11 | 1:H:3281:PHE:CZ | 2.43 | 0.53 |
| 1:I:16:VAL:HG21 | 1:I:105:ARG:HH22 | 1.73 | 0.53 |
| 1:J:328:VAL:HG12 | 1:J:386:VAL:HG22 | 1.90 | 0.53 |
| 1:J:1865:LYS:HE3 | 1:J:1867:HIS:H | 1.72 | 0.53 |
| 1:K:129:GLU:HA | 1:K:140:SER:HA | 1.90 | 0.53 |
| 1:K:203:LEU:HD21 | 1:K:351:LEU:HB3 | 1.91 | 0.53 |
| 1:L:1579:THR:HG21 | 1:L:1585:ASN:HB3 | 1.91 | 0.53 |
| 1:L:1932:ASP:OD2 | 1:L:1935:THR:N | 2.28 | 0.53 |
| 1:M:1159:ARG:C | 1:M:1160:LYS:HD3 | 2.33 | 0.53 |
| 1:M:3358:THR:H | 1:N:3329:LYS:HE3 | 1.73 | 0.53 |
| 1:N:231:LYS:HB3 | 1:N:237:TYR:HE1 | 1.72 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:N:313:PHE:HB3 | 1:N:315:LEU:HD23 | 1.90 | 0.53 |
| 1:N:2530:LYS:HB2 | 1:N:2533:ARG:HH22 | 1.73 | 0.53 |
| 1:O:27:GLU:O | 1:O:30:LYS:NZ | 2.29 | 0.53 |
| 1:O:259:ASN:ND2 | 1:O:264:THR:OG1 | 2.42 | 0.53 |
| 1:P:328:VAL:HG12 | 1:P:386:VAL:HG22 | 1.90 | 0.53 |
| 1:P:744:ASN:HB3 | 1:P:779:TRP:CE2 | 2.44 | 0.53 |
| 1:P:2217:ILE:HG22 | 1:P:2220:SER:H | 1.73 | 0.53 |
| 1:Q:204:GLU:OE2 | 1:Q:354:ALA:N | 2.36 | 0.53 |
| 1:Q:2108:LYS:O | 1:Q:2112:ARG:NH1 | 2.42 | 0.53 |
| 1:R:1274:GLY:O | 1:R:1277:GLU:HG3 | 2.09 | 0.53 |
| 1:R:1890:ARG:NH1 | 1:R:1957:THR:O | 2.41 | 0.53 |
| 1:S:418:ASP:OD2 | 1:S:662:TYR:N | 2.41 | 0.53 |
| 1:S:1008:GLN:N | 1:S:1008:GLN:OE1 | 2.40 | 0.53 |
| 1:S:2078:LYS:HB2 | 1:S:2080:ARG:HH12 | 1.72 | 0.53 |
| 1:S:2961:GLY:HA2 | 1:S:3106:LEU:HD23 | 1.91 | 0.53 |
| 1:T:2542:ARG:HD3 | 1:T:2591:LEU:HD22 | 1.89 | 0.53 |
| 1:A:24:ARG:NH2 | 1:A:123:ASN:HA | 2.23 | 0.53 |
| 1:A:2090:ASN:C | 1:A:2091:ARG:HD3 | 2.33 | 0.53 |
| 1:B:859:VAL:HG12 | 1:B:863:ARG:NE | 2.23 | 0.53 |
| 1:B:2210:ASN:HD21 | 1:B:2212:PHE:HB2 | 1.74 | 0.53 |
| 1:B:2745:GLU:OE1 | 1:B:2749:TRP:NE1 | 2.41 | 0.53 |
| 1:B:2785:THR:OG1 | 1:B:2788:GLN:OE1 | 2.17 | 0.53 |
| 1:B:2984:PHE:O | 1:B:2988:HIS:ND1 | 2.40 | 0.53 |
| 1:C:44:GLU:N | 1:C:204:GLU:O | 2.38 | 0.53 |
| 1:C:1307:HIS:CG | 1:C:1602:MET:HE1 | 2.43 | 0.53 |
| 1:C:2093:ARG:NH1 | 1:C:2177:ALA:O | 2.41 | 0.53 |
| 1:C:2095:GLU:CD | 1:C:2097:SER:H | 2.16 | 0.53 |
| 1:C:2882:THR:OG1 | 4:C:3501:NAG:N2 | 2.34 | 0.53 |
| 1:D:200:LEU:HD21 | 1:D:209:ASP:HB3 | 1.90 | 0.53 |
| 1:E:44:GLU:N | 1:E:204:GLU:O | 2.38 | 0.53 |
| 1:E:182:GLU:O | 1:E:186:ASN:ND2 | 2.41 | 0.53 |
| 1:E:539:GLU:HA | 1:E:555:PHE:HB2 | 1.90 | 0.53 |
| 1:E:1811:ARG:HH22 | 1:E:1880:ILE:HB | 1.74 | 0.53 |
| 1:E:2802:VAL:HG12 | 1:E:2856:THR:HG22 | 1.89 | 0.53 |
| 1:F:1126:LEU:H | 1:F:1126:LEU:HD23 | 1.73 | 0.53 |
| 1:G:9:ASP:OD1 | 1:G:9:ASP:N | 2.40 | 0.53 |
| 1:G:390:LEU:HD22 | 1:G:398:LEU:HB3 | 1.88 | 0.53 |
| 1:G:2213:ALA:O | 1:G:2226:ARG:NH1 | 2.38 | 0.53 |
| 1:G:2981:MET:HG3 | 1:G:2982:PRO:HD2 | 1.90 | 0.53 |
| 1:H:2876:ILE:HB | 1:H:2884:LEU:HB2 | 1.89 | 0.53 |
| 1:H:3303:VAL:HG13 | 1:H:3305:ILE:HD11 | 1.91 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:I:292:ASN:H | 1:I:295:GLN:NE2 | 2.07 | 0.53 |
| 1:I:1091:PHE:O | 1:I:1107:SER:OG | 2.25 | 0.53 |
| 1:I:1865:LYS:HB3 | 1:I:1868:SER:HB3 | 1.90 | 0.53 |
| 1:I:1900:ARG:O | 1:I:1900:ARG:NH1 | 2.42 | 0.53 |
| 1:I:2421:ARG:HH22 | 1:I:2424:ALA:HB2 | 1.73 | 0.53 |
| 1:J:188:ILE:HD13 | 1:J:215:HIS:NE2 | 2.24 | 0.53 |
| 1:J:674:LEU:HA | 1:J:695:ARG:HH12 | 1.73 | 0.53 |
| 1:J:1067:GLN:HA | 1:J:1070:ARG:HG2 | 1.89 | 0.53 |
| 1:J:1272:SER:N | 1:J:1275:GLU:OE2 | 2.35 | 0.53 |
| 1:J:2985:PRO:HB2 | 1:J:2989:ARG:NH2 | 2.23 | 0.53 |
| 1:K:752:ILE:O | 1:K:808:LEU:HA | 2.08 | 0.53 |
| 1:K:2421:ARG:HH22 | 1:K:2424:ALA:HB2 | 1.72 | 0.53 |
| 1:L:960:THR:OG1 | 1:L:964:GLU:OE2 | 2.25 | 0.53 |
| 1:L:1299:HIS:ND1 | 1:L:1299:HIS:O | 2.42 | 0.53 |
| 1:L:1728:ARG:NH2 | 4:N:3501:NAG:O7 | 2.42 | 0.53 |
| 1:M:508:GLU:OE2 | 1:M:520:ILE:N | 2.40 | 0.53 |
| 1:M:1506:GLU:HG3 | 1:M:1507:PHE:N | 2.22 | 0.53 |
| 1:M:1671:THR:O | 1:M:1673:ARG:NH2 | 2.39 | 0.53 |
| 1:M:2378:ASP:OD1 | 1:M:2378:ASP:N | 2.41 | 0.53 |
| 1:O:1903:GLY:HA3 | 1:P:1667:GLN:HB2 | 1.89 | 0.53 |
| 1:O:2729:ASP:OD1 | 1:O:2916:THR:OG1 | 2.25 | 0.53 |
| 1:P:453:SER:HB3 | 1:P:553:PRO:HG3 | 1.91 | 0.53 |
| 1:P:1848:VAL:HG12 | 1:P:2026:PHE:HD2 | 1.74 | 0.53 |
| 1:P:2831:ALA:HA | 1:P:2858:VAL:HG11 | 1.90 | 0.53 |
| 1:Q:1328:LEU:HB3 | 1:Q:1499:PHE:HE2 | 1.73 | 0.53 |
| 1:Q:2215:GLY:N | 1:Q:2224:THR:OG1 | 2.36 | 0.53 |
| 1:R:1736:MET:HG2 | 1:R:1738:THR:H | 1.73 | 0.53 |
| 1:S:1359:PRO:HB2 | 1:S:1362:ILE:HG12 | 1.89 | 0.53 |
| 1:T:24:ARG:HD3 | 1:T:123:ASN:HA | 1.90 | 0.53 |
| 1:T:176:HIS:HA | 1:T:179:VAL:HG12 | 1.91 | 0.53 |
| 1:T:594:LEU:HA | 1:T:602:PHE:CE1 | 2.40 | 0.53 |
| 1:T:1011:PHE:HA | 1:T:1063:TRP:HH2 | 1.73 | 0.53 |
| 1:T:1365:ALA:HA | 1:T:1378:ASN:HB3 | 1.89 | 0.53 |
| 1:T:2602:ASP:OD1 | 1:T:2603:TRP:N | 2.42 | 0.53 |
| 1:T:2820:ASP:OD1 | 1:T:2829:SER:N | 2.41 | 0.53 |
| 1:A:392:SER:OG | 1:A:393:VAL:N | 2.40 | 0.53 |
| 1:A:1244:ARG:HD3 | 1:A:1245:PRO:HD2 | 1.91 | 0.53 |
| 1:B:1564:ASN:HB3 | 1:B:1604:PHE:CE1 | 2.43 | 0.53 |
| 1:B:2666:ASP:OD1 | 1:B:2667:TYR:N | 2.40 | 0.53 |
| 1:B:2675:GLU:O | 1:B:2679:ASN:ND2 | 2.42 | 0.53 |
| 1:C:2345:ASN:HD21 | 1:C:2347:PHE:HB3 | 1.72 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:D:1143:ARG:O | 1:D:1148:ARG:NH1 | 2.33 | 0.53 |
| 1:D:3122:ILE:HG13 | 1:D:3125:ILE:HD11 | 1.91 | 0.53 |
| 1:E:60:VAL:HG13 | 1:E:63:MET:HE2 | 1.91 | 0.53 |
| 1:E:1189:GLU:N | 1:E:1189:GLU:OE1 | 2.42 | 0.53 |
| 1:E:1585:ASN:OD1 | 1:E:1586:CYS:N | 2.42 | 0.53 |
| 1:E:2454:HIS:O | 1:E:2456:ARG:NH1 | 2.41 | 0.53 |
| 1:F:3015:ARG:HD3 | 1:F:3016:PRO:HD2 | 1.91 | 0.53 |
| 1:H:662:TYR:CE2 | 1:H:700:TYR:HB3 | 2.44 | 0.53 |
| 1:H:2718:ILE:HD13 | 1:H:2779:LEU:HD12 | 1.90 | 0.53 |
| 1:I:866:LEU:HD22 | 1:I:968:PHE:CE1 | 2.44 | 0.53 |
| 1:I:1404:ASP:O | 1:I:1408:ASN:ND2 | 2.42 | 0.53 |
| 1:I:1413:ALA:HB1 | 1:I:1425:GLN:OE1 | 2.09 | 0.53 |
| 1:I:2532:LEU:HG | 1:I:2536:GLN:NE2 | 2.24 | 0.53 |
| 1:I:3091:ILE:HA | 1:I:3094:LEU:HD23 | 1.90 | 0.53 |
| 1:J:737:PHE:HB2 | 1:J:829:ILE:HB | 1.89 | 0.53 |
| 1:J:2044:SER:N | 1:J:2047:ASP:OD2 | 2.41 | 0.53 |
| 1:K:2805:ASN:HB3 | 1:K:2850:LEU:HD11 | 1.90 | 0.53 |
| 1:K:3133:GLN:HE21 | 1:K:3138:ARG:HB3 | 1.73 | 0.53 |
| 1:L:337:GLN:HB2 | 1:S:1588:HIS:CE1 | 2.43 | 0.53 |
| 1:L:662:TYR:CE2 | 1:L:700:TYR:HB3 | 2.43 | 0.53 |
| 1:L:1420:CYS:SG | 1:L:1485:SER:OG | 2.66 | 0.53 |
| 1:L:2988:HIS:HA | 1:L:2991:LEU:HD12 | 1.90 | 0.53 |
| 1:M:148:ARG:HA | 1:M:151:GLN:HE22 | 1.72 | 0.53 |
| 1:M:1383:VAL:H | 1:M:1392:THR:HG22 | 1.74 | 0.53 |
| 1:M:3213:VAL:HG23 | 1:M:3306:SER:HB2 | 1.90 | 0.53 |
| 1:N:38:LEU:O | 1:N:73:TYR:OH | 2.22 | 0.53 |
| 1:N:461:VAL:HG22 | 1:N:1277:GLU:OE2 | 2.08 | 0.53 |
| 1:N:1495:PRO:HA | 1:N:1515:ARG:NH2 | 2.24 | 0.53 |
| 1:O:1244:ARG:HD3 | 1:O:1245:PRO:HD2 | 1.91 | 0.53 |
| 1:O:2534:ALA:HA | 1:O:2537:GLN:HE22 | 1.74 | 0.53 |
| 1:O:2623:GLU:OE1 | 1:O:2623:GLU:N | 2.33 | 0.53 |
| 1:O:3268:ASP:N | 1:O:3268:ASP:OD1 | 2.41 | 0.53 |
| 1:P:848:ARG:HB3 | 1:P:933:GLY:HA3 | 1.89 | 0.53 |
| 1:P:860:GLN:HE21 | 1:P:864:GLU:HG2 | 1.74 | 0.53 |
| 1:P:2802:VAL:HG23 | 1:P:2855:VAL:HG23 | 1.90 | 0.53 |
| 1:Q:728:ASP:OD2 | 1:Q:836:HIS:ND1 | 2.41 | 0.53 |
| 1:Q:2470:ARG:NH2 | 1:Q:2471:TYR:O | 2.38 | 0.53 |
| 1:R:8:VAL:HA | 1:R:11:LEU:HD23 | 1.90 | 0.53 |
| 1:R:1701:ASP:N | 1:R:1701:ASP:OD1 | 2.42 | 0.53 |
| 1:R:2666:ASP:OD2 | 1:R:2849:ARG:NH2 | 2.41 | 0.53 |
| 1:R:2752:ASN:HD21 | 1:R:2757:ILE:HG13 | 1.73 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:R:2789:LEU:O | 1:R:2793:ILE:HG12 | 2.08 | 0.53 |
| 1:S:204:GLU:OE2 | 1:S:354:ALA:N | 2.39 | 0.53 |
| 1:S:584:THR:HG23 | 1:S:587:PHE:H | 1.73 | 0.53 |
| 1:S:2249:LEU:HD23 | 1:S:2383:GLU:CD | 2.34 | 0.53 |
| 1:S:2796:ARG:HG3 | 1:S:2801:ARG:HH21 | 1.74 | 0.53 |
| 1:T:452:LEU:HD23 | 1:T:554:PHE:CE1 | 2.43 | 0.53 |
| 1:T:1086:LYS:HZ3 | 1:T:1087:PRO:HD2 | 1.73 | 0.53 |
| 1:T:2164:GLN:NE2 | 1:T:2164:GLN:O | 2.41 | 0.53 |
| 1:A:229:LEU:HD11 | 1:A:297:TYR:HD1 | 1.73 | 0.53 |
| 1:A:915:ARG:NH1 | 1:A:1057:ASP:OD1 | 2.42 | 0.53 |
| 1:B:247:PHE:HB3 | 1:B:271:LYS:HD2 | 1.91 | 0.53 |
| 1:B:480:PRO:O | 1:B:485:ARG:NH1 | 2.42 | 0.53 |
| 1:B:2169:LEU:HB3 | 1:B:2174:SER:HB3 | 1.89 | 0.53 |
| 1:B:3232:LEU:HD23 | 1:B:3234:PRO:HD3 | 1.90 | 0.53 |
| 1:C:754:SER:OG | 1:C:762:SER:OG | 2.19 | 0.53 |
| 1:C:1189:GLU:N | 1:C:1189:GLU:OE1 | 2.42 | 0.53 |
| 1:C:1775:LEU:HD12 | 1:C:1779:PHE:HE1 | 1.73 | 0.53 |
| 1:C:2047:ASP:N | 1:D:1493:ARG:HH22 | 2.07 | 0.53 |
| 1:C:2095:GLU:HB3 | 1:C:2098:HIS:ND1 | 2.24 | 0.53 |
| 1:D:420:LYS:NZ | 1:D:422:SER:OG | 2.42 | 0.53 |
| 1:D:1726:ASN:OD1 | 1:D:1727:GLN:N | 2.42 | 0.53 |
| 1:D:2363:LEU:HB2 | 1:D:2365:PHE:HE1 | 1.74 | 0.53 |
| 1:E:674:LEU:HD22 | 1:E:695:ARG:NH2 | 2.24 | 0.53 |
| 1:E:2551:HIS:HB2 | 1:E:2581:PHE:CZ | 2.44 | 0.53 |
| 1:F:468:ALA:HB1 | 1:F:633:PHE:HA | 1.90 | 0.53 |
| 1:F:654:LEU:HD13 | 1:F:723:LEU:HD11 | 1.91 | 0.53 |
| 1:F:1087:PRO:HA | 1:F:1109:PRO:HD3 | 1.91 | 0.53 |
| 1:G:1721:PRO:HD3 | 1:G:1729:TYR:CZ | 2.43 | 0.53 |
| 1:G:2088:PRO:O | 1:G:2090:ASN:N | 2.37 | 0.53 |
| 1:G:2556:LEU:H | 1:G:2556:LEU:HD23 | 1.74 | 0.53 |
| 1:H:3106:LEU:HA | 1:H:3109:SER:HB3 | 1.89 | 0.53 |
| 1:I:5:ARG:HE | 1:I:90:GLY:HA3 | 1.73 | 0.53 |
| 1:I:454:ARG:NH2 | 1:I:514:ARG:O | 2.42 | 0.53 |
| 1:I:1835:LEU:HA | 1:I:1838:LEU:HD12 | 1.91 | 0.53 |
| 1:I:1910:ASN:ND2 | 1:J:1657:PHE:O | 2.42 | 0.53 |
| 1:I:2456:ARG:N | 1:I:2459:ASP:OD2 | 2.42 | 0.53 |
| 1:K:2556:LEU:H | 1:K:2556:LEU:HD23 | 1.74 | 0.53 |
| 1:M:613:PRO:HB2 | 1:M:640:HIS:NE2 | 2.23 | 0.53 |
| 1:M:2959:PHE:HE1 | 1:M:3162:LYS:HE2 | 1.74 | 0.53 |
| 1:M:3142:TYR:HE2 | 1:M:3144:ARG:HD3 | 1.73 | 0.53 |
| 1:M:3301:THR:HB | 1:M:3325:LYS:HB3 | 1.90 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:N:435:LYS:HG2 | 1:N:436:ASP:H | 1.72 | 0.53 |
| 1:N:658:ARG:HH12 | 1:N:727:ILE:HD11 | 1.73 | 0.53 |
| 1:N:2164:GLN:O | 1:N:2164:GLN:NE2 | 2.42 | 0.53 |
| 1:N:2313:GLN:HG2 | 1:N:2320:TYR:HB3 | 1.89 | 0.53 |
| 1:N:3071:THR:HB | 1:N:3072:LEU:HD12 | 1.90 | 0.53 |
| 1:O:2234:LYS:HG3 | 1:O:2243:VAL:HG11 | 1.90 | 0.53 |
| 1:O:3015:ARG:HG2 | 1:O:3016:PRO:HD2 | 1.90 | 0.53 |
| 1:P:169:LEU:HD12 | 1:P:177:PHE:HZ | 1.73 | 0.53 |
| 1:P:1023:ASN:HB3 | 1:P:1182:TYR:HD2 | 1.74 | 0.53 |
| 1:P:1150:PHE:HB3 | 1:P:1199:GLN:OE1 | 2.09 | 0.53 |
| 1:P:2666:ASP:OD1 | 1:P:2667:TYR:N | 2.42 | 0.53 |
| 1:P:2944:LEU:HD22 | 1:P:2999:LEU:HD23 | 1.90 | 0.53 |
| 1:Q:284:ASP:OD1 | 1:Q:285:ASP:N | 2.41 | 0.53 |
| 1:Q:1093:GLN:HB2 | 1:Q:1097:ILE:HG21 | 1.91 | 0.53 |
| 1:Q:2105:MET:HA | 1:Q:2108:LYS:HG2 | 1.91 | 0.53 |
| 1:Q:2577:TRP:NE1 | 1:Q:2745:GLU:O | 2.37 | 0.53 |
| 1:R:938:ASP:OD1 | 1:R:1055:ASN:ND2 | 2.39 | 0.53 |
| 1:R:1268:LEU:HD23 | 1:R:1268:LEU:H | 1.73 | 0.53 |
| 1:R:1775:LEU:HD12 | 1:R:1776:PRO:HD2 | 1.90 | 0.53 |
| 1:R:1785:ARG:NH1 | 1:R:1786:ASP:O | 2.41 | 0.53 |
| 1:R:2340:VAL:HA | 1:R:2349:ARG:NH1 | 2.24 | 0.53 |
| 1:R:2967:PRO:O | 1:R:2973:ARG:NH1 | 2.42 | 0.53 |
| 1:R:3026:SER:OG | 1:R:3030:ASN:ND2 | 2.38 | 0.53 |
| 1:R:3079:ASP:OD1 | 1:R:3260:ARG:NH1 | 2.41 | 0.53 |
| 1:S:1225:ASP:HB3 | 1:S:1231:ILE:HD11 | 1.90 | 0.53 |
| 1:S:1328:LEU:HD21 | 1:S:1519:VAL:HG22 | 1.91 | 0.53 |
| 1:T:662:TYR:HE2 | 1:T:700:TYR:HB3 | 1.74 | 0.53 |
| 1:T:739:GLY:HA3 | 1:T:784:LEU:HB3 | 1.91 | 0.53 |
| 1:T:795:LYS:HD3 | 1:T:796:LYS:HD3 | 1.91 | 0.53 |
| 1:A:752:ILE:O | 1:A:808:LEU:HA | 2.07 | 0.53 |
| 1:A:3052:LEU:O | 1:A:3055:ARG:NH2 | 2.41 | 0.53 |
| 1:B:60:VAL:HG23 | 1:B:63:MET:HE2 | 1.90 | 0.53 |
| 1:B:149:LEU:HD21 | 1:B:191:LEU:HB3 | 1.90 | 0.53 |
| 1:B:499:TRP:HB3 | 1:B:500:HIS:CD2 | 2.44 | 0.53 |
| 1:B:2681:ILE:HD12 | 1:B:2708:HIS:HE1 | 1.73 | 0.53 |
| 1:C:482:ALA:O | 1:C:485:ARG:NH2 | 2.40 | 0.53 |
| 1:D:461:VAL:HG12 | 1:D:1371:ARG:HB2 | 1.91 | 0.53 |
| 1:D:2602:ASP:HA | 1:D:2711:ASN:ND2 | 2.23 | 0.53 |
| 1:E:221:ARG:NH2 | 1:E:287:SER:O | 2.41 | 0.53 |
| 1:E:2315:ARG:HH21 | 1:E:2377:LEU:HD12 | 1.73 | 0.53 |
| 1:E:2780:ASN:OD1 | 1:E:2784:LEU:N | 2.41 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:F:869:LEU:HB3 | 1:F:928:LYS:HE3 | 1.90 | 0.53 |
| 1:F:1348:TYR:OH | 1:F:1466:ARG:NH1 | 2.42 | 0.53 |
| 1:F:1785:ARG:HH12 | 1:F:1790:ASP:HA | 1.73 | 0.53 |
| 1:F:3125:ILE:HA | 1:F:3128:ILE:HG12 | 1.90 | 0.53 |
| 1:G:460:SER:O | 1:G:1371:ARG:NH1 | 2.42 | 0.53 |
| 1:G:494:ALA:HA | 1:G:603:GLU:OE2 | 2.09 | 0.53 |
| 1:G:1189:GLU:N | 1:G:1189:GLU:OE1 | 2.42 | 0.53 |
| 1:G:1394:ARG:NE | 1:G:1456:LEU:HD11 | 2.24 | 0.53 |
| 1:G:2147:CYS:O | 1:G:2149:HIS:ND1 | 2.36 | 0.53 |
| 1:G:3329:LYS:HD2 | 1:H:3357:TYR:HB3 | 1.90 | 0.53 |
| 1:H:24:ARG:HD3 | 1:H:123:ASN:HA | 1.89 | 0.53 |
| 1:I:1307:HIS:HB3 | 1:I:1312:VAL:HG11 | 1.90 | 0.53 |
| 1:I:1715:ALA:HB1 | 1:I:1873:HIS:HA | 1.91 | 0.53 |
| 1:I:2602:ASP:OD1 | 1:I:2604:THR:HG22 | 2.09 | 0.53 |
| 1:J:48:CYS:H | 1:J:58:CYS:HB2 | 1.74 | 0.53 |
| 1:J:1011:PHE:HA | 1:J:1063:TRP:HH2 | 1.73 | 0.53 |
| 1:K:259:ASN:ND2 | 1:K:264:THR:OG1 | 2.41 | 0.53 |
| 1:K:514:ARG:HH12 | 1:K:1343:ALA:HA | 1.72 | 0.53 |
| 1:K:3086:MET:O | 1:K:3090:THR:HG23 | 2.09 | 0.53 |
| 1:L:1539:THR:HG22 | 1:L:1542:GLN:NE2 | 2.24 | 0.53 |
| 1:L:1847:GLU:O | 1:L:1851:GLU:HG2 | 2.09 | 0.53 |
| 1:L:2044:SER:N | 1:L:2047:ASP:OD2 | 2.41 | 0.53 |
| 1:L:2675:GLU:O | 1:L:2679:ASN:ND2 | 2.41 | 0.53 |
| 1:L:2714:ARG:O | 1:L:2718:ILE:HG12 | 2.09 | 0.53 |
| 1:M:69:TRP:CD1 | 1:M:251:LEU:HD12 | 2.42 | 0.53 |
| 1:M:755:ILE:HG23 | 1:M:765:VAL:HG21 | 1.88 | 0.53 |
| 1:M:2567:CYS:HA | 1:M:2577:TRP:CE2 | 2.44 | 0.53 |
| 1:N:848:ARG:HB3 | 1:N:933:GLY:HA3 | 1.91 | 0.53 |
| 1:N:2273:TYR:HB3 | 1:N:2426:PHE:CD1 | 2.44 | 0.53 |
| 1:O:1345:SER:OG | 1:O:1346:VAL:N | 2.42 | 0.53 |
| 1:O:2849:ARG:HA | 1:O:2849:ARG:HH11 | 1.73 | 0.53 |
| 1:P:1238:LYS:NZ | 1:P:1239:VAL:O | 2.42 | 0.53 |
| 1:P:3008:ILE:HD13 | 1:P:3116:MET:HB3 | 1.91 | 0.53 |
| 1:Q:71:ARG:HA | 1:Q:74:VAL:HG12 | 1.91 | 0.53 |
| 1:Q:735:ARG:HE | 1:Q:737:PHE:HZ | 1.55 | 0.53 |
| 1:Q:1244:ARG:HD3 | 1:Q:1245:PRO:HD2 | 1.91 | 0.53 |
| 1:Q:1932:ASP:OD2 | 1:Q:1934:ILE:HG22 | 2.09 | 0.53 |
| 1:Q:2740:LEU:HB3 | 1:Q:2764:VAL:HG22 | 1.91 | 0.53 |
| 1:R:958:PRO:HA | 1:R:961:ASN:HA | 1.91 | 0.53 |
| 1:R:2824:ALA:HB2 | 1:R:2869:VAL:HG23 | 1.90 | 0.53 |
| 1:S:44:GLU:N | 1:S:204:GLU:O | 2.37 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:S:1930:ASN:HB3 | 1:S:1936:LYS:HZ3 | 1.72 | 0.53 |
| 1:S:1978:LYS:HA | 1:S:2078:LYS:HG2 | 1.91 | 0.53 |
| 1:S:2962:ALA:HB2 | 1:S:3107:GLU:HG2 | 1.91 | 0.53 |
| 1:T:196:HIS:O | 1:T:199:SER:OG | 2.26 | 0.53 |
| 1:T:392:SER:OG | 1:T:394:ASN:OD1 | 2.23 | 0.53 |
| 1:T:461:VAL:HG12 | 1:T:1371:ARG:HB2 | 1.91 | 0.53 |
| 1:T:1221:TYR:OH | 1:T:1233:SER:O | 2.27 | 0.53 |
| 1:T:1492:MET:HB3 | 1:T:1517:ILE:HG23 | 1.89 | 0.53 |
| 1:T:1857:ILE:HD12 | 1:T:1884:HIS:CD2 | 2.44 | 0.53 |
| 1:T:2330:MET:HE1 | 1:T:2355:LYS:HD3 | 1.91 | 0.53 |
| 3:LA:1:NAG:H62 | 3:LA:2:NAG:HN2 | 1.73 | 0.53 |
| 1:A:171:GLU:OE2 | 1:A:173:ASP:N | 2.41 | 0.53 |
| 1:A:1195:ASP:OD1 | 1:A:1196:ARG:N | 2.42 | 0.53 |
| 1:A:1433:LEU:HD11 | 1:A:1460:HIS:CE1 | 2.43 | 0.53 |
| 1:A:2681:ILE:O | 1:A:2685:ILE:HG22 | 2.08 | 0.53 |
| 1:A:2805:ASN:HB3 | 1:A:2850:LEU:HD11 | 1.91 | 0.53 |
| 1:A:3227:THR:OG1 | 1:A:3245:PHE:O | 2.26 | 0.53 |
| 1:B:459:THR:OG1 | 1:B:1285:ARG:NH1 | 2.42 | 0.53 |
| 1:B:2579:ARG:NH2 | 1:B:2769:TYR:HB3 | 2.23 | 0.53 |
| 1:C:24:ARG:NH2 | 1:C:123:ASN:HA | 2.24 | 0.53 |
| 1:C:1026:HIS:HA | 1:C:1037:MET:HE2 | 1.91 | 0.53 |
| 1:C:1272:SER:OG | 1:C:1275:GLU:OE1 | 2.23 | 0.53 |
| 1:C:1508:ASP:CG | 1:C:1509:LEU:H | 2.17 | 0.53 |
| 1:C:2282:SER:H | 1:C:2285:SER:HB2 | 1.73 | 0.53 |
| 1:D:597:ARG:HH22 | 1:D:655:GLN:HA | 1.73 | 0.53 |
| 1:E:1466:ARG:NH2 | 1:E:1534:ASN:O | 2.42 | 0.53 |
| 1:E:1865:LYS:HB3 | 1:E:1868:SER:HB3 | 1.90 | 0.53 |
| 1:E:3212:ARG:NE | 1:E:3214:TYR:OH | 2.42 | 0.53 |
| 1:F:2235:LEU:HD12 | 1:F:2239:GLY:HA2 | 1.91 | 0.53 |
| 1:G:17:LEU:O | 1:G:20:GLU:HG3 | 2.08 | 0.53 |
| 1:G:595:GLU:O | 1:G:597:ARG:NE | 2.42 | 0.53 |
| 1:G:1587:ASN:OD1 | 1:G:1588:HIS:ND1 | 2.42 | 0.53 |
| 1:G:2215:GLY:N | 1:G:2224:THR:OG1 | 2.36 | 0.53 |
| 1:G:2414:GLN:HE21 | 1:G:2453:LEU:HD22 | 1.74 | 0.53 |
| 1:G:2602:ASP:HA | 1:G:2711:ASN:ND2 | 2.24 | 0.53 |
| 1:H:913:TRP:HD1 | 1:H:1088:LEU:HD12 | 1.74 | 0.53 |
| 1:H:1222:SER:HB3 | 1:H:1230:LYS:HZ1 | 1.72 | 0.53 |
| 1:H:1431:ASN:HB3 | 1:H:1596:LEU:HD22 | 1.90 | 0.53 |
| 1:H:1763:ILE:HD12 | 1:H:1764:PRO:HD2 | 1.90 | 0.53 |
| 1:H:2343:ASN:HB3 | 1:H:2349:ARG:NH2 | 2.24 | 0.53 |
| 1:I:854:LEU:HD12 | 1:I:858:GLN:HG3 | 1.89 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:I:1426:PHE:HE1 | 1:I:1464:VAL:HG13 | 1.74 | 0.53 |
| 1:I:2579:ARG:NE | 1:I:2774:TYR:HH | 2.04 | 0.53 |
| 1:J:2695:THR:OG1 | 1:J:2697:GLU:OE1 | 2.25 | 0.53 |
| 1:K:17:LEU:O | 1:K:20:GLU:HG3 | 2.09 | 0.53 |
| 1:K:170:GLU:HG3 | 1:K:304:ARG:HH11 | 1.74 | 0.53 |
| 1:K:1418:SER:OG | 1:K:1419:PHE:N | 2.42 | 0.53 |
| 1:K:3037:ILE:HG12 | 1:K:3039:PHE:H | 1.74 | 0.53 |
| 1:M:44:GLU:HG3 | 1:M:135:MET:HE1 | 1.91 | 0.53 |
| 1:M:2254:GLN:N | 1:M:2254:GLN:OE1 | 2.42 | 0.53 |
| 1:N:1599:GLU:OE2 | 1:N:1600:THR:OG1 | 2.27 | 0.53 |
| 1:N:1836:PHE:O | 1:N:1840:GLN:NE2 | 2.24 | 0.53 |
| 1:N:3102:SER:O | 1:N:3105:THR:OG1 | 2.25 | 0.53 |
| 1:O:937:TRP:CD1 | 1:O:938:ASP:H | 2.26 | 0.53 |
| 1:O:1890:ARG:NH2 | 1:O:1959:GLU:O | 2.42 | 0.53 |
| 1:O:2152:PRO:HA | 1:O:2261:GLU:HG3 | 1.90 | 0.53 |
| 1:O:2736:ASN:HD22 | 1:O:2738:GLN:HE22 | 1.56 | 0.53 |
| 1:O:3304:VAL:HG23 | 1:O:3317:ILE:HB | 1.91 | 0.53 |
| 1:P:284:ASP:OD1 | 1:P:285:ASP:N | 2.42 | 0.53 |
| 1:P:2450:LEU:HD12 | 1:P:2455:ILE:HB | 1.90 | 0.53 |
| 1:Q:1037:MET:HA | 1:Q:1043:THR:HA | 1.91 | 0.53 |
| 1:Q:1742:TRP:CD1 | 1:Q:1920:LEU:HD12 | 2.44 | 0.53 |
| 1:Q:2802:VAL:HG12 | 1:Q:2856:THR:HG22 | 1.89 | 0.53 |
| 1:Q:3226:ALA:HA | 1:Q:3289:LYS:HA | 1.89 | 0.53 |
| 1:R:998:ILE:HA | 1:R:1001:MET:HG3 | 1.90 | 0.53 |
| 1:R:1785:ARG:HH12 | 1:R:1790:ASP:HA | 1.74 | 0.53 |
| 1:S:2155:PRO:HB2 | 1:S:2159:ARG:NH2 | 2.24 | 0.53 |
| 1:S:2990:LEU:HA | 1:S:2993:VAL:HG12 | 1.89 | 0.53 |
| 1:T:2231:GLU:CD | 1:T:2231:GLU:H | 2.16 | 0.53 |
| 1:T:3114:PHE:HA | 1:T:3117:ILE:HG12 | 1.89 | 0.53 |
| 1:A:1572:GLN:HB2 | 1:A:1636:LYS:HB2 | 1.89 | 0.53 |
| 1:A:3011:TRP:CZ3 | 1:A:3013:TRP:HB3 | 2.44 | 0.53 |
| 1:A:3105:THR:O | 1:A:3109:SER:HB3 | 2.09 | 0.53 |
| 1:B:312:SER:HA | 1:B:365:TYR:O | 2.09 | 0.53 |
| 1:B:499:TRP:NE1 | 1:B:676:LYS:O | 2.42 | 0.53 |
| 1:B:3144:ARG:NH2 | 1:B:3407:ASP:OD1 | 2.42 | 0.53 |
| 1:B:3342:SER:OG | 1:B:3344:VAL:O | 2.26 | 0.53 |
| 1:C:559:VAL:N | 1:C:564:GLU:O | 2.29 | 0.53 |
| 1:C:2414:GLN:HE21 | 1:C:2453:LEU:HD22 | 1.74 | 0.53 |
| 1:D:98:LYS:HZ1 | 1:D:289:ASN:H | 1.57 | 0.53 |
| 1:D:454:ARG:HH21 | 1:D:1339:ALA:HA | 1.74 | 0.53 |
| 1:E:64:ALA:O | 1:E:174:TYR:OH | 2.27 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:F:1726:ASN:OD1 | 1:F:1727:GLN:N | 2.42 | 0.53 |
| 1:F:3079:ASP:O | 1:F:3083:GLN:NE2 | 2.38 | 0.53 |
| 1:G:699:ILE:HG13 | 1:G:706:LEU:HD21 | 1.91 | 0.53 |
| 1:G:2315:ARG:NH2 | 1:G:2381:GLU:OE2 | 2.41 | 0.53 |
| 1:G:2446:ILE:HD11 | 1:G:2491:ILE:HD11 | 1.90 | 0.53 |
| 1:H:312:SER:HA | 1:H:365:TYR:O | 2.09 | 0.53 |
| 1:H:378:LYS:NZ | 1:H:383:ASP:O | 2.40 | 0.53 |
| 1:H:1626:ASP:OD1 | 1:H:1627:SER:N | 2.41 | 0.53 |
| 1:H:2817:VAL:HG22 | 1:H:2876:ILE:HD12 | 1.91 | 0.53 |
| 1:I:650:ILE:HG22 | 1:I:713:LEU:HD12 | 1.91 | 0.53 |
| 1:J:474:PRO:HB2 | 1:J:476:ARG:HH12 | 1.74 | 0.53 |
| 1:J:1286:MET:HE1 | 1:J:1292:PHE:HB2 | 1.90 | 0.53 |
| 1:J:1706:GLY:O | 1:J:1710:LEU:HG | 2.08 | 0.53 |
| 1:J:2164:GLN:NE2 | 1:J:2164:GLN:O | 2.41 | 0.53 |
| 1:K:418:ASP:OD2 | 1:K:662:TYR:N | 2.42 | 0.53 |
| 1:K:460:SER:O | 1:K:1371:ARG:NH1 | 2.42 | 0.53 |
| 1:K:799:LYS:N | 1:K:802:ASP:OD2 | 2.41 | 0.53 |
| 1:K:855:THR:HG22 | 1:K:858:GLN:HE22 | 1.72 | 0.53 |
| 1:K:1144:GLN:HA | 1:K:1148:ARG:HH22 | 1.73 | 0.53 |
| 1:K:2393:VAL:HG13 | 1:K:2446:ILE:HG13 | 1.91 | 0.53 |
| 1:L:913:TRP:CD1 | 1:L:1088:LEU:HD12 | 2.44 | 0.53 |
| 1:L:1284:ARG:NH2 | 1:L:1379:PRO:HB3 | 2.23 | 0.53 |
| 1:L:2602:ASP:OD2 | 1:L:2604:THR:OG1 | 2.24 | 0.53 |
| 1:L:3018:LYS:HA | 1:L:3055:ARG:HH12 | 1.73 | 0.53 |
| 1:L:3229:ASN:H | 1:L:3286:THR:HG22 | 1.74 | 0.53 |
| 1:M:5:ARG:HE | 1:M:90:GLY:HA3 | 1.73 | 0.53 |
| 1:M:1122:HIS:ND1 | 1:M:1123:TYR:O | 2.42 | 0.53 |
| 1:M:1189:GLU:N | 1:M:1189:GLU:OE1 | 2.42 | 0.53 |
| 1:M:2805:ASN:ND2 | 1:M:2852:GLN:OE1 | 2.42 | 0.53 |
| 1:M:3074:GLU:OE1 | 1:M:3076:ASN:N | 2.38 | 0.53 |
| 1:M:3091:ILE:HA | 1:M:3094:LEU:HD12 | 1.90 | 0.53 |
| 1:N:159:THR:O | 1:N:162:PHE:N | 2.41 | 0.53 |
| 1:N:887:GLN:NE2 | 1:N:889:ASN:HB2 | 2.24 | 0.53 |
| 1:N:1785:ARG:HH12 | 1:N:1790:ASP:HA | 1.74 | 0.53 |
| 1:N:2652:SER:O | 1:N:2656:ARG:NH1 | 2.41 | 0.53 |
| 1:O:608:VAL:HG11 | 1:O:785:VAL:HG21 | 1.91 | 0.53 |
| 1:O:1684:THR:OG1 | 1:O:1687:GLU:OE1 | 2.21 | 0.53 |
| 1:O:3114:PHE:HA | 1:O:3117:ILE:HG12 | 1.89 | 0.53 |
| 1:P:60:VAL:HG23 | 1:P:63:MET:HE2 | 1.91 | 0.53 |
| 1:Q:399:ASN:HD21 | 1:Q:401:ASN:HD21 | 1.56 | 0.53 |
| 1:Q:482:ALA:O | 1:Q:485:ARG:NH2 | 2.41 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:Q:866:LEU:HD23 | 1:Q:967:PRO:HB2 | 1.91 | 0.53 |
| 1:Q:914:HIS:CE1 | 1:Q:1053:HIS:CE1 | 2.96 | 0.53 |
| 1:Q:1576:CYS:HA | 1:T:337:GLN:OE1 | 2.09 | 0.53 |
| 1:Q:2603:TRP:HD1 | 1:Q:2711:ASN:HD22 | 1.57 | 0.53 |
| 1:R:166:LEU:HA | 1:R:169:LEU:HG | 1.91 | 0.53 |
| 1:R:1896:GLN:NE2 | 1:R:1906:PRO:O | 2.41 | 0.53 |
| 1:S:1081:ILE:HD13 | 1:T:2460:VAL:HG12 | 1.91 | 0.53 |
| 1:S:1153:PHE:HE2 | 1:S:1166:LEU:HD21 | 1.74 | 0.53 |
| 1:S:1572:GLN:HB2 | 1:S:1636:LYS:HB2 | 1.89 | 0.53 |
| 1:S:3157:PHE:HD2 | 1:S:3168:THR:HB | 1.74 | 0.53 |
| 1:T:996:THR:HG23 | 1:T:999:ALA:H | 1.72 | 0.53 |
| 1:T:1568:SER:OG | 1:T:1597:GLY:O | 2.26 | 0.53 |
| 1:T:3102:SER:HG | 1:T:3104:SER:HG | 1.57 | 0.53 |
| 1:A:2286:LEU:HD12 | 1:A:2429:GLY:HA2 | 1.90 | 0.53 |
| 1:B:680:PHE:O | 1:B:685:ASN:ND2 | 2.39 | 0.53 |
| 1:C:484:VAL:O | 1:C:485:ARG:NH1 | 2.42 | 0.53 |
| 1:C:1544:GLU:OE1 | 1:C:1544:GLU:N | 2.33 | 0.53 |
| 1:D:142:ALA:HB3 | 1:D:196:HIS:CE1 | 2.44 | 0.53 |
| 1:D:737:PHE:HB2 | 1:D:829:ILE:HB | 1.89 | 0.53 |
| 1:D:1960:LEU:N | 1:D:1963:ILE:O | 2.40 | 0.53 |
| 1:E:714:GLN:OE1 | 1:E:718:MET:N | 2.34 | 0.53 |
| 1:E:1225:ASP:HB3 | 1:E:1231:ILE:HD11 | 1.91 | 0.53 |
| 1:E:1317:HIS:HA | 1:E:1322:PHE:HD1 | 1.73 | 0.53 |
| 1:E:1495:PRO:HA | 1:E:1516:PRO:HD3 | 1.91 | 0.53 |
| 1:E:1509:LEU:HD23 | 1:E:1526:PHE:HD1 | 1.74 | 0.53 |
| 1:E:2078:LYS:HB3 | 1:E:2080:ARG:HH22 | 1.74 | 0.53 |
| 1:F:1008:GLN:OE1 | 1:F:1008:GLN:N | 2.37 | 0.53 |
| 1:F:2377:LEU:HA | 1:F:2380:LEU:HD12 | 1.90 | 0.53 |
| 1:G:1638:ARG:HD2 | 1:G:1644:TYR:HE1 | 1.74 | 0.53 |
| 1:G:2661:ALA:O | 1:G:2664:GLN:NE2 | 2.42 | 0.53 |
| 1:H:1284:ARG:HH12 | 1:H:1379:PRO:HB3 | 1.74 | 0.53 |
| 1:I:306:ARG:O | 1:I:411:ARG:NH2 | 2.42 | 0.53 |
| 1:I:984:ASP:OD1 | 1:I:984:ASP:N | 2.41 | 0.53 |
| 1:I:1551:ARG:HG3 | 1:I:1661:GLU:HG3 | 1.91 | 0.53 |
| 1:I:1896:GLN:NE2 | 1:I:1906:PRO:O | 2.28 | 0.53 |
| 1:I:2056:ARG:NH1 | 1:I:2061:SER:O | 2.41 | 0.53 |
| 1:I:2723:GLN:HE22 | 1:I:2728:LEU:HD23 | 1.73 | 0.53 |
| 1:I:2797:ARG:HA | 1:I:2801:ARG:HH22 | 1.74 | 0.53 |
| 1:I:2959:PHE:HE1 | 1:I:3162:LYS:HE2 | 1.74 | 0.53 |
| 1:J:1169:CYS:HA | 1:J:1175:CYS:HA | 1.91 | 0.53 |
| 1:J:1827:ASP:O | 1:J:1832:LYS:NZ | 2.41 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:J:2313:GLN:NE2 | 1:J:2320:TYR:HB3 | 2.23 | 0.53 |
| 1:K:1324:HIS:HD2 | 1:K:1519:VAL:HB | 1.74 | 0.53 |
| 1:K:3213:VAL:HG23 | 1:K:3306:SER:HB2 | 1.90 | 0.53 |
| 1:L:74:VAL:HA | 1:L:77:LEU:HD23 | 1.91 | 0.53 |
| 1:L:1539:THR:H | 1:L:1542:GLN:NE2 | 2.07 | 0.53 |
| 1:L:1763:ILE:HD12 | 1:L:1764:PRO:HD2 | 1.89 | 0.53 |
| 1:L:3119:HIS:O | 1:L:3122:ILE:HG22 | 2.09 | 0.53 |
| 1:M:181:PHE:HE2 | 1:M:219:VAL:HG13 | 1.74 | 0.53 |
| 1:M:736:THR:N | 1:M:790:THR:OG1 | 2.40 | 0.53 |
| 1:M:1560:PHE:HZ | 1:M:1573:LEU:HD21 | 1.73 | 0.53 |
| 1:M:1578:ALA:HA | 1:M:1584:ARG:HD3 | 1.91 | 0.53 |
| 1:N:1012:CYS:SG | 1:N:1196:ARG:NH1 | 2.75 | 0.53 |
| 1:N:2923:ARG:HE | 1:N:2924:TYR:H | 1.57 | 0.53 |
| 1:N:2948:ASP:N | 1:N:2948:ASP:OD1 | 2.42 | 0.53 |
| 1:O:126:PHE:O | 1:O:143:ARG:NH1 | 2.39 | 0.53 |
| 1:O:1684:THR:N | 1:O:1687:GLU:OE2 | 2.33 | 0.53 |
| 1:O:2621:PRO:HA | 1:O:2624:HIS:CE1 | 2.44 | 0.53 |
| 1:O:3087:LEU:O | 1:O:3090:THR:OG1 | 2.27 | 0.53 |
| 1:P:3203:ILE:HG22 | 1:P:3207:LEU:HD23 | 1.90 | 0.53 |
| 1:Q:972:LEU:HA | 1:Q:977:LYS:HA | 1.90 | 0.53 |
| 1:Q:1312:VAL:HG22 | 1:Q:1313:ALA:H | 1.73 | 0.53 |
| 1:Q:1782:PRO:O | 1:Q:1795:ASN:N | 2.38 | 0.53 |
| 1:Q:2959:PHE:HE1 | 1:Q:3162:LYS:HE2 | 1.74 | 0.53 |
| 1:R:936:TYR:OH | 1:R:1124:ASP:OD1 | 2.25 | 0.53 |
| 1:R:1433:LEU:O | 1:R:1437:VAL:HG22 | 2.09 | 0.53 |
| 1:R:2580:LEU:HA | 1:R:2583:VAL:HG12 | 1.91 | 0.53 |
| 1:R:3211:ASP:OD1 | 1:R:3309:ALA:N | 2.42 | 0.53 |
| 1:S:3118:HIS:O | 1:S:3122:ILE:HG12 | 2.09 | 0.53 |
| 1:S:3268:ASP:N | 1:S:3268:ASP:OD1 | 2.42 | 0.53 |
| 1:T:1284:ARG:HH22 | 1:T:1379:PRO:HB3 | 1.73 | 0.53 |
| 1:T:2967:PRO:O | 1:T:2973:ARG:NH1 | 2.42 | 0.53 |
| 1:A:409:VAL:HG13 | 1:A:666:CYS:HA | 1.89 | 0.52 |
| 1:B:625:LEU:HA | 1:B:631:SER:HB2 | 1.90 | 0.52 |
| 1:B:1809:VAL:HG22 | 1:B:1811:ARG:HH12 | 1.74 | 0.52 |
| 1:B:2433:GLU:N | 1:B:2433:GLU:OE1 | 2.41 | 0.52 |
| 1:C:699:ILE:HG13 | 1:C:706:LEU:HD21 | 1.91 | 0.52 |
| 1:C:1328:LEU:HB3 | 1:C:1499:PHE:HE2 | 1.72 | 0.52 |
| 1:C:2183:TRP:O | 1:C:2242:SER:OG | 2.22 | 0.52 |
| 1:D:461:VAL:HG22 | 1:D:1277:GLU:OE2 | 2.10 | 0.52 |
| 1:D:1965:ALA:HA | 1:D:1968:LEU:HB2 | 1.92 | 0.52 |
| 1:D:2526:GLU:HA | 1:D:2529:LYS:HG2 | 1.91 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:F:374:GLU:OE1 | 1:F:374:GLU:N | 2.33 | 0.52 |
| 1:F:1001:MET:HA | 1:F:1004:LEU:HD23 | 1.91 | 0.52 |
| 1:H:185:HIS:O | 1:H:188:ILE:HG22 | 2.09 | 0.52 |
| 1:H:672:HIS:O | 1:H:695:ARG:NH1 | 2.42 | 0.52 |
| 1:H:2340:VAL:HA | 1:H:2349:ARG:HH11 | 1.73 | 0.52 |
| 1:H:2522:VAL:O | 1:H:2526:GLU:HG2 | 2.09 | 0.52 |
| 1:H:3079:ASP:OD1 | 1:H:3260:ARG:NH1 | 2.42 | 0.52 |
| 1:I:2919:LYS:O | 1:I:2919:LYS:HD2 | 2.09 | 0.52 |
| 1:I:2956:ILE:HD12 | 1:I:2959:PHE:HE2 | 1.73 | 0.52 |
| 1:J:928:LYS:HG3 | 1:J:929:GLY:H | 1.74 | 0.52 |
| 1:J:950:VAL:HA | 1:J:968:PHE:HB3 | 1.90 | 0.52 |
| 1:J:2263:GLN:HE22 | 1:J:2443:LYS:H | 1.56 | 0.52 |
| 1:J:2812:LYS:HG2 | 1:J:2840:PRO:HA | 1.90 | 0.52 |
| 1:K:24:ARG:NH2 | 1:K:123:ASN:HA | 2.24 | 0.52 |
| 1:K:957:ASN:HD21 | 1:K:959:GLU:HB3 | 1.74 | 0.52 |
| 1:K:2191:PRO:O | 1:K:2195:THR:HG23 | 2.09 | 0.52 |
| 1:K:2439:ASP:N | 1:K:2439:ASP:OD1 | 2.40 | 0.52 |
| 1:K:2864:LEU:HD11 | 1:K:2870:TYR:HB3 | 1.91 | 0.52 |
| 1:K:3125:ILE:HA | 1:K:3128:ILE:HG12 | 1.91 | 0.52 |
| 1:L:674:LEU:HD12 | 1:L:695:ARG:NH2 | 2.24 | 0.52 |
| 1:M:1007:GLU:OE1 | 1:M:1007:GLU:N | 2.31 | 0.52 |
| 1:M:1008:GLN:N | 1:M:1008:GLN:OE1 | 2.39 | 0.52 |
| 1:M:1407:LEU:O | 1:M:1411:LEU:HD23 | 2.09 | 0.52 |
| 1:M:1812:ASP:HB3 | 1:M:1863:GLY:HA3 | 1.90 | 0.52 |
| 1:O:114:ASP:OD2 | 1:O:117:GLY:N | 2.40 | 0.52 |
| 1:P:245:GLU:HA | 1:P:248:ARG:HD2 | 1.91 | 0.52 |
| 1:P:845:LEU:O | 1:P:926:ARG:NH1 | 2.42 | 0.52 |
| 1:P:1884:HIS:O | 1:P:1887:SER:OG | 2.24 | 0.52 |
| 1:Q:782:ASP:OD1 | 1:Q:783:ARG:N | 2.43 | 0.52 |
| 1:Q:1284:ARG:NH2 | 1:Q:1377:SER:O | 2.42 | 0.52 |
| 1:Q:3231:LYS:HB2 | 1:Q:3284:GLN:HE21 | 1.74 | 0.52 |
| 1:R:313:PHE:HB3 | 1:R:315:LEU:HD23 | 1.91 | 0.52 |
| 1:R:1111:GLU:N | 1:R:1111:GLU:OE1 | 2.41 | 0.52 |
| 1:R:1718:PRO:HG2 | 1:R:1728:ARG:HB3 | 1.89 | 0.52 |
| 1:R:1926:GLY:HA2 | 1:R:1936:LYS:HE2 | 1.90 | 0.52 |
| 1:R:2164:GLN:O | 1:R:2164:GLN:NE2 | 2.42 | 0.52 |
| 1:R:2371:LYS:HD3 | 1:R:2376:ASN:HA | 1.91 | 0.52 |
| 1:S:2095:GLU:OE2 | 1:S:2097:SER:OG | 2.19 | 0.52 |
| 1:S:2857:SER:O | 1:S:2861:GLN:HG3 | 2.09 | 0.52 |
| 1:A:731:ARG:HH12 | 1:A:737:PHE:HZ | 1.57 | 0.52 |
| 1:A:1585:ASN:OD1 | 1:A:1586:CYS:N | 2.40 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:2328:ASN:HD21 | 1:B:1240:THR:HA | 1.75 | 0.52 |
| 1:A:3200:ILE:HA | 1:A:3203:ILE:HG22 | 1.90 | 0.52 |
| 1:B:228:GLU:HA | 1:B:231:LYS:HG3 | 1.90 | 0.52 |
| 1:B:1100:ASP:O | 1:B:1104:ARG:NH1 | 2.42 | 0.52 |
| 1:B:1978:LYS:NZ | 1:B:1979:SER:O | 2.41 | 0.52 |
| 1:C:1677:ARG:C | 1:C:1678:LYS:HD3 | 2.35 | 0.52 |
| 1:C:1732:CYS:C | 1:C:1734:HIS:HD1 | 2.16 | 0.52 |
| 1:C:1839:GLU:HA | 1:C:1902:ARG:HH22 | 1.73 | 0.52 |
| 1:D:169:LEU:HA | 1:D:177:PHE:HE1 | 1.74 | 0.52 |
| 1:D:524:ASP:OD2 | 1:D:526:THR:OG1 | 2.23 | 0.52 |
| 1:D:848:ARG:HB2 | 1:D:1123:TYR:HD2 | 1.74 | 0.52 |
| 1:E:24:ARG:NH2 | 1:E:123:ASN:HA | 2.24 | 0.52 |
| 1:F:996:THR:HG23 | 1:F:999:ALA:H | 1.74 | 0.52 |
| 1:F:2217:ILE:HG22 | 1:F:2220:SER:H | 1.74 | 0.52 |
| 1:G:255:ASP:OD1 | 1:G:255:ASP:N | 2.41 | 0.52 |
| 1:G:972:LEU:HD23 | 1:G:977:LYS:HB3 | 1.90 | 0.52 |
| 1:G:2059:ASN:OD1 | 1:G:2061:SER:N | 2.43 | 0.52 |
| 1:G:2109:ALA:HA | 1:G:2112:ARG:NH2 | 2.24 | 0.52 |
| 1:G:2553:TYR:H | 1:G:2697:GLU:HB3 | 1.73 | 0.52 |
| 1:G:3263:LYS:HD2 | 1:G:3305:ILE:HD11 | 1.91 | 0.52 |
| 1:H:2413:CYS:SG | 1:H:2470:ARG:NE | 2.82 | 0.52 |
| 1:H:3164:PRO:HA | 1:H:3169:ARG:HH21 | 1.74 | 0.52 |
| 1:I:1407:LEU:O | 1:I:1411:LEU:HD23 | 2.09 | 0.52 |
| 1:I:1535:PHE:N | 1:I:1538:TRP:O | 2.40 | 0.52 |
| 1:I:2974:TYR:HB3 | 1:J:3367:PRO:HB2 | 1.91 | 0.52 |
| 1:J:881:ILE:HD12 | 1:J:920:GLN:HE22 | 1.74 | 0.52 |
| 1:J:1349:TRP:O | 1:J:1463:ASN:ND2 | 2.36 | 0.52 |
| 1:J:2109:ALA:HA | 1:J:2112:ARG:HG2 | 1.92 | 0.52 |
| 1:J:2338:ASN:OD1 | 1:J:2339:SER:N | 2.42 | 0.52 |
| 1:J:2997:MET:HA | 1:J:2997:MET:HE3 | 1.90 | 0.52 |
| 1:J:3058:GLN:NE2 | 1:J:3268:ASP:OD2 | 2.43 | 0.52 |
| 1:L:38:LEU:HG | 1:L:73:TYR:CZ | 2.44 | 0.52 |
| 1:L:925:LEU:HD22 | 1:L:928:LYS:HZ3 | 1.74 | 0.52 |
| 1:L:1289:ASP:OD2 | 1:L:1340:ARG:NH2 | 2.43 | 0.52 |
| 1:L:1676:ILE:HG13 | 1:L:1761:VAL:HG23 | 1.91 | 0.52 |
| 1:L:2264:PHE:HZ | 1:L:2302:VAL:HG13 | 1.73 | 0.52 |
| 1:L:3402:VAL:HG13 | 1:L:3404:ILE:HD11 | 1.90 | 0.52 |
| 1:M:586:LEU:HD12 | 1:M:586:LEU:H | 1.74 | 0.52 |
| 1:M:1032:ASN:HA | 1:M:1226:LEU:HD12 | 1.91 | 0.52 |
| 1:M:3037:ILE:HD11 | 1:M:3039:PHE:HB2 | 1.92 | 0.52 |
| 1:N:474:PRO:HB2 | 1:N:476:ARG:NH1 | 2.24 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:N:1698:LEU:HD21 | 1:N:1757:ARG:HG3 | 1.90 | 0.52 |
| 1:N:2253:GLU:OE2 | 1:N:2388:GLN:NE2 | 2.42 | 0.52 |
| 1:N:3287:LEU:HD21 | 1:N:3299:LEU:HD21 | 1.92 | 0.52 |
| 1:O:2331:SER:HA | 1:O:2355:LYS:HZ1 | 1.74 | 0.52 |
| 1:O:2383:GLU:O | 1:O:2387:HIS:ND1 | 2.38 | 0.52 |
| 1:O:2820:ASP:OD1 | 1:O:2831:ALA:N | 2.38 | 0.52 |
| 1:P:38:LEU:O | 1:P:73:TYR:OH | 2.27 | 0.52 |
| 1:P:1056:THR:HA | 1:P:1059:ILE:HD12 | 1.91 | 0.52 |
| 1:P:1539:THR:HG22 | 1:P:1542:GLN:NE2 | 2.24 | 0.52 |
| 1:P:1706:GLY:O | 1:P:1710:LEU:HG | 2.08 | 0.52 |
| 1:P:2757:ILE:O | 1:P:2761:ALA:HB2 | 2.09 | 0.52 |
| 1:Q:231:LYS:HD3 | 1:Q:237:TYR:HE1 | 1.74 | 0.52 |
| 1:Q:1684:THR:OG1 | 1:Q:1687:GLU:OE1 | 2.21 | 0.52 |
| 1:Q:2201:ASP:OD1 | 1:Q:2203:TRP:N | 2.37 | 0.52 |
| 1:Q:2641:GLN:NE2 | 1:Q:2645:ASP:OD1 | 2.34 | 0.52 |
| 1:Q:3089:ASN:ND2 | 1:Q:3247:ILE:HD12 | 2.24 | 0.52 |
| 1:R:552:ASN:HD21 | 1:R:554:PHE:HB2 | 1.74 | 0.52 |
| 1:R:581:GLY:N | 1:R:856:ARG:HH22 | 2.02 | 0.52 |
| 1:R:1011:PHE:HA | 1:R:1063:TRP:HH2 | 1.72 | 0.52 |
| 1:R:1745:LEU:HD23 | 1:R:1923:PHE:HD2 | 1.75 | 0.52 |
| 1:R:1881:PHE:O | 1:R:1885:HIS:ND1 | 2.38 | 0.52 |
| 1:S:1189:GLU:N | 1:S:1189:GLU:OE1 | 2.42 | 0.52 |
| 1:S:1684:THR:N | 1:S:1687:GLU:OE2 | 2.39 | 0.52 |
| 1:S:2664:GLN:OE1 | 1:S:2664:GLN:N | 2.39 | 0.52 |
| 1:S:2929:LEU:HD22 | 1:S:2933:GLN:HG3 | 1.90 | 0.52 |
| 1:S:3086:MET:O | 1:S:3090:THR:HG23 | 2.10 | 0.52 |
| 1:S:3317:ILE:HA | 1:S:3339:ARG:O | 2.08 | 0.52 |
| 1:T:130:ILE:O | 1:T:138:HIS:HA | 2.09 | 0.52 |
| 1:T:259:ASN:O | 1:T:265:ARG:NH2 | 2.41 | 0.52 |
| 1:T:980:ARG:NH2 | 1:T:1046:ASP:OD1 | 2.39 | 0.52 |
| 1:T:1364:GLU:OE2 | 1:T:1365:ALA:N | 2.41 | 0.52 |
| 1:T:1847:GLU:CD | 1:T:1847:GLU:H | 2.17 | 0.52 |
| 1:T:2671:GLU:OE1 | 1:T:2671:GLU:N | 2.30 | 0.52 |
| 1:T:3352:LYS:HG2 | 1:T:3365:ILE:HG23 | 1.90 | 0.52 |
| 1:A:913:TRP:HD1 | 1:A:1088:LEU:HD23 | 1.73 | 0.52 |
| 1:A:1434:HIS:NE2 | 1:A:1460:HIS:HD2 | 2.07 | 0.52 |
| 1:A:1865:LYS:HZ2 | 1:A:1867:HIS:H | 1.56 | 0.52 |
| 1:A:2331:SER:HA | 1:A:2355:LYS:HZ1 | 1.73 | 0.52 |
| 1:B:1305:CYS:SG | 1:B:1314:CYS:N | 2.82 | 0.52 |
| 1:B:1959:GLU:OE1 | 1:B:1962:GLY:N | 2.41 | 0.52 |
| 1:B:2985:PRO:HB2 | 1:B:2989:ARG:NH2 | 2.23 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:3122:ILE:HA | 1:B:3125:ILE:HG12 | 1.90 | 0.52 |
| 1:C:5:ARG:HD2 | 1:C:91:VAL:O | 2.08 | 0.52 |
| 1:C:849:SER:OG | 1:C:850:ASP:N | 2.42 | 0.52 |
| 1:C:1312:VAL:HG22 | 1:C:1313:ALA:H | 1.75 | 0.52 |
| 1:C:2566:CYS:O | 1:C:2577:TRP:NE1 | 2.42 | 0.52 |
| 1:C:2980:GLY:HA2 | 1:C:3258:TYR:HE2 | 1.74 | 0.52 |
| 1:D:997:LYS:HG3 | 1:D:998:ILE:HD12 | 1.92 | 0.52 |
| 1:D:2287:HIS:HE1 | 1:D:2432:LEU:HB2 | 1.74 | 0.52 |
| 1:D:3142:TYR:CE2 | 1:D:3144:ARG:HB2 | 2.45 | 0.52 |
| 1:E:539:GLU:N | 1:E:539:GLU:OE1 | 2.43 | 0.52 |
| 1:E:1730:ALA:N | 1:E:2020:ALA:O | 2.40 | 0.52 |
| 1:E:1828:ASN:OD1 | 1:E:1829:TRP:N | 2.42 | 0.52 |
| 1:F:581:GLY:H | 1:F:856:ARG:NH2 | 2.06 | 0.52 |
| 1:F:924:ALA:O | 1:F:928:LYS:HG2 | 2.09 | 0.52 |
| 1:F:956:VAL:HA | 1:F:963:PRO:HA | 1.91 | 0.52 |
| 1:F:1995:HIS:ND1 | 1:F:2013:PHE:O | 2.42 | 0.52 |
| 1:F:2433:GLU:N | 1:F:2433:GLU:OE1 | 2.41 | 0.52 |
| 1:F:2578:HIS:HB3 | 1:F:2709:HIS:HD2 | 1.74 | 0.52 |
| 1:G:1091:PHE:O | 1:G:1107:SER:OG | 2.27 | 0.52 |
| 1:G:3021:PRO:HD2 | 1:G:3024:LEU:HD21 | 1.91 | 0.52 |
| 1:H:458:ASP:HB2 | 1:H:1341:GLY:HA3 | 1.91 | 0.52 |
| 1:H:468:ALA:HB1 | 1:H:633:PHE:HA | 1.91 | 0.52 |
| 1:H:956:VAL:HA | 1:H:963:PRO:HA | 1.91 | 0.52 |
| 1:I:986:LEU:HD12 | 1:I:1028:LEU:HG | 1.91 | 0.52 |
| 1:I:2155:PRO:HB2 | 1:I:2306:TRP:CZ3 | 2.44 | 0.52 |
| 1:I:2981:MET:HG3 | 1:I:2983:VAL:HG22 | 1.92 | 0.52 |
| 1:J:378:LYS:NZ | 1:J:383:ASP:H | 2.08 | 0.52 |
| 1:J:379:LYS:HD3 | 1:J:381:ASN:H | 1.74 | 0.52 |
| 1:J:499:TRP:NE1 | 1:J:676:LYS:O | 2.40 | 0.52 |
| 1:J:635:PRO:O | 1:J:638:ILE:HG22 | 2.09 | 0.52 |
| 1:J:2481:LEU:HD21 | 3:GA:1:NAG:H62 | 1.91 | 0.52 |
| 1:K:5:ARG:HD2 | 1:K:283:TYR:HE1 | 1.74 | 0.52 |
| 1:M:24:ARG:NH2 | 1:M:123:ASN:HA | 2.24 | 0.52 |
| 1:M:1091:PHE:O | 1:M:1107:SER:OG | 2.27 | 0.52 |
| 1:M:1223:VAL:HG13 | 1:M:1231:ILE:HB | 1.91 | 0.52 |
| 1:M:2370:MET:SD | 1:M:2370:MET:N | 2.82 | 0.52 |
| 1:M:2962:ALA:HB2 | 1:M:3107:GLU:HG2 | 1.91 | 0.52 |
| 1:M:3339:ARG:NH2 | 1:M:3376:ASP:O | 2.42 | 0.52 |
| 1:N:2552:GLY:HA3 | 1:N:2697:GLU:HA | 1.90 | 0.52 |
| 1:N:2964:LYS:HG2 | 1:N:2973:ARG:HB2 | 1.91 | 0.52 |
| 1:N:3270:LEU:HD22 | 1:N:3275:LEU:HB2 | 1.92 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:O:1163:LEU:HG | 1:O:1182:TYR:HD1 | 1.74 | 0.52 |
| 1:O:1195:ASP:OD1 | 1:O:1196:ARG:N | 2.42 | 0.52 |
| 1:O:1978:LYS:HA | 1:O:2078:LYS:HG2 | 1.91 | 0.52 |
| 1:O:2000:VAL:O | 1:O:2041:LYS:NZ | 2.40 | 0.52 |
| 1:O:2780:ASN:OD1 | 1:O:2784:LEU:N | 2.43 | 0.52 |
| 1:P:2626:GLU:OE1 | 1:P:2633:LYS:NZ | 2.33 | 0.52 |
| 1:Q:17:LEU:O | 1:Q:20:GLU:HG3 | 2.08 | 0.52 |
| 1:Q:646:ARG:HA | 1:Q:710:TYR:HE2 | 1.74 | 0.52 |
| 1:Q:855:THR:HG23 | 1:Q:857:GLU:OE1 | 2.10 | 0.52 |
| 1:Q:953:GLU:HG3 | 1:Q:954:THR:HG23 | 1.90 | 0.52 |
| 1:Q:1404:ASP:O | 1:Q:1408:ASN:ND2 | 2.42 | 0.52 |
| 1:R:501:ARG:NE | 1:R:645:ASP:OD1 | 2.40 | 0.52 |
| 1:R:913:TRP:CD1 | 1:R:1088:LEU:HD12 | 2.44 | 0.52 |
| 1:R:1507:PHE:CE2 | 1:R:1509:LEU:HB3 | 2.45 | 0.52 |
| 1:T:655:GLN:HG2 | 1:T:662:TYR:HB3 | 1.90 | 0.52 |
| 1:T:1063:TRP:NE1 | 1:T:1067:GLN:HE22 | 2.07 | 0.52 |
| 1:T:1286:MET:O | 1:T:1291:THR:OG1 | 2.27 | 0.52 |
| 1:T:3106:LEU:HA | 1:T:3109:SER:HB3 | 1.91 | 0.52 |
| 1:T:3395:ARG:NE | 1:T:3398:GLN:OE1 | 2.43 | 0.52 |
| 1:A:1723:PRO:O | 1:A:1728:ARG:NH1 | 2.42 | 0.52 |
| 1:A:1914:GLU:CD | 1:A:1914:GLU:H | 2.18 | 0.52 |
| 1:A:2085:GLN:CD | 1:A:2087:LEU:H | 2.18 | 0.52 |
| 1:B:920:GLN:HB3 | 1:B:1103:THR:HG21 | 1.92 | 0.52 |
| 1:B:2217:ILE:HG22 | 1:B:2220:SER:H | 1.75 | 0.52 |
| 1:B:2487:SER:OG | 1:B:2488:LYS:N | 2.43 | 0.52 |
| 1:B:2729:ASP:OD2 | 1:B:2732:SER:OG | 2.26 | 0.52 |
| 1:B:2876:ILE:HB | 1:B:2884:LEU:HB2 | 1.91 | 0.52 |
| 1:C:81:LEU:HD21 | 1:C:86:LEU:HD23 | 1.92 | 0.52 |
| 1:D:913:TRP:CD1 | 1:D:1088:LEU:HD12 | 2.44 | 0.52 |
| 1:D:1898:LEU:HD21 | 1:D:1965:ALA:HB1 | 1.91 | 0.52 |
| 1:D:3350:ASN:OD1 | 1:D:3351:VAL:N | 2.42 | 0.52 |
| 1:E:418:ASP:OD2 | 1:E:662:TYR:N | 2.42 | 0.52 |
| 1:E:1025:ILE:HG21 | 1:E:1052:HIS:CE1 | 2.44 | 0.52 |
| 1:E:1201:GLU:OE2 | 1:E:1203:THR:N | 2.39 | 0.52 |
| 1:E:1802:ILE:HD12 | 1:E:1805:GLU:HB2 | 1.92 | 0.52 |
| 1:E:2156:HIS:CD2 | 1:E:2159:ARG:HH21 | 2.27 | 0.52 |
| 1:E:3151:TYR:O | 1:E:3173:ARG:NH2 | 2.42 | 0.52 |
| 1:E:3395:ARG:NE | 1:E:3398:GLN:OE1 | 2.43 | 0.52 |
| 1:F:1277:GLU:HA | 1:F:1280:LYS:HG2 | 1.91 | 0.52 |
| 1:F:1538:TRP:CD1 | 1:F:1542:GLN:HG3 | 2.44 | 0.52 |
| 1:F:1990:ILE:O | 1:F:1991:LYS:HG2 | 2.10 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:F:3110:ALA:HA | 1:F:3115:PHE:CD2 | 2.44 | 0.52 |
| 1:G:310:LEU:HD23 | 1:G:366:HIS:HB3 | 1.90 | 0.52 |
| 1:G:913:TRP:HD1 | 1:G:1088:LEU:HD23 | 1.74 | 0.52 |
| 1:G:1881:PHE:HE2 | 1:G:1885:HIS:CE1 | 2.27 | 0.52 |
| 1:G:2387:HIS:O | 1:G:2392:ARG:NH1 | 2.42 | 0.52 |
| 1:G:3086:MET:O | 1:G:3090:THR:HG23 | 2.09 | 0.52 |
| 1:G:3227:THR:OG1 | 1:G:3245:PHE:O | 2.23 | 0.52 |
| 1:H:1324:HIS:HB3 | 1:H:1519:VAL:HG21 | 1.92 | 0.52 |
| 1:H:1514:SER:OG | 1:H:1515:ARG:NH2 | 2.41 | 0.52 |
| 1:H:3350:ASN:OD1 | 1:H:3351:VAL:N | 2.43 | 0.52 |
| 1:I:501:ARG:NH1 | 1:I:702:TYR:HB3 | 2.24 | 0.52 |
| 1:I:2580:LEU:HA | 1:I:2583:VAL:HG12 | 1.92 | 0.52 |
| 1:I:3015:ARG:HH22 | 1:I:3192:LEU:HA | 1.74 | 0.52 |
| 1:J:103:LEU:HD12 | 1:J:104:PRO:HD2 | 1.91 | 0.52 |
| 1:J:848:ARG:HB3 | 1:J:934:LEU:O | 2.10 | 0.52 |
| 1:J:1294:LYS:O | 1:J:1297:SER:OG | 2.22 | 0.52 |
| 1:K:1872:LEU:HD21 | 1:K:2016:LEU:HD13 | 1.92 | 0.52 |
| 1:M:64:ALA:O | 1:M:174:TYR:OH | 2.27 | 0.52 |
| 1:M:1677:ARG:C | 1:M:1678:LYS:HD3 | 2.35 | 0.52 |
| 1:M:2544:TYR:OH | 1:M:2701:TYR:O | 2.25 | 0.52 |
| 1:M:2723:GLN:HE21 | 1:M:2726:ARG:HH21 | 1.57 | 0.52 |
| 1:N:1172:SER:HG | 1:N:1216:ARG:HH22 | 1.56 | 0.52 |
| 1:N:1372:SER:O | 1:N:1374:THR:OG1 | 2.27 | 0.52 |
| 1:O:914:HIS:CE1 | 1:O:1053:HIS:CE1 | 2.98 | 0.52 |
| 1:O:1662:ASP:OD1 | 1:O:1662:ASP:N | 2.41 | 0.52 |
| 1:O:3151:TYR:O | 1:O:3173:ARG:NH2 | 2.42 | 0.52 |
| 1:P:379:LYS:HD3 | 1:P:381:ASN:H | 1.73 | 0.52 |
| 1:P:711:ASP:N | 1:P:711:ASP:OD1 | 2.41 | 0.52 |
| 1:P:757:PRO:HB2 | 1:P:760:GLY:H | 1.75 | 0.52 |
| 1:P:956:VAL:HA | 1:P:963:PRO:HA | 1.91 | 0.52 |
| 1:Q:580:TYR:HE2 | 1:Q:856:ARG:HD3 | 1.75 | 0.52 |
| 1:Q:1671:THR:O | 1:Q:1673:ARG:NH1 | 2.42 | 0.52 |
| 1:Q:1899:GLN:NE2 | 1:Q:1904:HIS:HB2 | 2.22 | 0.52 |
| 1:Q:2271:ILE:HG13 | 1:Q:2298:HIS:HE1 | 1.74 | 0.52 |
| 1:Q:2553:TYR:CD1 | 1:Q:2554:PRO:HA | 2.45 | 0.52 |
| 1:R:1286:MET:O | 1:R:1291:THR:OG1 | 2.24 | 0.52 |
| 1:R:1433:LEU:HD21 | 1:R:1460:HIS:NE2 | 2.24 | 0.52 |
| 1:S:2287:HIS:CD2 | 1:S:2430:GLY:HA3 | 2.45 | 0.52 |
| 1:T:254:PHE:HD2 | 1:T:264:THR:HB | 1.74 | 0.52 |
| 1:A:129:GLU:HA | 1:A:140:SER:HA | 1.91 | 0.52 |
| 1:A:624:SER:HG | 1:A:626:SER:HG | 1.56 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:507:VAL:HG21 | 1:B:638:ILE:HD11 | 1.92 | 0.52 |
| 1:B:1126:LEU:H | 1:B:1126:LEU:HD23 | 1.74 | 0.52 |
| 1:B:1599:GLU:OE2 | 1:B:1600:THR:OG1 | 2.26 | 0.52 |
| 1:B:3010:TYR:OH | 1:B:3189:ASN:OD1 | 2.24 | 0.52 |
| 1:C:501:ARG:NH1 | 1:C:702:TYR:HB3 | 2.25 | 0.52 |
| 1:C:1731:CYS:HA | 1:C:2022:MET:HE1 | 1.91 | 0.52 |
| 1:C:2930:SER:OG | 1:C:2933:GLN:OE1 | 2.20 | 0.52 |
| 1:C:3240:VAL:HG21 | 1:C:3272:LYS:NZ | 2.25 | 0.52 |
| 1:D:950:VAL:HA | 1:D:968:PHE:HB3 | 1.90 | 0.52 |
| 1:D:1008:GLN:N | 1:D:1008:GLN:OE1 | 2.42 | 0.52 |
| 1:D:2675:GLU:O | 1:D:2679:ASN:ND2 | 2.42 | 0.52 |
| 1:E:2095:GLU:OE2 | 1:E:2097:SER:OG | 2.19 | 0.52 |
| 1:F:1147:GLU:OE1 | 1:F:1245:PRO:HA | 2.10 | 0.52 |
| 1:F:1694:ALA:O | 1:F:1697:SER:OG | 2.21 | 0.52 |
| 1:F:1978:LYS:NZ | 1:F:1979:SER:O | 2.42 | 0.52 |
| 1:G:47:MET:C | 1:G:55:ARG:HH12 | 2.17 | 0.52 |
| 1:G:608:VAL:HG11 | 1:G:785:VAL:HG21 | 1.92 | 0.52 |
| 1:G:903:CYS:O | 1:G:905:HIS:ND1 | 2.36 | 0.52 |
| 1:G:1342:SER:OG | 1:G:1344:VAL:O | 2.25 | 0.52 |
| 1:G:1554:ASP:OD1 | 1:G:1554:ASP:N | 2.42 | 0.52 |
| 1:G:2961:GLY:HA2 | 1:G:3106:LEU:HD23 | 1.90 | 0.52 |
| 1:G:3203:ILE:HA | 1:G:3206:ASN:HB2 | 1.92 | 0.52 |
| 1:G:3333:SER:OG | 1:G:3336:THR:OG1 | 2.23 | 0.52 |
| 1:H:1010:ASP:OD1 | 1:H:1011:PHE:N | 2.42 | 0.52 |
| 1:H:1706:GLY:O | 1:H:1710:LEU:HG | 2.09 | 0.52 |
| 1:H:2269:ASN:CG | 1:H:2428:LEU:HD13 | 2.34 | 0.52 |
| 1:I:1349:TRP:NE1 | 1:I:1359:PRO:HG3 | 2.25 | 0.52 |
| 1:I:2454:HIS:O | 1:I:2456:ARG:NH1 | 2.43 | 0.52 |
| 1:I:2930:SER:H | 1:I:2933:GLN:NE2 | 2.07 | 0.52 |
| 1:I:3289:LYS:HD2 | 1:I:3291:ASN:HD22 | 1.73 | 0.52 |
| 1:J:1501:ASP:OD2 | 1:J:1504:GLN:N | 2.41 | 0.52 |
| 1:J:2378:ASP:O | 1:J:2381:GLU:HG2 | 2.10 | 0.52 |
| 1:K:593:ALA:HA | 1:K:605:GLN:HG3 | 1.91 | 0.52 |
| 1:M:181:PHE:CE2 | 1:M:219:VAL:HG13 | 2.44 | 0.52 |
| 1:M:460:SER:O | 1:M:1371:ARG:NH1 | 2.41 | 0.52 |
| 1:M:1980:ARG:HE | 1:M:1982:PHE:HZ | 1.57 | 0.52 |
| 1:M:2249:LEU:HD23 | 1:M:2383:GLU:CD | 2.33 | 0.52 |
| 1:M:2981:MET:SD | 1:M:2982:PRO:HD2 | 2.49 | 0.52 |
| 1:N:2369:ASP:OD1 | 1:N:2369:ASP:N | 2.43 | 0.52 |
| 1:N:2602:ASP:OD1 | 1:N:2603:TRP:N | 2.42 | 0.52 |
| 1:N:2673:GLN:HA | 1:N:2676:VAL:HG22 | 1.91 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:N:3092:HIS:O | 1:N:3104:SER:OG | 2.27 | 0.52 |
| 1:O:2439:ASP:OD1 | 1:O:2439:ASP:N | 2.43 | 0.52 |
| 1:P:142:ALA:HB3 | 1:P:196:HIS:CG | 2.45 | 0.52 |
| 1:P:1149:VAL:HG13 | 1:P:1202:ILE:HG23 | 1.90 | 0.52 |
| 1:P:1277:GLU:HA | 1:P:1280:LYS:HG2 | 1.91 | 0.52 |
| 1:P:1466:ARG:O | 1:P:1470:ILE:HG12 | 2.09 | 0.52 |
| 1:Q:2037:VAL:HA | 1:Q:2040:LYS:HG2 | 1.92 | 0.52 |
| 1:Q:2929:LEU:HD22 | 1:Q:2933:GLN:HG3 | 1.91 | 0.52 |
| 1:R:444:GLU:O | 1:R:447:GLU:HG2 | 2.10 | 0.52 |
| 1:R:860:GLN:NE2 | 1:R:860:GLN:O | 2.43 | 0.52 |
| 1:R:1638:ARG:HG2 | 1:R:1644:TYR:CE1 | 2.44 | 0.52 |
| 1:R:2602:ASP:HA | 1:R:2711:ASN:ND2 | 2.24 | 0.52 |
| 1:R:2723:GLN:HG2 | 1:R:2728:LEU:HD21 | 1.90 | 0.52 |
| 1:R:3058:GLN:N | 1:R:3061:LEU:O | 2.29 | 0.52 |
| 1:S:939:TRP:HE1 | 1:S:998:ILE:HG21 | 1.74 | 0.52 |
| 1:S:1742:TRP:CD1 | 1:S:1920:LEU:HD12 | 2.45 | 0.52 |
| 1:T:1011:PHE:HA | 1:T:1063:TRP:CH2 | 2.44 | 0.52 |
| 1:T:1015:GLU:OE1 | 1:T:1015:GLU:N | 2.35 | 0.52 |
| 1:T:2343:ASN:HB3 | 1:T:2349:ARG:NH2 | 2.25 | 0.52 |
| 1:T:2536:GLN:HA | 1:T:2544:TYR:HB3 | 1.92 | 0.52 |
| 1:T:2693:MET:HE1 | 1:T:2705:PHE:N | 2.25 | 0.52 |
| 1:A:884:PHE:CE1 | 1:A:1090:PRO:HG2 | 2.44 | 0.52 |
| 1:B:159:THR:O | 1:B:162:PHE:N | 2.42 | 0.52 |
| 1:B:2536:GLN:HA | 1:B:2544:TYR:HB3 | 1.91 | 0.52 |
| 1:C:672:HIS:O | 1:C:695:ARG:NH1 | 2.39 | 0.52 |
| 1:C:1195:ASP:OD2 | 1:C:1196:ARG:NH1 | 2.43 | 0.52 |
| 1:D:307:GLU:HG3 | 1:D:413:ALA:HA | 1.92 | 0.52 |
| 1:D:642:SER:O | 1:D:645:ASP:HB3 | 2.08 | 0.52 |
| 1:D:1785:ARG:HH12 | 1:D:1790:ASP:HA | 1.74 | 0.52 |
| 1:D:1884:HIS:O | 1:D:1887:SER:OG | 2.21 | 0.52 |
| 1:D:2740:LEU:HD23 | 1:D:2763:ALA:HB3 | 1.90 | 0.52 |
| 1:D:3008:ILE:HG21 | 1:D:3116:MET:HB3 | 1.90 | 0.52 |
| 1:E:330:ASP:OD1 | 1:E:331:HIS:N | 2.42 | 0.52 |
| 1:E:1420:CYS:HB2 | 1:E:1608:ARG:HH21 | 1.75 | 0.52 |
| 1:E:1732:CYS:O | 1:E:1734:HIS:ND1 | 2.28 | 0.52 |
| 1:E:1865:LYS:NZ | 1:E:1867:HIS:H | 2.08 | 0.52 |
| 1:E:2273:TYR:HB2 | 1:E:2428:LEU:HD11 | 1.91 | 0.52 |
| 1:E:3033:SER:O | 1:E:3046:ARG:NH2 | 2.43 | 0.52 |
| 1:F:112:PHE:HB3 | 1:F:121:GLN:O | 2.09 | 0.52 |
| 1:F:267:TYR:HB3 | 1:F:273:LEU:HD21 | 1.91 | 0.52 |
| 1:F:1775:LEU:HD12 | 1:F:1776:PRO:HD2 | 1.90 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:F:2044:SER:N | 1:F:2047:ASP:OD2 | 2.43 | 0.52 |
| 1:F:2824:ALA:HB2 | 1:F:2869:VAL:HG23 | 1.91 | 0.52 |
| 1:F:3232:LEU:HD23 | 1:F:3234:PRO:HD3 | 1.91 | 0.52 |
| 1:G:13:ASP:OD2 | 1:G:14:GLN:N | 2.42 | 0.52 |
| 1:G:586:LEU:H | 1:G:586:LEU:HD12 | 1.74 | 0.52 |
| 1:G:1025:ILE:HD12 | 1:G:1028:LEU:HD23 | 1.92 | 0.52 |
| 1:H:46:SER:O | 1:H:55:ARG:NE | 2.36 | 0.52 |
| 1:H:1507:PHE:CE2 | 1:H:1509:LEU:HB3 | 2.44 | 0.52 |
| 1:H:1539:THR:H | 1:H:1542:GLN:NE2 | 2.08 | 0.52 |
| 1:H:1769:VAL:O | 1:H:1828:ASN:ND2 | 2.42 | 0.52 |
| 1:I:376:LEU:HB3 | 1:I:378:LYS:HZ3 | 1.75 | 0.52 |
| 1:I:586:LEU:HD12 | 1:I:586:LEU:H | 1.74 | 0.52 |
| 1:I:2567:CYS:HA | 1:I:2577:TRP:CE2 | 2.44 | 0.52 |
| 1:I:2990:LEU:HA | 1:I:2993:VAL:HG12 | 1.91 | 0.52 |
| 1:J:696:PRO:HA | 1:J:699:ILE:HD13 | 1.92 | 0.52 |
| 1:J:1142:HIS:HE1 | 1:J:1524:ASN:HA | 1.75 | 0.52 |
| 1:J:1397:GLN:HB2 | 1:J:1400:LEU:HD23 | 1.92 | 0.52 |
| 1:J:1560:PHE:HZ | 1:J:1573:LEU:HD11 | 1.75 | 0.52 |
| 1:J:1626:ASP:OD1 | 1:J:1627:SER:N | 2.42 | 0.52 |
| 1:J:3350:ASN:OD1 | 1:J:3351:VAL:N | 2.42 | 0.52 |
| 1:K:2313:GLN:OE1 | 1:K:2318:LEU:HB2 | 2.08 | 0.52 |
| 1:K:2986:HIS:HB3 | 1:K:3177:ILE:HG21 | 1.91 | 0.52 |
| 1:L:937:TRP:H | 1:L:1051:LEU:HB2 | 1.75 | 0.52 |
| 1:L:2247:GLU:OE2 | 1:L:2267:THR:OG1 | 2.28 | 0.52 |
| 1:M:129:GLU:HA | 1:M:140:SER:HA | 1.91 | 0.52 |
| 1:M:1163:LEU:HG | 1:M:1182:TYR:HD1 | 1.75 | 0.52 |
| 1:M:1268:LEU:HB3 | 1:M:1347:PRO:HB2 | 1.91 | 0.52 |
| 1:N:1350:ASP:HA | 1:N:1463:ASN:ND2 | 2.25 | 0.52 |
| 1:N:1884:HIS:O | 1:N:1887:SER:OG | 2.20 | 0.52 |
| 1:N:3229:ASN:H | 1:N:3286:THR:HG22 | 1.73 | 0.52 |
| 1:N:3270:LEU:HD11 | 1:N:3281:PHE:CZ | 2.45 | 0.52 |
| 1:O:363:LEU:HD12 | 1:O:364:PRO:HD2 | 1.91 | 0.52 |
| 1:O:1400:LEU:HD21 | 1:O:1436:LEU:HB3 | 1.92 | 0.52 |
| 1:P:1452:ALA:HA | 1:P:1457:PHE:CD2 | 2.45 | 0.52 |
| 1:P:2271:ILE:HD12 | 1:P:2298:HIS:NE2 | 2.24 | 0.52 |
| 1:P:3296:ASP:OD1 | 1:P:3296:ASP:N | 2.42 | 0.52 |
| 1:Q:1736:MET:HB3 | 1:Q:1915:LEU:HD13 | 1.92 | 0.52 |
| 1:R:374:GLU:OE1 | 1:R:374:GLU:N | 2.35 | 0.52 |
| 1:R:2630:LEU:HD11 | 1:R:2698:TYR:HE1 | 1.74 | 0.52 |
| 1:R:2867:ASP:HA | 1:S:2741:ARG:CZ | 2.40 | 0.52 |
| 1:S:383:ASP:OD1 | 1:S:383:ASP:N | 2.42 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:S:1815:ARG:HA | 1:S:1818:LEU:HG | 1.90 | 0.52 |
| 1:T:480:PRO:HA | 1:T:485:ARG:HH22 | 1.72 | 0.52 |
| 1:T:1282:ALA:O | 1:T:1286:MET:HG3 | 2.09 | 0.52 |
| 1:A:17:LEU:O | 1:A:20:GLU:HG3 | 2.09 | 0.52 |
| 1:A:306:ARG:O | 1:A:411:ARG:NH2 | 2.42 | 0.52 |
| 1:A:1568:SER:HB2 | 1:A:1597:GLY:H | 1.74 | 0.52 |
| 1:A:2159:ARG:HH22 | 1:A:2360:TYR:HD2 | 1.57 | 0.52 |
| 1:B:2714:ARG:NH2 | 1:B:2780:ASN:O | 2.43 | 0.52 |
| 1:B:2862:MET:HB3 | 1:B:2864:LEU:HD23 | 1.92 | 0.52 |
| 1:C:248:ARG:NH1 | 1:C:803:GLU:OE1 | 2.43 | 0.52 |
| 1:C:913:TRP:CD1 | 1:C:1088:LEU:HD21 | 2.45 | 0.52 |
| 1:C:2345:ASN:O | 1:C:2349:ARG:HG2 | 2.09 | 0.52 |
| 1:C:3071:THR:HG21 | 1:C:3087:LEU:HD11 | 1.92 | 0.52 |
| 1:C:3144:ARG:HA | 1:C:3147:LEU:HD21 | 1.92 | 0.52 |
| 1:E:255:ASP:OD1 | 1:E:255:ASP:N | 2.43 | 0.52 |
| 1:E:590:MET:HE3 | 1:E:647:LEU:HD13 | 1.92 | 0.52 |
| 1:E:1931:LEU:HD23 | 1:F:2102:ARG:HA | 1.92 | 0.52 |
| 1:E:2329:TYR:HE1 | 1:F:1238:LYS:HZ2 | 1.56 | 0.52 |
| 1:F:256:ARG:O | 1:F:265:ARG:NH1 | 2.36 | 0.52 |
| 1:F:703:GLU:N | 1:F:703:GLU:OE1 | 2.42 | 0.52 |
| 1:F:848:ARG:NH2 | 1:F:922:GLU:HG3 | 2.24 | 0.52 |
| 1:F:3088:HIS:NE2 | 1:F:3119:HIS:HE1 | 2.08 | 0.52 |
| 1:G:1315:CYS:HA | 1:G:1325:TRP:CH2 | 2.45 | 0.52 |
| 1:G:3289:LYS:HB3 | 1:G:3295:LEU:HD11 | 1.92 | 0.52 |
| 1:H:866:LEU:O | 1:H:869:LEU:HG | 2.10 | 0.52 |
| 1:H:1127:GLU:OE2 | 1:H:1131:PHE:N | 2.43 | 0.52 |
| 1:H:1539:THR:HG22 | 1:H:1542:GLN:NE2 | 2.24 | 0.52 |
| 1:H:1547:LEU:O | 1:H:1550:GLN:HG3 | 2.10 | 0.52 |
| 1:H:3392:ASN:HB3 | 1:H:3395:ARG:HG2 | 1.91 | 0.52 |
| 1:I:24:ARG:NH2 | 1:I:123:ASN:HA | 2.25 | 0.52 |
| 1:I:1532:THR:OG1 | 1:I:1534:ASN:OD1 | 2.23 | 0.52 |
| 1:I:3103:MET:HA | 1:I:3109:SER:HA | 1.92 | 0.52 |
| 1:J:859:VAL:HG12 | 1:J:863:ARG:NE | 2.25 | 0.52 |
| 1:J:2948:ASP:N | 1:J:2948:ASP:OD1 | 2.42 | 0.52 |
| 1:K:811:LYS:HD2 | 1:K:815:GLY:HA2 | 1.92 | 0.52 |
| 1:K:2232:LEU:HD13 | 1:K:2274:LEU:HD21 | 1.91 | 0.52 |
| 1:K:2780:ASN:OD1 | 1:K:2784:LEU:N | 2.43 | 0.52 |
| 1:K:3353:GLU:HG3 | 1:K:3386:TYR:HD2 | 1.74 | 0.52 |
| 1:L:1008:GLN:N | 1:L:1008:GLN:OE1 | 2.43 | 0.52 |
| 1:L:1023:ASN:HD21 | 1:L:1184:LEU:HD22 | 1.74 | 0.52 |
| 1:L:1965:ALA:HA | 1:L:1968:LEU:HG | 1.91 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:L:2413:CYS:SG | 1:L:2470:ARG:NH2 | 2.82 | 0.52 |
| 1:M:250:LYS:HD2 | 1:M:268:SER:HB3 | 1.91 | 0.52 |
| 1:M:1404:ASP:O | 1:M:1408:ASN:ND2 | 2.43 | 0.52 |
| 1:M:2390:LYS:O | 1:M:2392:ARG:NH1 | 2.42 | 0.52 |
| 1:M:2872:PHE:HD2 | 1:M:2892:PRO:HG2 | 1.74 | 0.52 |
| 1:M:3271:GLU:N | 1:M:3271:GLU:OE1 | 2.42 | 0.52 |
| 1:N:176:HIS:HA | 1:N:179:VAL:HG12 | 1.92 | 0.52 |
| 1:N:1056:THR:HA | 1:N:1059:ILE:HD12 | 1.91 | 0.52 |
| 1:N:1286:MET:O | 1:N:1291:THR:OG1 | 2.26 | 0.52 |
| 1:N:2800:ASP:OD1 | 1:N:2899:GLY:N | 2.42 | 0.52 |
| 1:N:3008:ILE:HD13 | 1:N:3116:MET:HB3 | 1.91 | 0.52 |
| 1:O:602:PHE:HA | 1:O:605:GLN:NE2 | 2.25 | 0.52 |
| 1:O:651:TRP:CZ3 | 1:O:655:GLN:HG3 | 2.45 | 0.52 |
| 1:O:794:ASN:OD1 | 1:O:795:LYS:N | 2.43 | 0.52 |
| 1:O:1812:ASP:HB3 | 1:O:1863:GLY:HA3 | 1.92 | 0.52 |
| 1:O:1814:LYS:HE2 | 1:O:1860:TRP:HZ3 | 1.74 | 0.52 |
| 1:P:444:GLU:O | 1:P:447:GLU:HG2 | 2.10 | 0.52 |
| 1:P:3147:LEU:HD23 | 1:P:3150:LEU:HD12 | 1.92 | 0.52 |
| 1:Q:734:ASP:OD1 | 1:Q:734:ASP:N | 2.42 | 0.52 |
| 1:Q:1081:ILE:HD13 | 1:R:2460:VAL:HG12 | 1.91 | 0.52 |
| 1:Q:2569:HIS:HA | 1:Q:2574:PHE:CE2 | 2.45 | 0.52 |
| 1:R:1281:SER:O | 1:R:1285:ARG:HG2 | 2.10 | 0.52 |
| 1:R:1713:PHE:HE1 | 1:R:1929:TYR:HB3 | 1.75 | 0.52 |
| 1:R:3102:SER:O | 1:R:3105:THR:OG1 | 2.26 | 0.52 |
| 1:R:3314:ASP:O | 1:R:3336:THR:HA | 2.10 | 0.52 |
| 1:R:3317:ILE:HG13 | 1:R:3339:ARG:HB3 | 1.92 | 0.52 |
| 1:R:3342:SER:OG | 1:R:3344:VAL:O | 2.27 | 0.52 |
| 1:S:1731:CYS:HA | 1:S:2022:MET:HE1 | 1.91 | 0.52 |
| 1:S:2360:TYR:HA | 1:S:2363:LEU:HB2 | 1.92 | 0.52 |
| 1:S:2696:LEU:HD21 | 1:S:2839:GLY:HA3 | 1.91 | 0.52 |
| 1:S:2802:VAL:HG12 | 1:S:2856:THR:HG22 | 1.91 | 0.52 |
| 1:T:740:LEU:HB3 | 1:T:785:VAL:HB | 1.92 | 0.52 |
| 1:T:1143:ARG:HB3 | 1:T:1148:ARG:HH22 | 1.74 | 0.52 |
| 1:T:1268:LEU:HD23 | 1:T:1268:LEU:H | 1.75 | 0.52 |
| 1:T:1332:GLN:OE1 | 1:T:1505:ASN:ND2 | 2.39 | 0.52 |
| 1:T:2922:VAL:HG22 | 1:T:3186:ASN:OD1 | 2.10 | 0.52 |
| 1:A:1240:THR:HA | 1:B:2328:ASN:HD21 | 1.75 | 0.52 |
| 1:A:1495:PRO:HD2 | 1:A:1500:ASN:HD21 | 1.74 | 0.52 |
| 1:A:1590:ALA:HB1 | 1:A:1617:PRO:HG3 | 1.92 | 0.52 |
| 1:A:2000:VAL:HG12 | 1:A:2051:VAL:HG22 | 1.91 | 0.52 |
| 1:A:2108:LYS:O | 1:A:2112:ARG:NH1 | 2.43 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:458:ASP:OD1 | 1:B:459:THR:N | 2.43 | 0.52 |
| 1:B:475:ALA:HB3 | 1:B:485:ARG:HB3 | 1.90 | 0.52 |
| 1:B:2898:PRO:HB3 | 1:C:2917:LYS:HZ1 | 1.75 | 0.52 |
| 1:B:3119:HIS:O | 1:B:3122:ILE:HG22 | 2.10 | 0.52 |
| 1:B:3266:VAL:HG21 | 1:B:3283:PHE:CE2 | 2.45 | 0.52 |
| 1:C:17:LEU:O | 1:C:20:GLU:HG3 | 2.09 | 0.52 |
| 1:C:275:SER:HB3 | 1:C:278:GLN:HE22 | 1.75 | 0.52 |
| 1:C:1244:ARG:HD3 | 1:C:1245:PRO:HD2 | 1.91 | 0.52 |
| 1:C:2500:ARG:NH1 | 1:C:2502:GLU:OE2 | 2.43 | 0.52 |
| 1:C:3301:THR:HB | 1:C:3325:LYS:HB3 | 1.92 | 0.52 |
| 1:D:536:ALA:HB2 | 1:D:554:PHE:HD2 | 1.73 | 0.52 |
| 1:D:1087:PRO:HA | 1:D:1109:PRO:HD3 | 1.91 | 0.52 |
| 1:D:3317:ILE:HG13 | 1:D:3339:ARG:HB3 | 1.90 | 0.52 |
| 1:E:202:THR:OG1 | 1:E:204:GLU:OE1 | 2.27 | 0.52 |
| 1:E:3208:ARG:HA | 1:E:3212:ARG:HH12 | 1.74 | 0.52 |
| 1:F:866:LEU:HD23 | 1:F:967:PRO:HG2 | 1.91 | 0.52 |
| 1:F:1862:GLY:HA3 | 1:F:1870:ALA:HB2 | 1.92 | 0.52 |
| 1:F:2165:VAL:HG11 | 1:F:2296:PHE:CE2 | 2.45 | 0.52 |
| 1:F:3122:ILE:HG13 | 1:F:3125:ILE:HD11 | 1.91 | 0.52 |
| 1:G:183:VAL:HG21 | 1:G:365:TYR:CZ | 2.45 | 0.52 |
| 1:G:399:ASN:HD21 | 1:G:401:ASN:HD21 | 1.56 | 0.52 |
| 1:G:555:PHE:HA | 1:G:568:ARG:HH22 | 1.75 | 0.52 |
| 1:G:1404:ASP:O | 1:G:1408:ASN:ND2 | 2.42 | 0.52 |
| 1:G:1730:ALA:N | 1:G:2020:ALA:O | 2.43 | 0.52 |
| 1:G:2273:TYR:HB2 | 1:G:2428:LEU:HD21 | 1.91 | 0.52 |
| 1:H:887:GLN:NE2 | 1:H:889:ASN:HB2 | 2.24 | 0.52 |
| 1:H:1557:PHE:HD2 | 1:H:1611:LYS:HD2 | 1.74 | 0.52 |
| 1:H:2064:SER:HG | 1:H:2066:SER:HG | 1.53 | 0.52 |
| 1:H:3124:ARG:HD2 | 1:H:3187:PHE:CD2 | 2.45 | 0.52 |
| 1:H:3133:GLN:HB3 | 1:H:3138:ARG:HB2 | 1.91 | 0.52 |
| 1:H:3225:SER:O | 1:H:3290:TYR:N | 2.42 | 0.52 |
| 1:I:391:TYR:HA | 1:I:397:SER:HA | 1.91 | 0.52 |
| 1:I:1223:VAL:HG13 | 1:I:1231:ILE:HB | 1.90 | 0.52 |
| 1:I:1388:THR:OG1 | 1:I:1390:LYS:NZ | 2.42 | 0.52 |
| 1:I:1834:PHE:HE2 | 1:I:1891:ILE:HG13 | 1.75 | 0.52 |
| 1:J:559:VAL:N | 1:J:564:GLU:O | 2.41 | 0.52 |
| 1:J:618:GLY:HA3 | 1:J:626:SER:N | 2.25 | 0.52 |
| 1:J:934:LEU:HD23 | 1:J:1054:SER:HB3 | 1.92 | 0.52 |
| 1:J:1274:GLY:O | 1:J:1277:GLU:HG3 | 2.10 | 0.52 |
| 1:J:1547:LEU:O | 1:J:1550:GLN:HG3 | 2.09 | 0.52 |
| 1:J:1736:MET:HG2 | 1:J:1738:THR:H | 1.75 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:J:1869:MET:HE1 | 1:J:1878:ASP:HB3 | 1.91 | 0.52 |
| 1:J:1913:LEU:HA | 1:J:1916:MET:HG3 | 1.90 | 0.52 |
| 1:J:2283:LEU:HD21 | 1:J:2292:ASP:HB3 | 1.91 | 0.52 |
| 1:K:574:LEU:HB3 | 1:K:616:LEU:HD21 | 1.91 | 0.52 |
| 1:K:1910:ASN:OD1 | 1:K:1911:CYS:N | 2.43 | 0.52 |
| 1:K:3149:ASN:HD22 | 1:K:3152:ARG:NH2 | 2.07 | 0.52 |
| 1:L:594:LEU:HA | 1:L:602:PHE:CE1 | 2.44 | 0.52 |
| 1:L:956:VAL:HA | 1:L:963:PRO:HA | 1.91 | 0.52 |
| 1:L:1716:VAL:HG23 | 1:L:1718:PRO:HD3 | 1.92 | 0.52 |
| 1:L:3017:SER:O | 1:L:3055:ARG:NH2 | 2.35 | 0.52 |
| 1:L:3085:GLU:O | 1:L:3089:ASN:ND2 | 2.42 | 0.52 |
| 1:L:3390:SER:H | 1:L:3401:ARG:HH21 | 1.55 | 0.52 |
| 1:M:493:MET:HG2 | 1:M:494:ALA:H | 1.75 | 0.52 |
| 1:M:1322:PHE:HB3 | 1:M:1323:PRO:HD3 | 1.92 | 0.52 |
| 1:M:1756:ARG:HH12 | 1:N:2175:THR:HB | 1.74 | 0.52 |
| 1:M:1887:SER:O | 1:M:1890:ARG:HG2 | 2.10 | 0.52 |
| 1:M:2941:LEU:HD12 | 1:M:2944:LEU:HD11 | 1.92 | 0.52 |
| 1:N:7:ASN:HB3 | 1:N:10:LEU:HG | 1.90 | 0.52 |
| 1:N:711:ASP:OD1 | 1:N:711:ASP:N | 2.43 | 0.52 |
| 1:N:1147:GLU:OE1 | 1:N:1245:PRO:HA | 2.10 | 0.52 |
| 1:O:383:ASP:N | 1:O:383:ASP:OD1 | 2.42 | 0.52 |
| 1:P:3142:TYR:HA | 1:P:3144:ARG:HH12 | 1.73 | 0.52 |
| 1:Q:44:GLU:N | 1:Q:204:GLU:O | 2.43 | 0.52 |
| 1:Q:1220:LYS:NZ | 1:Q:1222:SER:HB2 | 2.25 | 0.52 |
| 1:R:1159:ARG:HH22 | 1:R:1160:LYS:HB3 | 1.75 | 0.52 |
| 1:R:1205:ILE:HD12 | 1:R:1208:LYS:HE3 | 1.92 | 0.52 |
| 1:R:2258:CYS:O | 1:R:2261:GLU:HG3 | 2.09 | 0.52 |
| 1:R:2414:GLN:HA | 1:R:2467:PHE:HA | 1.90 | 0.52 |
| 1:R:2487:SER:OG | 1:R:2488:LYS:N | 2.40 | 0.52 |
| 1:R:2655:TYR:CD2 | 1:R:2659:LEU:HD23 | 2.45 | 0.52 |
| 1:S:230:GLN:HA | 1:S:233:ARG:HG2 | 1.90 | 0.52 |
| 1:S:601:ASP:O | 1:S:604:VAL:HG22 | 2.10 | 0.52 |
| 1:S:1404:ASP:O | 1:S:1408:ASN:ND2 | 2.43 | 0.52 |
| 1:S:1577:VAL:O | 1:S:1584:ARG:NH2 | 2.43 | 0.52 |
| 1:S:1730:ALA:N | 1:S:2020:ALA:O | 2.43 | 0.52 |
| 1:S:2534:ALA:HA | 1:S:2537:GLN:HE22 | 1.75 | 0.52 |
| 1:S:3088:HIS:HD2 | 1:S:3122:ILE:HG13 | 1.74 | 0.52 |
| 1:S:3315:VAL:HA | 1:S:3337:ARG:O | 2.10 | 0.52 |
| 1:A:986:LEU:HD12 | 1:A:1028:LEU:HG | 1.92 | 0.52 |
| 1:A:1684:THR:N | 1:A:1687:GLU:OE2 | 2.31 | 0.52 |
| 1:B:38:LEU:O | 1:B:73:TYR:OH | 2.28 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:444:GLU:O | 1:B:447:GLU:HG2 | 2.10 | 0.52 |
| 1:B:468:ALA:HB1 | 1:B:633:PHE:HA | 1.90 | 0.52 |
| 1:B:1124:ASP:N | 1:B:1124:ASP:OD1 | 2.43 | 0.52 |
| 1:B:3058:GLN:N | 1:B:3061:LEU:O | 2.41 | 0.52 |
| 1:C:2569:HIS:HA | 1:C:2574:PHE:CZ | 2.45 | 0.52 |
| 1:D:188:ILE:HG21 | 1:D:215:HIS:CE1 | 2.44 | 0.52 |
| 1:E:363:LEU:HD12 | 1:E:364:PRO:HD2 | 1.92 | 0.52 |
| 1:F:538:LYS:HE3 | 1:F:541:TYR:HB3 | 1.92 | 0.52 |
| 1:F:1881:PHE:O | 1:F:1885:HIS:ND1 | 2.40 | 0.52 |
| 1:F:3234:PRO:HG2 | 1:F:3237:GLY:HA3 | 1.91 | 0.52 |
| 1:G:593:ALA:HA | 1:G:605:GLN:HG3 | 1.92 | 0.52 |
| 1:G:2191:PRO:O | 1:G:2195:THR:HG23 | 2.10 | 0.52 |
| 1:G:2456:ARG:N | 1:G:2459:ASP:OD2 | 2.43 | 0.52 |
| 1:G:2673:GLN:HE22 | 1:G:2852:GLN:H | 1.57 | 0.52 |
| 1:H:196:HIS:O | 1:H:199:SER:OG | 2.25 | 0.52 |
| 1:H:420:LYS:HD2 | 1:H:422:SER:O | 2.10 | 0.52 |
| 1:H:523:TRP:HB3 | 1:H:639:LEU:HD13 | 1.91 | 0.52 |
| 1:H:991:LYS:H | 1:H:994:ARG:CZ | 2.23 | 0.52 |
| 1:H:2112:ARG:HE | 1:H:2116:LYS:NZ | 2.08 | 0.52 |
| 1:H:2159:ARG:NE | 1:H:2303:ASP:OD1 | 2.22 | 0.52 |
| 1:H:2657:GLN:N | 1:H:2657:GLN:OE1 | 2.42 | 0.52 |
| 1:H:3321:LEU:O | 1:H:3395:ARG:NH2 | 2.35 | 0.52 |
| 1:I:471:HIS:HB3 | 1:I:632:ALA:HB2 | 1.91 | 0.52 |
| 1:I:2129:PHE:HE1 | 1:I:2342:LEU:HD13 | 1.75 | 0.52 |
| 1:I:2750:ASP:HA | 1:I:2758:ARG:HD2 | 1.92 | 0.52 |
| 1:J:176:HIS:HA | 1:J:179:VAL:HG12 | 1.92 | 0.52 |
| 1:J:1007:GLU:N | 1:J:1008:GLN:OE1 | 2.42 | 0.52 |
| 1:J:2265:GLU:OE1 | 1:J:2268:HIS:NE2 | 2.37 | 0.52 |
| 1:J:2311:GLU:OE1 | 1:J:2315:ARG:NH1 | 2.43 | 0.52 |
| 1:J:2336:PRO:HB2 | 1:J:2342:LEU:HD12 | 1.91 | 0.52 |
| 1:J:2602:ASP:OD1 | 1:J:2603:TRP:N | 2.42 | 0.52 |
| 1:K:1721:PRO:HD3 | 1:K:1729:TYR:CZ | 2.44 | 0.52 |
| 1:K:2000:VAL:O | 1:K:2041:LYS:NZ | 2.41 | 0.52 |
| 1:K:2569:HIS:HA | 1:K:2574:PHE:CE2 | 2.45 | 0.52 |
| 1:K:3049:GLN:HG2 | 1:K:3050:PRO:HD2 | 1.92 | 0.52 |
| 1:L:471:HIS:ND1 | 1:L:471:HIS:O | 2.43 | 0.52 |
| 1:L:2508:VAL:HG12 | 1:L:2590:THR:HG23 | 1.91 | 0.52 |
| 1:M:327:LYS:HE2 | 1:M:342:CYS:SG | 2.50 | 0.52 |
| 1:M:866:LEU:HD22 | 1:M:968:PHE:CE1 | 2.45 | 0.52 |
| 1:M:1732:CYS:C | 1:M:1734:HIS:HD1 | 2.17 | 0.52 |
| 1:M:2044:SER:OG | 1:M:2046:ASP:OD1 | 2.28 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:M:3395:ARG:NE | 1:M:3398:GLN:OE1 | 2.30 | 0.52 |
| 1:N:1008:GLN:N | 1:N:1008:GLN:OE1 | 2.43 | 0.52 |
| 1:N:1736:MET:HG2 | 1:N:1738:THR:H | 1.75 | 0.52 |
| 1:N:2304:LYS:HE2 | 1:N:2367:TYR:CG | 2.45 | 0.52 |
| 1:O:392:SER:OG | 1:O:393:VAL:N | 2.43 | 0.52 |
| 1:O:539:GLU:N | 1:O:539:GLU:OE1 | 2.43 | 0.52 |
| 1:O:953:GLU:HG3 | 1:O:954:THR:HG23 | 1.91 | 0.52 |
| 1:O:1775:LEU:HD12 | 1:O:1779:PHE:HE1 | 1.74 | 0.52 |
| 1:O:2990:LEU:HA | 1:O:2993:VAL:HG12 | 1.91 | 0.52 |
| 1:O:3113:PRO:HA | 1:O:3116:MET:HG3 | 1.91 | 0.52 |
| 1:P:914:HIS:O | 1:P:918:THR:HG23 | 2.08 | 0.52 |
| 1:P:1284:ARG:NH2 | 1:P:1287:GLN:HG2 | 2.25 | 0.52 |
| 1:P:3232:LEU:HD23 | 1:P:3234:PRO:HD3 | 1.91 | 0.52 |
| 1:Q:9:ASP:OD1 | 1:Q:9:ASP:N | 2.42 | 0.52 |
| 1:Q:275:SER:HB3 | 1:Q:278:GLN:HE22 | 1.73 | 0.52 |
| 1:Q:582:ASP:O | 1:Q:583:HIS:ND1 | 2.43 | 0.52 |
| 1:Q:2974:TYR:HB3 | 1:R:3367:PRO:HB2 | 1.92 | 0.52 |
| 1:Q:3334:ARG:NH2 | 1:Q:3407:ASP:OD1 | 2.42 | 0.52 |
| 1:R:1490:ASN:HA | 1:R:1493:ARG:NH1 | 2.25 | 0.52 |
| 1:R:1716:VAL:HG23 | 1:R:1718:PRO:HD3 | 1.92 | 0.52 |
| 1:R:1932:ASP:OD2 | 1:R:1935:THR:N | 2.31 | 0.52 |
| 1:R:2264:PHE:CZ | 1:R:2302:VAL:HG13 | 2.45 | 0.52 |
| 1:R:2582:VAL:HA | 1:R:2706:PHE:HE2 | 1.74 | 0.52 |
| 1:S:1739:PHE:HB3 | 1:S:1740:PRO:HD3 | 1.92 | 0.52 |
| 1:T:198:HIS:HA | 1:T:205:TRP:CD1 | 2.45 | 0.52 |
| 1:T:1169:CYS:HA | 1:T:1175:CYS:HA | 1.92 | 0.52 |
| 1:A:309:ALA:H | 1:A:370:SER:HG | 1.57 | 0.52 |
| 1:A:2797:ARG:HA | 1:A:2801:ARG:HH22 | 1.74 | 0.52 |
| 1:A:2801:ARG:HD3 | 1:A:2803:PHE:CZ | 2.45 | 0.52 |
| 1:B:495:THR:HG23 | 1:B:670:MET:HE3 | 1.92 | 0.52 |
| 1:B:1827:ASP:HA | 1:B:1831:TRP:CD1 | 2.45 | 0.52 |
| 1:B:1851:GLU:O | 1:B:1855:ASN:ND2 | 2.42 | 0.52 |
| 1:B:2788:GLN:HA | 1:B:2791:GLU:OE2 | 2.09 | 0.52 |
| 1:C:311:ALA:HB2 | 1:C:369:ILE:HD13 | 1.91 | 0.52 |
| 1:C:525:TRP:CE3 | 1:C:586:LEU:HD23 | 2.45 | 0.52 |
| 1:D:170:GLU:HG3 | 1:D:304:ARG:HH22 | 1.75 | 0.52 |
| 1:E:288:LEU:N | 1:E:291:LEU:O | 2.40 | 0.52 |
| 1:E:650:ILE:HG22 | 1:E:713:LEU:HD12 | 1.92 | 0.52 |
| 1:E:953:GLU:O | 1:E:966:ASN:N | 2.32 | 0.52 |
| 1:E:2148:LEU:HB3 | 1:E:2151:VAL:HG11 | 1.90 | 0.52 |
| 1:E:2696:LEU:HD21 | 1:E:2839:GLY:HA3 | 1.92 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:F:3131:THR:HA | 1:F:3134:LYS:NZ | 2.25 | 0.52 |
| 1:F:3213:VAL:HG12 | 1:F:3267:THR:HA | 1.92 | 0.52 |
| 1:F:3232:LEU:HD12 | 1:F:3283:PHE:CZ | 2.45 | 0.52 |
| 1:H:221:ARG:O | 1:H:225:ILE:HG12 | 2.10 | 0.52 |
| 1:H:2376:ASN:O | 1:H:2379:GLU:HG3 | 2.10 | 0.52 |
| 1:I:17:LEU:O | 1:I:20:GLU:HG3 | 2.10 | 0.52 |
| 1:I:44:GLU:N | 1:I:204:GLU:O | 2.41 | 0.52 |
| 1:I:2370:MET:SD | 1:I:2370:MET:N | 2.83 | 0.52 |
| 1:I:3385:ASP:H | 1:J:3148:ARG:HH21 | 1.58 | 0.52 |
| 1:J:244:VAL:HG23 | 1:J:248:ARG:HE | 1.75 | 0.52 |
| 1:J:379:LYS:HD3 | 1:J:380:LEU:N | 2.25 | 0.52 |
| 1:J:580:TYR:CG | 1:J:958:PRO:HG2 | 2.45 | 0.52 |
| 1:J:1845:ASP:HB3 | 1:J:2028:ARG:HD2 | 1.92 | 0.52 |
| 1:J:2330:MET:HE1 | 1:J:2355:LYS:HD3 | 1.90 | 0.52 |
| 1:K:1388:THR:HG23 | 1:K:1390:LYS:H | 1.74 | 0.52 |
| 1:K:2227:ASP:OD1 | 1:N:113:LYS:NZ | 2.29 | 0.52 |
| 1:K:2331:SER:HA | 1:K:2355:LYS:HZ1 | 1.75 | 0.52 |
| 1:L:105:ARG:HD2 | 1:L:106:LEU:HD22 | 1.91 | 0.52 |
| 1:L:303:ARG:HD3 | 1:L:306:ARG:HD3 | 1.91 | 0.52 |
| 1:L:901:ALA:HB2 | 1:L:1188:TYR:HB3 | 1.92 | 0.52 |
| 1:L:1142:HIS:CE1 | 1:L:1524:ASN:HA | 2.45 | 0.52 |
| 1:L:1624:LYS:NZ | 1:L:1626:ASP:OD2 | 2.36 | 0.52 |
| 1:L:2273:TYR:HE1 | 1:L:2476:VAL:HG12 | 1.75 | 0.52 |
| 1:L:2559:ASP:N | 1:L:2559:ASP:OD2 | 2.43 | 0.52 |
| 1:L:3324:ASN:OD1 | 1:L:3395:ARG:NH2 | 2.40 | 0.52 |
| 1:M:971:GLY:N | 1:M:978:THR:OG1 | 2.34 | 0.52 |
| 1:M:1785:ARG:HH12 | 1:M:1787:PRO:HA | 1.73 | 0.52 |
| 1:M:2456:ARG:N | 1:M:2459:ASP:OD2 | 2.43 | 0.52 |
| 1:N:956:VAL:HA | 1:N:963:PRO:HA | 1.92 | 0.52 |
| 1:N:1452:ALA:HA | 1:N:1457:PHE:CD2 | 2.44 | 0.52 |
| 1:N:1742:TRP:CD1 | 1:N:1920:LEU:HD12 | 2.45 | 0.52 |
| 1:O:1100:ASP:OD2 | 1:O:1102:ILE:HG22 | 2.10 | 0.52 |
| 1:O:2108:LYS:O | 1:O:2112:ARG:NH1 | 2.43 | 0.52 |
| 1:O:2153:THR:HA | 1:O:2156:HIS:ND1 | 2.24 | 0.52 |
| 1:O:2393:VAL:H | 1:O:2447:THR:HG22 | 1.75 | 0.52 |
| 1:O:3052:LEU:O | 1:O:3055:ARG:NH2 | 2.43 | 0.52 |
| 1:P:739:GLY:HA3 | 1:P:784:LEU:HB3 | 1.92 | 0.52 |
| 1:P:848:ARG:HD2 | 1:P:1123:TYR:CE2 | 2.45 | 0.52 |
| 1:P:1718:PRO:HG2 | 1:P:1728:ARG:HB3 | 1.92 | 0.52 |
| 1:P:1857:ILE:HB | 1:P:1884:HIS:CE1 | 2.45 | 0.52 |
| 1:Q:60:VAL:HG13 | 1:Q:63:MET:HE2 | 1.92 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:Q:1026:HIS:HA | 1:Q:1037:MET:HE2 | 1.91 | 0.52 |
| 1:Q:3211:ASP:HB2 | 1:Q:3309:ALA:HB2 | 1.90 | 0.52 |
| 1:R:450:GLN:O | 1:R:454:ARG:HG2 | 2.09 | 0.52 |
| 1:R:1148:ARG:HD3 | 1:R:1150:PHE:CZ | 2.45 | 0.52 |
| 1:R:2552:GLY:O | 1:R:2555:GLY:N | 2.43 | 0.52 |
| 1:S:1057:ASP:OD1 | 1:S:1123:TYR:OH | 2.24 | 0.52 |
| 1:S:2108:LYS:O | 1:S:2112:ARG:NH1 | 2.43 | 0.52 |
| 1:S:2345:ASN:O | 1:S:2349:ARG:HG2 | 2.10 | 0.52 |
| 1:S:2603:TRP:NE1 | 1:S:2711:ASN:HD22 | 2.08 | 0.52 |
| 1:S:3165:ASN:HD21 | 1:S:3167:VAL:HB | 1.75 | 0.52 |
| 1:T:74:VAL:HA | 1:T:77:LEU:HD23 | 1.92 | 0.52 |
| 1:T:435:LYS:HG2 | 1:T:436:ASP:H | 1.74 | 0.52 |
| 1:T:735:ARG:NH2 | 1:T:790:THR:H | 2.07 | 0.52 |
| 1:T:924:ALA:O | 1:T:928:LYS:HG2 | 2.10 | 0.52 |
| 1:T:2414:GLN:HE22 | 1:T:2453:LEU:HD22 | 1.75 | 0.52 |
| 1:A:699:ILE:HG13 | 1:A:706:LEU:HD21 | 1.92 | 0.51 |
| 1:A:884:PHE:HE1 | 1:A:1090:PRO:HG2 | 1.75 | 0.51 |
| 1:A:1189:GLU:N | 1:A:1189:GLU:OE1 | 2.43 | 0.51 |
| 1:A:2796:ARG:NH1 | 1:A:2799:GLU:OE2 | 2.42 | 0.51 |
| 1:B:488:CYS:HB3 | 1:B:677:PRO:HD3 | 1.91 | 0.51 |
| 1:B:956:VAL:HA | 1:B:963:PRO:HA | 1.92 | 0.51 |
| 1:B:1277:GLU:HA | 1:B:1280:LYS:HG2 | 1.93 | 0.51 |
| 1:C:1914:GLU:OE1 | 1:D:1654:SER:HA | 2.10 | 0.51 |
| 1:D:848:ARG:HB3 | 1:D:934:LEU:O | 2.10 | 0.51 |
| 1:D:1270:ASP:OD1 | 1:D:1271:LEU:N | 2.43 | 0.51 |
| 1:D:2567:CYS:C | 1:D:2569:HIS:HD1 | 2.17 | 0.51 |
| 1:D:3392:ASN:HB3 | 1:D:3395:ARG:HG2 | 1.92 | 0.51 |
| 1:E:191:LEU:HG | 1:E:349:PHE:HE2 | 1.74 | 0.51 |
| 1:E:728:ASP:CG | 1:E:836:HIS:HB2 | 2.36 | 0.51 |
| 1:E:2583:VAL:HG21 | 1:E:2772:PHE:HB3 | 1.91 | 0.51 |
| 1:E:3036:GLN:HB2 | 1:E:3043:GLN:HE22 | 1.74 | 0.51 |
| 1:F:6:LYS:HD2 | 1:F:11:LEU:HA | 1.92 | 0.51 |
| 1:F:474:PRO:HB2 | 1:F:476:ARG:NH1 | 2.22 | 0.51 |
| 1:F:2757:ILE:O | 1:F:2761:ALA:HB2 | 2.09 | 0.51 |
| 1:G:418:ASP:OD2 | 1:G:662:TYR:N | 2.43 | 0.51 |
| 1:G:855:THR:O | 1:G:859:VAL:HG23 | 2.10 | 0.51 |
| 1:G:1756:ARG:HH22 | 1:H:2175:THR:HB | 1.74 | 0.51 |
| 1:G:3105:THR:O | 1:G:3109:SER:HB3 | 2.10 | 0.51 |
| 1:H:680:PHE:O | 1:H:685:ASN:ND2 | 2.40 | 0.51 |
| 1:H:740:LEU:HB2 | 1:H:785:VAL:HB | 1.91 | 0.51 |
| 1:H:1088:LEU:HD22 | 1:H:1109:PRO:HG3 | 1.92 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:H:2666:ASP:HB3 | 1:H:2669:ASN:HD22 | 1.74 | 0.51 |
| 1:H:2779:LEU:H | 1:H:2779:LEU:HD23 | 1.75 | 0.51 |
| 1:I:390:LEU:HD22 | 1:I:398:LEU:HB3 | 1.91 | 0.51 |
| 1:I:674:LEU:HD22 | 1:I:695:ARG:NH2 | 2.25 | 0.51 |
| 1:J:1967:LEU:HD23 | 1:J:1967:LEU:H | 1.75 | 0.51 |
| 1:K:71:ARG:HA | 1:K:74:VAL:HG12 | 1.92 | 0.51 |
| 1:K:76:GLN:OE1 | 1:K:254:PHE:HE1 | 1.93 | 0.51 |
| 1:K:595:GLU:N | 1:K:595:GLU:OE1 | 2.43 | 0.51 |
| 1:K:2614:LEU:HB3 | 1:K:2636:ARG:HH12 | 1.74 | 0.51 |
| 1:L:103:LEU:HD23 | 1:L:108:GLN:HB3 | 1.91 | 0.51 |
| 1:L:166:LEU:HA | 1:L:169:LEU:HG | 1.92 | 0.51 |
| 1:L:176:HIS:HA | 1:L:179:VAL:HG12 | 1.92 | 0.51 |
| 1:L:312:SER:HB3 | 1:L:407:VAL:HG23 | 1.91 | 0.51 |
| 1:M:2090:ASN:C | 1:M:2091:ARG:HD3 | 2.34 | 0.51 |
| 1:M:2622:PHE:HA | 1:M:2703:PRO:HG2 | 1.92 | 0.51 |
| 1:M:2786:ILE:HD13 | 1:M:2789:LEU:HD21 | 1.90 | 0.51 |
| 1:N:1143:ARG:HB3 | 1:N:1148:ARG:NH2 | 2.25 | 0.51 |
| 1:N:1225:ASP:OD1 | 1:N:1226:LEU:N | 2.35 | 0.51 |
| 1:N:2041:LYS:HG3 | 1:N:2043:LEU:HD23 | 1.92 | 0.51 |
| 1:N:2263:GLN:HE22 | 1:N:2443:LYS:H | 1.57 | 0.51 |
| 1:P:196:HIS:O | 1:P:199:SER:OG | 2.27 | 0.51 |
| 1:P:1963:ILE:HD11 | 1:P:1967:LEU:HD11 | 1.93 | 0.51 |
| 1:P:3125:ILE:HA | 1:P:3128:ILE:HG22 | 1.91 | 0.51 |
| 1:Q:704:HIS:ND1 | 1:Q:705:GLU:OE2 | 2.43 | 0.51 |
| 1:Q:1294:LYS:O | 1:Q:1297:SER:OG | 2.25 | 0.51 |
| 1:Q:3114:PHE:HA | 1:Q:3117:ILE:HG12 | 1.92 | 0.51 |
| 1:R:1362:ILE:HD13 | 1:R:1456:LEU:HD11 | 1.92 | 0.51 |
| 1:R:3127:GLN:O | 1:R:3130:GLN:HG3 | 2.09 | 0.51 |
| 1:R:3147:LEU:HA | 1:R:3150:LEU:HD12 | 1.92 | 0.51 |
| 1:R:3164:PRO:HA | 1:R:3169:ARG:HH21 | 1.73 | 0.51 |
| 1:S:330:ASP:OD1 | 1:S:331:HIS:N | 2.44 | 0.51 |
| 1:S:1910:ASN:ND2 | 1:T:1657:PHE:O | 2.43 | 0.51 |
| 1:T:540:THR:HG22 | 1:T:551:HIS:HA | 1.92 | 0.51 |
| 1:T:1564:ASN:HB3 | 1:T:1604:PHE:CE1 | 2.44 | 0.51 |
| 1:T:2109:ALA:HA | 1:T:2112:ARG:HG2 | 1.92 | 0.51 |
| 1:T:2856:THR:HG22 | 1:T:2860:ASN:HD22 | 1.74 | 0.51 |
| 1:A:734:ASP:OD1 | 1:A:734:ASP:N | 2.42 | 0.51 |
| 1:A:2446:ILE:HD11 | 1:A:2491:ILE:HD11 | 1.92 | 0.51 |
| 1:B:2182:ASP:HA | 1:B:2301:PHE:CE2 | 2.45 | 0.51 |
| 1:C:950:VAL:HG12 | 1:C:968:PHE:CD2 | 2.45 | 0.51 |
| 1:C:1689:ARG:NE | 1:C:1786:ASP:OD1 | 2.42 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:D:434:ARG:HB3 | 1:D:710:TYR:CD1 | 2.44 | 0.51 |
| 1:D:703:GLU:N | 1:D:703:GLU:OE1 | 2.43 | 0.51 |
| 1:D:848:ARG:HD3 | 1:D:934:LEU:HB3 | 1.92 | 0.51 |
| 1:D:1143:ARG:HB3 | 1:D:1148:ARG:HH22 | 1.75 | 0.51 |
| 1:D:1356:ARG:NH2 | 1:D:1402:ASN:OD1 | 2.43 | 0.51 |
| 1:D:2095:GLU:OE1 | 1:D:2097:SER:N | 2.44 | 0.51 |
| 1:E:63:MET:HB3 | 1:E:246:LEU:HD21 | 1.91 | 0.51 |
| 1:E:2090:ASN:ND2 | 1:E:2175:THR:O | 2.43 | 0.51 |
| 1:E:2126:LEU:O | 1:E:2161:TYR:OH | 2.28 | 0.51 |
| 1:E:2495:PRO:HB2 | 1:E:2500:ARG:HD2 | 1.92 | 0.51 |
| 1:F:2739:GLU:HA | 1:F:2742:GLN:HE22 | 1.75 | 0.51 |
| 1:G:24:ARG:NH2 | 1:G:123:ASN:HA | 2.25 | 0.51 |
| 1:G:1910:ASN:ND2 | 1:H:1657:PHE:O | 2.42 | 0.51 |
| 1:G:2328:ASN:HD21 | 1:H:1240:THR:HA | 1.75 | 0.51 |
| 1:G:2570:GLY:HA2 | 1:G:2847:PHE:CE1 | 2.45 | 0.51 |
| 1:G:3205:GLU:HA | 1:G:3208:ARG:HB2 | 1.91 | 0.51 |
| 1:G:3385:ASP:OD1 | 1:G:3403:GLN:NE2 | 2.44 | 0.51 |
| 1:H:1963:ILE:HG23 | 1:H:1967:LEU:HD21 | 1.92 | 0.51 |
| 1:I:13:ASP:OD2 | 1:I:14:GLN:N | 2.44 | 0.51 |
| 1:I:204:GLU:OE2 | 1:I:354:ALA:N | 2.43 | 0.51 |
| 1:I:811:LYS:HD2 | 1:I:815:GLY:HA2 | 1.92 | 0.51 |
| 1:I:954:THR:HG22 | 1:I:965:PRO:HA | 1.92 | 0.51 |
| 1:I:1859:ALA:HB3 | 1:I:2014:ASP:OD2 | 2.10 | 0.51 |
| 1:I:2659:LEU:O | 1:I:2663:GLU:HG3 | 2.09 | 0.51 |
| 1:J:238:ASP:OD1 | 1:J:239:HIS:ND1 | 2.43 | 0.51 |
| 1:J:1284:ARG:NH2 | 1:J:1287:GLN:HG2 | 2.24 | 0.51 |
| 1:J:1489:LEU:O | 1:J:1493:ARG:NH1 | 2.24 | 0.51 |
| 1:J:2232:LEU:HD12 | 1:J:2274:LEU:HB3 | 1.90 | 0.51 |
| 1:K:330:ASP:OD1 | 1:K:331:HIS:N | 2.43 | 0.51 |
| 1:K:348:ILE:HD11 | 1:K:367:PHE:CD2 | 2.45 | 0.51 |
| 1:K:737:PHE:HE1 | 1:K:788:GLU:HG2 | 1.74 | 0.51 |
| 1:K:1315:CYS:HA | 1:K:1325:TRP:CH2 | 2.44 | 0.51 |
| 1:K:2345:ASN:O | 1:K:2349:ARG:HG2 | 2.10 | 0.51 |
| 1:K:2718:ILE:HD13 | 1:K:2779:LEU:HB3 | 1.90 | 0.51 |
| 1:L:598:ASP:HB3 | 1:L:601:ASP:HB3 | 1.92 | 0.51 |
| 1:L:1108:VAL:HG13 | 1:L:1111:GLU:OE1 | 2.11 | 0.51 |
| 1:L:2948:ASP:OD1 | 1:L:2948:ASP:N | 2.42 | 0.51 |
| 1:M:204:GLU:OE2 | 1:M:354:ALA:N | 2.43 | 0.51 |
| 1:M:752:ILE:O | 1:M:808:LEU:HA | 2.10 | 0.51 |
| 1:M:1362:ILE:HD12 | 1:M:1394:ARG:HH12 | 1.75 | 0.51 |
| 1:M:1554:ASP:N | 1:M:1554:ASP:OD2 | 2.43 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:M:1871:HIS:HD2 | 1:M:1873:HIS:HB2 | 1.75 | 0.51 |
| 1:N:1679:SER:OG | 1:N:1680:VAL:N | 2.43 | 0.51 |
| 1:N:1706:GLY:O | 1:N:1710:LEU:HG | 2.10 | 0.51 |
| 1:N:1995:HIS:ND1 | 1:N:2013:PHE:O | 2.43 | 0.51 |
| 1:N:3390:SER:HB3 | 1:N:3395:ARG:HG3 | 1.92 | 0.51 |
| 1:O:304:ARG:HA | 1:O:304:ARG:NE | 2.24 | 0.51 |
| 1:O:583:HIS:HB3 | 1:O:587:PHE:HD2 | 1.74 | 0.51 |
| 1:O:1189:GLU:N | 1:O:1189:GLU:OE1 | 2.43 | 0.51 |
| 1:O:1760:LEU:HD12 | 1:O:1761:VAL:HB | 1.91 | 0.51 |
| 1:P:1067:GLN:HA | 1:P:1070:ARG:HG2 | 1.91 | 0.51 |
| 1:P:3092:HIS:CG | 1:P:3103:MET:HE1 | 2.44 | 0.51 |
| 1:P:3270:LEU:HD12 | 1:P:3275:LEU:HB2 | 1.91 | 0.51 |
| 1:Q:24:ARG:NH2 | 1:Q:123:ASN:HA | 2.25 | 0.51 |
| 1:Q:738:VAL:HG23 | 1:Q:789:ILE:HG21 | 1.92 | 0.51 |
| 1:Q:1495:PRO:HA | 1:Q:1516:PRO:HD3 | 1.93 | 0.51 |
| 1:Q:3021:PRO:HD2 | 1:Q:3024:LEU:HD21 | 1.92 | 0.51 |
| 1:Q:3068:THR:O | 1:Q:3071:THR:OG1 | 2.27 | 0.51 |
| 1:R:654:LEU:HD13 | 1:R:723:LEU:HD11 | 1.92 | 0.51 |
| 1:R:1564:ASN:HB3 | 1:R:1604:PHE:CE1 | 2.45 | 0.51 |
| 1:S:1325:TRP:HE1 | 1:S:1498:PRO:HG3 | 1.75 | 0.51 |
| 1:S:2666:ASP:OD1 | 1:S:2669:ASN:HB2 | 2.10 | 0.51 |
| 1:A:704:HIS:ND1 | 1:A:705:GLU:OE2 | 2.44 | 0.51 |
| 1:A:1144:GLN:HA | 1:A:1148:ARG:HH22 | 1.76 | 0.51 |
| 1:A:2044:SER:OG | 1:A:2046:ASP:OD1 | 2.29 | 0.51 |
| 1:A:2201:ASP:OD1 | 1:A:2203:TRP:N | 2.35 | 0.51 |
| 1:A:3015:ARG:HG2 | 1:A:3016:PRO:HD2 | 1.91 | 0.51 |
| 1:B:456:GLN:NE2 | 1:B:553:PRO:O | 2.40 | 0.51 |
| 1:B:3103:MET:HA | 1:B:3109:SER:HA | 1.91 | 0.51 |
| 1:C:598:ASP:OD1 | 1:C:599:PHE:N | 2.44 | 0.51 |
| 1:C:2026:PHE:O | 1:D:1651:ARG:NH1 | 2.43 | 0.51 |
| 1:C:2960:HIS:HE1 | 1:C:3119:HIS:HE1 | 1.59 | 0.51 |
| 1:C:3171:ASN:HA | 1:C:3176:GLN:NE2 | 2.25 | 0.51 |
| 1:D:759:ASP:OD1 | 1:D:759:ASP:N | 2.43 | 0.51 |
| 1:D:787:VAL:HG23 | 1:D:789:ILE:HD11 | 1.92 | 0.51 |
| 1:D:855:THR:OG1 | 1:D:857:GLU:OE2 | 2.25 | 0.51 |
| 1:D:1421:ASP:O | 1:D:1424:ILE:HG22 | 2.11 | 0.51 |
| 1:D:2303:ASP:OD2 | 1:D:2367:TYR:OH | 2.25 | 0.51 |
| 1:E:734:ASP:OD1 | 1:E:734:ASP:N | 2.42 | 0.51 |
| 1:E:3118:HIS:O | 1:E:3121:SER:OG | 2.28 | 0.51 |
| 1:F:1415:GLU:OE2 | 1:F:1555:ARG:NH2 | 2.42 | 0.51 |
| 1:F:1827:ASP:HA | 1:F:1831:TRP:HD1 | 1.75 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:G:648:TRP:NE1 | 1:G:652:GLN:HE22 | 2.08 | 0.51 |
| 1:G:1815:ARG:HA | 1:G:1818:LEU:HG | 1.93 | 0.51 |
| 1:G:2080:ARG:HD3 | 1:G:2314:LYS:HE3 | 1.90 | 0.51 |
| 1:G:2376:ASN:O | 1:G:2379:GLU:HG2 | 2.10 | 0.51 |
| 1:H:79:GLN:O | 1:H:83:LYS:NZ | 2.43 | 0.51 |
| 1:H:378:LYS:NZ | 1:H:383:ASP:H | 2.09 | 0.51 |
| 1:H:3214:TYR:HB2 | 1:H:3263:LYS:HE2 | 1.92 | 0.51 |
| 1:I:1187:GLU:N | 1:I:1187:GLU:OE1 | 2.44 | 0.51 |
| 1:I:2557:CYS:HB3 | 1:I:2564:VAL:HG23 | 1.91 | 0.51 |
| 1:J:444:GLU:O | 1:J:447:GLU:HG2 | 2.11 | 0.51 |
| 1:J:722:GLN:NE2 | 1:J:932:ASP:OD1 | 2.43 | 0.51 |
| 1:J:2287:HIS:HE1 | 1:J:2432:LEU:HB2 | 1.75 | 0.51 |
| 1:J:3032:PHE:HA | 1:J:3113:PRO:HG2 | 1.92 | 0.51 |
| 1:K:50:LYS:NZ | 1:K:357:MET:SD | 2.80 | 0.51 |
| 1:K:699:ILE:HG13 | 1:K:706:LEU:HD21 | 1.92 | 0.51 |
| 1:K:1100:ASP:OD2 | 1:K:1102:ILE:HG22 | 2.11 | 0.51 |
| 1:K:2254:GLN:N | 1:K:2254:GLN:OE1 | 2.42 | 0.51 |
| 1:K:2273:TYR:HA | 1:K:2284:SER:OG | 2.11 | 0.51 |
| 1:L:859:VAL:HG12 | 1:L:863:ARG:NE | 2.25 | 0.51 |
| 1:L:934:LEU:HD23 | 1:L:1054:SER:HB3 | 1.93 | 0.51 |
| 1:L:1277:GLU:HA | 1:L:1280:LYS:HG2 | 1.92 | 0.51 |
| 1:L:1547:LEU:O | 1:L:1550:GLN:HG3 | 2.10 | 0.51 |
| 1:L:1602:MET:HE3 | 1:L:1603:PRO:HD2 | 1.92 | 0.51 |
| 1:L:2265:GLU:OE1 | 1:L:2268:HIS:NE2 | 2.33 | 0.51 |
| 1:M:143:ARG:NH2 | 1:M:209:ASP:OD2 | 2.43 | 0.51 |
| 1:M:647:LEU:O | 1:M:650:ILE:HG12 | 2.11 | 0.51 |
| 1:M:855:THR:O | 1:M:858:GLN:HG2 | 2.11 | 0.51 |
| 1:M:953:GLU:HG3 | 1:M:954:THR:HG23 | 1.93 | 0.51 |
| 1:M:1057:ASP:OD2 | 1:M:1123:TYR:OH | 2.26 | 0.51 |
| 1:M:2287:HIS:CD2 | 1:M:2430:GLY:HA3 | 2.45 | 0.51 |
| 1:N:244:VAL:HG22 | 1:N:828:ILE:HG21 | 1.92 | 0.51 |
| 1:N:784:LEU:O | 1:N:786:LYS:NZ | 2.31 | 0.51 |
| 1:N:1507:PHE:CE2 | 1:N:1509:LEU:HB3 | 2.46 | 0.51 |
| 1:N:2227:ASP:HB3 | 1:N:2277:GLY:HA3 | 1.92 | 0.51 |
| 1:O:624:SER:OG | 1:O:626:SER:OG | 2.26 | 0.51 |
| 1:O:1889:ASP:OD2 | 1:O:1955:TYR:OH | 2.25 | 0.51 |
| 1:O:2551:HIS:HB2 | 1:O:2581:PHE:CE1 | 2.43 | 0.51 |
| 1:P:434:ARG:HD2 | 1:P:710:TYR:CE1 | 2.46 | 0.51 |
| 1:P:1941:PRO:O | 1:P:1944:VAL:HG22 | 2.10 | 0.51 |
| 1:P:2044:SER:N | 1:P:2047:ASP:OD2 | 2.40 | 0.51 |
| 1:P:2296:PHE:O | 1:P:2300:THR:HG23 | 2.09 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:P:2583:VAL:HG21 | 1:P:2772:PHE:HD2 | 1.74 | 0.51 |
| 1:Q:452:LEU:HD23 | 1:Q:553:PRO:HB2 | 1.92 | 0.51 |
| 1:Q:767:LYS:HD3 | 1:Q:768:LEU:H | 1.74 | 0.51 |
| 1:Q:1756:ARG:NH2 | 1:R:2176:VAL:HG13 | 2.24 | 0.51 |
| 1:Q:2960:HIS:HA | 1:Q:2987:TRP:HH2 | 1.75 | 0.51 |
| 1:Q:3203:ILE:HA | 1:Q:3206:ASN:HB2 | 1.92 | 0.51 |
| 1:R:403:LEU:O | 1:R:405:ARG:NH1 | 2.43 | 0.51 |
| 1:R:571:GLN:NE2 | 1:R:616:LEU:O | 2.28 | 0.51 |
| 1:R:1254:ILE:HG23 | 1:R:1256:LYS:H | 1.74 | 0.51 |
| 1:R:1709:ALA:O | 1:R:1712:SER:OG | 2.23 | 0.51 |
| 1:R:1845:ASP:HB3 | 1:R:2028:ARG:HD2 | 1.93 | 0.51 |
| 1:R:3103:MET:HA | 1:R:3109:SER:HA | 1.93 | 0.51 |
| 1:R:3132:LEU:HG | 1:R:3136:ARG:NH1 | 2.26 | 0.51 |
| 1:S:674:LEU:HD22 | 1:S:695:ARG:NH2 | 2.25 | 0.51 |
| 1:S:915:ARG:HH21 | 1:S:1115:TYR:HB3 | 1.75 | 0.51 |
| 1:S:1946:ASP:OD1 | 1:S:1946:ASP:N | 2.39 | 0.51 |
| 1:S:2044:SER:OG | 1:S:2046:ASP:OD1 | 2.29 | 0.51 |
| 1:S:2328:ASN:HB3 | 1:T:1241:VAL:HB | 1.92 | 0.51 |
| 1:T:1535:PHE:O | 1:T:1538:TRP:HB2 | 2.11 | 0.51 |
| 1:T:2296:PHE:O | 1:T:2300:THR:HG23 | 2.11 | 0.51 |
| 1:T:2454:HIS:HA | 1:T:2456:ARG:HH22 | 1.75 | 0.51 |
| 1:T:2736:ASN:HB3 | 1:T:2739:GLU:HB2 | 1.93 | 0.51 |
| 1:A:304:ARG:HA | 1:A:304:ARG:NE | 2.25 | 0.51 |
| 1:A:949:ILE:HG23 | 1:A:950:VAL:HG13 | 1.92 | 0.51 |
| 1:A:1426:PHE:CE1 | 1:A:1464:VAL:HG13 | 2.42 | 0.51 |
| 1:B:1084:LEU:HB3 | 1:B:1110:PHE:HE2 | 1.75 | 0.51 |
| 1:B:2740:LEU:O | 1:B:2763:ALA:HB3 | 2.10 | 0.51 |
| 1:C:1030:GLY:HA3 | 1:C:1038:ALA:HB2 | 1.92 | 0.51 |
| 1:C:2027:ASP:HA | 1:D:1651:ARG:HH12 | 1.75 | 0.51 |
| 1:C:2443:LYS:HG3 | 1:C:2492:ILE:HD11 | 1.92 | 0.51 |
| 1:C:3229:ASN:OD1 | 1:C:3231:LYS:NZ | 2.35 | 0.51 |
| 1:D:848:ARG:H | 1:D:1123:TYR:HA | 1.75 | 0.51 |
| 1:D:1967:LEU:HD23 | 1:D:1967:LEU:H | 1.75 | 0.51 |
| 1:D:2273:TYR:HE2 | 1:D:2407:GLU:HB2 | 1.76 | 0.51 |
| 1:D:2587:ARG:HH22 | 1:D:2753:PRO:HG2 | 1.75 | 0.51 |
| 1:D:2630:LEU:HG | 1:D:2632:GLU:OE1 | 2.10 | 0.51 |
| 1:D:3155:GLU:OE2 | 1:D:3158:ASN:ND2 | 2.43 | 0.51 |
| 1:E:540:THR:HG22 | 1:E:551:HIS:HA | 1.93 | 0.51 |
| 1:E:1268:LEU:HD12 | 1:E:1361:LEU:HD13 | 1.92 | 0.51 |
| 1:E:2956:ILE:HD12 | 1:E:2959:PHE:HE2 | 1.75 | 0.51 |
| 1:E:3131:THR:HA | 1:E:3134:LYS:HG2 | 1.92 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:F:170:GLU:OE1 | 1:F:170:GLU:N | 2.41 | 0.51 |
| 1:F:1848:VAL:HA | 1:F:2026:PHE:HE2 | 1.75 | 0.51 |
| 1:F:2152:PRO:HD2 | 1:F:2329:TYR:CD2 | 2.46 | 0.51 |
| 1:F:3144:ARG:HG3 | 1:F:3147:LEU:HD11 | 1.92 | 0.51 |
| 1:G:1100:ASP:OD2 | 1:G:1102:ILE:HG22 | 2.10 | 0.51 |
| 1:G:1221:TYR:OH | 1:G:1236:PHE:N | 2.41 | 0.51 |
| 1:G:1568:SER:HB2 | 1:G:1597:GLY:H | 1.75 | 0.51 |
| 1:H:741:HIS:CE1 | 1:H:780:ASN:HD21 | 2.26 | 0.51 |
| 1:H:859:VAL:HG12 | 1:H:863:ARG:NE | 2.24 | 0.51 |
| 1:H:991:LYS:HB3 | 1:H:994:ARG:HE | 1.74 | 0.51 |
| 1:H:1917:ARG:O | 1:H:1940:LYS:NZ | 2.43 | 0.51 |
| 1:H:2488:LYS:NZ | 1:H:2489:PRO:O | 2.42 | 0.51 |
| 1:J:257:ASP:HA | 1:J:265:ARG:HD3 | 1.93 | 0.51 |
| 1:J:1363:ASN:OD1 | 1:J:1364:GLU:N | 2.43 | 0.51 |
| 1:J:2273:TYR:HB3 | 1:J:2426:PHE:CD1 | 2.44 | 0.51 |
| 1:J:2376:ASN:OD1 | 1:J:2377:LEU:N | 2.42 | 0.51 |
| 1:J:2610:LEU:HG | 1:J:2614:LEU:HD23 | 1.91 | 0.51 |
| 1:K:592:LEU:HD22 | 1:K:788:GLU:HG3 | 1.92 | 0.51 |
| 1:M:2509:SER:HB3 | 1:M:3138:ARG:HH12 | 1.75 | 0.51 |
| 1:N:188:ILE:HD13 | 1:N:215:HIS:NE2 | 2.25 | 0.51 |
| 1:N:525:TRP:CD1 | 1:N:586:LEU:HD13 | 2.45 | 0.51 |
| 1:N:2535:VAL:HA | 1:N:2538:GLN:HG3 | 1.93 | 0.51 |
| 1:O:1742:TRP:CD1 | 1:O:1920:LEU:HD12 | 2.45 | 0.51 |
| 1:P:1026:HIS:HB3 | 1:P:1037:MET:HE1 | 1.93 | 0.51 |
| 1:P:2338:ASN:OD1 | 1:P:2339:SER:N | 2.43 | 0.51 |
| 1:P:2357:VAL:HG13 | 1:P:2363:LEU:HD11 | 1.92 | 0.51 |
| 1:P:2602:ASP:OD1 | 1:P:2603:TRP:N | 2.43 | 0.51 |
| 1:Q:1830:LEU:HG | 1:Q:1834:PHE:CE2 | 2.46 | 0.51 |
| 1:Q:2556:LEU:HD23 | 1:Q:2556:LEU:H | 1.75 | 0.51 |
| 1:Q:2569:HIS:HA | 1:Q:2574:PHE:CZ | 2.45 | 0.51 |
| 1:R:859:VAL:HG12 | 1:R:863:ARG:NE | 2.24 | 0.51 |
| 1:R:936:TYR:HA | 1:R:1051:LEU:HB2 | 1.92 | 0.51 |
| 1:R:2610:LEU:HG | 1:R:2614:LEU:HD23 | 1.90 | 0.51 |
| 1:S:454:ARG:HH21 | 1:S:514:ARG:HB3 | 1.76 | 0.51 |
| 1:S:602:PHE:HA | 1:S:605:GLN:NE2 | 2.24 | 0.51 |
| 1:S:1017:GLN:HA | 1:S:1020:ILE:HG22 | 1.93 | 0.51 |
| 1:S:1313:ALA:H | 1:S:1600:THR:HG22 | 1.76 | 0.51 |
| 1:S:1585:ASN:OD1 | 1:S:1586:CYS:N | 2.43 | 0.51 |
| 1:S:1828:ASN:OD1 | 1:S:1829:TRP:N | 2.43 | 0.51 |
| 1:S:1890:ARG:HB2 | 1:S:1955:TYR:CE2 | 2.46 | 0.51 |
| 1:S:2147:CYS:O | 1:S:2149:HIS:ND1 | 2.37 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:S:2673:GLN:NE2 | 1:S:2852:GLN:H | 2.08 | 0.51 |
| 1:T:200:LEU:HD23 | 1:T:206:SER:HA | 1.93 | 0.51 |
| 1:T:2159:ARG:NE | 1:T:2303:ASP:OD1 | 2.28 | 0.51 |
| 1:A:193:GLY:HA3 | 1:A:201:SER:H | 1.74 | 0.51 |
| 1:A:580:TYR:CG | 1:A:958:PRO:HG2 | 2.45 | 0.51 |
| 1:A:1739:PHE:HB3 | 1:A:1740:PRO:HD3 | 1.92 | 0.51 |
| 1:A:2439:ASP:OD1 | 1:A:2439:ASP:N | 2.42 | 0.51 |
| 1:A:2696:LEU:HD21 | 1:A:2839:GLY:HA3 | 1.93 | 0.51 |
| 1:A:3276:ASN:OD1 | 1:A:3277:ALA:N | 2.42 | 0.51 |
| 1:B:950:VAL:HA | 1:B:968:PHE:HB3 | 1.91 | 0.51 |
| 1:C:1026:HIS:HD2 | 1:C:1184:LEU:HD11 | 1.74 | 0.51 |
| 1:C:1767:ASP:OD2 | 1:C:1890:ARG:NH1 | 2.44 | 0.51 |
| 1:C:2981:MET:SD | 1:C:2982:PRO:HD2 | 2.51 | 0.51 |
| 1:D:994:ARG:HE | 1:D:995:LEU:H | 1.59 | 0.51 |
| 1:D:1232:SER:OG | 1:D:1234:GLU:OE1 | 2.29 | 0.51 |
| 1:D:1274:GLY:O | 1:D:1277:GLU:HG3 | 2.10 | 0.51 |
| 1:D:2017:GLY:HA2 | 1:D:2021:GLU:OE2 | 2.10 | 0.51 |
| 1:E:866:LEU:HD22 | 1:E:968:PHE:CE1 | 2.46 | 0.51 |
| 1:E:1153:PHE:HE1 | 1:E:1166:LEU:HD21 | 1.75 | 0.51 |
| 1:E:2383:GLU:O | 1:E:2387:HIS:ND1 | 2.40 | 0.51 |
| 1:E:2805:ASN:ND2 | 1:E:2852:GLN:OE1 | 2.43 | 0.51 |
| 1:F:188:ILE:HD13 | 1:F:215:HIS:NE2 | 2.24 | 0.51 |
| 1:F:2991:LEU:HA | 1:F:2994:GLN:HE21 | 1.75 | 0.51 |
| 1:F:3144:ARG:HA | 1:F:3147:LEU:HG | 1.93 | 0.51 |
| 1:G:584:THR:HG23 | 1:G:587:PHE:H | 1.76 | 0.51 |
| 1:G:1166:LEU:HD22 | 1:G:1200:TYR:HD2 | 1.76 | 0.51 |
| 1:G:1577:VAL:HG12 | 1:J:337:GLN:HB3 | 1.92 | 0.51 |
| 1:G:1621:LEU:O | 1:H:2786:ILE:HD13 | 2.10 | 0.51 |
| 1:G:1646:GLU:OE1 | 1:G:1646:GLU:N | 2.42 | 0.51 |
| 1:G:1742:TRP:CD1 | 1:G:1920:LEU:HD12 | 2.46 | 0.51 |
| 1:G:2164:GLN:OE1 | 1:G:2167:GLN:NE2 | 2.43 | 0.51 |
| 1:G:2601:TRP:CD1 | 1:G:2611:PRO:HB3 | 2.45 | 0.51 |
| 1:G:3399:GLY:HA2 | 1:G:3401:ARG:HH21 | 1.75 | 0.51 |
| 1:H:434:ARG:NH2 | 1:H:508:GLU:OE2 | 2.43 | 0.51 |
| 1:H:1169:CYS:HA | 1:H:1175:CYS:HA | 1.93 | 0.51 |
| 1:H:1172:SER:HG | 1:H:1216:ARG:HH22 | 1.58 | 0.51 |
| 1:H:2636:ARG:HH21 | 1:H:2702:ASP:CG | 2.19 | 0.51 |
| 1:H:3389:VAL:HG12 | 1:H:3401:ARG:HE | 1.74 | 0.51 |
| 1:I:2246:ASP:N | 1:I:2246:ASP:OD1 | 2.43 | 0.51 |
| 1:J:81:LEU:HB3 | 1:J:86:LEU:HB2 | 1.92 | 0.51 |
| 1:J:1539:THR:HG22 | 1:J:1542:GLN:NE2 | 2.26 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:J:1576:CYS:N | 1:J:1632:ASP:O | 2.44 | 0.51 |
| 1:J:2817:VAL:O | 1:J:2833:THR:OG1 | 2.18 | 0.51 |
| 1:K:794:ASN:OD1 | 1:K:795:LYS:N | 2.43 | 0.51 |
| 1:K:2126:LEU:O | 1:K:2161:TYR:OH | 2.29 | 0.51 |
| 1:M:1166:LEU:HD22 | 1:M:1200:TYR:HD2 | 1.76 | 0.51 |
| 1:N:581:GLY:H | 1:N:856:ARG:NH2 | 2.08 | 0.51 |
| 1:N:2283:LEU:HD21 | 1:N:2292:ASP:HB3 | 1.92 | 0.51 |
| 1:N:3017:SER:O | 1:N:3055:ARG:NH2 | 2.39 | 0.51 |
| 1:O:938:ASP:HA | 1:O:1055:ASN:HD21 | 1.76 | 0.51 |
| 1:O:1495:PRO:HA | 1:O:1516:PRO:HD3 | 1.93 | 0.51 |
| 1:O:1809:VAL:HG23 | 1:O:1868:SER:HA | 1.91 | 0.51 |
| 1:O:2454:HIS:O | 1:O:2456:ARG:NH1 | 2.44 | 0.51 |
| 1:O:2827:HIS:ND1 | 1:O:2827:HIS:O | 2.44 | 0.51 |
| 1:P:217:SER:O | 1:P:283:TYR:OH | 2.20 | 0.51 |
| 1:P:468:ALA:HB1 | 1:P:633:PHE:HA | 1.92 | 0.51 |
| 1:P:1978:LYS:HD2 | 1:P:2078:LYS:HZ1 | 1.75 | 0.51 |
| 1:P:3092:HIS:CD2 | 1:P:3103:MET:HE1 | 2.45 | 0.51 |
| 1:Q:231:LYS:HD3 | 1:Q:237:TYR:CE1 | 2.45 | 0.51 |
| 1:Q:718:MET:HE1 | 1:Q:723:LEU:HG | 1.92 | 0.51 |
| 1:Q:1189:GLU:N | 1:Q:1189:GLU:OE1 | 2.44 | 0.51 |
| 1:Q:1324:HIS:HD2 | 1:Q:1519:VAL:HB | 1.76 | 0.51 |
| 1:Q:2328:ASN:HB3 | 1:R:1241:VAL:HB | 1.93 | 0.51 |
| 1:Q:2579:ARG:HH12 | 1:Q:2769:TYR:HB3 | 1.75 | 0.51 |
| 1:Q:3085:GLU:HG3 | 1:Q:3086:MET:HE2 | 1.92 | 0.51 |
| 1:R:231:LYS:HB3 | 1:R:237:TYR:HE2 | 1.75 | 0.51 |
| 1:R:505:VAL:HG21 | 1:R:706:LEU:HD12 | 1.93 | 0.51 |
| 1:R:2865:ARG:HG3 | 1:R:2867:ASP:H | 1.76 | 0.51 |
| 1:R:3127:GLN:HE22 | 1:R:3190:LEU:HD21 | 1.76 | 0.51 |
| 1:R:3296:ASP:N | 1:R:3296:ASP:OD1 | 2.44 | 0.51 |
| 1:S:255:ASP:OD1 | 1:S:255:ASP:N | 2.43 | 0.51 |
| 1:S:539:GLU:N | 1:S:539:GLU:OE1 | 2.42 | 0.51 |
| 1:S:2729:ASP:OD1 | 1:S:2916:THR:OG1 | 2.27 | 0.51 |
| 1:S:2780:ASN:OD1 | 1:S:2784:LEU:N | 2.44 | 0.51 |
| 1:S:3205:GLU:HA | 1:S:3208:ARG:HB2 | 1.93 | 0.51 |
| 1:A:1388:THR:OG1 | 1:A:1390:LYS:NZ | 2.44 | 0.51 |
| 1:A:1708:GLN:HE21 | 1:A:1803:ALA:HB2 | 1.74 | 0.51 |
| 1:A:1914:GLU:OE1 | 1:B:1655:LEU:HD23 | 2.10 | 0.51 |
| 1:B:571:GLN:NE2 | 1:B:616:LEU:O | 2.32 | 0.51 |
| 1:B:1910:ASN:OD1 | 1:B:1911:CYS:N | 2.44 | 0.51 |
| 1:B:2041:LYS:HG3 | 1:B:2043:LEU:HD23 | 1.93 | 0.51 |
| 1:B:3020:LEU:HD13 | 1:B:3024:LEU:HB2 | 1.93 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:418:ASP:OD2 | 1:C:662:TYR:N | 2.44 | 0.51 |
| 1:C:539:GLU:HA | 1:C:555:PHE:HB2 | 1.93 | 0.51 |
| 1:C:580:TYR:CG | 1:C:958:PRO:HG2 | 2.45 | 0.51 |
| 1:C:582:ASP:O | 1:C:583:HIS:ND1 | 2.43 | 0.51 |
| 1:C:675:LEU:HD11 | 1:C:696:PRO:HG3 | 1.93 | 0.51 |
| 1:C:714:GLN:OE1 | 1:C:718:MET:N | 2.44 | 0.51 |
| 1:C:1048:ILE:HA | 1:C:1051:LEU:HD12 | 1.92 | 0.51 |
| 1:C:1568:SER:HB2 | 1:C:1597:GLY:H | 1.75 | 0.51 |
| 1:D:3020:LEU:HD13 | 1:D:3024:LEU:HB2 | 1.93 | 0.51 |
| 1:E:1420:CYS:HB2 | 1:E:1608:ARG:NH2 | 2.25 | 0.51 |
| 1:E:2328:ASN:HB3 | 1:F:1241:VAL:HB | 1.91 | 0.51 |
| 1:F:307:GLU:O | 1:F:308:ARG:NE | 2.44 | 0.51 |
| 1:F:313:PHE:CE2 | 1:F:406:PRO:HB3 | 2.46 | 0.51 |
| 1:F:859:VAL:HG12 | 1:F:863:ARG:NE | 2.26 | 0.51 |
| 1:F:974:GLU:OE2 | 1:F:1035:TYR:OH | 2.28 | 0.51 |
| 1:G:449:ARG:HD3 | 1:G:541:TYR:CZ | 2.46 | 0.51 |
| 1:G:734:ASP:OD1 | 1:G:734:ASP:N | 2.42 | 0.51 |
| 1:H:780:ASN:OD1 | 1:H:781:PHE:N | 2.44 | 0.51 |
| 1:H:1560:PHE:HZ | 1:H:1573:LEU:HD11 | 1.74 | 0.51 |
| 1:I:2225:VAL:HG13 | 1:I:2279:GLN:HG3 | 1.93 | 0.51 |
| 1:I:3036:GLN:HB2 | 1:I:3043:GLN:HE22 | 1.76 | 0.51 |
| 1:I:3308:PRO:HG2 | 1:I:3311:ALA:HB3 | 1.92 | 0.51 |
| 1:J:699:ILE:H | 1:J:699:ILE:HD12 | 1.75 | 0.51 |
| 1:K:1651:ARG:NH1 | 1:L:2025:SER:OG | 2.43 | 0.51 |
| 1:L:842:HIS:NE2 | 1:L:844:GLU:HB2 | 2.26 | 0.51 |
| 1:L:1276:VAL:HG12 | 1:L:1280:LYS:HE3 | 1.93 | 0.51 |
| 1:L:1744:ARG:NE | 1:L:1889:ASP:OD1 | 2.43 | 0.51 |
| 1:L:3124:ARG:O | 1:L:3128:ILE:HG12 | 2.11 | 0.51 |
| 1:M:1919:PRO:O | 1:M:1921:LYS:NZ | 2.34 | 0.51 |
| 1:M:2473:ILE:HD12 | 1:M:2483:PRO:HA | 1.93 | 0.51 |
| 1:M:2556:LEU:HD23 | 1:M:2556:LEU:H | 1.75 | 0.51 |
| 1:M:2604:THR:HA | 1:M:2654:PHE:CE1 | 2.45 | 0.51 |
| 1:M:2974:TYR:HB3 | 1:N:3367:PRO:HB2 | 1.93 | 0.51 |
| 1:N:737:PHE:HB2 | 1:N:829:ILE:HB | 1.92 | 0.51 |
| 1:N:3296:ASP:OD1 | 1:N:3296:ASP:N | 2.42 | 0.51 |
| 1:O:1698:LEU:HD13 | 1:O:1757:ARG:HD2 | 1.91 | 0.51 |
| 1:O:2569:HIS:HA | 1:O:2574:PHE:CE1 | 2.45 | 0.51 |
| 1:O:2693:MET:HG2 | 1:O:2699:SER:HA | 1.93 | 0.51 |
| 1:P:1979:SER:H | 1:P:2078:LYS:HZ1 | 1.56 | 0.51 |
| 1:Q:811:LYS:HD2 | 1:Q:815:GLY:HA2 | 1.91 | 0.51 |
| 1:Q:888:PRO:HG2 | 1:Q:890:TRP:CH2 | 2.46 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:Q:2080:ARG:HD3 | 1:Q:2314:LYS:HE3 | 1.93 | 0.51 |
| 1:Q:2345:ASN:O | 1:Q:2349:ARG:HG2 | 2.11 | 0.51 |
| 1:Q:2598:ILE:HD11 | 1:Q:2707:ILE:HD13 | 1.92 | 0.51 |
| 1:R:848:ARG:HD2 | 1:R:1123:TYR:CE1 | 2.46 | 0.51 |
| 1:R:1232:SER:OG | 1:R:1234:GLU:OE1 | 2.28 | 0.51 |
| 1:R:2589:LEU:O | 1:R:2592:GLN:NE2 | 2.25 | 0.51 |
| 1:R:3081:GLU:OE1 | 1:R:3081:GLU:N | 2.44 | 0.51 |
| 1:R:3163:ASN:ND2 | 1:R:3168:THR:OG1 | 2.44 | 0.51 |
| 1:S:1093:GLN:HB2 | 1:S:1097:ILE:HG21 | 1.92 | 0.51 |
| 1:S:1187:GLU:N | 1:S:1187:GLU:OE1 | 2.44 | 0.51 |
| 1:S:1518:ASP:OD1 | 1:S:1525:HIS:ND1 | 2.36 | 0.51 |
| 1:S:2117:ASP:OD1 | 1:S:2119:THR:OG1 | 2.25 | 0.51 |
| 1:T:196:HIS:HE1 | 1:T:198:HIS:HB2 | 1.76 | 0.51 |
| 1:T:571:GLN:NE2 | 1:T:616:LEU:O | 2.31 | 0.51 |
| 1:T:859:VAL:HG12 | 1:T:863:ARG:NE | 2.25 | 0.51 |
| 1:T:953:GLU:HA | 1:T:969:HIS:HB2 | 1.92 | 0.51 |
| 1:T:1067:GLN:HA | 1:T:1070:ARG:HG2 | 1.93 | 0.51 |
| 1:T:2856:THR:O | 1:T:2860:ASN:ND2 | 2.43 | 0.51 |
| 1:A:2802:VAL:H | 1:A:2856:THR:HG22 | 1.76 | 0.51 |
| 1:B:735:ARG:NH2 | 1:B:790:THR:H | 2.09 | 0.51 |
| 1:B:1111:GLU:N | 1:B:1111:GLU:OE1 | 2.44 | 0.51 |
| 1:B:1149:VAL:H | 1:B:1203:THR:HG1 | 1.59 | 0.51 |
| 1:B:2111:LEU:HD13 | 1:B:2212:PHE:CE1 | 2.46 | 0.51 |
| 1:B:2551:HIS:HB2 | 1:B:2700:ALA:HB2 | 1.92 | 0.51 |
| 1:B:2695:THR:HG21 | 1:B:2698:TYR:CD2 | 2.46 | 0.51 |
| 1:C:1124:ASP:OD1 | 1:C:1125:ASP:N | 2.41 | 0.51 |
| 1:D:188:ILE:HA | 1:D:191:LEU:HB2 | 1.92 | 0.51 |
| 1:D:1579:THR:HG21 | 1:D:1585:ASN:HB3 | 1.93 | 0.51 |
| 1:E:2147:CYS:O | 1:E:2149:HIS:ND1 | 2.44 | 0.51 |
| 1:F:499:TRP:NE1 | 1:F:676:LYS:O | 2.38 | 0.51 |
| 1:F:2254:GLN:HE21 | 1:F:2260:PHE:HA | 1.76 | 0.51 |
| 1:F:2343:ASN:HB3 | 1:F:2349:ARG:HH22 | 1.75 | 0.51 |
| 1:G:849:SER:OG | 1:G:850:ASP:N | 2.44 | 0.51 |
| 1:G:938:ASP:HA | 1:G:1055:ASN:HD21 | 1.76 | 0.51 |
| 1:G:1100:ASP:O | 1:G:1104:ARG:NH1 | 2.44 | 0.51 |
| 1:G:1522:TYR:HA | 1:G:1526:PHE:HD2 | 1.76 | 0.51 |
| 1:H:220:ASP:OD1 | 1:H:221:ARG:N | 2.44 | 0.51 |
| 1:H:444:GLU:O | 1:H:447:GLU:HG2 | 2.11 | 0.51 |
| 1:H:1136:LEU:O | 1:H:1140:ILE:HG12 | 2.11 | 0.51 |
| 1:H:1742:TRP:CD1 | 1:H:1920:LEU:HD12 | 2.43 | 0.51 |
| 1:H:2124:GLN:HG2 | 1:H:2125:ALA:N | 2.26 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:I:255:ASP:OD1 | 1:I:255:ASP:N | 2.43 | 0.51 |
| 1:I:595:GLU:N | 1:I:595:GLU:OE1 | 2.44 | 0.51 |
| 1:J:2820:ASP:OD1 | 1:J:2829:SER:N | 2.44 | 0.51 |
| 1:K:2529:LYS:HD3 | 1:K:2613:LEU:HD11 | 1.93 | 0.51 |
| 1:L:597:ARG:NH2 | 1:L:658:ARG:HB2 | 2.25 | 0.51 |
| 1:L:604:VAL:O | 1:L:608:VAL:HG23 | 2.10 | 0.51 |
| 1:L:887:GLN:HE22 | 1:L:889:ASN:HB2 | 1.75 | 0.51 |
| 1:L:950:VAL:HA | 1:L:968:PHE:HB3 | 1.92 | 0.51 |
| 1:L:1397:GLN:HB2 | 1:L:1400:LEU:HD23 | 1.92 | 0.51 |
| 1:L:2191:PRO:HG2 | 1:L:2194:PHE:HD2 | 1.75 | 0.51 |
| 1:L:3133:GLN:HB3 | 1:L:3138:ARG:HB2 | 1.92 | 0.51 |
| 1:M:1359:PRO:HB2 | 1:M:1362:ILE:HG12 | 1.93 | 0.51 |
| 1:M:1466:ARG:HA | 1:M:1530:TYR:HE2 | 1.75 | 0.51 |
| 1:M:1903:GLY:HA3 | 1:N:1667:GLN:HB2 | 1.93 | 0.51 |
| 1:N:1126:LEU:H | 1:N:1126:LEU:HD23 | 1.76 | 0.51 |
| 1:N:2558:LYS:HD2 | 1:N:2563:THR:HA | 1.93 | 0.51 |
| 1:P:196:HIS:CE1 | 1:P:198:HIS:HB2 | 2.46 | 0.51 |
| 1:P:496:PHE:HB3 | 1:P:497:PRO:HD3 | 1.93 | 0.51 |
| 1:P:1015:GLU:N | 1:P:1015:GLU:OE1 | 2.42 | 0.51 |
| 1:P:1299:HIS:HB3 | 1:P:1452:ALA:HB2 | 1.92 | 0.51 |
| 1:P:1356:ARG:HH12 | 1:P:1402:ASN:H | 1.59 | 0.51 |
| 1:P:2433:GLU:N | 1:P:2433:GLU:OE1 | 2.44 | 0.51 |
| 1:Q:1710:LEU:HB3 | 1:Q:1750:PHE:CE1 | 2.45 | 0.51 |
| 1:Q:1733:VAL:HG23 | 1:Q:1736:MET:HE2 | 1.92 | 0.51 |
| 1:Q:2511:ILE:H | 1:Q:2596:VAL:HG12 | 1.75 | 0.51 |
| 1:R:2210:ASN:HD21 | 1:R:2212:PHE:HB2 | 1.76 | 0.51 |
| 1:S:288:LEU:N | 1:S:291:LEU:O | 2.39 | 0.51 |
| 1:S:1489:LEU:HD11 | 1:T:2075:TYR:HB2 | 1.93 | 0.51 |
| 1:S:1568:SER:HB2 | 1:S:1597:GLY:H | 1.75 | 0.51 |
| 1:S:2570:GLY:H | 1:S:2574:PHE:HE2 | 1.58 | 0.51 |
| 1:S:3015:ARG:HE | 1:S:3016:PRO:HD2 | 1.76 | 0.51 |
| 1:S:3339:ARG:NH2 | 1:S:3376:ASP:O | 2.44 | 0.51 |
| 1:T:1742:TRP:CD1 | 1:T:1920:LEU:HD12 | 2.46 | 0.51 |
| 1:T:3200:ILE:HA | 1:T:3203:ILE:HD12 | 1.93 | 0.51 |
| 1:A:794:ASN:OD1 | 1:A:795:LYS:N | 2.44 | 0.51 |
| 1:A:1433:LEU:HD21 | 1:A:1460:HIS:CE1 | 2.46 | 0.51 |
| 1:B:618:GLY:HA3 | 1:B:626:SER:N | 2.26 | 0.51 |
| 1:B:887:GLN:HE22 | 1:B:889:ASN:HB2 | 1.75 | 0.51 |
| 1:B:917:LEU:O | 1:B:920:GLN:NE2 | 2.37 | 0.51 |
| 1:B:1167:GLU:HA | 1:B:1177:PRO:HA | 1.92 | 0.51 |
| 1:B:1365:ALA:HA | 1:B:1378:ASN:HB3 | 1.93 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:2660:LEU:HD21 | 1:B:2803:PHE:HE1 | 1.76 | 0.51 |
| 1:B:3270:LEU:HD12 | 1:B:3275:LEU:HB2 | 1.93 | 0.51 |
| 1:C:481:ASP:OD1 | 1:F:1644:TYR:N | 2.43 | 0.51 |
| 1:C:513:SER:OG | 1:C:514:ARG:NH1 | 2.41 | 0.51 |
| 1:C:1159:ARG:NE | 1:C:1186:ASP:O | 2.41 | 0.51 |
| 1:C:1324:HIS:HD2 | 1:C:1519:VAL:HB | 1.76 | 0.51 |
| 1:C:2663:GLU:HA | 1:C:2793:ILE:HD11 | 1.92 | 0.51 |
| 1:C:2861:GLN:OE1 | 1:D:1538:TRP:NE1 | 2.39 | 0.51 |
| 1:C:3226:ALA:HA | 1:C:3289:LYS:HA | 1.90 | 0.51 |
| 1:C:3312:ASP:OD1 | 1:C:3313:TYR:N | 2.43 | 0.51 |
| 1:D:1281:SER:O | 1:D:1285:ARG:HG2 | 2.11 | 0.51 |
| 1:D:2433:GLU:N | 1:D:2433:GLU:OE1 | 2.43 | 0.51 |
| 1:D:2639:ARG:HD3 | 1:D:2641:GLN:HE22 | 1.76 | 0.51 |
| 1:E:1114:ASP:N | 1:E:1114:ASP:OD1 | 2.44 | 0.51 |
| 1:F:646:ARG:O | 1:F:650:ILE:HG12 | 2.10 | 0.51 |
| 1:F:1075:ASN:HB2 | 1:F:1113:PHE:HB3 | 1.93 | 0.51 |
| 1:F:1847:GLU:CD | 1:F:1847:GLU:H | 2.19 | 0.51 |
| 1:F:2338:ASN:OD1 | 1:F:2339:SER:N | 2.43 | 0.51 |
| 1:F:2602:ASP:OD1 | 1:F:2603:TRP:N | 2.43 | 0.51 |
| 1:F:2820:ASP:HB3 | 1:F:2873:ASP:OD1 | 2.11 | 0.51 |
| 1:F:3000:ARG:NH2 | 1:F:3004:ALA:O | 2.44 | 0.51 |
| 1:F:3017:SER:O | 1:F:3055:ARG:NH2 | 2.44 | 0.51 |
| 1:F:3058:GLN:N | 1:F:3061:LEU:O | 2.35 | 0.51 |
| 1:F:3389:VAL:HG12 | 1:F:3401:ARG:HE | 1.76 | 0.51 |
| 1:G:1367:TYR:CZ | 1:G:1376:GLU:HB3 | 2.46 | 0.51 |
| 1:G:1430:HIS:CD2 | 1:G:1460:HIS:HE1 | 2.29 | 0.51 |
| 1:G:2246:ASP:OD1 | 1:G:2246:ASP:N | 2.43 | 0.51 |
| 1:G:2392:ARG:HB3 | 1:G:2394:PHE:HE1 | 1.76 | 0.51 |
| 1:G:2461:PHE:HE1 | 1:H:1081:ILE:HG12 | 1.75 | 0.51 |
| 1:G:3301:THR:HB | 1:G:3325:LYS:HB3 | 1.93 | 0.51 |
| 1:H:920:GLN:HB2 | 1:H:1103:THR:HG21 | 1.93 | 0.51 |
| 1:H:2938:ARG:NH2 | 1:H:3029:ASN:OD1 | 2.43 | 0.51 |
| 1:H:3260:ARG:HH12 | 1:H:3333:SER:HA | 1.75 | 0.51 |
| 1:I:2090:ASN:C | 1:I:2091:ARG:HD3 | 2.36 | 0.51 |
| 1:I:2796:ARG:HH22 | 1:I:2801:ARG:HE | 1.58 | 0.51 |
| 1:I:3228:ALA:O | 1:I:3245:PHE:N | 2.44 | 0.51 |
| 1:J:493:MET:HE1 | 1:J:495:THR:HG22 | 1.92 | 0.51 |
| 1:J:960:THR:OG1 | 1:J:964:GLU:OE2 | 2.25 | 0.51 |
| 1:J:1321:VAL:HG11 | 1:J:1491:ILE:HG21 | 1.93 | 0.51 |
| 1:J:3119:HIS:O | 1:J:3122:ILE:HG22 | 2.11 | 0.51 |
| 1:K:47:MET:C | 1:K:55:ARG:HH12 | 2.19 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:K:1067:GLN:NE2 | 1:K:1073:PRO:O | 2.41 | 0.51 |
| 1:K:1189:GLU:N | 1:K:1189:GLU:OE1 | 2.43 | 0.51 |
| 1:K:2724:ARG:NH1 | 1:K:2730:TYR:OH | 2.44 | 0.51 |
| 1:K:2737:ILE:H | 1:K:2737:ILE:HD12 | 1.75 | 0.51 |
| 1:L:1286:MET:O | 1:L:1291:THR:OG1 | 2.25 | 0.51 |
| 1:L:2623:GLU:N | 1:L:2623:GLU:OE1 | 2.43 | 0.51 |
| 1:L:2919:LYS:HD3 | 1:L:3184:HIS:HB2 | 1.91 | 0.51 |
| 1:M:1016:VAL:O | 1:M:1019:GLU:HG3 | 2.10 | 0.51 |
| 1:M:2334:MET:SD | 1:M:2334:MET:N | 2.84 | 0.51 |
| 1:N:2368:ASP:N | 1:N:2368:ASP:OD1 | 2.43 | 0.51 |
| 1:N:2777:ASP:OD1 | 1:N:2777:ASP:N | 2.42 | 0.51 |
| 1:O:293:ILE:H | 1:O:293:ILE:HD12 | 1.76 | 0.51 |
| 1:O:844:GLU:HB2 | 1:O:846:HIS:CE1 | 2.46 | 0.51 |
| 1:P:2514:ARG:HE | 1:P:2774:TYR:HD2 | 1.58 | 0.51 |
| 1:P:2526:GLU:HA | 1:P:2529:LYS:HG2 | 1.93 | 0.51 |
| 1:P:2602:ASP:HA | 1:P:2711:ASN:ND2 | 2.26 | 0.51 |
| 1:Q:436:ASP:HB3 | 1:Q:522:TYR:CZ | 2.46 | 0.51 |
| 1:Q:1221:TYR:OH | 1:Q:1236:PHE:N | 2.38 | 0.51 |
| 1:Q:2864:LEU:HD21 | 1:Q:2870:TYR:CD1 | 2.46 | 0.51 |
| 1:Q:3386:TYR:HB2 | 1:Q:3404:ILE:HG22 | 1.92 | 0.51 |
| 1:R:658:ARG:HH12 | 1:R:727:ILE:HD11 | 1.75 | 0.51 |
| 1:R:1153:PHE:C | 1:R:1154:MET:HE2 | 2.36 | 0.51 |
| 1:R:1193:GLN:OE1 | 1:R:1194:TYR:N | 2.44 | 0.51 |
| 1:R:1221:TYR:OH | 1:R:1233:SER:O | 2.29 | 0.51 |
| 1:R:1706:GLY:O | 1:R:1710:LEU:HG | 2.10 | 0.51 |
| 1:S:2778:ASP:OD1 | 1:S:2779:LEU:N | 2.43 | 0.51 |
| 1:S:3333:SER:OG | 1:S:3336:THR:OG1 | 2.25 | 0.51 |
| 1:T:1677:ARG:HD2 | 1:T:1763:ILE:O | 2.10 | 0.51 |
| 1:T:3020:LEU:HD13 | 1:T:3024:LEU:HB2 | 1.91 | 0.51 |
| 1:T:3058:GLN:NE2 | 1:T:3268:ASP:OD2 | 2.44 | 0.51 |
| 1:A:182:GLU:O | 1:A:186:ASN:ND2 | 2.43 | 0.51 |
| 1:A:514:ARG:HH12 | 1:A:1343:ALA:HA | 1.76 | 0.51 |
| 1:A:606:PHE:CZ | 1:A:644:VAL:HG13 | 2.45 | 0.51 |
| 1:A:1082:ALA:HB2 | 1:B:2491:ILE:HG12 | 1.93 | 0.51 |
| 1:A:2101:ALA:O | 1:A:2105:MET:HE2 | 2.10 | 0.51 |
| 1:B:54:LYS:NZ | 1:B:355:ASN:OD1 | 2.43 | 0.51 |
| 1:B:3149:ASN:HA | 1:B:3152:ARG:HD3 | 1.93 | 0.51 |
| 1:C:202:THR:OG1 | 1:C:204:GLU:OE1 | 2.28 | 0.51 |
| 1:C:1249:THR:O | 1:C:1251:LYS:NZ | 2.29 | 0.51 |
| 1:D:80:LYS:NZ | 1:D:261:ILE:HG13 | 2.25 | 0.51 |
| 1:D:860:GLN:O | 1:D:860:GLN:NE2 | 2.44 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:D:2714:ARG:O | 1:D:2718:ILE:HG12 | 2.10 | 0.51 |
| 1:D:3266:VAL:HG21 | 1:D:3283:PHE:HE1 | 1.75 | 0.51 |
| 1:E:250:LYS:HD2 | 1:E:268:SER:HB3 | 1.93 | 0.51 |
| 1:E:752:ILE:HG23 | 1:E:767:LYS:HZ3 | 1.76 | 0.51 |
| 1:E:2845:TRP:HZ3 | 1:E:2847:PHE:CE1 | 2.29 | 0.51 |
| 1:F:188:ILE:HG21 | 1:F:215:HIS:NE2 | 2.26 | 0.51 |
| 1:F:458:ASP:HB2 | 1:F:1341:GLY:HA3 | 1.93 | 0.51 |
| 1:F:940:THR:HG21 | 1:F:1128:PHE:HE1 | 1.76 | 0.51 |
| 1:F:1088:LEU:HD22 | 1:F:1109:PRO:HG3 | 1.93 | 0.51 |
| 1:F:1169:CYS:HA | 1:F:1175:CYS:HA | 1.93 | 0.51 |
| 1:F:3203:ILE:HG22 | 1:F:3207:LEU:HD23 | 1.92 | 0.51 |
| 1:G:1159:ARG:C | 1:G:1160:LYS:HD3 | 2.36 | 0.51 |
| 1:G:2059:ASN:ND2 | 1:G:2061:SER:OG | 2.42 | 0.51 |
| 1:G:2864:LEU:HD21 | 1:G:2870:TYR:CD1 | 2.46 | 0.51 |
| 1:H:409:VAL:HG13 | 1:H:666:CYS:HA | 1.93 | 0.51 |
| 1:H:471:HIS:ND1 | 1:H:471:HIS:O | 2.43 | 0.51 |
| 1:H:842:HIS:NE2 | 1:H:844:GLU:HB2 | 2.26 | 0.51 |
| 1:H:1271:LEU:HB2 | 1:H:1275:GLU:HG3 | 1.93 | 0.51 |
| 1:H:1345:SER:OG | 1:H:1346:VAL:N | 2.43 | 0.51 |
| 1:H:1560:PHE:CE1 | 1:H:1653:PRO:HB3 | 2.46 | 0.51 |
| 1:H:1679:SER:OG | 1:H:1680:VAL:N | 2.44 | 0.51 |
| 1:I:129:GLU:HA | 1:I:140:SER:HA | 1.91 | 0.51 |
| 1:I:501:ARG:CZ | 1:I:648:TRP:HZ3 | 2.22 | 0.51 |
| 1:I:1122:HIS:ND1 | 1:I:1123:TYR:O | 2.44 | 0.51 |
| 1:I:1284:ARG:NH2 | 1:I:1376:GLU:OE2 | 2.44 | 0.51 |
| 1:I:2328:ASN:HD21 | 1:J:1240:THR:HA | 1.76 | 0.51 |
| 1:J:245:GLU:HA | 1:J:248:ARG:HD2 | 1.92 | 0.51 |
| 1:J:312:SER:HA | 1:J:365:TYR:O | 2.11 | 0.51 |
| 1:K:50:LYS:HG3 | 1:K:52:ASP:H | 1.76 | 0.51 |
| 1:K:555:PHE:HA | 1:K:568:ARG:HH22 | 1.76 | 0.51 |
| 1:K:3064:LEU:O | 1:K:3067:GLN:HG3 | 2.10 | 0.51 |
| 1:K:3211:ASP:HB2 | 1:K:3309:ALA:HB2 | 1.92 | 0.51 |
| 1:L:111:ILE:HG13 | 1:S:2214:ARG:HH11 | 1.76 | 0.51 |
| 1:L:699:ILE:HD12 | 1:L:699:ILE:H | 1.76 | 0.51 |
| 1:L:866:LEU:O | 1:L:869:LEU:HG | 2.11 | 0.51 |
| 1:L:1087:PRO:HA | 1:L:1109:PRO:HD3 | 1.92 | 0.51 |
| 1:L:1284:ARG:HH12 | 1:L:1379:PRO:HB3 | 1.76 | 0.51 |
| 1:L:1307:HIS:CD2 | 1:L:1602:MET:HE1 | 2.46 | 0.51 |
| 1:L:1677:ARG:HD2 | 1:L:1763:ILE:O | 2.11 | 0.51 |
| 1:L:2416:ASN:ND2 | 1:L:2418:LYS:O | 2.40 | 0.51 |
| 1:L:3132:LEU:HG | 1:L:3136:ARG:NH1 | 2.25 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:M:17:LEU:O | 1:M:20:GLU:HG3 | 2.11 | 0.51 |
| 1:M:714:GLN:OE1 | 1:M:718:MET:N | 2.44 | 0.51 |
| 1:M:794:ASN:OD1 | 1:M:795:LYS:N | 2.44 | 0.51 |
| 1:M:1872:LEU:HD21 | 1:M:2016:LEU:HD13 | 1.93 | 0.51 |
| 1:M:1883:LEU:O | 1:M:1886:SER:OG | 2.26 | 0.51 |
| 1:M:2580:LEU:HA | 1:M:2583:VAL:HG12 | 1.93 | 0.51 |
| 1:N:1153:PHE:HZ | 1:N:1166:LEU:HD13 | 1.74 | 0.51 |
| 1:N:2754:ASN:OD1 | 1:N:2755:ASP:N | 2.44 | 0.51 |
| 1:O:1630:ASP:O | 1:P:1917:ARG:NH2 | 2.43 | 0.51 |
| 1:P:130:ILE:O | 1:P:138:HIS:HA | 2.10 | 0.51 |
| 1:P:1777:ALA:HB1 | 1:P:1781:GLU:HG3 | 1.92 | 0.51 |
| 1:P:3080:PHE:N | 1:P:3081:GLU:OE1 | 2.44 | 0.51 |
| 1:P:3147:LEU:HA | 1:P:3150:LEU:HD12 | 1.93 | 0.51 |
| 1:Q:1384:LYS:HA | 1:Q:1391:VAL:HG12 | 1.92 | 0.51 |
| 1:Q:2078:LYS:HB2 | 1:Q:2080:ARG:HH12 | 1.76 | 0.51 |
| 1:Q:2190:LEU:HD21 | 1:Q:2194:PHE:CD2 | 2.46 | 0.51 |
| 1:Q:2345:ASN:HD22 | 1:Q:2348:THR:HG23 | 1.74 | 0.51 |
| 1:Q:3103:MET:HA | 1:Q:3109:SER:HA | 1.92 | 0.51 |
| 1:R:379:LYS:HD3 | 1:R:380:LEU:N | 2.26 | 0.51 |
| 1:R:542:VAL:HA | 1:R:549:SER:HA | 1.93 | 0.51 |
| 1:S:47:MET:C | 1:S:55:ARG:HH12 | 2.19 | 0.51 |
| 1:S:1671:THR:O | 1:S:1673:ARG:NH1 | 2.44 | 0.51 |
| 1:S:2345:ASN:HD22 | 1:S:2348:THR:HG23 | 1.76 | 0.51 |
| 1:S:2521:THR:O | 1:S:2525:THR:OG1 | 2.26 | 0.51 |
| 1:T:379:LYS:HD3 | 1:T:381:ASN:H | 1.76 | 0.51 |
| 1:T:596:GLN:CD | 1:T:598:ASP:H | 2.19 | 0.51 |
| 1:T:1126:LEU:HD23 | 1:T:1126:LEU:H | 1.75 | 0.51 |
| 1:T:3062:ASP:OD2 | 1:T:3065:PHE:N | 2.34 | 0.51 |
| 1:A:1084:LEU:HG | 1:A:1110:PHE:CE1 | 2.46 | 0.51 |
| 1:A:3095:VAL:HG13 | 1:A:3103:MET:SD | 2.51 | 0.51 |
| 1:B:471:HIS:ND1 | 1:B:471:HIS:O | 2.44 | 0.51 |
| 1:B:1777:ALA:HA | 1:B:1780:ASN:HB3 | 1.93 | 0.51 |
| 1:B:1857:ILE:HB | 1:B:1884:HIS:CE1 | 2.46 | 0.51 |
| 1:B:1965:ALA:HA | 1:B:1968:LEU:HD13 | 1.93 | 0.51 |
| 1:B:2802:VAL:HG23 | 1:B:2855:VAL:HG23 | 1.93 | 0.51 |
| 1:C:915:ARG:HD2 | 1:C:1060:TRP:HZ3 | 1.76 | 0.51 |
| 1:C:1221:TYR:OH | 1:C:1236:PHE:N | 2.34 | 0.51 |
| 1:C:2439:ASP:OD2 | 1:C:2440:ARG:NE | 2.41 | 0.51 |
| 1:C:2557:CYS:HB3 | 1:C:2564:VAL:HG23 | 1.93 | 0.51 |
| 1:C:3105:THR:O | 1:C:3109:SER:HB3 | 2.11 | 0.51 |
| 1:D:60:VAL:HG23 | 1:D:63:MET:HE2 | 1.92 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:D:1067:GLN:HG3 | 1:D:1070:ARG:HH21 | 1.75 | 0.51 |
| 1:D:2262:VAL:HG23 | 1:D:2438:PHE:CD1 | 2.46 | 0.51 |
| 1:D:2757:ILE:O | 1:D:2761:ALA:HB2 | 2.11 | 0.51 |
| 1:E:291:LEU:HA | 1:E:295:GLN:HE21 | 1.75 | 0.51 |
| 1:E:1736:MET:HB3 | 1:E:1915:LEU:HD22 | 1.93 | 0.51 |
| 1:E:1752:ASP:OD1 | 1:E:1753:ALA:N | 2.43 | 0.51 |
| 1:E:1812:ASP:HB3 | 1:E:1863:GLY:HA3 | 1.93 | 0.51 |
| 1:F:1457:PHE:CE2 | 1:F:1461:HIS:HE1 | 2.28 | 0.51 |
| 1:F:1541:PRO:O | 1:F:1544:GLU:HG3 | 2.10 | 0.51 |
| 1:F:1775:LEU:HD11 | 1:F:1779:PHE:HE1 | 1.75 | 0.51 |
| 1:F:2984:PHE:O | 1:F:2988:HIS:ND1 | 2.39 | 0.51 |
| 1:F:3023:LEU:O | 1:F:3030:ASN:ND2 | 2.42 | 0.51 |
| 1:G:306:ARG:O | 1:G:411:ARG:NH2 | 2.44 | 0.51 |
| 1:G:2090:ASN:ND2 | 1:G:2175:THR:O | 2.42 | 0.51 |
| 1:G:3251:ASP:OD1 | 1:G:3251:ASP:N | 2.44 | 0.51 |
| 1:H:1135:GLN:O | 1:H:1138:ARG:HG2 | 2.10 | 0.51 |
| 1:H:1254:ILE:HG23 | 1:H:1256:LYS:H | 1.75 | 0.51 |
| 1:H:1884:HIS:O | 1:H:1887:SER:OG | 2.23 | 0.51 |
| 1:H:2637:SER:HB2 | 1:H:2687:GLY:HA3 | 1.93 | 0.51 |
| 1:H:2714:ARG:O | 1:H:2718:ILE:HG12 | 2.11 | 0.51 |
| 1:I:438:ASP:OD1 | 1:I:438:ASP:N | 2.43 | 0.51 |
| 1:I:1919:PRO:HB2 | 1:I:1924:SER:HB2 | 1.93 | 0.51 |
| 1:I:2556:LEU:HD23 | 1:I:2556:LEU:H | 1.76 | 0.51 |
| 1:I:2663:GLU:HA | 1:I:2793:ILE:HD11 | 1.92 | 0.51 |
| 1:I:2960:HIS:HE1 | 1:I:3119:HIS:CE1 | 2.28 | 0.51 |
| 1:I:3015:ARG:CZ | 1:I:3193:ASN:H | 2.25 | 0.51 |
| 1:J:1225:ASP:OD1 | 1:J:1226:LEU:N | 2.36 | 0.51 |
| 1:J:2923:ARG:HD3 | 1:J:3008:ILE:O | 2.11 | 0.51 |
| 1:K:1535:PHE:N | 1:K:1538:TRP:O | 2.34 | 0.51 |
| 1:K:2232:LEU:HB2 | 1:K:2274:LEU:HD11 | 1.93 | 0.51 |
| 1:K:2234:LYS:HG3 | 1:K:2243:VAL:HG11 | 1.92 | 0.51 |
| 1:K:2988:HIS:HD2 | 1:K:3119:HIS:CE1 | 2.29 | 0.51 |
| 1:K:3216:GLY:HA2 | 1:K:3262:TYR:O | 2.11 | 0.51 |
| 1:M:438:ASP:OD1 | 1:M:438:ASP:N | 2.43 | 0.51 |
| 1:M:1531:ASP:OD1 | 1:M:1532:THR:N | 2.44 | 0.51 |
| 1:M:2570:GLY:HA2 | 1:M:2847:PHE:CE2 | 2.46 | 0.51 |
| 1:M:3150:LEU:N | 1:M:3152:ARG:HH12 | 2.09 | 0.51 |
| 1:N:444:GLU:O | 1:N:447:GLU:HG2 | 2.11 | 0.51 |
| 1:N:1773:ASN:OD1 | 1:N:1774:SER:N | 2.44 | 0.51 |
| 1:N:2111:LEU:HD13 | 1:N:2212:PHE:CE1 | 2.46 | 0.51 |
| 1:N:2655:TYR:CD2 | 1:N:2659:LEU:HD23 | 2.46 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:O:1815:ARG:HA | 1:O:1818:LEU:HG | 1.93 | 0.51 |
| 1:P:471:HIS:O | 1:P:471:HIS:ND1 | 2.44 | 0.51 |
| 1:P:600:CYS:HB3 | 1:P:783:ARG:HH12 | 1.76 | 0.51 |
| 1:P:672:HIS:O | 1:P:695:ARG:NH1 | 2.44 | 0.51 |
| 1:P:680:PHE:O | 1:P:685:ASN:ND2 | 2.42 | 0.51 |
| 1:P:1008:GLN:N | 1:P:1008:GLN:OE1 | 2.44 | 0.51 |
| 1:P:1328:LEU:HD21 | 1:P:1499:PHE:HD2 | 1.76 | 0.51 |
| 1:P:1881:PHE:O | 1:P:1885:HIS:ND1 | 2.36 | 0.51 |
| 1:P:1896:GLN:NE2 | 1:P:1906:PRO:O | 2.41 | 0.51 |
| 1:P:2820:ASP:HB3 | 1:P:2873:ASP:OD1 | 2.11 | 0.51 |
| 1:Q:794:ASN:OD1 | 1:Q:795:LYS:N | 2.44 | 0.51 |
| 1:Q:1195:ASP:OD2 | 1:Q:1196:ARG:NH2 | 2.43 | 0.51 |
| 1:Q:1551:ARG:HB3 | 1:Q:1661:GLU:HG3 | 1.92 | 0.51 |
| 1:Q:1752:ASP:OD1 | 1:Q:1753:ALA:N | 2.44 | 0.51 |
| 1:Q:2112:ARG:NH2 | 1:Q:2208:LEU:HD21 | 2.26 | 0.51 |
| 1:Q:2514:ARG:HD3 | 1:Q:2598:ILE:HG23 | 1.92 | 0.51 |
| 1:Q:3289:LYS:HD2 | 1:Q:3291:ASN:HD22 | 1.76 | 0.51 |
| 1:R:3225:SER:O | 1:R:3290:TYR:N | 2.44 | 0.51 |
| 1:S:13:ASP:OD1 | 1:S:14:GLN:N | 2.43 | 0.51 |
| 1:S:636:ILE:H | 1:S:636:ILE:HD12 | 1.76 | 0.51 |
| 1:S:2059:ASN:OD1 | 1:S:2061:SER:N | 2.43 | 0.51 |
| 1:T:914:HIS:HA | 1:T:917:LEU:HG | 1.93 | 0.51 |
| 1:T:956:VAL:HA | 1:T:963:PRO:HA | 1.92 | 0.51 |
| 1:T:1024:TYR:CE1 | 1:T:1028:LEU:HD11 | 2.46 | 0.51 |
| 1:T:3125:ILE:HA | 1:T:3128:ILE:HG12 | 1.93 | 0.51 |
| 1:A:997:LYS:O | 1:A:1000:GLU:HG3 | 2.12 | 0.50 |
| 1:A:2108:LYS:HE2 | 1:A:2211:PRO:HD2 | 1.91 | 0.50 |
| 1:A:2621:PRO:HA | 1:A:2624:HIS:CE1 | 2.46 | 0.50 |
| 1:A:3205:GLU:O | 1:B:1117:ARG:NH1 | 2.37 | 0.50 |
| 1:A:3395:ARG:HH21 | 1:A:3398:GLN:HE22 | 1.59 | 0.50 |
| 1:B:69:TRP:HD1 | 1:B:251:LEU:HD22 | 1.74 | 0.50 |
| 1:B:144:ALA:HB3 | 1:B:194:GLY:HA3 | 1.92 | 0.50 |
| 1:B:1457:PHE:CE1 | 1:B:1461:HIS:HE1 | 2.28 | 0.50 |
| 1:B:1521:ASP:HB3 | 1:B:1525:HIS:CD2 | 2.46 | 0.50 |
| 1:B:3082:VAL:O | 1:B:3086:MET:HG2 | 2.11 | 0.50 |
| 1:C:454:ARG:HH21 | 1:C:514:ARG:HB3 | 1.76 | 0.50 |
| 1:C:568:ARG:HH11 | 1:C:636:ILE:HD11 | 1.75 | 0.50 |
| 1:C:732:THR:HA | 1:C:836:HIS:NE2 | 2.26 | 0.50 |
| 1:C:953:GLU:OE1 | 1:C:969:HIS:ND1 | 2.44 | 0.50 |
| 1:C:1991:LYS:O | 1:C:1991:LYS:HD2 | 2.11 | 0.50 |
| 1:C:2874:VAL:HG21 | 1:C:2889:LEU:HD22 | 1.92 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:D:444:GLU:O | 1:D:447:GLU:HG2 | 2.11 | 0.50 |
| 1:D:2109:ALA:HA | 1:D:2112:ARG:HG2 | 1.92 | 0.50 |
| 1:D:2264:PHE:CZ | 1:D:2302:VAL:HG13 | 2.46 | 0.50 |
| 1:D:2286:LEU:HD23 | 1:D:2428:LEU:HG | 1.93 | 0.50 |
| 1:E:304:ARG:HA | 1:E:304:ARG:NE | 2.26 | 0.50 |
| 1:E:911:PRO:HG3 | 1:E:1011:PHE:HZ | 1.76 | 0.50 |
| 1:E:1489:LEU:HA | 1:E:1492:MET:HG2 | 1.93 | 0.50 |
| 1:E:1651:ARG:NH2 | 1:F:2027:ASP:OD1 | 2.45 | 0.50 |
| 1:F:737:PHE:HB3 | 1:F:786:LYS:HB3 | 1.92 | 0.50 |
| 1:F:752:ILE:HB | 1:F:809:SER:HB3 | 1.93 | 0.50 |
| 1:F:1795:ASN:HD21 | 1:F:1797:TRP:HB2 | 1.77 | 0.50 |
| 1:F:3160:GLU:CD | 1:F:3160:GLU:H | 2.19 | 0.50 |
| 1:G:632:ALA:HA | 1:G:637:PHE:CD2 | 2.47 | 0.50 |
| 1:G:1585:ASN:OD1 | 1:G:1586:CYS:N | 2.41 | 0.50 |
| 1:G:2648:ARG:HH11 | 1:G:2656:ARG:NH2 | 2.09 | 0.50 |
| 1:H:245:GLU:HA | 1:H:248:ARG:HD2 | 1.92 | 0.50 |
| 1:H:2165:VAL:HG11 | 1:H:2296:PHE:CE2 | 2.46 | 0.50 |
| 1:H:3296:ASP:OD1 | 1:H:3296:ASP:N | 2.45 | 0.50 |
| 1:I:1710:LEU:HB3 | 1:I:1750:PHE:CE1 | 2.43 | 0.50 |
| 1:I:2446:ILE:HD11 | 1:I:2491:ILE:HD11 | 1.92 | 0.50 |
| 1:J:956:VAL:HA | 1:J:963:PRO:HA | 1.93 | 0.50 |
| 1:K:69:TRP:HD1 | 1:K:251:LEU:HD12 | 1.76 | 0.50 |
| 1:K:1687:GLU:HB2 | 1:K:1760:LEU:HD11 | 1.92 | 0.50 |
| 1:K:2525:THR:O | 1:K:2529:LYS:HG2 | 2.11 | 0.50 |
| 1:K:2802:VAL:HG12 | 1:K:2856:THR:HG22 | 1.91 | 0.50 |
| 1:L:1111:GLU:OE1 | 1:L:1111:GLU:N | 2.44 | 0.50 |
| 1:L:2820:ASP:OD1 | 1:L:2821:LEU:N | 2.44 | 0.50 |
| 1:M:574:LEU:HD23 | 1:M:616:LEU:HG | 1.93 | 0.50 |
| 1:M:2191:PRO:O | 1:M:2195:THR:HG23 | 2.11 | 0.50 |
| 1:N:3092:HIS:ND1 | 1:N:3103:MET:HE1 | 2.25 | 0.50 |
| 1:O:1568:SER:HB2 | 1:O:1597:GLY:H | 1.77 | 0.50 |
| 1:O:2009:ASP:OD1 | 1:O:2010:ALA:N | 2.44 | 0.50 |
| 1:O:2021:GLU:N | 1:O:2021:GLU:OE1 | 2.44 | 0.50 |
| 1:O:2405:SER:HB3 | 1:O:2426:PHE:HE1 | 1.76 | 0.50 |
| 1:P:859:VAL:HG12 | 1:P:863:ARG:NE | 2.25 | 0.50 |
| 1:P:1415:GLU:HA | 1:P:1547:LEU:HD21 | 1.93 | 0.50 |
| 1:P:1420:CYS:SG | 1:P:1485:SER:OG | 2.66 | 0.50 |
| 1:P:2556:LEU:HD11 | 1:P:2746:PRO:HG3 | 1.92 | 0.50 |
| 1:P:3122:ILE:HG13 | 1:P:3125:ILE:HD11 | 1.92 | 0.50 |
| 1:P:3163:ASN:ND2 | 1:P:3168:THR:OG1 | 2.44 | 0.50 |
| 1:Q:611:ASN:HD22 | 1:Q:771:LEU:H | 1.57 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:Q:973:VAL:N | 1:Q:976:LYS:O | 2.33 | 0.50 |
| 1:Q:2114:LEU:HG | 1:Q:2123:TRP:HB2 | 1.93 | 0.50 |
| 1:R:1247:SER:OG | 1:R:1250:LYS:NZ | 2.44 | 0.50 |
| 1:R:3392:ASN:HB3 | 1:R:3395:ARG:HG2 | 1.93 | 0.50 |
| 1:S:171:GLU:OE2 | 1:S:173:ASP:N | 2.43 | 0.50 |
| 1:S:792:ALA:HA | 1:S:795:LYS:HG2 | 1.92 | 0.50 |
| 1:S:1622:GLY:HA2 | 1:T:2779:LEU:HD21 | 1.93 | 0.50 |
| 1:S:2091:ARG:HA | 1:S:2093:ARG:HH21 | 1.76 | 0.50 |
| 1:S:2556:LEU:H | 1:S:2556:LEU:HD23 | 1.76 | 0.50 |
| 1:T:1706:GLY:O | 1:T:1710:LEU:HG | 2.10 | 0.50 |
| 1:T:2101:ALA:O | 1:T:2105:MET:HG3 | 2.11 | 0.50 |
| 1:T:2569:HIS:HD2 | 1:T:2837:LEU:HD23 | 1.76 | 0.50 |
| 1:T:2645:ASP:CG | 1:T:2656:ARG:HH22 | 2.18 | 0.50 |
| 1:C:143:ARG:NH2 | 1:C:209:ASP:OD2 | 2.43 | 0.50 |
| 1:C:278:GLN:OE1 | 1:C:278:GLN:N | 2.41 | 0.50 |
| 1:C:820:GLU:OE1 | 1:C:820:GLU:N | 2.41 | 0.50 |
| 1:C:2393:VAL:H | 1:C:2447:THR:HG22 | 1.75 | 0.50 |
| 1:C:2462:ASN:O | 1:D:1085:ARG:NH1 | 2.35 | 0.50 |
| 1:C:2867:ASP:OD1 | 1:C:2867:ASP:N | 2.43 | 0.50 |
| 1:C:3350:ASN:O | 1:C:3391:SER:N | 2.44 | 0.50 |
| 1:D:2948:ASP:OD1 | 1:D:2948:ASP:N | 2.42 | 0.50 |
| 1:E:1091:PHE:O | 1:E:1104:ARG:HA | 2.12 | 0.50 |
| 1:E:1318:GLY:HA2 | 1:E:1606:PHE:CE1 | 2.47 | 0.50 |
| 1:E:3217:PHE:HB2 | 1:E:3262:TYR:HD2 | 1.76 | 0.50 |
| 1:F:735:ARG:NH2 | 1:F:790:THR:H | 2.09 | 0.50 |
| 1:F:866:LEU:O | 1:F:869:LEU:HG | 2.11 | 0.50 |
| 1:F:2296:PHE:O | 1:F:2300:THR:HG23 | 2.11 | 0.50 |
| 1:F:2620:ASN:HB3 | 1:F:2623:GLU:OE1 | 2.11 | 0.50 |
| 1:G:2587:ARG:HA | 1:G:2590:THR:HG22 | 1.93 | 0.50 |
| 1:H:391:TYR:HE1 | 1:H:397:SER:HB2 | 1.77 | 0.50 |
| 1:H:913:TRP:NE1 | 1:H:1089:GLN:O | 2.44 | 0.50 |
| 1:I:392:SER:OG | 1:I:393:VAL:N | 2.45 | 0.50 |
| 1:I:1161:SER:OG | 1:I:1185:GLY:N | 2.24 | 0.50 |
| 1:I:1701:ASP:OD1 | 1:I:1702:SER:N | 2.43 | 0.50 |
| 1:J:185:HIS:O | 1:J:188:ILE:HG22 | 2.11 | 0.50 |
| 1:J:1024:TYR:CE1 | 1:J:1028:LEU:HD11 | 2.47 | 0.50 |
| 1:J:1324:HIS:HB3 | 1:J:1519:VAL:HG21 | 1.93 | 0.50 |
| 1:J:3035:TYR:H | 1:J:3044:VAL:HG22 | 1.76 | 0.50 |
| 1:K:1161:SER:N | 1:K:1185:GLY:O | 2.44 | 0.50 |
| 1:K:2587:ARG:HA | 1:K:2590:THR:HG22 | 1.94 | 0.50 |
| 1:L:3321:LEU:O | 1:L:3395:ARG:NH2 | 2.34 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:M:44:GLU:N | 1:M:204:GLU:O | 2.42 | 0.50 |
| 1:M:2520:LEU:HD13 | 1:M:2613:LEU:HD21 | 1.93 | 0.50 |
| 1:N:166:LEU:O | 1:N:169:LEU:N | 2.44 | 0.50 |
| 1:N:185:HIS:O | 1:N:188:ILE:HG22 | 2.11 | 0.50 |
| 1:N:259:ASN:O | 1:N:265:ARG:NH2 | 2.45 | 0.50 |
| 1:N:1281:SER:O | 1:N:1285:ARG:HG2 | 2.11 | 0.50 |
| 1:N:1865:LYS:O | 1:N:1868:SER:OG | 2.28 | 0.50 |
| 1:N:2695:THR:OG1 | 1:N:2697:GLU:OE1 | 2.28 | 0.50 |
| 1:N:2812:LYS:HG2 | 1:N:2840:PRO:HA | 1.93 | 0.50 |
| 1:N:3052:LEU:O | 1:N:3055:ARG:NH1 | 2.41 | 0.50 |
| 1:O:606:PHE:HZ | 1:O:644:VAL:HG13 | 1.76 | 0.50 |
| 1:O:1174:PRO:HG2 | 1:O:1176:HIS:CE1 | 2.46 | 0.50 |
| 1:O:1671:THR:O | 1:O:1673:ARG:NH1 | 2.45 | 0.50 |
| 1:P:2462:ASN:OD1 | 1:P:2463:ALA:N | 2.45 | 0.50 |
| 1:Q:1775:LEU:HD12 | 1:Q:1779:PHE:HE1 | 1.76 | 0.50 |
| 1:Q:2460:VAL:O | 1:R:1085:ARG:NH2 | 2.44 | 0.50 |
| 1:R:471:HIS:ND1 | 1:R:471:HIS:O | 2.44 | 0.50 |
| 1:R:532:VAL:HG13 | 1:R:537:SER:HB3 | 1.92 | 0.50 |
| 1:S:64:ALA:O | 1:S:174:TYR:OH | 2.29 | 0.50 |
| 1:S:2056:ARG:HH22 | 1:S:2060:GLY:HA2 | 1.76 | 0.50 |
| 1:T:866:LEU:O | 1:T:869:LEU:HG | 2.11 | 0.50 |
| 1:T:2064:SER:OG | 1:T:2066:SER:OG | 2.29 | 0.50 |
| 1:A:225:ILE:O | 1:A:228:GLU:HG3 | 2.11 | 0.50 |
| 1:A:293:ILE:H | 1:A:293:ILE:HD12 | 1.77 | 0.50 |
| 1:A:326:ILE:O | 1:A:345:ALA:HB3 | 2.12 | 0.50 |
| 1:B:474:PRO:HB2 | 1:B:476:ARG:HH12 | 1.76 | 0.50 |
| 1:B:2939:ASN:HB3 | 1:B:2943:LYS:NZ | 2.26 | 0.50 |
| 1:C:493:MET:HG3 | 1:C:494:ALA:H | 1.76 | 0.50 |
| 1:C:585:ALA:HA | 1:C:588:ASP:OD2 | 2.11 | 0.50 |
| 1:C:792:ALA:O | 1:C:795:LYS:HG2 | 2.11 | 0.50 |
| 1:C:1093:GLN:HB2 | 1:C:1097:ILE:HG21 | 1.94 | 0.50 |
| 1:C:1809:VAL:HG23 | 1:C:1868:SER:HA | 1.92 | 0.50 |
| 1:C:2189:GLN:HA | 1:C:2233:PHE:HE1 | 1.76 | 0.50 |
| 1:C:2248:VAL:HG13 | 1:C:2249:LEU:HD12 | 1.93 | 0.50 |
| 1:D:859:VAL:HG12 | 1:D:863:ARG:NE | 2.25 | 0.50 |
| 1:D:887:GLN:NE2 | 1:D:889:ASN:HB2 | 2.25 | 0.50 |
| 1:D:1108:VAL:HG13 | 1:D:1111:GLU:OE1 | 2.11 | 0.50 |
| 1:E:328:VAL:HG13 | 1:E:376:LEU:HD11 | 1.93 | 0.50 |
| 1:E:855:THR:HG22 | 1:E:858:GLN:NE2 | 2.26 | 0.50 |
| 1:E:2465:ALA:HB2 | 1:F:1085:ARG:HD2 | 1.93 | 0.50 |
| 1:F:1004:LEU:O | 1:F:1008:GLN:NE2 | 2.43 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:F:2462:ASN:OD1 | 1:F:2463:ALA:N | 2.45 | 0.50 |
| 1:G:307:GLU:OE2 | 1:G:413:ALA:N | 2.42 | 0.50 |
| 1:G:1195:ASP:OD2 | 1:G:1196:ARG:NE | 2.42 | 0.50 |
| 1:G:2473:ILE:HD12 | 1:G:2483:PRO:HA | 1.93 | 0.50 |
| 1:G:2777:ASP:O | 1:G:3137:HIS:NE2 | 2.44 | 0.50 |
| 1:H:60:VAL:HG23 | 1:H:63:MET:HE2 | 1.94 | 0.50 |
| 1:H:475:ALA:HB3 | 1:H:485:ARG:HB3 | 1.94 | 0.50 |
| 1:H:627:THR:HG21 | 1:H:630:TYR:HD2 | 1.74 | 0.50 |
| 1:H:1881:PHE:O | 1:H:1885:HIS:ND1 | 2.43 | 0.50 |
| 1:H:3320:LEU:N | 1:H:3341:HIS:O | 2.45 | 0.50 |
| 1:I:277:ARG:NH2 | 1:O:836:HIS:O | 2.41 | 0.50 |
| 1:I:754:SER:HA | 1:I:765:VAL:HG23 | 1.94 | 0.50 |
| 1:I:2390:LYS:O | 1:I:2392:ARG:NH1 | 2.44 | 0.50 |
| 1:I:3056:ARG:NH1 | 1:I:3058:GLN:OE1 | 2.44 | 0.50 |
| 1:J:744:ASN:HB3 | 1:J:779:TRP:NE1 | 2.27 | 0.50 |
| 1:J:845:LEU:HD21 | 1:J:932:ASP:HA | 1.94 | 0.50 |
| 1:J:1283:LEU:HD12 | 1:J:1286:MET:SD | 2.52 | 0.50 |
| 1:J:3124:ARG:O | 1:J:3128:ILE:HG12 | 2.11 | 0.50 |
| 1:K:1328:LEU:HD21 | 1:K:1519:VAL:HG22 | 1.92 | 0.50 |
| 1:L:461:VAL:HG22 | 1:L:1277:GLU:CD | 2.36 | 0.50 |
| 1:L:991:LYS:H | 1:L:994:ARG:CZ | 2.24 | 0.50 |
| 1:L:1540:ILE:H | 1:L:1540:ILE:HD12 | 1.76 | 0.50 |
| 1:L:1750:PHE:HD2 | 1:L:1882:LEU:HD11 | 1.76 | 0.50 |
| 1:L:1947:TYR:CZ | 1:L:1948:LYS:HG3 | 2.47 | 0.50 |
| 1:L:2194:PHE:HD1 | 1:L:2212:PHE:HB3 | 1.77 | 0.50 |
| 1:L:2252:LEU:HD23 | 1:L:2309:TRP:HD1 | 1.77 | 0.50 |
| 1:M:222:ILE:HA | 1:M:225:ILE:HG22 | 1.92 | 0.50 |
| 1:M:582:ASP:O | 1:M:583:HIS:ND1 | 2.45 | 0.50 |
| 1:M:1124:ASP:OD1 | 1:M:1125:ASP:N | 2.43 | 0.50 |
| 1:M:1246:GLY:O | 1:M:1249:THR:OG1 | 2.24 | 0.50 |
| 1:M:1684:THR:N | 1:M:1687:GLU:OE2 | 2.34 | 0.50 |
| 1:M:3174:PRO:HA | 1:M:3177:ILE:HD12 | 1.92 | 0.50 |
| 1:N:63:MET:SD | 1:N:64:ALA:N | 2.85 | 0.50 |
| 1:N:460:SER:HB2 | 1:N:1277:GLU:OE2 | 2.12 | 0.50 |
| 1:N:1141:LEU:HD11 | 1:N:1258:ILE:HD13 | 1.92 | 0.50 |
| 1:N:1268:LEU:HD23 | 1:N:1268:LEU:H | 1.76 | 0.50 |
| 1:N:1978:LYS:NZ | 1:N:1979:SER:O | 2.44 | 0.50 |
| 1:N:2513:VAL:HG21 | 1:N:2515:LYS:HZ3 | 1.77 | 0.50 |
| 1:N:2939:ASN:HB3 | 1:N:2943:LYS:NZ | 2.27 | 0.50 |
| 1:N:3332:VAL:HG21 | 1:N:3406:ILE:HD13 | 1.94 | 0.50 |
| 1:O:13:ASP:OD1 | 1:O:14:GLN:N | 2.45 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:O:143:ARG:NH2 | 1:O:209:ASP:OD2 | 2.44 | 0.50 |
| 1:O:995:LEU:HB3 | 1:O:999:ALA:HB3 | 1.92 | 0.50 |
| 1:O:1388:THR:OG1 | 1:O:1390:LYS:NZ | 2.45 | 0.50 |
| 1:O:2096:ILE:HD13 | 1:O:2179:PRO:HG2 | 1.93 | 0.50 |
| 1:P:312:SER:HA | 1:P:365:TYR:O | 2.12 | 0.50 |
| 1:P:378:LYS:NZ | 1:P:383:ASP:O | 2.41 | 0.50 |
| 1:P:755:ILE:HD11 | 1:P:804:TYR:HB2 | 1.94 | 0.50 |
| 1:Q:169:LEU:HA | 1:Q:177:PHE:HE1 | 1.76 | 0.50 |
| 1:Q:611:ASN:HA | 1:Q:614:HIS:HD2 | 1.76 | 0.50 |
| 1:Q:2575:PRO:O | 1:Q:2579:ARG:HB2 | 2.10 | 0.50 |
| 1:Q:2626:GLU:OE2 | 1:Q:2633:LYS:NZ | 2.43 | 0.50 |
| 1:Q:3072:LEU:HA | 1:Q:3080:PHE:HE2 | 1.76 | 0.50 |
| 1:Q:3125:ILE:HG13 | 1:Q:3128:ILE:HD11 | 1.93 | 0.50 |
| 1:R:719:THR:HG22 | 1:R:722:GLN:CD | 2.36 | 0.50 |
| 1:R:744:ASN:ND2 | 1:R:777:MET:O | 2.44 | 0.50 |
| 1:R:1433:LEU:HD23 | 1:R:1433:LEU:H | 1.75 | 0.50 |
| 1:S:293:ILE:H | 1:S:293:ILE:HD12 | 1.77 | 0.50 |
| 1:S:580:TYR:HE1 | 1:S:856:ARG:HD2 | 1.77 | 0.50 |
| 1:S:1301:PHE:CD1 | 1:S:1302:PRO:HA | 2.47 | 0.50 |
| 1:S:2521:THR:HG23 | 1:S:2524:GLU:H | 1.76 | 0.50 |
| 1:T:299:LEU:HD13 | 1:T:302:GLN:HE21 | 1.77 | 0.50 |
| 1:T:999:ALA:HA | 1:T:1002:VAL:HG22 | 1.93 | 0.50 |
| 1:T:2513:VAL:HG11 | 1:T:2515:LYS:NZ | 2.27 | 0.50 |
| 1:T:3132:LEU:HG | 1:T:3136:ARG:NH1 | 2.26 | 0.50 |
| 1:A:915:ARG:HD2 | 1:A:1060:TRP:HZ3 | 1.76 | 0.50 |
| 1:A:1815:ARG:HD2 | 1:A:1818:LEU:HD21 | 1.93 | 0.50 |
| 1:A:2585:LEU:HG | 1:A:2589:LEU:HD23 | 1.93 | 0.50 |
| 1:B:699:ILE:H | 1:B:699:ILE:HD12 | 1.76 | 0.50 |
| 1:B:914:HIS:O | 1:B:917:LEU:HG | 2.11 | 0.50 |
| 1:B:1351:TRP:HZ3 | 1:B:1463:ASN:HB3 | 1.77 | 0.50 |
| 1:B:1397:GLN:HB2 | 1:B:1400:LEU:HD23 | 1.93 | 0.50 |
| 1:B:2602:ASP:HA | 1:B:2711:ASN:ND2 | 2.27 | 0.50 |
| 1:B:2602:ASP:OD1 | 1:B:2603:TRP:N | 2.45 | 0.50 |
| 1:B:3132:LEU:HG | 1:B:3136:ARG:HH12 | 1.74 | 0.50 |
| 1:C:225:ILE:O | 1:C:228:GLU:HG3 | 2.10 | 0.50 |
| 1:C:1852:ILE:HD13 | 1:C:2030:TYR:CZ | 2.46 | 0.50 |
| 1:C:2251:VAL:HG22 | 1:C:2263:GLN:HB3 | 1.94 | 0.50 |
| 1:C:3385:ASP:O | 1:D:3148:ARG:NH2 | 2.45 | 0.50 |
| 1:D:1742:TRP:CD1 | 1:D:1920:LEU:HD12 | 2.45 | 0.50 |
| 1:D:2464:ASP:OD1 | 1:D:2465:ALA:N | 2.45 | 0.50 |
| 1:D:2481:LEU:HD21 | 3:m:1:NAG:H62 | 1.93 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:E:3095:VAL:HG13 | 1:E:3103:MET:SD | 2.52 | 0.50 |
| 1:F:284:ASP:OD1 | 1:F:284:ASP:N | 2.44 | 0.50 |
| 1:F:1271:LEU:HB2 | 1:F:1275:GLU:HG3 | 1.92 | 0.50 |
| 1:G:613:PRO:HB2 | 1:G:640:HIS:CE1 | 2.46 | 0.50 |
| 1:G:2663:GLU:HA | 1:G:2793:ILE:HD11 | 1.92 | 0.50 |
| 1:H:1995:HIS:ND1 | 1:H:2013:PHE:O | 2.44 | 0.50 |
| 1:H:3052:LEU:O | 1:H:3055:ARG:NH1 | 2.38 | 0.50 |
| 1:I:56:VAL:HG22 | 1:I:57:ALA:H | 1.77 | 0.50 |
| 1:I:794:ASN:OD1 | 1:I:795:LYS:N | 2.45 | 0.50 |
| 1:I:2088:PRO:O | 1:I:2090:ASN:N | 2.38 | 0.50 |
| 1:I:2231:GLU:O | 1:I:2234:LYS:HG2 | 2.12 | 0.50 |
| 1:I:2583:VAL:HG21 | 1:I:2772:PHE:HB3 | 1.93 | 0.50 |
| 1:I:3337:ARG:HH21 | 1:I:3379:TYR:C | 2.19 | 0.50 |
| 1:J:7:ASN:HB3 | 1:J:10:LEU:HG | 1.92 | 0.50 |
| 1:J:81:LEU:HD12 | 1:J:86:LEU:HD13 | 1.93 | 0.50 |
| 1:J:600:CYS:HB3 | 1:J:783:ARG:HH12 | 1.76 | 0.50 |
| 1:J:1802:ILE:HG22 | 1:J:1877:TYR:CD1 | 2.47 | 0.50 |
| 1:J:1892:TYR:O | 1:J:1896:GLN:HG2 | 2.12 | 0.50 |
| 1:J:2152:PRO:HD2 | 1:J:2329:TYR:CD1 | 2.45 | 0.50 |
| 1:K:304:ARG:HA | 1:K:304:ARG:NE | 2.26 | 0.50 |
| 1:K:307:GLU:OE2 | 1:K:413:ALA:N | 2.44 | 0.50 |
| 1:K:1100:ASP:O | 1:K:1104:ARG:NH1 | 2.44 | 0.50 |
| 1:K:2583:VAL:HG21 | 1:K:2772:PHE:HB3 | 1.93 | 0.50 |
| 1:M:1654:SER:OG | 1:M:1655:LEU:N | 2.43 | 0.50 |
| 1:M:2109:ALA:HA | 1:M:2112:ARG:NH2 | 2.26 | 0.50 |
| 1:N:508:GLU:O | 1:N:512:LYS:HG3 | 2.12 | 0.50 |
| 1:N:2831:ALA:HA | 1:N:2858:VAL:HG11 | 1.94 | 0.50 |
| 1:P:257:ASP:HA | 1:P:265:ARG:HD3 | 1.92 | 0.50 |
| 1:P:811:LYS:NZ | 1:P:815:GLY:O | 2.45 | 0.50 |
| 1:P:1111:GLU:N | 1:P:1111:GLU:OE1 | 2.44 | 0.50 |
| 1:P:2923:ARG:NH1 | 1:P:3007:GLY:O | 2.43 | 0.50 |
| 1:Q:390:LEU:HD22 | 1:Q:398:LEU:HB3 | 1.93 | 0.50 |
| 1:Q:449:ARG:HD3 | 1:Q:541:TYR:CZ | 2.46 | 0.50 |
| 1:Q:501:ARG:NH1 | 1:Q:702:TYR:HB3 | 2.26 | 0.50 |
| 1:Q:602:PHE:HA | 1:Q:605:GLN:NE2 | 2.26 | 0.50 |
| 1:Q:889:ASN:HB3 | 1:Q:900:PHE:O | 2.11 | 0.50 |
| 1:Q:1475:GLN:HB3 | 1:Q:1482:ASP:HB3 | 1.93 | 0.50 |
| 1:Q:2348:THR:HG1 | 1:Q:2349:ARG:NH1 | 2.08 | 0.50 |
| 1:Q:2516:ASN:HD21 | 1:Q:2602:ASP:HB2 | 1.77 | 0.50 |
| 1:Q:3055:ARG:HH12 | 1:Q:3064:LEU:HD12 | 1.76 | 0.50 |
| 1:R:188:ILE:HA | 1:R:191:LEU:HB2 | 1.93 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:R:554:PHE:O | 1:R:568:ARG:NH2 | 2.45 | 0.50 |
| 1:R:1086:LYS:HZ3 | 1:R:1087:PRO:HD2 | 1.77 | 0.50 |
| 1:R:2111:LEU:HD13 | 1:R:2212:PHE:HE1 | 1.76 | 0.50 |
| 1:R:3010:TYR:OH | 1:R:3189:ASN:OD1 | 2.26 | 0.50 |
| 1:S:77:LEU:HD13 | 1:S:213:PHE:CE1 | 2.47 | 0.50 |
| 1:S:111:ILE:HD13 | 1:S:122:LYS:HA | 1.93 | 0.50 |
| 1:S:1872:LEU:HD21 | 1:S:2016:LEU:HD13 | 1.94 | 0.50 |
| 1:S:2407:GLU:HB2 | 1:S:2426:PHE:CE2 | 2.47 | 0.50 |
| 1:T:1238:LYS:NZ | 1:T:1239:VAL:O | 2.44 | 0.50 |
| 1:T:1363:ASN:OD1 | 1:T:1364:GLU:N | 2.45 | 0.50 |
| 1:T:1694:ALA:O | 1:T:1697:SER:OG | 2.27 | 0.50 |
| 1:T:1775:LEU:HD12 | 1:T:1776:PRO:HD2 | 1.92 | 0.50 |
| 1:T:1795:ASN:HD21 | 1:T:1797:TRP:HB2 | 1.76 | 0.50 |
| 1:A:13:ASP:OD1 | 1:A:14:GLN:N | 2.44 | 0.50 |
| 1:A:636:ILE:H | 1:A:636:ILE:HD12 | 1.76 | 0.50 |
| 1:A:757:PRO:HB3 | 1:A:798:LEU:HD11 | 1.93 | 0.50 |
| 1:A:1868:SER:O | 1:A:1874:TYR:HB2 | 2.11 | 0.50 |
| 1:B:38:LEU:HG | 1:B:73:TYR:CZ | 2.47 | 0.50 |
| 1:B:371:LYS:HD3 | 1:B:371:LYS:C | 2.36 | 0.50 |
| 1:B:646:ARG:HA | 1:B:710:TYR:HE2 | 1.77 | 0.50 |
| 1:B:934:LEU:HD23 | 1:B:1054:SER:HB3 | 1.92 | 0.50 |
| 1:B:1785:ARG:NH1 | 1:B:1786:ASP:O | 2.44 | 0.50 |
| 1:B:2044:SER:N | 1:B:2047:ASP:OD2 | 2.42 | 0.50 |
| 1:C:972:LEU:HA | 1:C:977:LYS:HA | 1.94 | 0.50 |
| 1:C:1007:GLU:HB3 | 1:C:1140:ILE:HG12 | 1.93 | 0.50 |
| 1:C:2091:ARG:HH21 | 1:C:2364:ASN:HD21 | 1.60 | 0.50 |
| 1:C:2191:PRO:O | 1:C:2195:THR:HG23 | 2.12 | 0.50 |
| 1:C:2604:THR:HA | 1:C:2654:PHE:HE1 | 1.76 | 0.50 |
| 1:C:2800:ASP:OD1 | 1:C:2899:GLY:N | 2.38 | 0.50 |
| 1:C:3095:VAL:HG13 | 1:C:3103:MET:SD | 2.51 | 0.50 |
| 1:C:3211:ASP:OD1 | 1:C:3212:ARG:N | 2.44 | 0.50 |
| 1:D:1913:LEU:HA | 1:D:1916:MET:HG3 | 1.94 | 0.50 |
| 1:E:738:VAL:HG23 | 1:E:789:ILE:HG21 | 1.92 | 0.50 |
| 1:E:1081:ILE:HD13 | 1:F:2460:VAL:HG12 | 1.93 | 0.50 |
| 1:E:2522:VAL:O | 1:E:2526:GLU:HG3 | 2.11 | 0.50 |
| 1:E:2977:CYS:SG | 1:E:3106:LEU:HD11 | 2.52 | 0.50 |
| 1:F:887:GLN:NE2 | 1:F:889:ASN:HB2 | 2.27 | 0.50 |
| 1:F:1294:LYS:O | 1:F:1297:SER:OG | 2.24 | 0.50 |
| 1:F:1493:ARG:HH21 | 1:F:1515:ARG:HD2 | 1.77 | 0.50 |
| 1:F:1626:ASP:OD1 | 1:F:1627:SER:N | 2.44 | 0.50 |
| 1:G:148:ARG:HB2 | 1:G:151:GLN:HE22 | 1.77 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:G:583:HIS:HB3 | 1:G:587:PHE:HD2 | 1.77 | 0.50 |
| 1:G:1917:ARG:NH2 | 1:H:1631:ILE:O | 2.39 | 0.50 |
| 1:G:3174:PRO:HA | 1:G:3177:ILE:HD12 | 1.93 | 0.50 |
| 1:H:371:LYS:HD3 | 1:H:371:LYS:C | 2.37 | 0.50 |
| 1:H:924:ALA:O | 1:H:928:LYS:HG2 | 2.12 | 0.50 |
| 1:H:2958:SER:HB3 | 1:H:2963:PRO:HD3 | 1.93 | 0.50 |
| 1:H:3163:ASN:ND2 | 1:H:3168:THR:OG1 | 2.44 | 0.50 |
| 1:I:1709:ALA:O | 1:I:1712:SER:OG | 2.27 | 0.50 |
| 1:I:2603:TRP:CD1 | 1:I:2711:ASN:HD22 | 2.29 | 0.50 |
| 1:I:3045:THR:HG21 | 1:I:3099:GLY:HA3 | 1.94 | 0.50 |
| 1:I:3133:GLN:HA | 1:I:3136:ARG:HE | 1.74 | 0.50 |
| 1:J:276:TYR:O | 1:J:280:GLY:N | 2.42 | 0.50 |
| 1:J:1995:HIS:ND1 | 1:J:2013:PHE:O | 2.45 | 0.50 |
| 1:J:2754:ASN:OD1 | 1:J:2755:ASP:N | 2.44 | 0.50 |
| 1:K:399:ASN:HD21 | 1:K:401:ASN:HD21 | 1.59 | 0.50 |
| 1:K:1494:GLN:NE2 | 1:K:1495:PRO:O | 2.44 | 0.50 |
| 1:K:2109:ALA:HA | 1:K:2112:ARG:NH2 | 2.26 | 0.50 |
| 1:K:2460:VAL:O | 1:L:1085:ARG:NH2 | 2.44 | 0.50 |
| 1:L:57:ALA:H | 1:L:355:ASN:HB3 | 1.76 | 0.50 |
| 1:L:2530:LYS:HB2 | 1:L:2533:ARG:HH22 | 1.76 | 0.50 |
| 1:M:376:LEU:HB3 | 1:M:378:LYS:NZ | 2.26 | 0.50 |
| 1:M:954:THR:HA | 1:M:965:PRO:HA | 1.94 | 0.50 |
| 1:M:1195:ASP:OD1 | 1:M:1196:ARG:N | 2.45 | 0.50 |
| 1:M:2531:ALA:O | 1:M:2535:VAL:HG23 | 2.12 | 0.50 |
| 1:M:3056:ARG:NH1 | 1:M:3058:GLN:OE1 | 2.34 | 0.50 |
| 1:N:1299:HIS:CD2 | 1:N:1457:PHE:HZ | 2.28 | 0.50 |
| 1:N:2122:GLY:HA3 | 1:N:2124:GLN:HE22 | 1.76 | 0.50 |
| 1:N:2718:ILE:CD1 | 1:N:2779:LEU:HB2 | 2.41 | 0.50 |
| 1:N:3038:LYS:O | 1:N:3041:GLN:NE2 | 2.44 | 0.50 |
| 1:N:3320:LEU:N | 1:N:3341:HIS:O | 2.43 | 0.50 |
| 1:O:646:ARG:HA | 1:O:710:TYR:HE2 | 1.77 | 0.50 |
| 1:O:1900:ARG:O | 1:O:1900:ARG:NH1 | 2.45 | 0.50 |
| 1:O:1978:LYS:NZ | 1:O:1979:SER:O | 2.34 | 0.50 |
| 1:O:2152:PRO:HD2 | 1:O:2329:TYR:HD2 | 1.76 | 0.50 |
| 1:O:2313:GLN:HG2 | 1:O:2320:TYR:HB3 | 1.93 | 0.50 |
| 1:P:1270:ASP:OD1 | 1:P:1271:LEU:N | 2.44 | 0.50 |
| 1:P:1736:MET:HG2 | 1:P:1738:THR:H | 1.77 | 0.50 |
| 1:P:2967:PRO:O | 1:P:2973:ARG:NH1 | 2.44 | 0.50 |
| 1:P:2987:TRP:CD1 | 1:P:3154:LEU:HD12 | 2.46 | 0.50 |
| 1:P:3350:ASN:OD1 | 1:P:3351:VAL:N | 2.43 | 0.50 |
| 1:Q:475:ALA:HB3 | 1:Q:485:ARG:HB3 | 1.92 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:Q:1082:ALA:HB2 | 1:R:2491:ILE:HG13 | 1.92 | 0.50 |
| 1:R:225:ILE:O | 1:R:229:LEU:HG | 2.11 | 0.50 |
| 1:R:299:LEU:HD13 | 1:R:302:GLN:HE21 | 1.77 | 0.50 |
| 1:R:313:PHE:CE2 | 1:R:406:PRO:HB3 | 2.38 | 0.50 |
| 1:R:501:ARG:HG2 | 1:R:645:ASP:CG | 2.37 | 0.50 |
| 1:R:1325:TRP:HE3 | 1:R:1496:LEU:HD21 | 1.76 | 0.50 |
| 1:R:3117:ILE:O | 1:R:3120:SER:OG | 2.26 | 0.50 |
| 1:S:183:VAL:HG21 | 1:S:365:TYR:CE1 | 2.47 | 0.50 |
| 1:S:442:ASP:OD1 | 1:S:443:GLU:N | 2.45 | 0.50 |
| 1:S:910:PHE:HZ | 1:S:1022:HIS:ND1 | 2.10 | 0.50 |
| 1:S:1465:ASP:OD2 | 1:S:1528:TYR:OH | 2.28 | 0.50 |
| 1:T:71:ARG:NH1 | 1:T:273:LEU:O | 2.40 | 0.50 |
| 1:T:984:ASP:OD1 | 1:T:985:GLU:N | 2.44 | 0.50 |
| 1:A:579:GLU:HG3 | 1:A:582:ASP:CG | 2.36 | 0.50 |
| 1:A:2266:VAL:HG21 | 1:A:2442:TYR:CD1 | 2.47 | 0.50 |
| 1:B:782:ASP:OD1 | 1:B:782:ASP:N | 2.41 | 0.50 |
| 1:B:1284:ARG:HH11 | 1:B:1284:ARG:HG2 | 1.76 | 0.50 |
| 1:B:1284:ARG:HH21 | 1:B:1287:GLN:HG2 | 1.77 | 0.50 |
| 1:B:1746:TYR:CE2 | 1:B:1750:PHE:HE2 | 2.28 | 0.50 |
| 1:C:1693:LEU:O | 1:C:1696:GLN:HG3 | 2.12 | 0.50 |
| 1:C:1905:ASP:HB3 | 1:C:1908:GLU:HB2 | 1.91 | 0.50 |
| 1:D:1890:ARG:NH2 | 1:D:1959:GLU:OE2 | 2.42 | 0.50 |
| 1:E:1033:GLU:O | 1:E:1036:SER:OG | 2.24 | 0.50 |
| 1:E:1404:ASP:O | 1:E:1408:ASN:ND2 | 2.44 | 0.50 |
| 1:E:1742:TRP:CD1 | 1:E:1920:LEU:HD12 | 2.47 | 0.50 |
| 1:F:545:ASN:HD21 | 1:F:992:PHE:HE2 | 1.60 | 0.50 |
| 1:F:1722:TYR:CE2 | 1:F:1724:GLU:HB3 | 2.46 | 0.50 |
| 1:F:1963:ILE:HG23 | 1:F:1968:LEU:HD11 | 1.92 | 0.50 |
| 1:F:2777:ASP:OD1 | 1:F:2777:ASP:N | 2.40 | 0.50 |
| 1:G:111:ILE:HD13 | 1:G:122:LYS:HA | 1.94 | 0.50 |
| 1:G:1220:LYS:NZ | 1:G:1222:SER:HB2 | 2.27 | 0.50 |
| 1:G:1579:THR:OG1 | 1:G:1583:GLU:O | 2.22 | 0.50 |
| 1:H:667:ALA:O | 1:H:671:THR:HG23 | 2.12 | 0.50 |
| 1:H:742:LEU:HD23 | 1:H:781:PHE:CE2 | 2.47 | 0.50 |
| 1:H:1276:VAL:O | 1:H:1279:LEU:HG | 2.12 | 0.50 |
| 1:H:1324:HIS:HA | 1:H:1519:VAL:HG11 | 1.93 | 0.50 |
| 1:H:2661:ALA:HA | 1:H:2664:GLN:HE22 | 1.75 | 0.50 |
| 1:H:3058:GLN:NE2 | 1:H:3268:ASP:OD2 | 2.44 | 0.50 |
| 1:I:755:ILE:HG23 | 1:I:765:VAL:HG21 | 1.94 | 0.50 |
| 1:I:1058:ARG:NH1 | 1:I:1125:ASP:O | 2.44 | 0.50 |
| 1:I:1854:HIS:HE1 | 1:I:1885:HIS:CE1 | 2.30 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:I:3118:HIS:O | 1:I:3122:ILE:HG12 | 2.12 | 0.50 |
| 1:I:3334:ARG:NE | 1:I:3334:ARG:HA | 2.27 | 0.50 |
| 1:J:303:ARG:HD3 | 1:J:306:ARG:HG3 | 1.93 | 0.50 |
| 1:J:309:ALA:N | 1:J:370:SER:OG | 2.39 | 0.50 |
| 1:J:475:ALA:O | 1:J:476:ARG:NH1 | 2.43 | 0.50 |
| 1:J:836:HIS:NE2 | 1:J:838:GLU:OE1 | 2.44 | 0.50 |
| 1:J:1979:SER:H | 1:J:2078:LYS:NZ | 2.09 | 0.50 |
| 1:J:2589:LEU:O | 1:J:2592:GLN:NE2 | 2.28 | 0.50 |
| 1:J:2712:VAL:HA | 1:J:2715:GLN:CD | 2.36 | 0.50 |
| 1:J:3232:LEU:HD23 | 1:J:3234:PRO:HD3 | 1.92 | 0.50 |
| 1:J:3321:LEU:O | 1:J:3395:ARG:NH1 | 2.39 | 0.50 |
| 1:K:1278:SER:O | 1:K:1281:SER:OG | 2.27 | 0.50 |
| 1:K:1568:SER:HB2 | 1:K:1597:GLY:H | 1.75 | 0.50 |
| 1:L:313:PHE:HB3 | 1:L:315:LEU:HD23 | 1.93 | 0.50 |
| 1:L:998:ILE:HA | 1:L:1001:MET:HG3 | 1.93 | 0.50 |
| 1:L:1022:HIS:HD2 | 1:L:1026:HIS:HE1 | 1.60 | 0.50 |
| 1:L:3283:PHE:HB2 | 1:L:3302:PRO:HG2 | 1.93 | 0.50 |
| 1:M:1365:ALA:HA | 1:M:1381:PHE:CZ | 2.47 | 0.50 |
| 1:M:1756:ARG:HH21 | 1:N:2176:VAL:HG13 | 1.77 | 0.50 |
| 1:N:848:ARG:NE | 1:N:934:LEU:H | 2.06 | 0.50 |
| 1:N:984:ASP:OD1 | 1:N:985:GLU:N | 2.45 | 0.50 |
| 1:N:1086:LYS:NZ | 1:N:1087:PRO:O | 2.34 | 0.50 |
| 1:N:1821:ASP:OD1 | 1:N:1821:ASP:N | 2.43 | 0.50 |
| 1:N:2823:ASP:OD1 | 1:N:2823:ASP:N | 2.45 | 0.50 |
| 1:N:3225:SER:O | 1:N:3290:TYR:N | 2.44 | 0.50 |
| 1:O:341:HIS:NE2 | 1:O:343:GLU:OE2 | 2.42 | 0.50 |
| 1:P:1431:ASN:OD1 | 1:P:1594:SER:OG | 2.29 | 0.50 |
| 1:P:1847:GLU:H | 1:P:1847:GLU:CD | 2.20 | 0.50 |
| 1:P:2101:ALA:O | 1:P:2105:MET:HG3 | 2.12 | 0.50 |
| 1:P:2647:GLU:OE2 | 1:P:2656:ARG:NH2 | 2.35 | 0.50 |
| 1:Q:752:ILE:O | 1:Q:808:LEU:HA | 2.12 | 0.50 |
| 1:Q:2191:PRO:O | 1:Q:2195:THR:HG23 | 2.11 | 0.50 |
| 1:Q:2439:ASP:OD1 | 1:Q:2439:ASP:N | 2.44 | 0.50 |
| 1:R:1019:GLU:HA | 1:R:1022:HIS:NE2 | 2.27 | 0.50 |
| 1:R:1947:TYR:OH | 1:R:1948:LYS:NZ | 2.28 | 0.50 |
| 1:S:501:ARG:NH1 | 1:S:702:TYR:HB3 | 2.25 | 0.50 |
| 1:S:1316:VAL:HG11 | 1:S:1321:VAL:HG13 | 1.92 | 0.50 |
| 1:S:3337:ARG:HE | 1:S:3338:VAL:H | 1.60 | 0.50 |
| 1:T:231:LYS:HB3 | 1:T:237:TYR:HE2 | 1.77 | 0.50 |
| 1:T:703:GLU:N | 1:T:703:GLU:OE1 | 2.44 | 0.50 |
| 1:T:860:GLN:O | 1:T:860:GLN:NE2 | 2.44 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:T:1905:ASP:HB3 | 1:T:1908:GLU:HB2 | 1.94 | 0.50 |
| 1:T:2263:GLN:HE22 | 1:T:2443:LYS:H | 1.58 | 0.50 |
| 1:A:110:PRO:HA | 1:A:126:PHE:CG | 2.47 | 0.50 |
| 1:A:539:GLU:N | 1:A:539:GLU:OE1 | 2.44 | 0.50 |
| 1:B:197:ASP:OD1 | 1:B:197:ASP:N | 2.43 | 0.50 |
| 1:B:257:ASP:HA | 1:B:265:ARG:HD3 | 1.93 | 0.50 |
| 1:B:1775:LEU:HD12 | 1:B:1776:PRO:HD2 | 1.93 | 0.50 |
| 1:B:2326:ALA:O | 1:B:2330:MET:HG2 | 2.11 | 0.50 |
| 1:B:2945:GLN:HG3 | 1:B:3035:TYR:HE1 | 1.77 | 0.50 |
| 1:C:1980:ARG:HE | 1:C:1982:PHE:HZ | 1.60 | 0.50 |
| 1:D:551:HIS:HE1 | 1:D:555:PHE:HB3 | 1.77 | 0.50 |
| 1:D:739:GLY:HA3 | 1:D:784:LEU:HB3 | 1.93 | 0.50 |
| 1:D:2137:PRO:HD2 | 1:D:2143:LYS:HE2 | 1.94 | 0.50 |
| 1:D:2665:ARG:O | 1:D:2723:GLN:NE2 | 2.45 | 0.50 |
| 1:E:849:SER:OG | 1:E:850:ASP:N | 2.45 | 0.50 |
| 1:E:1284:ARG:NH1 | 1:E:1376:GLU:OE1 | 2.41 | 0.50 |
| 1:E:1322:PHE:HB3 | 1:E:1323:PRO:HD3 | 1.94 | 0.50 |
| 1:E:1433:LEU:HA | 1:E:1436:LEU:HB2 | 1.94 | 0.50 |
| 1:E:1652:ARG:HG2 | 1:E:1653:PRO:HD2 | 1.94 | 0.50 |
| 1:E:2580:LEU:HD12 | 1:E:2744:LEU:HD22 | 1.94 | 0.50 |
| 1:F:148:ARG:HA | 1:F:151:GLN:HG2 | 1.94 | 0.50 |
| 1:F:618:GLY:HA3 | 1:F:626:SER:N | 2.27 | 0.50 |
| 1:F:845:LEU:HD21 | 1:F:932:ASP:HA | 1.92 | 0.50 |
| 1:F:2720:GLN:NE2 | 1:F:2730:TYR:HB2 | 2.25 | 0.50 |
| 1:F:2948:ASP:OD1 | 1:F:2948:ASP:N | 2.43 | 0.50 |
| 1:G:1011:PHE:HA | 1:G:1014:PHE:HB3 | 1.94 | 0.50 |
| 1:G:2345:ASN:O | 1:G:2349:ARG:HG2 | 2.12 | 0.50 |
| 1:G:2672:VAL:HG23 | 1:G:2847:PHE:CD2 | 2.46 | 0.50 |
| 1:G:3160:GLU:HA | 1:G:3169:ARG:HH22 | 1.76 | 0.50 |
| 1:H:112:PHE:H | 1:H:122:LYS:HA | 1.76 | 0.50 |
| 1:H:1710:LEU:HD22 | 1:H:1750:PHE:CE1 | 2.47 | 0.50 |
| 1:H:2271:ILE:HD12 | 1:H:2298:HIS:NE2 | 2.27 | 0.50 |
| 1:H:2602:ASP:HA | 1:H:2711:ASN:ND2 | 2.27 | 0.50 |
| 1:I:47:MET:C | 1:I:55:ARG:HH12 | 2.19 | 0.50 |
| 1:I:47:MET:SD | 1:I:47:MET:N | 2.84 | 0.50 |
| 1:I:991:LYS:HE3 | 1:I:994:ARG:HE | 1.76 | 0.50 |
| 1:J:2393:VAL:HG11 | 1:J:2450:LEU:HD12 | 1.94 | 0.50 |
| 1:J:2674:TYR:OH | 1:J:2712:VAL:HB | 2.11 | 0.50 |
| 1:K:602:PHE:HA | 1:K:605:GLN:NE2 | 2.27 | 0.50 |
| 1:K:2551:HIS:HB2 | 1:K:2581:PHE:CE2 | 2.47 | 0.50 |
| 1:K:2598:ILE:HD11 | 1:K:2707:ILE:HD13 | 1.93 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:L:542:VAL:HA | 1:L:549:SER:HA | 1.93 | 0.50 |
| 1:L:1048:ILE:HA | 1:L:1051:LEU:HG | 1.92 | 0.50 |
| 1:L:2111:LEU:HD13 | 1:L:2212:PHE:CE1 | 2.47 | 0.50 |
| 1:L:3344:VAL:HG12 | 1:L:3346:SER:H | 1.77 | 0.50 |
| 1:M:47:MET:C | 1:M:55:ARG:HH12 | 2.19 | 0.50 |
| 1:M:811:LYS:HD2 | 1:M:815:GLY:HA2 | 1.94 | 0.50 |
| 1:M:851:VAL:HG12 | 1:M:935:PRO:HB2 | 1.93 | 0.50 |
| 1:M:936:TYR:OH | 1:M:1058:ARG:NH1 | 2.45 | 0.50 |
| 1:M:2604:THR:HG23 | 1:M:2782:HIS:NE2 | 2.27 | 0.50 |
| 1:M:2797:ARG:HA | 1:M:2801:ARG:NH2 | 2.27 | 0.50 |
| 1:M:3103:MET:HA | 1:M:3109:SER:HA | 1.94 | 0.50 |
| 1:N:1153:PHE:C | 1:N:1154:MET:HE2 | 2.37 | 0.50 |
| 1:N:1274:GLY:O | 1:N:1277:GLU:HG3 | 2.12 | 0.50 |
| 1:N:1414:LEU:HA | 1:N:1422:PHE:HE1 | 1.75 | 0.50 |
| 1:N:1492:MET:SD | 1:N:1492:MET:N | 2.85 | 0.50 |
| 1:N:1501:ASP:OD2 | 1:N:1504:GLN:N | 2.42 | 0.50 |
| 1:N:1547:LEU:O | 1:N:1550:GLN:HG3 | 2.12 | 0.50 |
| 1:N:2711:ASN:O | 1:N:2714:ARG:HB3 | 2.12 | 0.50 |
| 1:O:636:ILE:H | 1:O:636:ILE:HD12 | 1.75 | 0.50 |
| 1:O:2529:LYS:NZ | 1:O:2620:ASN:OD1 | 2.45 | 0.50 |
| 1:P:171:GLU:HB3 | 1:P:177:PHE:HD1 | 1.77 | 0.50 |
| 1:P:1283:LEU:HG | 1:P:1284:ARG:HH22 | 1.77 | 0.50 |
| 1:Q:2095:GLU:CD | 1:Q:2097:SER:H | 2.19 | 0.50 |
| 1:Q:2930:SER:OG | 1:Q:2933:GLN:OE1 | 2.16 | 0.50 |
| 1:Q:3133:GLN:OE1 | 1:Q:3140:PHE:HB3 | 2.10 | 0.50 |
| 1:Q:3229:ASN:OD1 | 1:Q:3231:LYS:NZ | 2.31 | 0.50 |
| 1:R:331:HIS:NE2 | 1:R:672:HIS:O | 2.42 | 0.50 |
| 1:R:1085:ARG:HD3 | 1:R:1110:PHE:HE2 | 1.77 | 0.50 |
| 1:R:1174:PRO:HG2 | 1:R:1176:HIS:HE1 | 1.77 | 0.50 |
| 1:R:1579:THR:HG21 | 1:R:1585:ASN:HB3 | 1.92 | 0.50 |
| 1:S:954:THR:HG22 | 1:S:965:PRO:HA | 1.94 | 0.50 |
| 1:S:1033:GLU:O | 1:S:1036:SER:OG | 2.24 | 0.50 |
| 1:S:1868:SER:O | 1:S:1874:TYR:HB2 | 2.12 | 0.50 |
| 1:S:2112:ARG:HH11 | 1:S:2211:PRO:HG3 | 1.77 | 0.50 |
| 1:S:2328:ASN:HD21 | 1:T:1240:THR:HA | 1.77 | 0.50 |
| 1:S:2542:ARG:NH1 | 1:S:2588:ALA:HA | 2.27 | 0.50 |
| 1:T:855:THR:O | 1:T:859:VAL:HG23 | 2.12 | 0.50 |
| 1:T:1224:ILE:HB | 1:T:1230:LYS:HZ2 | 1.77 | 0.50 |
| 1:T:1284:ARG:HH12 | 1:T:1379:PRO:HB3 | 1.77 | 0.50 |
| 1:T:1547:LEU:O | 1:T:1550:GLN:HG3 | 2.12 | 0.50 |
| 1:T:2287:HIS:HE1 | 1:T:2432:LEU:HB2 | 1.75 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:2521:THR:O | 1:A:2525:THR:OG1 | 2.18 | 0.50 |
| 1:A:3133:GLN:HE21 | 1:A:3138:ARG:HB3 | 1.76 | 0.50 |
| 1:B:188:ILE:HA | 1:B:191:LEU:HD12 | 1.93 | 0.50 |
| 1:B:757:PRO:HB2 | 1:B:760:GLY:H | 1.77 | 0.50 |
| 1:B:1842:ASN:OD1 | 1:B:1843:TYR:N | 2.44 | 0.50 |
| 1:B:2271:ILE:HD12 | 1:B:2298:HIS:NE2 | 2.27 | 0.50 |
| 1:B:2623:GLU:N | 1:B:2623:GLU:OE1 | 2.44 | 0.50 |
| 1:B:2674:TYR:HE1 | 1:B:2715:GLN:HE21 | 1.59 | 0.50 |
| 1:C:277:ARG:NH1 | 1:K:834:THR:O | 2.44 | 0.50 |
| 1:C:348:ILE:HD11 | 1:C:367:PHE:CD2 | 2.47 | 0.50 |
| 1:C:811:LYS:HD2 | 1:C:815:GLY:HA2 | 1.93 | 0.50 |
| 1:C:1590:ALA:HB1 | 1:C:1617:PRO:HG3 | 1.93 | 0.50 |
| 1:C:1756:ARG:HH12 | 1:D:2175:THR:HB | 1.77 | 0.50 |
| 1:C:2190:LEU:HD21 | 1:C:2194:PHE:CD2 | 2.47 | 0.50 |
| 1:C:2542:ARG:HH22 | 1:C:2591:LEU:HD13 | 1.77 | 0.50 |
| 1:D:1465:ASP:OD2 | 1:D:1528:TYR:OH | 2.26 | 0.50 |
| 1:D:2865:ARG:HH12 | 1:E:2741:ARG:NH2 | 2.10 | 0.50 |
| 1:D:3153:PRO:HB2 | 1:D:3158:ASN:HD22 | 1.76 | 0.50 |
| 1:E:1654:SER:OG | 1:E:1655:LEU:N | 2.45 | 0.50 |
| 1:E:1775:LEU:HD12 | 1:E:1779:PHE:HE1 | 1.77 | 0.50 |
| 1:E:2378:ASP:HA | 1:E:2381:GLU:OE1 | 2.12 | 0.50 |
| 1:E:3118:HIS:O | 1:E:3122:ILE:HG12 | 2.11 | 0.50 |
| 1:E:3308:PRO:HG2 | 1:E:3311:ALA:HB3 | 1.92 | 0.50 |
| 1:F:475:ALA:HB3 | 1:F:485:ARG:HB3 | 1.94 | 0.50 |
| 1:F:869:LEU:HD23 | 1:F:925:LEU:HD11 | 1.93 | 0.50 |
| 1:G:1817:ARG:HG3 | 1:G:1860:TRP:CH2 | 2.47 | 0.50 |
| 1:G:2639:ARG:HE | 1:G:2640:PRO:HD2 | 1.76 | 0.50 |
| 1:G:2750:ASP:HA | 1:G:2758:ARG:HH11 | 1.76 | 0.50 |
| 1:H:1433:LEU:O | 1:H:1437:VAL:HG22 | 2.12 | 0.50 |
| 1:H:1848:VAL:HA | 1:H:2026:PHE:CE1 | 2.47 | 0.50 |
| 1:H:3010:TYR:OH | 1:H:3189:ASN:OD1 | 2.25 | 0.50 |
| 1:I:971:GLY:N | 1:I:978:THR:OG1 | 2.36 | 0.50 |
| 1:I:2328:ASN:O | 1:I:2331:SER:OG | 2.30 | 0.50 |
| 1:I:2963:PRO:HD2 | 1:I:2965:LEU:HD23 | 1.94 | 0.50 |
| 1:I:3045:THR:N | 1:I:3101:TYR:O | 2.39 | 0.50 |
| 1:I:3081:GLU:HA | 1:I:3084:PHE:HB3 | 1.92 | 0.50 |
| 1:J:1452:ALA:HA | 1:J:1457:PHE:CG | 2.47 | 0.50 |
| 1:K:441:THR:OG1 | 1:K:443:GLU:OE1 | 2.28 | 0.50 |
| 1:K:752:ILE:HG13 | 1:K:767:LYS:NZ | 2.27 | 0.50 |
| 1:K:1221:TYR:OH | 1:K:1236:PHE:N | 2.38 | 0.50 |
| 1:K:1244:ARG:HD3 | 1:K:1245:PRO:HD2 | 1.93 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:K:1852:ILE:HD13 | 1:K:2030:TYR:CZ | 2.47 | 0.50 |
| 1:L:52:ASP:OD1 | 1:L:53:GLY:N | 2.45 | 0.50 |
| 1:L:658:ARG:NH2 | 1:L:724:ASP:OD1 | 2.45 | 0.50 |
| 1:L:795:LYS:HD3 | 1:L:796:LYS:HD3 | 1.94 | 0.50 |
| 1:L:1365:ALA:HA | 1:L:1378:ASN:HB3 | 1.91 | 0.50 |
| 1:L:2578:HIS:HB3 | 1:L:2709:HIS:HD2 | 1.77 | 0.50 |
| 1:M:442:ASP:N | 1:M:442:ASP:OD1 | 2.44 | 0.50 |
| 1:M:1033:GLU:O | 1:M:1036:SER:OG | 2.25 | 0.50 |
| 1:M:1067:GLN:NE2 | 1:M:1072:LEU:HB2 | 2.27 | 0.50 |
| 1:M:1742:TRP:CD1 | 1:M:1920:LEU:HD12 | 2.46 | 0.50 |
| 1:M:2525:THR:O | 1:M:2529:LYS:HG2 | 2.11 | 0.50 |
| 1:M:3086:MET:O | 1:M:3090:THR:HG23 | 2.12 | 0.50 |
| 1:M:3260:ARG:HE | 1:M:3261:VAL:H | 1.60 | 0.50 |
| 1:N:958:PRO:C | 1:N:961:ASN:H | 2.19 | 0.50 |
| 1:N:1271:LEU:HB2 | 1:N:1275:GLU:HG3 | 1.93 | 0.50 |
| 1:N:2226:ARG:NH1 | 1:N:2292:ASP:OD2 | 2.45 | 0.50 |
| 1:N:3245:PHE:HB3 | 1:N:3264:TYR:HE2 | 1.77 | 0.50 |
| 1:O:203:LEU:HD21 | 1:O:351:LEU:HB3 | 1.94 | 0.50 |
| 1:O:441:THR:OG1 | 1:O:444:GLU:OE1 | 2.30 | 0.50 |
| 1:O:596:GLN:HG2 | 1:O:605:GLN:NE2 | 2.27 | 0.50 |
| 1:O:846:HIS:H | 1:O:846:HIS:HD1 | 1.58 | 0.50 |
| 1:O:2112:ARG:HH11 | 1:O:2211:PRO:HG3 | 1.77 | 0.50 |
| 1:O:2624:HIS:HB2 | 1:O:2633:LYS:HZ1 | 1.76 | 0.50 |
| 1:P:1284:ARG:HH11 | 1:P:1284:ARG:HG2 | 1.77 | 0.50 |
| 1:P:2183:TRP:CD2 | 1:P:2271:ILE:HD11 | 2.47 | 0.50 |
| 1:P:2283:LEU:HD21 | 1:P:2292:ASP:HB3 | 1.93 | 0.50 |
| 1:Q:520:ILE:HD11 | 1:Q:638:ILE:HD12 | 1.93 | 0.50 |
| 1:Q:1557:PHE:CD2 | 1:Q:1611:LYS:HD3 | 2.47 | 0.50 |
| 1:Q:2786:ILE:HD13 | 1:Q:2789:LEU:HD21 | 1.92 | 0.50 |
| 1:R:435:LYS:O | 1:R:521:PRO:HA | 2.12 | 0.50 |
| 1:R:453:SER:HB3 | 1:R:553:PRO:HG3 | 1.93 | 0.50 |
| 1:R:2948:ASP:N | 1:R:2948:ASP:OD1 | 2.45 | 0.50 |
| 1:R:3008:ILE:HG21 | 1:R:3116:MET:HB3 | 1.93 | 0.50 |
| 1:S:922:GLU:HG3 | 1:S:934:LEU:HD23 | 1.94 | 0.50 |
| 1:S:3082:VAL:HG21 | 1:S:3260:ARG:HG2 | 1.94 | 0.50 |
| 1:S:3113:PRO:HA | 1:S:3116:MET:HG3 | 1.92 | 0.50 |
| 1:T:303:ARG:HD3 | 1:T:306:ARG:HD3 | 1.93 | 0.50 |
| 1:T:313:PHE:CE1 | 1:T:406:PRO:HB3 | 2.47 | 0.50 |
| 1:T:887:GLN:NE2 | 1:T:889:ASN:HB2 | 2.27 | 0.50 |
| 1:T:1305:CYS:SG | 1:T:1314:CYS:N | 2.85 | 0.50 |
| 1:T:1324:HIS:HB3 | 1:T:1519:VAL:HG21 | 1.94 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:T:2865:ARG:HD3 | 1:T:2867:ASP:H | 1.76 | 0.50 |
| 1:T:3122:ILE:HG13 | 1:T:3125:ILE:HD11 | 1.94 | 0.50 |
| 1:T:3147:LEU:HA | 1:T:3150:LEU:HD12 | 1.93 | 0.50 |
| 1:A:539:GLU:HA | 1:A:555:PHE:HB2 | 1.93 | 0.50 |
| 1:A:1322:PHE:HD2 | 1:A:1426:PHE:HE2 | 1.59 | 0.50 |
| 1:A:2153:THR:HA | 1:A:2156:HIS:ND1 | 2.26 | 0.50 |
| 1:B:188:ILE:HA | 1:B:191:LEU:HB2 | 1.93 | 0.50 |
| 1:B:1319:SER:OG | 1:B:1320:ALA:N | 2.45 | 0.50 |
| 1:B:1325:TRP:HE3 | 1:B:1496:LEU:HD21 | 1.77 | 0.50 |
| 1:B:2526:GLU:HA | 1:B:2529:LYS:HG2 | 1.93 | 0.50 |
| 1:B:2714:ARG:O | 1:B:2718:ILE:HG12 | 2.12 | 0.50 |
| 1:B:3106:LEU:HA | 1:B:3109:SER:HB3 | 1.93 | 0.50 |
| 1:C:2409:ARG:O | 1:C:2471:TYR:HA | 2.12 | 0.50 |
| 1:D:76:GLN:HE21 | 1:D:264:THR:HG22 | 1.76 | 0.50 |
| 1:D:543:ASP:OD2 | 1:D:546:SER:N | 2.39 | 0.50 |
| 1:D:2789:LEU:O | 1:D:2793:ILE:HG12 | 2.11 | 0.50 |
| 1:E:598:ASP:OD1 | 1:E:599:PHE:N | 2.45 | 0.50 |
| 1:E:938:ASP:HA | 1:E:1055:ASN:HD21 | 1.77 | 0.50 |
| 1:E:1809:VAL:HG23 | 1:E:1868:SER:HA | 1.94 | 0.50 |
| 1:E:2044:SER:OG | 1:E:2046:ASP:OD1 | 2.30 | 0.50 |
| 1:E:2400:HIS:NE2 | 1:E:2485:SER:O | 2.42 | 0.50 |
| 1:F:905:HIS:H | 1:F:907:MET:HE1 | 1.77 | 0.50 |
| 1:F:1268:LEU:HD23 | 1:F:1268:LEU:H | 1.77 | 0.50 |
| 1:F:2536:GLN:HA | 1:F:2544:TYR:HB3 | 1.93 | 0.50 |
| 1:G:1307:HIS:HB3 | 1:G:1312:VAL:HG11 | 1.92 | 0.50 |
| 1:G:3070:GLU:O | 1:G:3073:GLU:HG2 | 2.12 | 0.50 |
| 1:G:3086:MET:HB3 | 1:G:3245:PHE:HZ | 1.76 | 0.50 |
| 1:H:313:PHE:HB3 | 1:H:315:LEU:HD23 | 1.92 | 0.50 |
| 1:H:1162:ALA:HB3 | 1:H:1183:ILE:HD11 | 1.94 | 0.50 |
| 1:H:2018:GLY:O | 1:H:2021:GLU:HG2 | 2.12 | 0.50 |
| 1:H:2569:HIS:HA | 1:H:2574:PHE:CE1 | 2.46 | 0.50 |
| 1:I:442:ASP:N | 1:I:442:ASP:OD1 | 2.43 | 0.50 |
| 1:I:580:TYR:HE2 | 1:I:959:GLU:HB2 | 1.75 | 0.50 |
| 1:I:996:THR:HG23 | 1:I:999:ALA:H | 1.77 | 0.50 |
| 1:I:2329:TYR:OH | 1:J:1238:LYS:HD3 | 2.12 | 0.50 |
| 1:I:2996:GLU:OE1 | 1:I:3008:ILE:N | 2.42 | 0.50 |
| 1:J:193:GLY:HA3 | 1:J:201:SER:HB3 | 1.94 | 0.50 |
| 1:J:220:ASP:OD1 | 1:J:221:ARG:N | 2.45 | 0.50 |
| 1:J:325:ARG:HE | 1:J:391:TYR:HE2 | 1.60 | 0.50 |
| 1:J:914:HIS:O | 1:J:917:LEU:HG | 2.12 | 0.50 |
| 1:J:958:PRO:C | 1:J:961:ASN:H | 2.20 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:J:1788:VAL:HG12 | 1:J:1789:LEU:HD22 | 1.94 | 0.50 |
| 1:J:2939:ASN:HB3 | 1:J:2943:LYS:NZ | 2.27 | 0.50 |
| 1:K:1554:ASP:OD1 | 1:K:1554:ASP:N | 2.43 | 0.50 |
| 1:K:2360:TYR:HA | 1:K:2363:LEU:HD23 | 1.93 | 0.50 |
| 1:L:259:ASN:O | 1:L:265:ARG:NH2 | 2.45 | 0.50 |
| 1:L:1223:VAL:HG13 | 1:L:1231:ILE:HB | 1.94 | 0.50 |
| 1:L:2616:ASP:OD2 | 1:L:2620:ASN:HB2 | 2.12 | 0.50 |
| 1:M:651:TRP:CZ3 | 1:M:655:GLN:HG3 | 2.46 | 0.50 |
| 1:M:938:ASP:HA | 1:M:1055:ASN:HD21 | 1.76 | 0.50 |
| 1:M:3096:GLY:HA3 | 1:M:3104:SER:HB3 | 1.93 | 0.50 |
| 1:N:3015:ARG:HH12 | 1:N:3194:GLY:H | 1.60 | 0.50 |
| 1:O:1085:ARG:NH1 | 1:P:2462:ASN:O | 2.45 | 0.50 |
| 1:P:176:HIS:HA | 1:P:179:VAL:HG12 | 1.94 | 0.50 |
| 1:P:695:ARG:HH21 | 1:P:696:PRO:HD2 | 1.77 | 0.50 |
| 1:P:866:LEU:O | 1:P:869:LEU:HG | 2.12 | 0.50 |
| 1:P:2623:GLU:N | 1:P:2623:GLU:OE1 | 2.45 | 0.50 |
| 1:Q:1630:ASP:OD1 | 1:Q:1630:ASP:N | 2.41 | 0.50 |
| 1:R:224:VAL:HA | 1:R:227:GLN:OE1 | 2.11 | 0.50 |
| 1:R:1540:ILE:H | 1:R:1540:ILE:HD12 | 1.76 | 0.50 |
| 1:R:3148:ARG:HG2 | 1:R:3152:ARG:HH22 | 1.76 | 0.50 |
| 1:S:2136:CYS:HB3 | 1:S:2144:TYR:C | 2.37 | 0.50 |
| 1:S:2157:TRP:HE3 | 1:S:2158:HIS:HD2 | 1.60 | 0.50 |
| 1:S:2567:CYS:HA | 1:S:2577:TRP:CE2 | 2.47 | 0.50 |
| 1:T:1277:GLU:HA | 1:T:1280:LYS:HG2 | 1.94 | 0.50 |
| 1:A:583:HIS:HB3 | 1:A:587:PHE:HD2 | 1.77 | 0.49 |
| 1:A:3337:ARG:NH2 | 1:A:3380:SER:HB2 | 2.28 | 0.49 |
| 1:B:8:VAL:HG11 | 1:B:94:TRP:HB2 | 1.94 | 0.49 |
| 1:B:727:ILE:HG22 | 1:B:730:ARG:HH21 | 1.76 | 0.49 |
| 1:B:1356:ARG:NH2 | 1:B:1402:ASN:OD1 | 2.45 | 0.49 |
| 1:B:3075:THR:HA | 1:B:3133:GLN:HE22 | 1.75 | 0.49 |
| 1:B:3314:ASP:OD1 | 1:B:3315:VAL:N | 2.43 | 0.49 |
| 1:C:1890:ARG:NH2 | 1:C:1959:GLU:O | 2.39 | 0.49 |
| 1:C:2604:THR:HA | 1:C:2654:PHE:CE1 | 2.47 | 0.49 |
| 1:C:3047:ASP:HB2 | 1:C:3097:GLY:HA3 | 1.93 | 0.49 |
| 1:D:1324:HIS:HA | 1:D:1519:VAL:HG11 | 1.94 | 0.49 |
| 1:D:2469:LEU:HD11 | 1:D:2489:PRO:HG2 | 1.94 | 0.49 |
| 1:E:248:ARG:NH1 | 1:E:803:GLU:HA | 2.27 | 0.49 |
| 1:E:2345:ASN:HD22 | 1:E:2348:THR:HG23 | 1.77 | 0.49 |
| 1:E:3021:PRO:HD2 | 1:E:3024:LEU:HD21 | 1.94 | 0.49 |
| 1:F:855:THR:O | 1:F:859:VAL:HG23 | 2.11 | 0.49 |
| 1:F:1153:PHE:HB2 | 1:F:1198:PHE:HD2 | 1.77 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:F:1485:SER:OG | 1:F:1486:ASP:N | 2.44 | 0.49 |
| 1:F:1539:THR:H | 1:F:1542:GLN:NE2 | 2.10 | 0.49 |
| 1:G:481:ASP:OD1 | 1:J:1644:TYR:N | 2.45 | 0.49 |
| 1:G:1651:ARG:NH2 | 1:H:2025:SER:O | 2.45 | 0.49 |
| 1:G:1746:TYR:HE2 | 1:G:1881:PHE:HE1 | 1.59 | 0.49 |
| 1:G:2375:LEU:HB3 | 1:G:2379:GLU:HG3 | 1.94 | 0.49 |
| 1:G:2525:THR:O | 1:G:2529:LYS:HG2 | 2.11 | 0.49 |
| 1:H:551:HIS:ND1 | 1:H:552:ASN:O | 2.43 | 0.49 |
| 1:H:737:PHE:N | 1:H:829:ILE:O | 2.35 | 0.49 |
| 1:H:1223:VAL:HG13 | 1:H:1231:ILE:HB | 1.94 | 0.49 |
| 1:H:2111:LEU:HD13 | 1:H:2212:PHE:CE1 | 2.46 | 0.49 |
| 1:I:383:ASP:OD1 | 1:I:383:ASP:N | 2.43 | 0.49 |
| 1:I:2117:ASP:OD1 | 1:I:2119:THR:OG1 | 2.25 | 0.49 |
| 1:I:2371:LYS:HZ2 | 1:I:2376:ASN:HB3 | 1.77 | 0.49 |
| 1:I:2399:LEU:HB3 | 1:I:2436:TRP:HH2 | 1.77 | 0.49 |
| 1:I:2414:GLN:O | 1:I:2416:ASN:N | 2.45 | 0.49 |
| 1:J:197:ASP:N | 1:J:197:ASP:OD1 | 2.45 | 0.49 |
| 1:J:2389:SER:OG | 1:J:2390:LYS:N | 2.45 | 0.49 |
| 1:K:1709:ALA:O | 1:K:1712:SER:OG | 2.28 | 0.49 |
| 1:L:284:ASP:OD1 | 1:L:284:ASP:N | 2.44 | 0.49 |
| 1:L:428:SER:OG | 1:L:429:ALA:N | 2.44 | 0.49 |
| 1:L:1884:HIS:O | 1:L:1887:SER:OG | 2.23 | 0.49 |
| 1:L:2567:CYS:O | 1:L:2569:HIS:ND1 | 2.44 | 0.49 |
| 1:M:2295:PHE:O | 1:M:2299:HIS:ND1 | 2.44 | 0.49 |
| 1:N:1223:VAL:O | 1:N:1230:LYS:NZ | 2.34 | 0.49 |
| 1:O:193:GLY:HA3 | 1:O:201:SER:H | 1.77 | 0.49 |
| 1:O:482:ALA:O | 1:O:485:ARG:NH2 | 2.45 | 0.49 |
| 1:O:650:ILE:HG22 | 1:O:713:LEU:HD12 | 1.93 | 0.49 |
| 1:O:938:ASP:HA | 1:O:1055:ASN:ND2 | 2.26 | 0.49 |
| 1:O:954:THR:HG22 | 1:O:965:PRO:HA | 1.94 | 0.49 |
| 1:O:2392:ARG:HE | 1:O:2447:THR:HG21 | 1.77 | 0.49 |
| 1:O:2806:PHE:HB2 | 1:O:2851:PHE:HB3 | 1.93 | 0.49 |
| 1:O:2981:MET:SD | 1:O:2982:PRO:HD2 | 2.51 | 0.49 |
| 1:O:3301:THR:HG22 | 1:O:3327:PRO:HD3 | 1.92 | 0.49 |
| 1:P:153:VAL:HG21 | 1:P:159:THR:HA | 1.94 | 0.49 |
| 1:P:580:TYR:CG | 1:P:958:PRO:HG2 | 2.46 | 0.49 |
| 1:P:1325:TRP:HE3 | 1:P:1496:LEU:HD21 | 1.77 | 0.49 |
| 1:P:1851:GLU:O | 1:P:1855:ASN:ND2 | 2.45 | 0.49 |
| 1:P:1862:GLY:HA3 | 1:P:1870:ALA:HB2 | 1.93 | 0.49 |
| 1:P:2642:LEU:HD13 | 1:P:2684:TRP:HB3 | 1.93 | 0.49 |
| 1:Q:418:ASP:OD2 | 1:Q:662:TYR:N | 2.44 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:Q:750:LEU:HD21 | 1:Q:767:LYS:NZ | 2.27 | 0.49 |
| 1:Q:1723:PRO:HA | 1:Q:1728:ARG:HH12 | 1.77 | 0.49 |
| 1:Q:1890:ARG:HB2 | 1:Q:1955:TYR:CE2 | 2.47 | 0.49 |
| 1:Q:1977:GLU:O | 1:Q:2078:LYS:NZ | 2.34 | 0.49 |
| 1:R:144:ALA:HB3 | 1:R:194:GLY:HA3 | 1.93 | 0.49 |
| 1:R:1677:ARG:HD2 | 1:R:1763:ILE:O | 2.12 | 0.49 |
| 1:R:1827:ASP:HA | 1:R:1831:TRP:CD1 | 2.47 | 0.49 |
| 1:R:2165:VAL:HG11 | 1:R:2296:PHE:CE2 | 2.47 | 0.49 |
| 1:S:850:ASP:O | 1:S:853:SER:OG | 2.29 | 0.49 |
| 1:S:2073:VAL:HG23 | 1:T:1489:LEU:H | 1.77 | 0.49 |
| 1:S:2390:LYS:HB2 | 1:S:2392:ARG:HH12 | 1.77 | 0.49 |
| 1:S:2392:ARG:HE | 1:S:2447:THR:HG21 | 1.76 | 0.49 |
| 1:S:2977:CYS:HA | 1:S:2987:TRP:CZ3 | 2.47 | 0.49 |
| 1:T:252:GLU:OE1 | 1:T:256:ARG:NH2 | 2.45 | 0.49 |
| 1:T:284:ASP:OD1 | 1:T:284:ASP:N | 2.44 | 0.49 |
| 1:T:1319:SER:OG | 1:T:1320:ALA:N | 2.45 | 0.49 |
| 1:A:2553:TYR:CD2 | 1:A:2554:PRO:HA | 2.47 | 0.49 |
| 1:A:3381:LEU:HD23 | 1:A:3386:TYR:CD1 | 2.47 | 0.49 |
| 1:B:887:GLN:NE2 | 1:B:889:ASN:HB2 | 2.27 | 0.49 |
| 1:B:1108:VAL:HG13 | 1:B:1111:GLU:OE1 | 2.12 | 0.49 |
| 1:C:277:ARG:CZ | 1:K:835:THR:HA | 2.42 | 0.49 |
| 1:C:390:LEU:HD22 | 1:C:398:LEU:HB3 | 1.93 | 0.49 |
| 1:C:1025:ILE:O | 1:C:1029:VAL:HG12 | 2.12 | 0.49 |
| 1:C:1067:GLN:NE2 | 1:C:1072:LEU:HB2 | 2.26 | 0.49 |
| 1:C:1710:LEU:HB3 | 1:C:1750:PHE:CE1 | 2.45 | 0.49 |
| 1:C:2271:ILE:HA | 1:C:2274:LEU:HB3 | 1.95 | 0.49 |
| 1:C:2878:ALA:N | 1:C:2882:THR:O | 2.39 | 0.49 |
| 1:C:3113:PRO:HA | 1:C:3116:MET:HG3 | 1.93 | 0.49 |
| 1:D:1019:GLU:HA | 1:D:1022:HIS:CD2 | 2.47 | 0.49 |
| 1:D:1186:ASP:H | 1:D:1189:GLU:HB2 | 1.77 | 0.49 |
| 1:D:1433:LEU:O | 1:D:1437:VAL:HG22 | 2.12 | 0.49 |
| 1:D:1677:ARG:NH2 | 1:D:1751:GLU:OE2 | 2.45 | 0.49 |
| 1:D:2111:LEU:HD13 | 1:D:2212:PHE:CE1 | 2.46 | 0.49 |
| 1:E:146:ASP:OD2 | 1:E:148:ARG:NH1 | 2.45 | 0.49 |
| 1:E:972:LEU:HD23 | 1:E:977:LYS:HB3 | 1.94 | 0.49 |
| 1:E:1395:ASP:HB3 | 1:E:1439:GLY:HA3 | 1.95 | 0.49 |
| 1:E:1751:GLU:OE2 | 1:E:1763:ILE:N | 2.46 | 0.49 |
| 1:E:2345:ASN:O | 1:E:2349:ARG:HG2 | 2.11 | 0.49 |
| 1:F:80:LYS:HA | 1:F:83:LYS:HZ3 | 1.77 | 0.49 |
| 1:F:307:GLU:CD | 1:F:413:ALA:HA | 2.37 | 0.49 |
| 1:F:1280:LYS:HB2 | 1:F:1284:ARG:NH1 | 2.27 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:F:2164:GLN:NE2 | 1:F:2164:GLN:O | 2.45 | 0.49 |
| 1:F:2217:ILE:HG22 | 1:F:2219:GLU:H | 1.76 | 0.49 |
| 1:F:2341:VAL:HG12 | 1:F:2342:LEU:HD23 | 1.95 | 0.49 |
| 1:F:3395:ARG:O | 1:F:3401:ARG:NH1 | 2.36 | 0.49 |
| 1:G:478:PRO:HB2 | 1:G:676:LYS:HZ2 | 1.76 | 0.49 |
| 1:G:881:ILE:HA | 1:G:884:PHE:HD2 | 1.77 | 0.49 |
| 1:G:2164:GLN:HE22 | 1:G:2343:ASN:HD21 | 1.60 | 0.49 |
| 1:H:562:LEU:HB3 | 1:H:564:GLU:OE1 | 2.12 | 0.49 |
| 1:H:1540:ILE:H | 1:H:1540:ILE:HD12 | 1.77 | 0.49 |
| 1:H:1999:LYS:NZ | 1:H:2009:ASP:OD1 | 2.45 | 0.49 |
| 1:H:3314:ASP:O | 1:H:3336:THR:HA | 2.12 | 0.49 |
| 1:I:523:TRP:CH2 | 1:I:525:TRP:HB3 | 2.47 | 0.49 |
| 1:I:1531:ASP:OD1 | 1:I:1532:THR:N | 2.44 | 0.49 |
| 1:I:1914:GLU:CD | 1:I:1914:GLU:H | 2.20 | 0.49 |
| 1:I:2962:ALA:HB2 | 1:I:3107:GLU:HG2 | 1.93 | 0.49 |
| 1:J:848:ARG:HD2 | 1:J:1123:TYR:CE2 | 2.46 | 0.49 |
| 1:J:1098:ASN:O | 1:J:1104:ARG:NH1 | 2.45 | 0.49 |
| 1:J:1362:ILE:HD13 | 1:J:1456:LEU:HD11 | 1.94 | 0.49 |
| 1:J:1745:LEU:HA | 1:J:1748:VAL:HG12 | 1.94 | 0.49 |
| 1:J:3400:THR:HG22 | 1:J:3401:ARG:HH21 | 1.76 | 0.49 |
| 1:K:583:HIS:HB3 | 1:K:587:PHE:HD2 | 1.78 | 0.49 |
| 1:K:972:LEU:HD23 | 1:K:977:LYS:HB3 | 1.94 | 0.49 |
| 1:K:1138:ARG:HD3 | 1:K:1260:ALA:HA | 1.94 | 0.49 |
| 1:K:2414:GLN:O | 1:K:2416:ASN:N | 2.45 | 0.49 |
| 1:L:371:LYS:HD3 | 1:L:371:LYS:C | 2.37 | 0.49 |
| 1:L:1192:TRP:HZ3 | 1:L:1194:TYR:HB2 | 1.77 | 0.49 |
| 1:L:1638:ARG:HH11 | 1:L:1644:TYR:HE1 | 1.60 | 0.49 |
| 1:M:383:ASP:OD1 | 1:M:383:ASP:N | 2.45 | 0.49 |
| 1:M:1295:ILE:HD12 | 1:M:1333:VAL:HG23 | 1.94 | 0.49 |
| 1:M:1698:LEU:HD13 | 1:M:1757:ARG:HD2 | 1.94 | 0.49 |
| 1:M:3037:ILE:HG13 | 1:M:3040:ALA:H | 1.78 | 0.49 |
| 1:M:3216:GLY:HA2 | 1:M:3262:TYR:O | 2.13 | 0.49 |
| 1:N:1142:HIS:HE1 | 1:N:1524:ASN:HA | 1.77 | 0.49 |
| 1:N:1149:VAL:HG11 | 1:N:1206:LEU:HD23 | 1.94 | 0.49 |
| 1:N:1313:ALA:H | 1:N:1600:THR:HG22 | 1.77 | 0.49 |
| 1:N:1683:LEU:O | 1:N:1688:ARG:NH1 | 2.45 | 0.49 |
| 1:O:539:GLU:HA | 1:O:555:PHE:HB2 | 1.92 | 0.49 |
| 1:O:1040:LEU:HD12 | 1:O:1184:LEU:HD21 | 1.93 | 0.49 |
| 1:O:1868:SER:O | 1:O:1874:TYR:HB2 | 2.11 | 0.49 |
| 1:P:190:TYR:CD2 | 1:P:349:PHE:HD2 | 2.30 | 0.49 |
| 1:P:2645:ASP:HB2 | 1:P:2649:GLY:O | 2.11 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:P:2865:ARG:NH1 | 1:P:2866:PRO:HG2 | 2.27 | 0.49 |
| 1:P:2964:LYS:HG2 | 1:P:2973:ARG:HB2 | 1.94 | 0.49 |
| 1:Q:306:ARG:O | 1:Q:411:ARG:NH2 | 2.45 | 0.49 |
| 1:Q:711:ASP:OD1 | 1:Q:712:ASN:N | 2.45 | 0.49 |
| 1:Q:1677:ARG:C | 1:Q:1678:LYS:HD3 | 2.37 | 0.49 |
| 1:Q:1991:LYS:O | 1:Q:1991:LYS:HD2 | 2.12 | 0.49 |
| 1:R:52:ASP:OD1 | 1:R:53:GLY:N | 2.45 | 0.49 |
| 1:R:223:PHE:HZ | 1:R:274:PHE:HD1 | 1.59 | 0.49 |
| 1:R:327:LYS:HG3 | 1:R:343:GLU:O | 2.12 | 0.49 |
| 1:R:529:GLY:HA2 | 1:R:575:SER:HA | 1.94 | 0.49 |
| 1:R:635:PRO:O | 1:R:638:ILE:HG22 | 2.12 | 0.49 |
| 1:R:1419:PHE:HE1 | 1:R:1468:TRP:HE1 | 1.60 | 0.49 |
| 1:R:1556:LEU:HB2 | 1:R:1625:LEU:HD21 | 1.94 | 0.49 |
| 1:R:1710:LEU:HD22 | 1:R:1750:PHE:HE1 | 1.76 | 0.49 |
| 1:R:2605:GLU:O | 1:R:2652:SER:OG | 2.30 | 0.49 |
| 1:R:2754:ASN:OD1 | 1:R:2755:ASP:N | 2.46 | 0.49 |
| 1:S:291:LEU:HA | 1:S:295:GLN:HE21 | 1.76 | 0.49 |
| 1:S:2216:TYR:CD1 | 1:S:2223:TYR:HB3 | 2.47 | 0.49 |
| 1:S:2471:TYR:OH | 1:S:2488:LYS:NZ | 2.43 | 0.49 |
| 1:T:859:VAL:O | 1:T:862:LEU:HG | 2.11 | 0.49 |
| 1:T:1540:ILE:H | 1:T:1540:ILE:HD12 | 1.78 | 0.49 |
| 1:T:1777:ALA:HB1 | 1:T:1781:GLU:HG3 | 1.94 | 0.49 |
| 1:T:2271:ILE:HD12 | 1:T:2298:HIS:NE2 | 2.27 | 0.49 |
| 1:T:3084:PHE:HD2 | 1:T:3122:ILE:HD11 | 1.76 | 0.49 |
| 1:T:3213:VAL:HA | 1:T:3306:SER:HA | 1.93 | 0.49 |
| 1:T:3317:ILE:HA | 1:T:3339:ARG:O | 2.12 | 0.49 |
| 1:A:255:ASP:OD1 | 1:A:255:ASP:N | 2.45 | 0.49 |
| 1:A:1016:VAL:O | 1:A:1019:GLU:HG3 | 2.12 | 0.49 |
| 1:A:1802:ILE:HD12 | 1:A:1805:GLU:HB2 | 1.94 | 0.49 |
| 1:A:2614:LEU:HD12 | 1:A:2636:ARG:NH1 | 2.28 | 0.49 |
| 1:A:2812:LYS:NZ | 1:A:2840:PRO:O | 2.45 | 0.49 |
| 1:B:188:ILE:HG21 | 1:B:215:HIS:CE1 | 2.47 | 0.49 |
| 1:B:855:THR:O | 1:B:859:VAL:HG23 | 2.12 | 0.49 |
| 1:B:1008:GLN:N | 1:B:1008:GLN:OE1 | 2.45 | 0.49 |
| 1:B:2991:LEU:HA | 1:B:2994:GLN:HE21 | 1.78 | 0.49 |
| 1:C:1016:VAL:O | 1:C:1019:GLU:HG3 | 2.12 | 0.49 |
| 1:C:2653:PHE:O | 1:C:2656:ARG:NH1 | 2.45 | 0.49 |
| 1:D:1809:VAL:HG22 | 1:D:1811:ARG:HH12 | 1.76 | 0.49 |
| 1:E:2567:CYS:O | 1:E:2569:HIS:ND1 | 2.45 | 0.49 |
| 1:F:795:LYS:HD3 | 1:F:796:LYS:HD3 | 1.94 | 0.49 |
| 1:F:2210:ASN:HD21 | 1:F:2212:PHE:HB2 | 1.76 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:F:2602:ASP:OD2 | 1:F:2604:THR:OG1 | 2.30 | 0.49 |
| 1:F:2602:ASP:HA | 1:F:2711:ASN:ND2 | 2.26 | 0.49 |
| 1:F:2714:ARG:O | 1:F:2718:ILE:HG12 | 2.12 | 0.49 |
| 1:F:2820:ASP:OD1 | 1:F:2821:LEU:N | 2.45 | 0.49 |
| 1:F:3124:ARG:HD2 | 1:F:3187:PHE:CD2 | 2.47 | 0.49 |
| 1:G:293:ILE:H | 1:G:293:ILE:HD12 | 1.77 | 0.49 |
| 1:G:1842:ASN:HB3 | 1:G:1845:ASP:HB2 | 1.94 | 0.49 |
| 1:H:1145:HIS:HD2 | 1:H:1248:GLU:OE1 | 1.94 | 0.49 |
| 1:H:1871:HIS:HE1 | 1:H:2018:GLY:HA3 | 1.77 | 0.49 |
| 1:I:1124:ASP:OD1 | 1:I:1125:ASP:N | 2.44 | 0.49 |
| 1:I:1518:ASP:OD1 | 1:I:1525:HIS:ND1 | 2.46 | 0.49 |
| 1:I:1622:GLY:HA2 | 1:J:2779:LEU:HD21 | 1.94 | 0.49 |
| 1:I:3015:ARG:NH1 | 1:I:3193:ASN:H | 2.11 | 0.49 |
| 1:I:3243:GLY:HA3 | 1:I:3264:TYR:OH | 2.12 | 0.49 |
| 1:J:8:VAL:HA | 1:J:11:LEU:HD23 | 1.93 | 0.49 |
| 1:J:259:ASN:O | 1:J:265:ARG:NH2 | 2.46 | 0.49 |
| 1:J:787:VAL:HG23 | 1:J:789:ILE:HD11 | 1.95 | 0.49 |
| 1:J:855:THR:O | 1:J:859:VAL:HG23 | 2.12 | 0.49 |
| 1:J:1372:SER:O | 1:J:1374:THR:OG1 | 2.30 | 0.49 |
| 1:K:220:ASP:OD1 | 1:K:283:TYR:OH | 2.24 | 0.49 |
| 1:K:391:TYR:HA | 1:K:397:SER:HA | 1.94 | 0.49 |
| 1:K:2216:TYR:HA | 1:K:2223:TYR:HB3 | 1.94 | 0.49 |
| 1:L:744:ASN:HB3 | 1:L:779:TRP:CD1 | 2.48 | 0.49 |
| 1:L:2958:SER:HB3 | 1:L:2963:PRO:HD3 | 1.94 | 0.49 |
| 1:M:2111:LEU:HD12 | 1:M:2211:PRO:HG2 | 1.94 | 0.49 |
| 1:N:245:GLU:HA | 1:N:248:ARG:HD2 | 1.93 | 0.49 |
| 1:N:571:GLN:NE2 | 1:N:616:LEU:O | 2.30 | 0.49 |
| 1:N:1722:TYR:HD2 | 1:N:1725:ALA:HB2 | 1.77 | 0.49 |
| 1:N:2112:ARG:HE | 1:N:2116:LYS:HE2 | 1.77 | 0.49 |
| 1:N:2137:PRO:HD2 | 1:N:2143:LYS:HE2 | 1.95 | 0.49 |
| 1:N:3350:ASN:OD1 | 1:N:3351:VAL:N | 2.45 | 0.49 |
| 1:O:1512:ARG:HH21 | 1:O:1513:TYR:HE1 | 1.60 | 0.49 |
| 1:O:2521:THR:O | 1:O:2525:THR:OG1 | 2.18 | 0.49 |
| 1:O:2583:VAL:HG21 | 1:O:2772:PHE:HB3 | 1.95 | 0.49 |
| 1:P:38:LEU:HG | 1:P:73:TYR:CZ | 2.48 | 0.49 |
| 1:P:334:ASP:OD1 | 1:P:334:ASP:N | 2.44 | 0.49 |
| 1:P:562:LEU:HB3 | 1:P:564:GLU:OE1 | 2.12 | 0.49 |
| 1:P:1139:GLU:O | 1:P:1143:ARG:HG2 | 2.12 | 0.49 |
| 1:P:1785:ARG:HH12 | 1:P:1790:ASP:HA | 1.77 | 0.49 |
| 1:Q:568:ARG:HH11 | 1:Q:636:ILE:HD11 | 1.77 | 0.49 |
| 1:Q:1058:ARG:O | 1:Q:1062:ILE:HG12 | 2.12 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:Q:1249:THR:O | 1:Q:1251:LYS:NZ | 2.30 | 0.49 |
| 1:Q:2392:ARG:HB3 | 1:Q:2394:PHE:CE1 | 2.48 | 0.49 |
| 1:R:284:ASP:OD1 | 1:R:284:ASP:N | 2.44 | 0.49 |
| 1:R:427:GLN:OE1 | 1:R:427:GLN:N | 2.44 | 0.49 |
| 1:R:1108:VAL:HG13 | 1:R:1111:GLU:OE1 | 2.12 | 0.49 |
| 1:R:1992:THR:CA | 1:R:2017:GLY:O | 2.60 | 0.49 |
| 1:R:2345:ASN:ND2 | 1:R:2348:THR:OG1 | 2.44 | 0.49 |
| 1:R:2866:PRO:O | 1:S:2741:ARG:NH1 | 2.45 | 0.49 |
| 1:S:114:ASP:OD2 | 1:S:117:GLY:N | 2.40 | 0.49 |
| 1:S:1085:ARG:NH1 | 1:T:2464:ASP:O | 2.45 | 0.49 |
| 1:S:1986:LEU:HB2 | 1:S:2069:PRO:HG2 | 1.95 | 0.49 |
| 1:S:2269:ASN:OD1 | 1:S:2428:LEU:HB2 | 2.12 | 0.49 |
| 1:S:2382:GLU:O | 1:S:2385:ARG:HG2 | 2.13 | 0.49 |
| 1:T:680:PHE:O | 1:T:685:ASN:ND2 | 2.42 | 0.49 |
| 1:T:1452:ALA:HA | 1:T:1457:PHE:CG | 2.46 | 0.49 |
| 1:T:1676:ILE:HG13 | 1:T:1761:VAL:HG23 | 1.93 | 0.49 |
| 1:T:1677:ARG:HH22 | 1:T:1751:GLU:CD | 2.19 | 0.49 |
| 1:T:2745:GLU:OE1 | 1:T:2749:TRP:NE1 | 2.45 | 0.49 |
| 1:A:257:ASP:O | 1:A:265:ARG:NH2 | 2.37 | 0.49 |
| 1:A:855:THR:O | 1:A:859:VAL:HG23 | 2.12 | 0.49 |
| 1:A:1890:ARG:HB2 | 1:A:1955:TYR:CE2 | 2.47 | 0.49 |
| 1:B:1223:VAL:HG13 | 1:B:1231:ILE:HB | 1.95 | 0.49 |
| 1:B:1427:GLU:O | 1:B:1431:ASN:ND2 | 2.45 | 0.49 |
| 1:B:1431:ASN:OD1 | 1:B:1594:SER:OG | 2.31 | 0.49 |
| 1:B:1540:ILE:HD12 | 1:B:1540:ILE:H | 1.77 | 0.49 |
| 1:B:2104:THR:HB | 1:B:2108:LYS:HZ1 | 1.77 | 0.49 |
| 1:B:2430:GLY:N | 1:B:2433:GLU:OE2 | 2.41 | 0.49 |
| 1:B:3096:GLY:HA3 | 1:B:3104:SER:HB3 | 1.93 | 0.49 |
| 1:C:197:ASP:OD1 | 1:C:197:ASP:N | 2.44 | 0.49 |
| 1:C:636:ILE:H | 1:C:636:ILE:HD12 | 1.78 | 0.49 |
| 1:C:750:LEU:HD11 | 1:C:767:LYS:HD2 | 1.94 | 0.49 |
| 1:C:1345:SER:OG | 1:C:1346:VAL:N | 2.45 | 0.49 |
| 1:C:2147:CYS:O | 1:C:2149:HIS:ND1 | 2.45 | 0.49 |
| 1:C:2354:PRO:O | 1:C:2357:VAL:HG22 | 2.12 | 0.49 |
| 1:C:2556:LEU:H | 1:C:2556:LEU:HD23 | 1.77 | 0.49 |
| 1:D:510:ALA:O | 1:D:514:ARG:HG2 | 2.12 | 0.49 |
| 1:D:711:ASP:OD1 | 1:D:712:ASN:N | 2.43 | 0.49 |
| 1:D:953:GLU:HA | 1:D:969:HIS:HB2 | 1.94 | 0.49 |
| 1:E:167:ASP:OD1 | 1:E:303:ARG:NH2 | 2.45 | 0.49 |
| 1:E:1638:ARG:HE | 1:E:1644:TYR:HE1 | 1.60 | 0.49 |
| 1:E:2090:ASN:O | 1:E:2091:ARG:HD3 | 2.13 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:E:2108:LYS:O | 1:E:2112:ARG:NH1 | 2.45 | 0.49 |
| 1:F:925:LEU:HD22 | 1:F:928:LYS:HZ3 | 1.77 | 0.49 |
| 1:F:1345:SER:OG | 1:F:1346:VAL:N | 2.45 | 0.49 |
| 1:F:1564:ASN:HB3 | 1:F:1604:PHE:CE1 | 2.47 | 0.49 |
| 1:G:574:LEU:HB3 | 1:G:616:LEU:HD21 | 1.94 | 0.49 |
| 1:G:954:THR:HA | 1:G:965:PRO:HA | 1.94 | 0.49 |
| 1:G:1750:PHE:HD2 | 1:G:1882:LEU:HD21 | 1.76 | 0.49 |
| 1:G:2464:ASP:O | 1:H:1085:ARG:NH1 | 2.46 | 0.49 |
| 1:G:2990:LEU:HA | 1:G:2993:VAL:HG12 | 1.93 | 0.49 |
| 1:H:1501:ASP:OD2 | 1:H:1504:GLN:N | 2.45 | 0.49 |
| 1:H:1926:GLY:HA2 | 1:H:1936:LYS:HE2 | 1.94 | 0.49 |
| 1:H:2620:ASN:HB3 | 1:H:2623:GLU:OE1 | 2.12 | 0.49 |
| 1:H:2926:VAL:HG12 | 1:H:3011:TRP:HB3 | 1.95 | 0.49 |
| 1:I:606:PHE:CZ | 1:I:644:VAL:HG13 | 2.47 | 0.49 |
| 1:I:1100:ASP:OD2 | 1:I:1102:ILE:HG22 | 2.12 | 0.49 |
| 1:J:98:LYS:HE3 | 1:J:289:ASN:H | 1.78 | 0.49 |
| 1:J:435:LYS:HG2 | 1:J:436:ASP:H | 1.77 | 0.49 |
| 1:J:458:ASP:HB2 | 1:J:1341:GLY:HA3 | 1.94 | 0.49 |
| 1:J:1839:GLU:HA | 1:J:1902:ARG:HH22 | 1.77 | 0.49 |
| 1:J:1854:HIS:O | 1:J:1884:HIS:HE1 | 1.95 | 0.49 |
| 1:K:193:GLY:HA2 | 1:K:199:SER:HB2 | 1.95 | 0.49 |
| 1:K:392:SER:OG | 1:K:393:VAL:N | 2.45 | 0.49 |
| 1:K:938:ASP:HA | 1:K:1055:ASN:ND2 | 2.27 | 0.49 |
| 1:K:3122:ILE:O | 1:K:3125:ILE:HG22 | 2.12 | 0.49 |
| 1:L:229:LEU:HB3 | 1:L:233:ARG:HH21 | 1.78 | 0.49 |
| 1:L:458:ASP:HB2 | 1:L:1341:GLY:HA3 | 1.94 | 0.49 |
| 1:L:658:ARG:NH2 | 1:L:728:ASP:OD1 | 2.45 | 0.49 |
| 1:L:674:LEU:HD12 | 1:L:695:ARG:HH22 | 1.77 | 0.49 |
| 1:L:758:LYS:HD3 | 1:L:803:GLU:HB3 | 1.95 | 0.49 |
| 1:L:810:ILE:HG23 | 1:L:818:TRP:HE3 | 1.77 | 0.49 |
| 1:L:887:GLN:NE2 | 1:L:889:ASN:HB2 | 2.28 | 0.49 |
| 1:L:1086:LYS:HZ3 | 1:L:1087:PRO:HD2 | 1.77 | 0.49 |
| 1:L:1126:LEU:HD23 | 1:L:1126:LEU:H | 1.77 | 0.49 |
| 1:L:1332:GLN:OE1 | 1:L:1505:ASN:ND2 | 2.45 | 0.49 |
| 1:M:490:VAL:HG13 | 1:M:493:MET:HB3 | 1.95 | 0.49 |
| 1:M:596:GLN:O | 1:M:658:ARG:NH2 | 2.44 | 0.49 |
| 1:M:1488:ALA:HB3 | 1:M:1492:MET:HE3 | 1.93 | 0.49 |
| 1:M:1751:GLU:OE2 | 1:M:1763:ILE:HB | 2.12 | 0.49 |
| 1:M:2626:GLU:OE2 | 1:M:2633:LYS:NZ | 2.45 | 0.49 |
| 1:M:2926:VAL:HG12 | 1:M:3009:PRO:HB2 | 1.94 | 0.49 |
| 1:M:2941:LEU:HD22 | 1:M:3032:PHE:CD1 | 2.47 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:N:801:ASP:OD1 | 1:N:801:ASP:N | 2.42 | 0.49 |
| 1:N:859:VAL:HG12 | 1:N:863:ARG:NE | 2.27 | 0.49 |
| 1:N:1540:ILE:HD12 | 1:N:1540:ILE:H | 1.78 | 0.49 |
| 1:N:3119:HIS:O | 1:N:3122:ILE:HG22 | 2.12 | 0.49 |
| 1:O:149:LEU:HD11 | 1:O:191:LEU:HB3 | 1.93 | 0.49 |
| 1:O:186:ASN:HB3 | 1:O:351:LEU:HD13 | 1.95 | 0.49 |
| 1:O:248:ARG:NH1 | 1:O:803:GLU:HA | 2.27 | 0.49 |
| 1:O:2604:THR:HG23 | 1:O:2782:HIS:NE2 | 2.27 | 0.49 |
| 1:O:2912:ASP:OD1 | 1:O:2912:ASP:N | 2.43 | 0.49 |
| 1:P:220:ASP:OD1 | 1:P:221:ARG:N | 2.45 | 0.49 |
| 1:P:1710:LEU:HD22 | 1:P:1750:PHE:CE1 | 2.47 | 0.49 |
| 1:Q:820:GLU:N | 1:Q:820:GLU:OE1 | 2.44 | 0.49 |
| 1:R:230:GLN:NE2 | 1:R:236:THR:O | 2.44 | 0.49 |
| 1:R:956:VAL:HA | 1:R:963:PRO:HA | 1.93 | 0.49 |
| 1:R:1466:ARG:O | 1:R:1470:ILE:HG12 | 2.12 | 0.49 |
| 1:R:1884:HIS:O | 1:R:1887:SER:OG | 2.24 | 0.49 |
| 1:R:2671:GLU:HA | 1:R:2674:TYR:HB3 | 1.95 | 0.49 |
| 1:S:885:HIS:ND1 | 1:S:885:HIS:O | 2.45 | 0.49 |
| 1:S:1395:ASP:HB3 | 1:S:1439:GLY:HA3 | 1.95 | 0.49 |
| 1:S:1730:ALA:H | 1:S:2020:ALA:HB1 | 1.78 | 0.49 |
| 1:S:2669:ASN:HA | 1:S:2672:VAL:HG12 | 1.93 | 0.49 |
| 1:T:200:LEU:HD21 | 1:T:209:ASP:HB3 | 1.92 | 0.49 |
| 1:T:744:ASN:HB3 | 1:T:779:TRP:NE1 | 2.28 | 0.49 |
| 1:T:848:ARG:HB3 | 1:T:934:LEU:O | 2.12 | 0.49 |
| 1:T:1367:TYR:CE2 | 1:T:1369:ASP:HB3 | 2.47 | 0.49 |
| 1:T:1367:TYR:HE2 | 1:T:1369:ASP:HB3 | 1.76 | 0.49 |
| 1:T:1521:ASP:HB3 | 1:T:1525:HIS:CD2 | 2.48 | 0.49 |
| 1:A:203:LEU:HD21 | 1:A:351:LEU:HB3 | 1.95 | 0.49 |
| 1:A:437:VAL:HG12 | 1:A:521:PRO:HB2 | 1.94 | 0.49 |
| 1:A:449:ARG:CZ | 1:A:552:ASN:HD21 | 2.25 | 0.49 |
| 1:A:2954:GLU:OE2 | 1:A:3035:TYR:OH | 2.29 | 0.49 |
| 1:B:1185:GLY:HA2 | 1:B:1189:GLU:HG3 | 1.94 | 0.49 |
| 1:B:1710:LEU:HD13 | 1:B:1750:PHE:HE1 | 1.74 | 0.49 |
| 1:B:1795:ASN:HD21 | 1:B:1797:TRP:HB2 | 1.77 | 0.49 |
| 1:B:3211:ASP:OD1 | 1:B:3309:ALA:N | 2.46 | 0.49 |
| 1:C:277:ARG:NH2 | 1:K:836:HIS:HD2 | 2.04 | 0.49 |
| 1:C:1919:PRO:HG3 | 1:C:1940:LYS:NZ | 2.27 | 0.49 |
| 1:C:2304:LYS:HB2 | 1:C:2367:TYR:HE2 | 1.78 | 0.49 |
| 1:D:842:HIS:NE2 | 1:D:844:GLU:HB2 | 2.28 | 0.49 |
| 1:D:1048:ILE:HA | 1:D:1051:LEU:HG | 1.94 | 0.49 |
| 1:D:1193:GLN:OE1 | 1:D:1194:TYR:N | 2.45 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:D:3071:THR:HB | 1:D:3072:LEU:HD12 | 1.95 | 0.49 |
| 1:E:169:LEU:HA | 1:E:177:PHE:HE1 | 1.76 | 0.49 |
| 1:E:1721:PRO:HD3 | 1:E:1729:TYR:CZ | 2.48 | 0.49 |
| 1:E:2021:GLU:N | 1:E:2021:GLU:OE1 | 2.45 | 0.49 |
| 1:E:2153:THR:HA | 1:E:2156:HIS:ND1 | 2.26 | 0.49 |
| 1:E:2488:LYS:HD2 | 1:E:2489:PRO:HD2 | 1.94 | 0.49 |
| 1:F:701:ASP:OD1 | 1:F:701:ASP:N | 2.45 | 0.49 |
| 1:F:2191:PRO:HG2 | 1:F:2194:PHE:CD2 | 2.47 | 0.49 |
| 1:G:441:THR:OG1 | 1:G:443:GLU:OE1 | 2.31 | 0.49 |
| 1:G:752:ILE:O | 1:G:808:LEU:HA | 2.12 | 0.49 |
| 1:G:3214:TYR:HD1 | 1:G:3265:ASP:HA | 1.76 | 0.49 |
| 1:H:52:ASP:OD1 | 1:H:53:GLY:N | 2.46 | 0.49 |
| 1:H:128:GLY:N | 1:H:141:THR:OG1 | 2.46 | 0.49 |
| 1:H:502:LEU:HA | 1:H:505:VAL:HG12 | 1.94 | 0.49 |
| 1:H:848:ARG:HB3 | 1:H:933:GLY:HA3 | 1.95 | 0.49 |
| 1:H:1284:ARG:NH2 | 1:H:1379:PRO:HB3 | 2.24 | 0.49 |
| 1:H:2194:PHE:HD1 | 1:H:2212:PHE:HB3 | 1.76 | 0.49 |
| 1:H:2513:VAL:HG21 | 1:H:2515:LYS:HE2 | 1.94 | 0.49 |
| 1:H:2626:GLU:OE1 | 1:H:2627:ILE:N | 2.46 | 0.49 |
| 1:H:2666:ASP:OD1 | 1:H:2667:TYR:N | 2.46 | 0.49 |
| 1:H:2789:LEU:O | 1:H:2793:ILE:HG12 | 2.12 | 0.49 |
| 1:I:938:ASP:HA | 1:I:1055:ASN:HD21 | 1.76 | 0.49 |
| 1:I:2762:ARG:HG3 | 1:I:2764:VAL:HG22 | 1.93 | 0.49 |
| 1:J:1745:LEU:HD23 | 1:J:1923:PHE:HD2 | 1.78 | 0.49 |
| 1:J:2413:CYS:SG | 1:J:2470:ARG:NE | 2.82 | 0.49 |
| 1:K:13:ASP:OD1 | 1:K:14:GLN:N | 2.45 | 0.49 |
| 1:K:938:ASP:HA | 1:K:1055:ASN:HD21 | 1.78 | 0.49 |
| 1:K:1486:ASP:N | 1:K:1486:ASP:OD1 | 2.45 | 0.49 |
| 1:K:2796:ARG:O | 1:K:2801:ARG:NH2 | 2.45 | 0.49 |
| 1:L:851:VAL:HG12 | 1:L:935:PRO:HB2 | 1.94 | 0.49 |
| 1:L:914:HIS:HA | 1:L:917:LEU:HG | 1.94 | 0.49 |
| 1:L:1325:TRP:HE3 | 1:L:1496:LEU:HD21 | 1.77 | 0.49 |
| 1:L:1492:MET:HA | 1:L:1516:PRO:HG2 | 1.94 | 0.49 |
| 1:L:1720:CYS:SG | 1:L:1731:CYS:N | 2.85 | 0.49 |
| 1:L:2330:MET:HE1 | 1:L:2355:LYS:HD3 | 1.94 | 0.49 |
| 1:M:399:ASN:HD21 | 1:M:401:ASN:HD21 | 1.60 | 0.49 |
| 1:M:2155:PRO:HB2 | 1:M:2306:TRP:CZ3 | 2.48 | 0.49 |
| 1:M:2983:VAL:HG11 | 1:M:3149:ASN:O | 2.12 | 0.49 |
| 1:N:255:ASP:N | 1:N:255:ASP:OD1 | 2.46 | 0.49 |
| 1:N:944:THR:HA | 1:N:987:PHE:CD1 | 2.47 | 0.49 |
| 1:N:1067:GLN:HG3 | 1:N:1070:ARG:HH21 | 1.76 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:N:1152:GLY:HA2 | 1:N:1198:PHE:O | 2.13 | 0.49 |
| 1:N:2252:LEU:HD23 | 1:N:2309:TRP:HD1 | 1.77 | 0.49 |
| 1:O:2008:LYS:NZ | 1:O:2037:VAL:O | 2.44 | 0.49 |
| 1:O:2111:LEU:HD12 | 1:O:2211:PRO:HG2 | 1.93 | 0.49 |
| 1:O:2345:ASN:O | 1:O:2349:ARG:HG2 | 2.12 | 0.49 |
| 1:P:1427:GLU:O | 1:P:1431:ASN:ND2 | 2.46 | 0.49 |
| 1:P:2124:GLN:HG2 | 1:P:2125:ALA:N | 2.28 | 0.49 |
| 1:Q:855:THR:HG22 | 1:Q:858:GLN:NE2 | 2.27 | 0.49 |
| 1:Q:2587:ARG:HD2 | 1:Q:2754:ASN:HD22 | 1.78 | 0.49 |
| 1:Q:2863:HIS:NE2 | 1:R:1536:ASN:OD1 | 2.39 | 0.49 |
| 1:R:887:GLN:HE22 | 1:R:889:ASN:HB2 | 1.77 | 0.49 |
| 1:S:1085:ARG:NH2 | 1:T:2463:ALA:O | 2.27 | 0.49 |
| 1:S:1828:ASN:HD21 | 1:S:1830:LEU:HB3 | 1.76 | 0.49 |
| 1:S:2370:MET:SD | 1:S:2370:MET:N | 2.85 | 0.49 |
| 1:S:2978:THR:N | 1:S:2987:TRP:HZ3 | 2.10 | 0.49 |
| 1:T:580:TYR:CG | 1:T:958:PRO:HG2 | 2.48 | 0.49 |
| 1:T:599:PHE:HA | 1:T:651:TRP:HH2 | 1.76 | 0.49 |
| 1:T:2112:ARG:HE | 1:T:2116:LYS:HZ2 | 1.61 | 0.49 |
| 1:T:3320:LEU:N | 1:T:3341:HIS:O | 2.45 | 0.49 |
| 1:A:1730:ALA:N | 1:A:2020:ALA:O | 2.45 | 0.49 |
| 1:A:1903:GLY:HA3 | 1:B:1667:GLN:HB2 | 1.95 | 0.49 |
| 1:A:3395:ARG:NE | 1:A:3398:GLN:OE1 | 2.42 | 0.49 |
| 1:B:1139:GLU:O | 1:B:1143:ARG:HG2 | 2.13 | 0.49 |
| 1:C:2773:ASN:HD21 | 1:C:3142:TYR:HB2 | 1.78 | 0.49 |
| 1:C:2912:ASP:OD1 | 1:C:2912:ASP:N | 2.44 | 0.49 |
| 1:D:7:ASN:HB3 | 1:D:10:LEU:HG | 1.93 | 0.49 |
| 1:D:1324:HIS:HB3 | 1:D:1519:VAL:HG21 | 1.94 | 0.49 |
| 1:D:1620:LYS:HE2 | 1:D:1620:LYS:HA | 1.95 | 0.49 |
| 1:D:2311:GLU:CD | 1:D:2377:LEU:HD22 | 2.37 | 0.49 |
| 1:D:2655:TYR:CD1 | 1:D:2659:LEU:HD23 | 2.46 | 0.49 |
| 1:E:811:LYS:HD2 | 1:E:815:GLY:HA2 | 1.94 | 0.49 |
| 1:E:986:LEU:HD12 | 1:E:1028:LEU:HG | 1.94 | 0.49 |
| 1:E:991:LYS:HE3 | 1:E:994:ARG:HE | 1.77 | 0.49 |
| 1:E:1100:ASP:OD2 | 1:E:1102:ILE:HG22 | 2.12 | 0.49 |
| 1:E:3075:THR:OG1 | 1:E:3138:ARG:NH1 | 2.46 | 0.49 |
| 1:F:1052:HIS:O | 1:F:1056:THR:HG23 | 2.13 | 0.49 |
| 1:F:1705:THR:HG23 | 1:F:1931:LEU:HD12 | 1.94 | 0.49 |
| 1:F:1713:PHE:CE1 | 1:F:1929:TYR:HB3 | 2.45 | 0.49 |
| 1:F:3303:VAL:HG13 | 1:F:3305:ILE:HD11 | 1.94 | 0.49 |
| 1:G:1174:PRO:HG2 | 1:G:1176:HIS:CE1 | 2.47 | 0.49 |
| 1:G:1246:GLY:O | 1:G:1249:THR:OG1 | 2.26 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:G:2802:VAL:HG12 | 1:G:2856:THR:HG22 | 1.94 | 0.49 |
| 1:I:757:PRO:HB3 | 1:I:798:LEU:HD11 | 1.94 | 0.49 |
| 1:I:1560:PHE:HZ | 1:I:1573:LEU:HD21 | 1.77 | 0.49 |
| 1:I:3268:ASP:OD1 | 1:I:3268:ASP:N | 2.45 | 0.49 |
| 1:J:1124:ASP:N | 1:J:1124:ASP:OD1 | 2.46 | 0.49 |
| 1:J:2087:LEU:HD13 | 1:J:2366:ARG:HD3 | 1.95 | 0.49 |
| 1:J:2092:VAL:HG13 | 1:J:2366:ARG:HG3 | 1.95 | 0.49 |
| 1:J:2595:ARG:HG3 | 1:J:2596:VAL:HG13 | 1.94 | 0.49 |
| 1:J:3127:GLN:HE22 | 1:J:3190:LEU:HD22 | 1.78 | 0.49 |
| 1:K:222:ILE:O | 1:K:225:ILE:HG22 | 2.13 | 0.49 |
| 1:K:231:LYS:HE3 | 1:K:237:TYR:HE1 | 1.77 | 0.49 |
| 1:K:539:GLU:N | 1:K:539:GLU:OE1 | 2.45 | 0.49 |
| 1:K:857:GLU:HG2 | 1:K:858:GLN:OE1 | 2.13 | 0.49 |
| 1:K:915:ARG:NH1 | 1:K:1115:TYR:HB3 | 2.27 | 0.49 |
| 1:K:2378:ASP:N | 1:K:2378:ASP:OD1 | 2.46 | 0.49 |
| 1:K:3251:ASP:OD1 | 1:K:3251:ASP:N | 2.46 | 0.49 |
| 1:L:567:SER:OG | 1:L:623:TYR:O | 2.29 | 0.49 |
| 1:L:1186:ASP:H | 1:L:1189:GLU:HB2 | 1.77 | 0.49 |
| 1:L:2124:GLN:HG2 | 1:L:2125:ALA:N | 2.27 | 0.49 |
| 1:L:2286:LEU:HD23 | 1:L:2286:LEU:H | 1.78 | 0.49 |
| 1:L:3211:ASP:OD1 | 1:L:3309:ALA:N | 2.46 | 0.49 |
| 1:M:390:LEU:HD22 | 1:M:398:LEU:HB3 | 1.94 | 0.49 |
| 1:M:1890:ARG:HB3 | 1:M:1955:TYR:CE2 | 2.48 | 0.49 |
| 1:M:2926:VAL:HB | 1:M:3023:LEU:HD21 | 1.95 | 0.49 |
| 1:N:80:LYS:HA | 1:N:83:LYS:HZ3 | 1.76 | 0.49 |
| 1:N:458:ASP:OD2 | 1:N:460:SER:OG | 2.30 | 0.49 |
| 1:N:845:LEU:HB3 | 1:N:926:ARG:CZ | 2.42 | 0.49 |
| 1:N:2377:LEU:HA | 1:N:2380:LEU:HB2 | 1.94 | 0.49 |
| 1:N:3232:LEU:HD23 | 1:N:3234:PRO:HD3 | 1.95 | 0.49 |
| 1:O:24:ARG:HH21 | 1:O:123:ASN:HA | 1.78 | 0.49 |
| 1:O:2027:ASP:HA | 1:P:1651:ARG:HH12 | 1.76 | 0.49 |
| 1:P:614:HIS:HA | 1:P:625:LEU:HG | 1.93 | 0.49 |
| 1:P:848:ARG:HH12 | 1:P:1121:TYR:HB2 | 1.77 | 0.49 |
| 1:P:3119:HIS:O | 1:P:3122:ILE:HG22 | 2.13 | 0.49 |
| 1:P:3320:LEU:N | 1:P:3341:HIS:O | 2.45 | 0.49 |
| 1:Q:513:SER:OG | 1:Q:514:ARG:NH1 | 2.41 | 0.49 |
| 1:R:329:CYS:HA | 1:R:342:CYS:CB | 2.43 | 0.49 |
| 1:R:454:ARG:NH2 | 1:R:1338:LEU:HG | 2.27 | 0.49 |
| 1:R:580:TYR:HE2 | 1:R:959:GLU:HB3 | 1.78 | 0.49 |
| 1:R:845:LEU:O | 1:R:926:ARG:NH1 | 2.45 | 0.49 |
| 1:R:1201:GLU:OE1 | 1:R:1202:ILE:N | 2.45 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:R:1728:ARG:HH21 | 4:T:3501:NAG:C8 | 2.25 | 0.49 |
| 1:R:2695:THR:HG21 | 1:R:2698:TYR:HD2 | 1.77 | 0.49 |
| 1:R:2720:GLN:HE22 | 1:R:2730:TYR:HB2 | 1.76 | 0.49 |
| 1:S:1138:ARG:NH1 | 1:S:1261:SER:HB3 | 2.28 | 0.49 |
| 1:S:1750:PHE:HD2 | 1:S:1882:LEU:HD21 | 1.78 | 0.49 |
| 1:S:2801:ARG:HD3 | 1:S:2803:PHE:CZ | 2.48 | 0.49 |
| 1:S:3148:ARG:HE | 1:T:3386:TYR:HE2 | 1.61 | 0.49 |
| 1:T:1205:ILE:HD12 | 1:T:1208:LYS:HE3 | 1.95 | 0.49 |
| 1:T:3303:VAL:HG13 | 1:T:3305:ILE:HD11 | 1.93 | 0.49 |
| 1:T:3317:ILE:HG13 | 1:T:3339:ARG:HB3 | 1.93 | 0.49 |
| 1:A:606:PHE:HZ | 1:A:644:VAL:HG13 | 1.78 | 0.49 |
| 1:A:672:HIS:O | 1:A:695:ARG:NH2 | 2.41 | 0.49 |
| 1:A:1295:ILE:HD12 | 1:A:1333:VAL:HG12 | 1.94 | 0.49 |
| 1:B:1136:LEU:HA | 1:B:1139:GLU:OE2 | 2.12 | 0.49 |
| 1:B:2462:ASN:OD1 | 1:B:2463:ALA:N | 2.45 | 0.49 |
| 1:C:169:LEU:HA | 1:C:177:PHE:HE1 | 1.78 | 0.49 |
| 1:C:988:GLU:OE2 | 1:C:996:THR:OG1 | 2.26 | 0.49 |
| 1:C:1122:HIS:ND1 | 1:C:1123:TYR:O | 2.45 | 0.49 |
| 1:C:1489:LEU:HA | 1:C:1492:MET:HG2 | 1.94 | 0.49 |
| 1:C:2037:VAL:HA | 1:C:2040:LYS:HG2 | 1.94 | 0.49 |
| 1:C:2439:ASP:N | 1:C:2439:ASP:OD1 | 2.46 | 0.49 |
| 1:C:3203:ILE:HD12 | 1:C:3206:ASN:HB2 | 1.93 | 0.49 |
| 1:D:2673:GLN:HA | 1:D:2676:VAL:HG22 | 1.95 | 0.49 |
| 1:E:938:ASP:HA | 1:E:1055:ASN:ND2 | 2.28 | 0.49 |
| 1:E:2848:ASP:OD1 | 1:E:2849:ARG:N | 2.46 | 0.49 |
| 1:F:1854:HIS:O | 1:F:1884:HIS:HE1 | 1.95 | 0.49 |
| 1:G:231:LYS:HE3 | 1:G:237:TYR:HE1 | 1.78 | 0.49 |
| 1:G:250:LYS:HD2 | 1:G:268:SER:HB3 | 1.93 | 0.49 |
| 1:G:663:LYS:HB2 | 1:G:665:HIS:NE2 | 2.28 | 0.49 |
| 1:G:887:GLN:HE21 | 1:G:889:ASN:HD21 | 1.61 | 0.49 |
| 1:G:1830:LEU:HG | 1:G:1834:PHE:CE2 | 2.47 | 0.49 |
| 1:G:2129:PHE:HE1 | 1:G:2342:LEU:HD13 | 1.78 | 0.49 |
| 1:H:705:GLU:N | 1:H:705:GLU:OE1 | 2.46 | 0.49 |
| 1:H:950:VAL:HA | 1:H:968:PHE:HB3 | 1.93 | 0.49 |
| 1:H:1143:ARG:HB3 | 1:H:1148:ARG:NH2 | 2.26 | 0.49 |
| 1:H:1223:VAL:O | 1:H:1230:LYS:NZ | 2.43 | 0.49 |
| 1:H:2158:HIS:HB3 | 1:H:2299:HIS:HD2 | 1.78 | 0.49 |
| 1:H:2182:ASP:HA | 1:H:2301:PHE:CE2 | 2.46 | 0.49 |
| 1:H:2738:GLN:O | 1:H:2742:GLN:NE2 | 2.45 | 0.49 |
| 1:I:245:GLU:HA | 1:I:248:ARG:HG2 | 1.94 | 0.49 |
| 1:I:693:HIS:CE1 | 1:I:705:GLU:HB3 | 2.47 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:I:1016:VAL:O | 1:I:1019:GLU:HG3 | 2.12 | 0.49 |
| 1:I:1426:PHE:CE1 | 1:I:1464:VAL:HG13 | 2.48 | 0.49 |
| 1:I:2587:ARG:HH12 | 1:I:2753:PRO:HB2 | 1.77 | 0.49 |
| 1:I:2676:VAL:HG21 | 1:I:2851:PHE:CZ | 2.47 | 0.49 |
| 1:J:503:PHE:HA | 1:J:678:PHE:HE1 | 1.76 | 0.49 |
| 1:J:674:LEU:HG | 1:J:676:LYS:HE3 | 1.93 | 0.49 |
| 1:J:1947:TYR:OH | 1:J:1948:LYS:NZ | 2.29 | 0.49 |
| 1:K:81:LEU:HD21 | 1:K:86:LEU:HD23 | 1.95 | 0.49 |
| 1:K:613:PRO:HA | 1:K:616:LEU:HB3 | 1.95 | 0.49 |
| 1:K:647:LEU:HA | 1:K:650:ILE:HG12 | 1.93 | 0.49 |
| 1:K:1539:THR:H | 1:K:1542:GLN:HE22 | 1.60 | 0.49 |
| 1:K:2044:SER:OG | 1:K:2046:ASP:OD1 | 2.30 | 0.49 |
| 1:K:2956:ILE:HA | 1:K:2959:PHE:HE2 | 1.76 | 0.49 |
| 1:K:3068:THR:O | 1:K:3071:THR:OG1 | 2.23 | 0.49 |
| 1:K:3142:TYR:CZ | 1:K:3144:ARG:HD3 | 2.47 | 0.49 |
| 1:L:2407:GLU:O | 1:L:2473:ILE:HA | 2.13 | 0.49 |
| 1:L:2626:GLU:OE1 | 1:L:2627:ILE:N | 2.45 | 0.49 |
| 1:L:2652:SER:O | 1:L:2656:ARG:NH1 | 2.46 | 0.49 |
| 1:M:221:ARG:NH2 | 1:M:287:SER:O | 2.45 | 0.49 |
| 1:M:255:ASP:OD1 | 1:M:255:ASP:N | 2.45 | 0.49 |
| 1:M:2152:PRO:HA | 1:M:2261:GLU:OE2 | 2.13 | 0.49 |
| 1:N:655:GLN:HG2 | 1:N:662:TYR:HB3 | 1.95 | 0.49 |
| 1:N:1018:TYR:CE1 | 1:N:1056:THR:HB | 2.46 | 0.49 |
| 1:N:2287:HIS:HE1 | 1:N:2432:LEU:HB2 | 1.78 | 0.49 |
| 1:N:3395:ARG:O | 1:N:3401:ARG:NH1 | 2.37 | 0.49 |
| 1:O:1008:GLN:OE1 | 1:O:1008:GLN:N | 2.41 | 0.49 |
| 1:O:2090:ASN:O | 1:O:2091:ARG:HD3 | 2.13 | 0.49 |
| 1:P:1142:HIS:HB3 | 1:P:1143:ARG:NH2 | 2.27 | 0.49 |
| 1:Q:1362:ILE:HB | 1:Q:1394:ARG:HH12 | 1.77 | 0.49 |
| 1:Q:1638:ARG:HG2 | 1:Q:1644:TYR:HE2 | 1.78 | 0.49 |
| 1:Q:1963:ILE:HG23 | 1:Q:1967:LEU:HD23 | 1.93 | 0.49 |
| 1:Q:3304:VAL:HG23 | 1:Q:3317:ILE:HB | 1.95 | 0.49 |
| 1:R:1024:TYR:O | 1:R:1028:LEU:HG | 2.13 | 0.49 |
| 1:R:1946:ASP:HB3 | 1:R:1950:HIS:CD2 | 2.48 | 0.49 |
| 1:R:3119:HIS:O | 1:R:3122:ILE:HG22 | 2.13 | 0.49 |
| 1:S:986:LEU:HD12 | 1:S:1028:LEU:HG | 1.95 | 0.49 |
| 1:T:1839:GLU:HA | 1:T:1902:ARG:NH2 | 2.27 | 0.49 |
| 1:T:2169:LEU:C | 1:T:2174:SER:HB3 | 2.37 | 0.49 |
| 1:T:2393:VAL:HG11 | 1:T:2450:LEU:HD12 | 1.95 | 0.49 |
| 1:T:2785:THR:OG1 | 1:T:2788:GLN:OE1 | 2.19 | 0.49 |
| 1:T:2865:ARG:NH1 | 1:T:2866:PRO:HG2 | 2.27 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:T:3131:THR:HA | 1:T:3134:LYS:HG2 | 1.95 | 0.49 |
| 1:A:524:ASP:OD1 | 1:A:526:THR:OG1 | 2.20 | 0.49 |
| 1:A:1418:SER:OG | 1:A:1419:PHE:N | 2.46 | 0.49 |
| 1:A:2059:ASN:OD1 | 1:A:2061:SER:N | 2.45 | 0.49 |
| 1:A:2090:ASN:O | 1:A:2091:ARG:HD3 | 2.13 | 0.49 |
| 1:B:79:GLN:O | 1:B:83:LYS:NZ | 2.46 | 0.49 |
| 1:B:105:ARG:HG2 | 1:B:105:ARG:O | 2.13 | 0.49 |
| 1:B:780:ASN:OD1 | 1:B:781:PHE:N | 2.45 | 0.49 |
| 1:B:845:LEU:HD22 | 1:B:926:ARG:HD3 | 1.94 | 0.49 |
| 1:C:12:THR:OG1 | 1:C:15:GLU:OE2 | 2.30 | 0.49 |
| 1:C:1322:PHE:HB3 | 1:C:1323:PRO:HD3 | 1.95 | 0.49 |
| 1:C:1588:HIS:ND1 | 1:C:1588:HIS:O | 2.46 | 0.49 |
| 1:C:2021:GLU:N | 1:C:2021:GLU:OE1 | 2.45 | 0.49 |
| 1:C:3276:ASN:OD1 | 1:C:3277:ALA:N | 2.45 | 0.49 |
| 1:D:1267:ASN:HB3 | 1:D:1348:TYR:CZ | 2.47 | 0.49 |
| 1:D:1568:SER:N | 1:D:1597:GLY:O | 2.46 | 0.49 |
| 1:D:1851:GLU:O | 1:D:1855:ASN:ND2 | 2.46 | 0.49 |
| 1:D:3077:TYR:OH | 1:D:3126:TRP:NE1 | 2.38 | 0.49 |
| 1:E:1579:THR:HG21 | 1:H:339:HIS:HA | 1.94 | 0.49 |
| 1:E:1684:THR:OG1 | 1:F:1962:GLY:HA3 | 2.11 | 0.49 |
| 1:E:1978:LYS:HA | 1:E:2078:LYS:HG2 | 1.95 | 0.49 |
| 1:E:2037:VAL:HA | 1:E:2040:LYS:HG2 | 1.95 | 0.49 |
| 1:E:2199:PHE:CE1 | 1:E:2208:LEU:HB3 | 2.48 | 0.49 |
| 1:F:188:ILE:HA | 1:F:191:LEU:HB3 | 1.95 | 0.49 |
| 1:F:913:TRP:NE1 | 1:F:1089:GLN:O | 2.45 | 0.49 |
| 1:F:1362:ILE:HD13 | 1:F:1456:LEU:HD11 | 1.95 | 0.49 |
| 1:F:2636:ARG:NH2 | 1:F:2702:ASP:OD1 | 2.36 | 0.49 |
| 1:F:2865:ARG:NH1 | 1:F:2866:PRO:HG2 | 2.28 | 0.49 |
| 1:F:3352:LYS:HB2 | 1:F:3389:VAL:HG23 | 1.95 | 0.49 |
| 1:G:363:LEU:HD12 | 1:G:364:PRO:HD2 | 1.95 | 0.49 |
| 1:G:1756:ARG:NH2 | 1:H:2176:VAL:HG13 | 2.28 | 0.49 |
| 1:G:3334:ARG:HH21 | 1:G:3406:ILE:HG23 | 1.78 | 0.49 |
| 1:H:451:ALA:HB1 | 1:H:514:ARG:HG2 | 1.94 | 0.49 |
| 1:H:594:LEU:HA | 1:H:602:PHE:CE2 | 2.47 | 0.49 |
| 1:H:1677:ARG:HD2 | 1:H:1763:ILE:O | 2.13 | 0.49 |
| 1:H:2414:GLN:HA | 1:H:2467:PHE:HA | 1.95 | 0.49 |
| 1:I:719:THR:HG21 | 1:I:847:VAL:HG21 | 1.95 | 0.49 |
| 1:J:32:VAL:HA | 1:J:37:ASN:HD21 | 1.78 | 0.49 |
| 1:J:542:VAL:HA | 1:J:549:SER:HA | 1.95 | 0.49 |
| 1:J:1150:PHE:HB3 | 1:J:1199:GLN:OE1 | 2.12 | 0.49 |
| 1:J:1492:MET:N | 1:J:1492:MET:HE2 | 2.27 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:J:1834:PHE:HE2 | 1:J:1891:ILE:HD13 | 1.77 | 0.49 |
| 1:J:2552:GLY:HA3 | 1:J:2697:GLU:HA | 1.95 | 0.49 |
| 1:K:612:LEU:HB2 | 1:K:613:PRO:HD3 | 1.94 | 0.49 |
| 1:K:939:TRP:HA | 1:K:943:MET:HE1 | 1.93 | 0.49 |
| 1:K:1585:ASN:OD1 | 1:K:1586:CYS:N | 2.44 | 0.49 |
| 1:K:1900:ARG:O | 1:K:1900:ARG:NH1 | 2.46 | 0.49 |
| 1:K:2124:GLN:OE1 | 1:K:2124:GLN:N | 2.38 | 0.49 |
| 1:L:111:ILE:HG23 | 1:L:122:LYS:HB2 | 1.94 | 0.49 |
| 1:L:196:HIS:CE1 | 1:L:198:HIS:HB2 | 2.47 | 0.49 |
| 1:L:614:HIS:HA | 1:L:625:LEU:HG | 1.94 | 0.49 |
| 1:L:872:ASP:HB3 | 1:L:877:GLY:HA2 | 1.93 | 0.49 |
| 1:L:1890:ARG:HH12 | 1:L:1959:GLU:HG3 | 1.78 | 0.49 |
| 1:L:2182:ASP:HA | 1:L:2301:PHE:CE2 | 2.47 | 0.49 |
| 1:L:2283:LEU:HD21 | 1:L:2292:ASP:HB3 | 1.93 | 0.49 |
| 1:M:2407:GLU:OE2 | 1:M:2424:ALA:HB1 | 2.13 | 0.49 |
| 1:M:2534:ALA:O | 1:M:2592:GLN:NE2 | 2.41 | 0.49 |
| 1:M:2655:TYR:O | 1:M:2658:ILE:HG22 | 2.13 | 0.49 |
| 1:N:143:ARG:HH22 | 1:N:209:ASP:CG | 2.21 | 0.49 |
| 1:N:228:GLU:HA | 1:N:231:LYS:HG3 | 1.93 | 0.49 |
| 1:N:2392:ARG:HH11 | 1:N:2394:PHE:HZ | 1.60 | 0.49 |
| 1:O:2603:TRP:NE1 | 1:O:2711:ASN:HD22 | 2.11 | 0.49 |
| 1:P:598:ASP:OD1 | 1:P:599:PHE:N | 2.46 | 0.49 |
| 1:P:845:LEU:HD21 | 1:P:932:ASP:HA | 1.94 | 0.49 |
| 1:P:1135:GLN:O | 1:P:1138:ARG:HG2 | 2.12 | 0.49 |
| 1:P:1271:LEU:HB2 | 1:P:1275:GLU:HG3 | 1.95 | 0.49 |
| 1:Q:470:PHE:HD2 | 1:Q:677:PRO:HG2 | 1.78 | 0.49 |
| 1:Q:1539:THR:H | 1:Q:1542:GLN:HE22 | 1.61 | 0.49 |
| 1:Q:1919:PRO:HG3 | 1:Q:1940:LYS:NZ | 2.28 | 0.49 |
| 1:Q:3211:ASP:OD1 | 1:Q:3212:ARG:N | 2.46 | 0.49 |
| 1:R:5:ARG:HB2 | 1:R:284:ASP:OD1 | 2.12 | 0.49 |
| 1:R:1420:CYS:O | 1:R:1608:ARG:NH1 | 2.46 | 0.49 |
| 1:R:2829:SER:OG | 1:R:2862:MET:HE1 | 2.13 | 0.49 |
| 1:S:363:LEU:HD12 | 1:S:364:PRO:HD2 | 1.95 | 0.49 |
| 1:S:972:LEU:HD23 | 1:S:977:LYS:HB3 | 1.95 | 0.49 |
| 1:S:1351:TRP:CZ3 | 1:S:1406:LEU:HD12 | 2.48 | 0.49 |
| 1:S:2581:PHE:O | 1:S:2584:THR:HG22 | 2.11 | 0.49 |
| 1:S:3142:TYR:HE2 | 1:S:3144:ARG:HH11 | 1.59 | 0.49 |
| 1:T:310:LEU:HD13 | 1:T:366:HIS:HB3 | 1.93 | 0.49 |
| 1:T:689:LYS:HG3 | 1:T:690:THR:N | 2.28 | 0.49 |
| 1:T:3350:ASN:OD1 | 1:T:3351:VAL:N | 2.46 | 0.49 |
| 1:A:425:ASP:OD1 | 1:A:426:VAL:N | 2.42 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:471:HIS:NE2 | 1:A:489:CYS:SG | 2.86 | 0.49 |
| 1:A:2111:LEU:HD12 | 1:A:2211:PRO:HG2 | 1.94 | 0.49 |
| 1:A:2515:LYS:HG3 | 1:A:2777:ASP:HB3 | 1.95 | 0.49 |
| 1:A:2556:LEU:HD23 | 1:A:2556:LEU:H | 1.78 | 0.49 |
| 1:A:2831:ALA:HA | 1:A:2858:VAL:HG11 | 1.95 | 0.49 |
| 1:A:2864:LEU:HD11 | 1:A:2870:TYR:HB3 | 1.95 | 0.49 |
| 1:B:795:LYS:HD3 | 1:B:796:LYS:HD3 | 1.94 | 0.49 |
| 1:B:1702:SER:O | 1:B:1702:SER:OG | 2.31 | 0.49 |
| 1:B:1834:PHE:O | 1:B:1838:LEU:HG | 2.13 | 0.49 |
| 1:B:2112:ARG:HH11 | 1:B:2208:LEU:HD22 | 1.77 | 0.49 |
| 1:B:2152:PRO:HD2 | 1:B:2329:TYR:CD2 | 2.48 | 0.49 |
| 1:C:913:TRP:HE3 | 1:C:914:HIS:HD2 | 1.60 | 0.49 |
| 1:C:1159:ARG:C | 1:C:1160:LYS:HD3 | 2.38 | 0.49 |
| 1:C:1868:SER:O | 1:C:1874:TYR:HB2 | 2.12 | 0.49 |
| 1:C:2345:ASN:HD22 | 1:C:2348:THR:HG23 | 1.78 | 0.49 |
| 1:C:2812:LYS:NZ | 1:C:2842:GLU:O | 2.36 | 0.49 |
| 1:D:479:ARG:NH2 | 1:D:481:ASP:O | 2.45 | 0.49 |
| 1:D:1014:PHE:CE1 | 1:D:1018:TYR:HB2 | 2.48 | 0.49 |
| 1:D:2169:LEU:C | 1:D:2174:SER:HB3 | 2.38 | 0.49 |
| 1:D:2787:PRO:HA | 1:D:2790:GLU:CD | 2.38 | 0.49 |
| 1:E:1883:LEU:O | 1:E:1886:SER:OG | 2.21 | 0.49 |
| 1:E:3268:ASP:OD1 | 1:E:3268:ASP:N | 2.46 | 0.49 |
| 1:E:3337:ARG:NH1 | 1:E:3379:TYR:O | 2.46 | 0.49 |
| 1:F:292:ASN:H | 1:F:295:GLN:HB2 | 1.78 | 0.49 |
| 1:F:457:ASN:HD22 | 3:t:1:NAG:H83 | 1.77 | 0.49 |
| 1:F:1286:MET:O | 1:F:1291:THR:OG1 | 2.29 | 0.49 |
| 1:F:1319:SER:OG | 1:F:1320:ALA:N | 2.42 | 0.49 |
| 1:F:2652:SER:O | 1:F:2656:ARG:NH1 | 2.46 | 0.49 |
| 1:F:3085:GLU:O | 1:F:3089:ASN:ND2 | 2.46 | 0.49 |
| 1:G:647:LEU:HA | 1:G:650:ILE:HG12 | 1.94 | 0.49 |
| 1:G:1247:SER:HA | 1:G:1250:LYS:HG2 | 1.95 | 0.49 |
| 1:H:284:ASP:OD1 | 1:H:284:ASP:N | 2.45 | 0.49 |
| 1:H:1775:LEU:HD12 | 1:H:1776:PRO:HD2 | 1.93 | 0.49 |
| 1:H:1938:TYR:HH | 1:H:1950:HIS:CG | 2.30 | 0.49 |
| 1:H:2263:GLN:HE22 | 1:H:2443:LYS:H | 1.58 | 0.49 |
| 1:H:3102:SER:O | 1:H:3105:THR:OG1 | 2.27 | 0.49 |
| 1:I:501:ARG:HA | 1:I:504:VAL:HG12 | 1.95 | 0.49 |
| 1:I:1365:ALA:HA | 1:I:1381:PHE:CZ | 2.47 | 0.49 |
| 1:I:1993:SER:HB2 | 1:I:2017:GLY:H | 1.77 | 0.49 |
| 1:I:2093:ARG:NH1 | 1:I:2177:ALA:O | 2.46 | 0.49 |
| 1:I:2570:GLY:H | 1:I:2574:PHE:HE2 | 1.61 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:J:1147:GLU:OE1 | 1:J:1245:PRO:HA | 2.13 | 0.49 |
| 1:J:1224:ILE:HB | 1:J:1230:LYS:HZ3 | 1.77 | 0.49 |
| 1:K:292:ASN:N | 1:K:295:GLN:OE1 | 2.38 | 0.49 |
| 1:K:2091:ARG:HH21 | 1:K:2364:ASN:HD21 | 1.61 | 0.49 |
| 1:K:2348:THR:HG1 | 1:K:2349:ARG:NH1 | 2.10 | 0.49 |
| 1:K:2529:LYS:HE3 | 1:K:2620:ASN:OD1 | 2.12 | 0.49 |
| 1:K:3358:THR:H | 1:L:3329:LYS:HE3 | 1.77 | 0.49 |
| 1:L:11:LEU:HD11 | 1:L:92:PRO:HG3 | 1.94 | 0.49 |
| 1:L:229:LEU:HB3 | 1:L:233:ARG:NH2 | 2.28 | 0.49 |
| 1:L:1350:ASP:HA | 1:L:1463:ASN:ND2 | 2.28 | 0.49 |
| 1:L:2312:LEU:O | 1:L:2316:ARG:NH1 | 2.46 | 0.49 |
| 1:M:436:ASP:HB3 | 1:M:522:TYR:CZ | 2.48 | 0.49 |
| 1:M:1100:ASP:OD2 | 1:M:1102:ILE:HG22 | 2.11 | 0.49 |
| 1:M:2532:LEU:HG | 1:M:2536:GLN:NE2 | 2.28 | 0.49 |
| 1:N:939:TRP:HZ3 | 1:N:1055:ASN:HB3 | 1.78 | 0.49 |
| 1:N:2152:PRO:HD2 | 1:N:2329:TYR:CD2 | 2.47 | 0.49 |
| 1:O:782:ASP:OD1 | 1:O:783:ARG:N | 2.44 | 0.49 |
| 1:O:2266:VAL:HG21 | 1:O:2442:TYR:CD1 | 2.47 | 0.49 |
| 1:O:2732:SER:HB3 | 1:O:2916:THR:HG21 | 1.95 | 0.49 |
| 1:O:3142:TYR:CZ | 1:O:3144:ARG:HD3 | 2.48 | 0.49 |
| 1:Q:129:GLU:HA | 1:Q:140:SER:HA | 1.94 | 0.49 |
| 1:Q:680:PHE:HB2 | 1:Q:684:LEU:HD22 | 1.94 | 0.49 |
| 1:Q:851:VAL:HG12 | 1:Q:935:PRO:HB2 | 1.94 | 0.49 |
| 1:Q:3351:VAL:HG21 | 1:Q:3388:PHE:HB3 | 1.95 | 0.49 |
| 1:Q:3389:VAL:HG22 | 1:Q:3401:ARG:HG2 | 1.95 | 0.49 |
| 1:R:705:GLU:N | 1:R:705:GLU:OE1 | 2.46 | 0.49 |
| 1:R:1048:ILE:HA | 1:R:1051:LEU:HG | 1.95 | 0.49 |
| 1:R:1420:CYS:SG | 1:R:1485:SER:OG | 2.70 | 0.49 |
| 1:R:1620:LYS:HE2 | 1:R:1620:LYS:HA | 1.95 | 0.49 |
| 1:R:2183:TRP:CD2 | 1:R:2271:ILE:HD11 | 2.48 | 0.49 |
| 1:R:2664:GLN:HG3 | 1:R:2669:ASN:HD21 | 1.77 | 0.49 |
| 1:S:225:ILE:O | 1:S:228:GLU:HG3 | 2.13 | 0.49 |
| 1:S:794:ASN:OD1 | 1:S:795:LYS:N | 2.45 | 0.49 |
| 1:S:881:ILE:HA | 1:S:884:PHE:CD2 | 2.47 | 0.49 |
| 1:S:913:TRP:HD1 | 1:S:1088:LEU:HD11 | 1.77 | 0.49 |
| 1:S:1732:CYS:O | 1:S:1734:HIS:ND1 | 2.46 | 0.49 |
| 1:S:1733:VAL:HG23 | 1:S:1736:MET:HE2 | 1.93 | 0.49 |
| 1:S:2446:ILE:HD11 | 1:S:2491:ILE:HD11 | 1.95 | 0.49 |
| 1:T:197:ASP:OD1 | 1:T:197:ASP:N | 2.46 | 0.49 |
| 1:T:496:PHE:HB3 | 1:T:497:PRO:HD3 | 1.95 | 0.49 |
| 1:T:735:ARG:HH22 | 1:T:790:THR:H | 1.59 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:T:997:LYS:HG3 | 1:T:998:ILE:HD12 | 1.95 | 0.49 |
| 1:A:345:ALA:HB1 | 1:A:369:ILE:HD11 | 1.94 | 0.49 |
| 1:A:396:THR:HB | 2:U:1:NAG:H82 | 1.95 | 0.49 |
| 1:A:792:ALA:O | 1:A:795:LYS:HG2 | 2.13 | 0.49 |
| 1:A:939:TRP:HZ3 | 1:A:1055:ASN:HB3 | 1.78 | 0.49 |
| 1:A:2334:MET:SD | 1:A:2334:MET:N | 2.86 | 0.49 |
| 1:A:2405:SER:HB3 | 1:A:2426:PHE:HE1 | 1.77 | 0.49 |
| 1:A:2641:GLN:NE2 | 1:A:2645:ASP:OD1 | 2.46 | 0.49 |
| 1:A:3076:ASN:HB2 | 1:A:3079:ASP:HB2 | 1.95 | 0.49 |
| 1:A:3196:SER:O | 1:A:3200:ILE:HD12 | 2.12 | 0.49 |
| 1:B:1271:LEU:HB2 | 1:B:1275:GLU:HG3 | 1.94 | 0.49 |
| 1:B:1694:ALA:O | 1:B:1697:SER:OG | 2.28 | 0.49 |
| 1:C:1186:ASP:N | 1:C:1189:GLU:OE2 | 2.33 | 0.49 |
| 1:C:1365:ALA:HA | 1:C:1381:PHE:CZ | 2.48 | 0.49 |
| 1:C:1508:ASP:OD1 | 1:C:1509:LEU:N | 2.44 | 0.49 |
| 1:C:1684:THR:OG1 | 1:C:1687:GLU:OE1 | 2.26 | 0.49 |
| 1:C:1883:LEU:O | 1:C:1886:SER:OG | 2.23 | 0.49 |
| 1:C:3103:MET:HA | 1:C:3109:SER:HA | 1.95 | 0.49 |
| 1:D:737:PHE:CG | 1:D:786:LYS:HB3 | 2.48 | 0.49 |
| 1:D:958:PRO:HA | 1:D:961:ASN:HA | 1.93 | 0.49 |
| 1:D:2124:GLN:HG2 | 1:D:2125:ALA:N | 2.27 | 0.49 |
| 1:E:71:ARG:HA | 1:E:74:VAL:HG12 | 1.94 | 0.49 |
| 1:E:794:ASN:OD1 | 1:E:795:LYS:N | 2.46 | 0.49 |
| 1:F:673:GLU:C | 1:F:695:ARG:HH22 | 2.18 | 0.49 |
| 1:F:2378:ASP:O | 1:F:2381:GLU:HG2 | 2.13 | 0.49 |
| 1:G:170:GLU:OE2 | 1:G:304:ARG:HD2 | 2.13 | 0.49 |
| 1:G:1494:GLN:NE2 | 1:G:1495:PRO:O | 2.46 | 0.49 |
| 1:G:2371:LYS:HZ2 | 1:G:2376:ASN:HB3 | 1.77 | 0.49 |
| 1:G:3114:PHE:HA | 1:G:3117:ILE:HG12 | 1.94 | 0.49 |
| 1:H:465:GLN:NE2 | 1:H:558:PRO:O | 2.30 | 0.49 |
| 1:H:1775:LEU:HD11 | 1:H:1779:PHE:HE1 | 1.78 | 0.49 |
| 1:H:1978:LYS:HA | 1:H:2078:LYS:NZ | 2.28 | 0.49 |
| 1:H:2416:ASN:ND2 | 1:H:2418:LYS:O | 2.39 | 0.49 |
| 1:H:3132:LEU:HG | 1:H:3136:ARG:HH12 | 1.78 | 0.49 |
| 1:I:945:ALA:HA | 1:I:987:PHE:CZ | 2.48 | 0.49 |
| 1:I:1852:ILE:HD13 | 1:I:2030:TYR:CZ | 2.48 | 0.49 |
| 1:J:531:THR:OG1 | 1:J:532:VAL:N | 2.46 | 0.49 |
| 1:J:674:LEU:HA | 1:J:695:ARG:NH1 | 2.28 | 0.49 |
| 1:J:2777:ASP:OD1 | 1:J:2777:ASP:N | 2.46 | 0.49 |
| 1:J:3058:GLN:N | 1:J:3061:LEU:O | 2.31 | 0.49 |
| 1:K:718:MET:HE1 | 1:K:723:LEU:HA | 1.94 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:K:855:THR:O | 1:K:859:VAL:HG23 | 2.13 | 0.49 |
| 1:K:1114:ASP:OD1 | 1:K:1114:ASP:N | 2.45 | 0.49 |
| 1:K:1466:ARG:NH2 | 1:K:1534:ASN:O | 2.46 | 0.49 |
| 1:K:2621:PRO:HA | 1:K:2624:HIS:CE1 | 2.48 | 0.49 |
| 1:K:3114:PHE:HA | 1:K:3117:ILE:HG12 | 1.94 | 0.49 |
| 1:L:1270:ASP:OD1 | 1:L:1271:LEU:N | 2.44 | 0.49 |
| 1:L:1457:PHE:CE1 | 1:L:1461:HIS:HE1 | 2.30 | 0.49 |
| 1:L:2425:ILE:HG21 | 1:L:2442:TYR:HE2 | 1.78 | 0.49 |
| 1:M:1982:PHE:HB2 | 1:M:2074:LEU:HB2 | 1.94 | 0.49 |
| 1:M:2663:GLU:HA | 1:M:2793:ILE:HD11 | 1.95 | 0.49 |
| 1:M:2996:GLU:OE1 | 1:M:3008:ILE:N | 2.43 | 0.49 |
| 1:N:703:GLU:N | 1:N:703:GLU:OE1 | 2.45 | 0.49 |
| 1:N:1019:GLU:HA | 1:N:1022:HIS:CD2 | 2.48 | 0.49 |
| 1:N:2312:LEU:O | 1:N:2316:ARG:NH1 | 2.45 | 0.49 |
| 1:O:409:VAL:HG13 | 1:O:666:CYS:HA | 1.94 | 0.49 |
| 1:O:612:LEU:HB2 | 1:O:613:PRO:HD3 | 1.94 | 0.49 |
| 1:O:2577:TRP:HA | 1:O:2744:LEU:HD11 | 1.94 | 0.49 |
| 1:O:2656:ARG:HD2 | 1:O:2656:ARG:N | 2.27 | 0.49 |
| 1:P:435:LYS:HG2 | 1:P:436:ASP:H | 1.76 | 0.49 |
| 1:P:527:ARG:O | 1:P:530:THR:OG1 | 2.25 | 0.49 |
| 1:P:1540:ILE:H | 1:P:1540:ILE:HD12 | 1.78 | 0.49 |
| 1:P:3080:PHE:HE2 | 1:P:3126:TRP:HD1 | 1.61 | 0.49 |
| 1:Q:953:GLU:O | 1:Q:966:ASN:N | 2.32 | 0.49 |
| 1:Q:2269:ASN:OD1 | 1:Q:2428:LEU:HB2 | 2.13 | 0.49 |
| 1:Q:2356:GLU:OE1 | 1:Q:2356:GLU:N | 2.41 | 0.49 |
| 1:Q:2542:ARG:NH1 | 1:Q:2588:ALA:HA | 2.28 | 0.49 |
| 1:Q:2990:LEU:HA | 1:Q:2993:VAL:HG12 | 1.94 | 0.49 |
| 1:R:806:VAL:HG11 | 1:R:825:HIS:O | 2.13 | 0.49 |
| 1:R:924:ALA:O | 1:R:928:LYS:HG2 | 2.13 | 0.49 |
| 1:R:1848:VAL:HG12 | 1:R:2026:PHE:CD1 | 2.48 | 0.49 |
| 1:R:1925:PHE:O | 1:R:1936:LYS:HE2 | 2.13 | 0.49 |
| 1:R:1995:HIS:ND1 | 1:R:2013:PHE:O | 2.44 | 0.49 |
| 1:R:2194:PHE:CD1 | 1:R:2212:PHE:HB3 | 2.46 | 0.49 |
| 1:R:2416:ASN:ND2 | 1:R:2418:LYS:O | 2.42 | 0.49 |
| 1:S:257:ASP:O | 1:S:265:ARG:NH2 | 2.36 | 0.49 |
| 1:T:503:PHE:HA | 1:T:678:PHE:HE1 | 1.77 | 0.49 |
| 1:T:618:GLY:HA3 | 1:T:626:SER:N | 2.27 | 0.49 |
| 1:T:1048:ILE:HA | 1:T:1051:LEU:HG | 1.94 | 0.49 |
| 1:A:629:HIS:HA | 1:A:775:LYS:HZ1 | 1.78 | 0.48 |
| 1:A:1815:ARG:HA | 1:A:1818:LEU:HG | 1.93 | 0.48 |
| 1:B:755:ILE:HD11 | 1:B:804:TYR:HB2 | 1.94 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:837:GLU:N | 1:B:837:GLU:OE1 | 2.46 | 0.48 |
| 1:B:1742:TRP:CD1 | 1:B:1920:LEU:HD12 | 2.47 | 0.48 |
| 1:B:1746:TYR:CD2 | 1:B:1750:PHE:HE2 | 2.31 | 0.48 |
| 1:B:2343:ASN:HD21 | 1:B:2345:ASN:HB3 | 1.78 | 0.48 |
| 1:C:9:ASP:OD1 | 1:C:9:ASP:N | 2.41 | 0.48 |
| 1:C:590:MET:HE1 | 1:C:647:LEU:HD13 | 1.95 | 0.48 |
| 1:C:767:LYS:HD3 | 1:C:768:LEU:H | 1.77 | 0.48 |
| 1:C:854:LEU:HD12 | 1:C:858:GLN:HG3 | 1.94 | 0.48 |
| 1:C:2034:ILE:O | 1:C:2038:LEU:HD23 | 2.13 | 0.48 |
| 1:C:2414:GLN:O | 1:C:2416:ASN:N | 2.46 | 0.48 |
| 1:C:3317:ILE:HG23 | 1:C:3339:ARG:HB3 | 1.94 | 0.48 |
| 1:D:221:ARG:O | 1:D:225:ILE:HG12 | 2.12 | 0.48 |
| 1:D:695:ARG:HG3 | 1:D:697:THR:HG23 | 1.95 | 0.48 |
| 1:D:944:THR:HA | 1:D:987:PHE:CD1 | 2.48 | 0.48 |
| 1:D:1428:ILE:HA | 1:D:1431:ASN:HD21 | 1.78 | 0.48 |
| 1:D:2626:GLU:OE1 | 1:D:2627:ILE:N | 2.46 | 0.48 |
| 1:D:3183:PHE:HB2 | 1:D:3185:TYR:CE1 | 2.48 | 0.48 |
| 1:E:954:THR:HG22 | 1:E:965:PRO:HA | 1.94 | 0.48 |
| 1:E:1539:THR:H | 1:E:1542:GLN:HE22 | 1.61 | 0.48 |
| 1:E:1811:ARG:HH12 | 1:E:1880:ILE:HD12 | 1.78 | 0.48 |
| 1:E:2577:TRP:NE1 | 1:E:2745:GLU:O | 2.46 | 0.48 |
| 1:E:2603:TRP:NE1 | 1:E:2711:ASN:HD22 | 2.10 | 0.48 |
| 1:F:1284:ARG:NH1 | 1:F:1379:PRO:HD3 | 2.28 | 0.48 |
| 1:F:1307:HIS:CG | 1:F:1602:MET:HE1 | 2.48 | 0.48 |
| 1:F:2623:GLU:OE1 | 1:F:2623:GLU:N | 2.46 | 0.48 |
| 1:F:2639:ARG:HD2 | 1:F:2641:GLN:HE22 | 1.78 | 0.48 |
| 1:F:2953:TYR:HE1 | 1:F:2995:PHE:HE1 | 1.61 | 0.48 |
| 1:F:2993:VAL:O | 1:F:2997:MET:HG2 | 2.13 | 0.48 |
| 1:G:589:GLY:HA2 | 1:G:592:LEU:HG | 1.94 | 0.48 |
| 1:G:1978:LYS:NZ | 1:G:1979:SER:O | 2.32 | 0.48 |
| 1:G:2378:ASP:OD1 | 1:G:2378:ASP:N | 2.46 | 0.48 |
| 1:G:2930:SER:H | 1:G:2933:GLN:NE2 | 2.12 | 0.48 |
| 1:G:3144:ARG:HA | 1:G:3147:LEU:HD21 | 1.94 | 0.48 |
| 1:H:38:LEU:HG | 1:H:73:TYR:CZ | 2.48 | 0.48 |
| 1:H:1012:CYS:O | 1:H:1196:ARG:NH1 | 2.46 | 0.48 |
| 1:H:2055:LEU:HB2 | 1:H:2063:LEU:HB2 | 1.94 | 0.48 |
| 1:H:2805:ASN:HD21 | 1:H:2850:LEU:HB3 | 1.78 | 0.48 |
| 1:I:1025:ILE:HG21 | 1:I:1052:HIS:NE2 | 2.28 | 0.48 |
| 1:I:1067:GLN:NE2 | 1:I:1072:LEU:HB2 | 2.28 | 0.48 |
| 1:I:1195:ASP:OD1 | 1:I:1196:ARG:N | 2.46 | 0.48 |
| 1:I:1316:VAL:HG11 | 1:I:1321:VAL:HG13 | 1.95 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:I:1418:SER:OG | 1:I:1419:PHE:N | 2.45 | 0.48 |
| 1:I:1654:SER:HB2 | 1:J:1914:GLU:CD | 2.37 | 0.48 |
| 1:I:1742:TRP:CD1 | 1:I:1920:LEU:HD12 | 2.48 | 0.48 |
| 1:I:2392:ARG:HE | 1:I:2447:THR:HG21 | 1.78 | 0.48 |
| 1:J:94:TRP:HB3 | 1:J:214:LEU:HD21 | 1.95 | 0.48 |
| 1:J:493:MET:SD | 1:J:670:MET:HE1 | 2.53 | 0.48 |
| 1:J:598:ASP:OD1 | 1:J:599:PHE:N | 2.46 | 0.48 |
| 1:J:1990:ILE:O | 1:J:1991:LYS:HG2 | 2.13 | 0.48 |
| 1:J:2786:ILE:H | 1:J:2786:ILE:HD12 | 1.77 | 0.48 |
| 1:K:453:SER:OG | 3:JA:1:NAG:O7 | 2.20 | 0.48 |
| 1:K:1622:GLY:HA3 | 1:L:2786:ILE:HD13 | 1.94 | 0.48 |
| 1:K:3196:SER:O | 1:K:3200:ILE:HD12 | 2.13 | 0.48 |
| 1:L:312:SER:HA | 1:L:365:TYR:O | 2.13 | 0.48 |
| 1:L:1276:VAL:O | 1:L:1279:LEU:HG | 2.12 | 0.48 |
| 1:M:914:HIS:CE1 | 1:M:1053:HIS:CE1 | 3.00 | 0.48 |
| 1:M:1350:ASP:OD1 | 1:M:1352:THR:N | 2.46 | 0.48 |
| 1:M:3074:GLU:OE1 | 1:M:3075:THR:N | 2.46 | 0.48 |
| 1:N:80:LYS:HZ1 | 1:N:261:ILE:HG13 | 1.78 | 0.48 |
| 1:N:454:ARG:NH2 | 1:N:1338:LEU:O | 2.46 | 0.48 |
| 1:N:744:ASN:HB3 | 1:N:779:TRP:NE1 | 2.27 | 0.48 |
| 1:N:1967:LEU:HD23 | 1:N:1967:LEU:H | 1.78 | 0.48 |
| 1:N:2655:TYR:HD2 | 1:N:2659:LEU:HD23 | 1.78 | 0.48 |
| 1:N:3208:ARG:HH12 | 1:N:3310:ASN:HA | 1.78 | 0.48 |
| 1:O:63:MET:HB3 | 1:O:246:LEU:HD21 | 1.94 | 0.48 |
| 1:O:1782:PRO:O | 1:O:1795:ASN:N | 2.41 | 0.48 |
| 1:O:2360:TYR:HA | 1:O:2363:LEU:HB2 | 1.94 | 0.48 |
| 1:P:939:TRP:HZ3 | 1:P:1055:ASN:HB3 | 1.78 | 0.48 |
| 1:P:2217:ILE:HG22 | 1:P:2219:GLU:H | 1.78 | 0.48 |
| 1:Q:750:LEU:HD21 | 1:Q:767:LYS:HZ2 | 1.77 | 0.48 |
| 1:Q:1732:CYS:C | 1:Q:1734:HIS:HD1 | 2.18 | 0.48 |
| 1:Q:1809:VAL:HG23 | 1:Q:1868:SER:HA | 1.95 | 0.48 |
| 1:Q:2124:GLN:H | 1:Q:2124:GLN:CD | 2.18 | 0.48 |
| 1:Q:2266:VAL:HG21 | 1:Q:2442:TYR:CD1 | 2.48 | 0.48 |
| 1:Q:2664:GLN:HE21 | 1:Q:2670:PHE:HA | 1.78 | 0.48 |
| 1:Q:3165:ASN:HD21 | 1:Q:3167:VAL:HB | 1.78 | 0.48 |
| 1:R:97:THR:HG22 | 1:R:165:VAL:HG21 | 1.96 | 0.48 |
| 1:R:836:HIS:NE2 | 1:R:838:GLU:OE2 | 2.46 | 0.48 |
| 1:R:1772:GLN:HB2 | 1:R:1818:LEU:HD21 | 1.94 | 0.48 |
| 1:R:2399:LEU:HD22 | 1:R:2438:PHE:CE2 | 2.48 | 0.48 |
| 1:R:2805:ASN:HD21 | 1:R:2850:LEU:HB3 | 1.78 | 0.48 |
| 1:R:3032:PHE:HA | 1:R:3113:PRO:HG2 | 1.95 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:R:3133:GLN:HB3 | 1:R:3138:ARG:HB2 | 1.95 | 0.48 |
| 1:S:608:VAL:HG11 | 1:S:785:VAL:HG21 | 1.93 | 0.48 |
| 1:S:3133:GLN:OE1 | 1:S:3140:PHE:HB3 | 2.13 | 0.48 |
| 1:S:3160:GLU:HG2 | 1:S:3169:ARG:HH22 | 1.78 | 0.48 |
| 1:S:3229:ASN:OD1 | 1:S:3231:LYS:NZ | 2.28 | 0.48 |
| 1:T:905:HIS:H | 1:T:907:MET:HE1 | 1.77 | 0.48 |
| 1:T:2377:LEU:HA | 1:T:2380:LEU:HB2 | 1.94 | 0.48 |
| 1:T:2715:GLN:HA | 1:T:2718:ILE:HG12 | 1.94 | 0.48 |
| 1:T:2857:SER:HA | 1:T:2860:ASN:HD21 | 1.78 | 0.48 |
| 1:A:436:ASP:OD1 | 1:A:436:ASP:N | 2.46 | 0.48 |
| 1:A:1084:LEU:HG | 1:A:1110:PHE:HE1 | 1.79 | 0.48 |
| 1:A:1220:LYS:NZ | 1:A:1222:SER:HB2 | 2.28 | 0.48 |
| 1:A:2345:ASN:O | 1:A:2349:ARG:HG2 | 2.13 | 0.48 |
| 1:B:313:PHE:HB3 | 1:B:315:LEU:HD23 | 1.96 | 0.48 |
| 1:B:1005:ALA:HB2 | 1:B:1017:GLN:HG3 | 1.95 | 0.48 |
| 1:B:1268:LEU:HD23 | 1:B:1268:LEU:H | 1.76 | 0.48 |
| 1:B:1742:TRP:HD1 | 1:B:1920:LEU:HD12 | 1.79 | 0.48 |
| 1:B:2595:ARG:HG3 | 1:B:2596:VAL:HG13 | 1.95 | 0.48 |
| 1:C:794:ASN:OD1 | 1:C:795:LYS:N | 2.46 | 0.48 |
| 1:C:954:THR:HA | 1:C:965:PRO:HA | 1.93 | 0.48 |
| 1:D:705:GLU:N | 1:D:705:GLU:OE1 | 2.46 | 0.48 |
| 1:D:806:VAL:HG11 | 1:D:825:HIS:O | 2.13 | 0.48 |
| 1:D:925:LEU:HD13 | 1:D:928:LYS:HE2 | 1.95 | 0.48 |
| 1:D:1488:ALA:HB1 | 1:D:1491:ILE:HD13 | 1.94 | 0.48 |
| 1:D:2162:THR:O | 1:D:2165:VAL:HG22 | 2.13 | 0.48 |
| 1:D:2657:GLN:OE1 | 1:D:2657:GLN:N | 2.40 | 0.48 |
| 1:D:2720:GLN:NE2 | 1:D:2730:TYR:HB2 | 2.28 | 0.48 |
| 1:D:2754:ASN:OD1 | 1:D:2755:ASP:N | 2.47 | 0.48 |
| 1:E:181:PHE:CE2 | 1:E:219:VAL:HG13 | 2.48 | 0.48 |
| 1:E:203:LEU:HD21 | 1:E:351:LEU:HB3 | 1.95 | 0.48 |
| 1:E:1305:CYS:HB3 | 1:E:1312:VAL:O | 2.13 | 0.48 |
| 1:E:1331:ASP:O | 1:E:1334:GLU:HG3 | 2.13 | 0.48 |
| 1:E:1345:SER:OG | 1:E:1346:VAL:N | 2.45 | 0.48 |
| 1:E:1868:SER:O | 1:E:1874:TYR:HB2 | 2.12 | 0.48 |
| 1:E:2393:VAL:H | 1:E:2447:THR:HG22 | 1.77 | 0.48 |
| 1:F:38:LEU:HG | 1:F:73:TYR:CZ | 2.48 | 0.48 |
| 1:F:310:LEU:HD13 | 1:F:366:HIS:HB3 | 1.95 | 0.48 |
| 1:F:636:ILE:O | 1:F:639:LEU:HG | 2.12 | 0.48 |
| 1:F:881:ILE:HD12 | 1:F:920:GLN:HE22 | 1.78 | 0.48 |
| 1:F:1267:ASN:HB3 | 1:F:1348:TYR:CZ | 2.48 | 0.48 |
| 1:F:1910:ASN:OD1 | 1:F:1911:CYS:N | 2.46 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:G:1278:SER:O | 1:G:1281:SER:OG | 2.27 | 0.48 |
| 1:G:1684:THR:N | 1:G:1687:GLU:OE2 | 2.37 | 0.48 |
| 1:G:2044:SER:OG | 1:G:2046:ASP:OD1 | 2.31 | 0.48 |
| 1:H:744:ASN:ND2 | 1:H:778:PRO:HA | 2.29 | 0.48 |
| 1:H:1356:ARG:HH12 | 1:H:1402:ASN:HD21 | 1.61 | 0.48 |
| 1:I:75:VAL:O | 1:I:78:GLU:HG3 | 2.13 | 0.48 |
| 1:I:2063:LEU:HD11 | 3:BA:1:NAG:H5 | 1.96 | 0.48 |
| 1:I:2101:ALA:O | 1:I:2105:MET:HG3 | 2.13 | 0.48 |
| 1:J:1845:ASP:OD1 | 1:J:1845:ASP:N | 2.45 | 0.48 |
| 1:J:2217:ILE:HG22 | 1:J:2219:GLU:H | 1.78 | 0.48 |
| 1:J:3245:PHE:HB3 | 1:J:3264:TYR:HE2 | 1.77 | 0.48 |
| 1:K:187:HIS:HA | 1:K:349:PHE:HD2 | 1.76 | 0.48 |
| 1:K:525:TRP:H | 1:K:525:TRP:CD1 | 2.31 | 0.48 |
| 1:K:2213:ALA:O | 1:K:2224:THR:OG1 | 2.24 | 0.48 |
| 1:K:2404:THR:HA | 1:K:2429:GLY:O | 2.12 | 0.48 |
| 1:K:3113:PRO:HA | 1:K:3116:MET:HG3 | 1.94 | 0.48 |
| 1:K:3359:SER:HA | 1:K:3362:LEU:HB2 | 1.95 | 0.48 |
| 1:L:246:LEU:HA | 1:L:249:LYS:HE2 | 1.95 | 0.48 |
| 1:L:1663:ASN:HD22 | 1:L:1665:GLN:HE21 | 1.60 | 0.48 |
| 1:L:1857:ILE:HB | 1:L:1884:HIS:CE1 | 2.48 | 0.48 |
| 1:M:126:PHE:O | 1:M:143:ARG:NH1 | 2.45 | 0.48 |
| 1:M:520:ILE:HD12 | 1:M:521:PRO:HD2 | 1.95 | 0.48 |
| 1:M:595:GLU:N | 1:M:595:GLU:OE1 | 2.46 | 0.48 |
| 1:M:754:SER:HA | 1:M:765:VAL:HG23 | 1.95 | 0.48 |
| 1:N:299:LEU:HD13 | 1:N:302:GLN:HE21 | 1.78 | 0.48 |
| 1:N:312:SER:HA | 1:N:365:TYR:O | 2.12 | 0.48 |
| 1:N:509:ASP:OD2 | 1:N:687:ASN:ND2 | 2.46 | 0.48 |
| 1:N:510:ALA:O | 1:N:514:ARG:HG2 | 2.13 | 0.48 |
| 1:N:855:THR:O | 1:N:859:VAL:HG23 | 2.12 | 0.48 |
| 1:N:1745:LEU:HA | 1:N:1748:VAL:HG12 | 1.94 | 0.48 |
| 1:O:436:ASP:HB3 | 1:O:522:TYR:CZ | 2.48 | 0.48 |
| 1:O:887:GLN:NE2 | 1:O:889:ASN:HD21 | 2.03 | 0.48 |
| 1:O:1212:GLU:CD | 1:O:1214:ASN:H | 2.22 | 0.48 |
| 1:O:1730:ALA:N | 1:O:2020:ALA:O | 2.46 | 0.48 |
| 1:O:3118:HIS:O | 1:O:3122:ILE:HG12 | 2.12 | 0.48 |
| 1:P:434:ARG:HD2 | 1:P:710:TYR:HE1 | 1.77 | 0.48 |
| 1:P:1022:HIS:HD2 | 1:P:1026:HIS:NE2 | 2.11 | 0.48 |
| 1:Q:954:THR:HG22 | 1:Q:965:PRO:HA | 1.95 | 0.48 |
| 1:Q:2694:SER:HB2 | 1:Q:2879:ILE:HG21 | 1.95 | 0.48 |
| 1:R:142:ALA:HB3 | 1:R:196:HIS:CE1 | 2.48 | 0.48 |
| 1:R:845:LEU:HD21 | 1:R:932:ASP:HA | 1.95 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:R:855:THR:O | 1:R:859:VAL:HG23 | 2.13 | 0.48 |
| 1:R:1992:THR:C | 1:R:2017:GLY:O | 2.55 | 0.48 |
| 1:R:2578:HIS:HB3 | 1:R:2709:HIS:HD2 | 1.78 | 0.48 |
| 1:R:2800:ASP:OD1 | 1:R:2899:GLY:N | 2.46 | 0.48 |
| 1:S:699:ILE:HG13 | 1:S:706:LEU:HD21 | 1.95 | 0.48 |
| 1:S:811:LYS:HD2 | 1:S:815:GLY:HA2 | 1.94 | 0.48 |
| 1:S:855:THR:O | 1:S:859:VAL:HG23 | 2.13 | 0.48 |
| 1:S:1467:ILE:HA | 1:S:1470:ILE:HD12 | 1.95 | 0.48 |
| 1:S:2576:GLN:NE2 | 1:S:2766:ALA:O | 2.47 | 0.48 |
| 1:T:596:GLN:NE2 | 1:T:598:ASP:H | 2.12 | 0.48 |
| 1:T:1274:GLY:O | 1:T:1277:GLU:HG3 | 2.13 | 0.48 |
| 1:T:2152:PRO:HD2 | 1:T:2329:TYR:CD2 | 2.48 | 0.48 |
| 1:T:2375:LEU:HD22 | 1:T:2379:GLU:HG2 | 1.95 | 0.48 |
| 3:uA:1:NAG:O3 | 3:uA:2:NAG:O6 | 2.31 | 0.48 |
| 1:A:953:GLU:O | 1:A:966:ASN:N | 2.30 | 0.48 |
| 1:A:2313:GLN:CD | 1:A:2318:LEU:HB2 | 2.38 | 0.48 |
| 1:A:2569:HIS:HA | 1:A:2574:PHE:CE2 | 2.47 | 0.48 |
| 1:A:3203:ILE:HA | 1:A:3206:ASN:HB2 | 1.96 | 0.48 |
| 1:B:2312:LEU:O | 1:B:2316:ARG:NH1 | 2.46 | 0.48 |
| 1:B:2752:ASN:HD21 | 1:B:2757:ILE:HG13 | 1.78 | 0.48 |
| 1:B:3183:PHE:HB2 | 1:B:3185:TYR:CE1 | 2.48 | 0.48 |
| 1:C:376:LEU:HB3 | 1:C:378:LYS:NZ | 2.28 | 0.48 |
| 1:C:580:TYR:HE2 | 1:C:959:GLU:HB2 | 1.78 | 0.48 |
| 1:C:1388:THR:HG23 | 1:C:1390:LYS:H | 1.76 | 0.48 |
| 1:C:1910:ASN:HB2 | 1:D:1657:PHE:HB3 | 1.96 | 0.48 |
| 1:C:2392:ARG:HB3 | 1:C:2394:PHE:CE1 | 2.48 | 0.48 |
| 1:C:2465:ALA:HB2 | 1:D:1085:ARG:HD2 | 1.95 | 0.48 |
| 1:C:2533:ARG:NH1 | 1:C:2621:PRO:HD3 | 2.29 | 0.48 |
| 1:C:2750:ASP:HA | 1:C:2758:ARG:HD2 | 1.94 | 0.48 |
| 1:D:2653:PHE:HA | 1:D:2656:ARG:HH22 | 1.77 | 0.48 |
| 1:D:2800:ASP:OD1 | 1:D:2899:GLY:N | 2.47 | 0.48 |
| 1:D:3071:THR:HG23 | 1:D:3083:GLN:HE21 | 1.79 | 0.48 |
| 1:E:718:MET:HE1 | 1:E:723:LEU:HG | 1.95 | 0.48 |
| 1:E:1739:PHE:HB3 | 1:E:1740:PRO:HD3 | 1.95 | 0.48 |
| 1:E:3011:TRP:CZ3 | 1:E:3013:TRP:HB3 | 2.48 | 0.48 |
| 1:F:1617:PRO:HA | 1:F:1620:LYS:HD2 | 1.95 | 0.48 |
| 1:F:2263:GLN:HE22 | 1:F:2443:LYS:H | 1.62 | 0.48 |
| 1:F:2675:GLU:O | 1:F:2679:ASN:ND2 | 2.45 | 0.48 |
| 1:F:3008:ILE:HG21 | 1:F:3116:MET:HB3 | 1.95 | 0.48 |
| 1:F:3200:ILE:HA | 1:F:3203:ILE:HD12 | 1.95 | 0.48 |
| 1:G:1489:LEU:HD11 | 1:H:2075:TYR:HB2 | 1.95 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:G:2614:LEU:HB3 | 1:G:2636:ARG:HH12 | 1.78 | 0.48 |
| 1:H:6:LYS:HD2 | 1:H:11:LEU:HD13 | 1.94 | 0.48 |
| 1:H:176:HIS:HA | 1:H:179:VAL:HG12 | 1.95 | 0.48 |
| 1:H:428:SER:OG | 1:H:429:ALA:N | 2.45 | 0.48 |
| 1:H:1736:MET:HG2 | 1:H:1738:THR:H | 1.78 | 0.48 |
| 1:H:2576:GLN:N | 1:H:2576:GLN:OE1 | 2.45 | 0.48 |
| 1:I:861:SER:OG | 1:I:929:GLY:O | 2.32 | 0.48 |
| 1:I:2405:SER:HB3 | 1:I:2426:PHE:CE1 | 2.49 | 0.48 |
| 1:J:81:LEU:HA | 1:J:84:LYS:HB2 | 1.95 | 0.48 |
| 1:K:170:GLU:CD | 1:K:304:ARG:HD2 | 2.39 | 0.48 |
| 1:K:501:ARG:NH1 | 1:K:702:TYR:HB3 | 2.28 | 0.48 |
| 1:K:1307:HIS:CD2 | 1:K:1602:MET:HE1 | 2.47 | 0.48 |
| 1:K:2091:ARG:NH2 | 1:K:2364:ASN:HD21 | 2.11 | 0.48 |
| 1:K:3231:LYS:HB2 | 1:K:3284:GLN:HG3 | 1.94 | 0.48 |
| 1:L:1018:TYR:CE1 | 1:L:1056:THR:HB | 2.48 | 0.48 |
| 1:L:2448:ASP:OD1 | 1:L:2449:THR:N | 2.46 | 0.48 |
| 1:L:2820:ASP:HB3 | 1:L:2873:ASP:OD1 | 2.13 | 0.48 |
| 1:L:3153:PRO:HB2 | 1:L:3158:ASN:HB3 | 1.96 | 0.48 |
| 1:L:3312:ASP:N | 1:L:3312:ASP:OD1 | 2.45 | 0.48 |
| 1:M:47:MET:SD | 1:M:47:MET:N | 2.86 | 0.48 |
| 1:M:436:ASP:OD1 | 1:M:436:ASP:N | 2.45 | 0.48 |
| 1:M:1324:HIS:HA | 1:M:1519:VAL:HG11 | 1.93 | 0.48 |
| 1:M:3022:SER:HA | 1:M:3025:THR:HG1 | 1.77 | 0.48 |
| 1:N:221:ARG:O | 1:N:225:ILE:HG12 | 2.12 | 0.48 |
| 1:N:1283:LEU:HD12 | 1:N:1286:MET:SD | 2.53 | 0.48 |
| 1:N:2303:ASP:OD2 | 1:N:2367:TYR:OH | 2.19 | 0.48 |
| 1:N:2738:GLN:NE2 | 1:O:2893:SER:HA | 2.21 | 0.48 |
| 1:O:299:LEU:O | 1:O:302:GLN:HG3 | 2.13 | 0.48 |
| 1:O:501:ARG:NH1 | 1:O:702:TYR:HB3 | 2.29 | 0.48 |
| 1:O:855:THR:O | 1:O:859:VAL:HG23 | 2.14 | 0.48 |
| 1:O:1742:TRP:HD1 | 1:O:1920:LEU:HD12 | 1.78 | 0.48 |
| 1:O:2570:GLY:HA3 | 1:O:2845:TRP:HB2 | 1.94 | 0.48 |
| 1:O:2940:ALA:HB2 | 1:O:3002:LYS:HZ1 | 1.78 | 0.48 |
| 1:P:1821:ASP:OD1 | 1:P:1821:ASP:N | 2.46 | 0.48 |
| 1:P:2194:PHE:HD1 | 1:P:2212:PHE:HB3 | 1.77 | 0.48 |
| 1:Q:1345:SER:OG | 1:Q:1346:VAL:N | 2.46 | 0.48 |
| 1:Q:2091:ARG:HH21 | 1:Q:2364:ASN:ND2 | 2.10 | 0.48 |
| 1:Q:2136:CYS:HB3 | 1:Q:2144:TYR:C | 2.39 | 0.48 |
| 1:Q:3214:TYR:HB3 | 1:Q:3264:TYR:O | 2.13 | 0.48 |
| 1:Q:3276:ASN:OD1 | 1:Q:3277:ALA:N | 2.45 | 0.48 |
| 1:Q:3359:SER:HA | 1:Q:3362:LEU:HB2 | 1.95 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:R:569:GLN:HB3 | 1:R:619:GLY:HA3 | 1.95 | 0.48 |
| 1:R:759:ASP:OD1 | 1:R:759:ASP:N | 2.45 | 0.48 |
| 1:R:1014:PHE:N | 1:R:1015:GLU:OE1 | 2.39 | 0.48 |
| 1:R:1280:LYS:O | 1:R:1284:ARG:HG2 | 2.13 | 0.48 |
| 1:R:1301:PHE:CD1 | 1:R:1302:PRO:HA | 2.48 | 0.48 |
| 1:R:1742:TRP:CD1 | 1:R:1920:LEU:HD12 | 2.46 | 0.48 |
| 1:R:1809:VAL:HG22 | 1:R:1811:ARG:HH12 | 1.78 | 0.48 |
| 1:R:2312:LEU:O | 1:R:2316:ARG:NH1 | 2.46 | 0.48 |
| 1:R:2602:ASP:OD1 | 1:R:2603:TRP:N | 2.45 | 0.48 |
| 1:R:3153:PRO:HA | 1:R:3173:ARG:HD3 | 1.93 | 0.48 |
| 1:S:259:ASN:ND2 | 1:S:264:THR:OG1 | 2.46 | 0.48 |
| 1:S:1619:ARG:HD2 | 1:T:2775:GLN:HE21 | 1.77 | 0.48 |
| 1:S:1900:ARG:O | 1:S:1900:ARG:NH1 | 2.46 | 0.48 |
| 1:S:2284:SER:HA | 1:S:2428:LEU:HD23 | 1.95 | 0.48 |
| 1:S:2709:HIS:HA | 1:S:2712:VAL:HG22 | 1.94 | 0.48 |
| 1:T:170:GLU:OE1 | 1:T:304:ARG:NH1 | 2.46 | 0.48 |
| 1:T:504:VAL:O | 1:T:507:VAL:HG22 | 2.12 | 0.48 |
| 1:A:4:VAL:HG13 | 1:A:6:LYS:HZ2 | 1.78 | 0.48 |
| 1:A:193:GLY:HA2 | 1:A:199:SER:HB2 | 1.95 | 0.48 |
| 1:A:343:GLU:OE1 | 1:A:375:HIS:ND1 | 2.46 | 0.48 |
| 1:A:650:ILE:HG22 | 1:A:713:LEU:HD12 | 1.94 | 0.48 |
| 1:A:1174:PRO:HG2 | 1:A:1176:HIS:CE1 | 2.48 | 0.48 |
| 1:A:1646:GLU:OE1 | 1:A:1646:GLU:N | 2.39 | 0.48 |
| 1:A:2037:VAL:HA | 1:A:2040:LYS:HG2 | 1.95 | 0.48 |
| 1:A:2746:PRO:O | 1:A:2749:TRP:HB2 | 2.13 | 0.48 |
| 1:A:2802:VAL:HG12 | 1:A:2856:THR:HG22 | 1.95 | 0.48 |
| 1:A:3068:THR:O | 1:A:3071:THR:OG1 | 2.27 | 0.48 |
| 1:B:1775:LEU:HD11 | 1:B:1779:PHE:HE1 | 1.77 | 0.48 |
| 1:B:3245:PHE:HB3 | 1:B:3264:TYR:HE2 | 1.78 | 0.48 |
| 1:C:50:LYS:HG3 | 1:C:52:ASP:H | 1.78 | 0.48 |
| 1:C:643:ASN:O | 1:C:647:LEU:HG | 2.13 | 0.48 |
| 1:C:1317:HIS:HA | 1:C:1322:PHE:CD1 | 2.49 | 0.48 |
| 1:C:3011:TRP:CZ3 | 1:C:3013:TRP:HB3 | 2.49 | 0.48 |
| 1:D:38:LEU:HG | 1:D:73:TYR:CZ | 2.49 | 0.48 |
| 1:D:554:PHE:O | 1:D:568:ARG:NH2 | 2.46 | 0.48 |
| 1:D:914:HIS:HA | 1:D:917:LEU:HG | 1.95 | 0.48 |
| 1:D:2715:GLN:HA | 1:D:2718:ILE:HG12 | 1.94 | 0.48 |
| 1:E:2557:CYS:HB3 | 1:E:2564:VAL:HG23 | 1.96 | 0.48 |
| 1:E:3083:GLN:OE1 | 1:E:3263:LYS:N | 2.41 | 0.48 |
| 1:F:635:PRO:O | 1:F:638:ILE:HG22 | 2.13 | 0.48 |
| 1:F:1085:ARG:HD3 | 1:F:1110:PHE:HE2 | 1.78 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:F:1165:THR:N | 1:F:1222:SER:O | 2.38 | 0.48 |
| 1:F:2101:ALA:O | 1:F:2105:MET:HG3 | 2.13 | 0.48 |
| 1:F:2754:ASN:OD1 | 1:F:2755:ASP:N | 2.47 | 0.48 |
| 1:F:2800:ASP:OD1 | 1:F:2899:GLY:N | 2.46 | 0.48 |
| 1:G:193:GLY:HA2 | 1:G:199:SER:HB2 | 1.95 | 0.48 |
| 1:G:761:ASP:OD1 | 1:G:761:ASP:N | 2.46 | 0.48 |
| 1:G:1161:SER:N | 1:G:1185:GLY:O | 2.46 | 0.48 |
| 1:G:1328:LEU:HB3 | 1:G:1499:PHE:CE2 | 2.42 | 0.48 |
| 1:G:2796:ARG:O | 1:G:2801:ARG:NH1 | 2.40 | 0.48 |
| 1:G:3226:ALA:HA | 1:G:3289:LYS:HA | 1.94 | 0.48 |
| 1:G:3350:ASN:O | 1:G:3391:SER:N | 2.39 | 0.48 |
| 1:H:658:ARG:NH2 | 1:H:728:ASP:OD1 | 2.47 | 0.48 |
| 1:H:811:LYS:NZ | 1:H:815:GLY:O | 2.35 | 0.48 |
| 1:H:968:PHE:O | 1:H:980:ARG:NH1 | 2.44 | 0.48 |
| 1:H:1205:ILE:HD12 | 1:H:1208:LYS:HE3 | 1.96 | 0.48 |
| 1:H:2585:LEU:HG | 1:H:2589:LEU:HD23 | 1.96 | 0.48 |
| 1:H:2820:ASP:HB3 | 1:H:2873:ASP:OD1 | 2.13 | 0.48 |
| 1:H:3127:GLN:O | 1:H:3130:GLN:HG3 | 2.13 | 0.48 |
| 1:H:3144:ARG:HA | 1:H:3147:LEU:HG | 1.95 | 0.48 |
| 1:I:436:ASP:HB3 | 1:I:522:TYR:CZ | 2.48 | 0.48 |
| 1:I:1246:GLY:O | 1:I:1249:THR:OG1 | 2.25 | 0.48 |
| 1:I:3087:LEU:O | 1:I:3090:THR:OG1 | 2.30 | 0.48 |
| 1:I:3276:ASN:OD1 | 1:I:3277:ALA:N | 2.46 | 0.48 |
| 1:J:471:HIS:ND1 | 1:J:471:HIS:O | 2.47 | 0.48 |
| 1:J:924:ALA:O | 1:J:928:LYS:HG2 | 2.13 | 0.48 |
| 1:J:954:THR:HB | 1:J:963:PRO:HB2 | 1.94 | 0.48 |
| 1:J:1018:TYR:CE1 | 1:J:1056:THR:HB | 2.48 | 0.48 |
| 1:J:1299:HIS:ND1 | 1:J:1299:HIS:O | 2.47 | 0.48 |
| 1:J:2536:GLN:HA | 1:J:2544:TYR:HB3 | 1.94 | 0.48 |
| 1:J:3038:LYS:O | 1:J:3041:GLN:NE2 | 2.47 | 0.48 |
| 1:K:1815:ARG:HA | 1:K:1818:LEU:HG | 1.94 | 0.48 |
| 1:K:1989:GLY:N | 1:K:2024:TRP:O | 2.47 | 0.48 |
| 1:K:2861:GLN:NE2 | 1:L:1538:TRP:HE1 | 2.11 | 0.48 |
| 1:K:3021:PRO:HD2 | 1:K:3024:LEU:HD21 | 1.95 | 0.48 |
| 1:K:3289:LYS:HD2 | 1:K:3291:ASN:HD22 | 1.77 | 0.48 |
| 1:L:536:ALA:HA | 1:L:552:ASN:HD21 | 1.78 | 0.48 |
| 1:L:743:GLN:HA | 1:L:780:ASN:HA | 1.95 | 0.48 |
| 1:L:913:TRP:NE1 | 1:L:1089:GLN:O | 2.46 | 0.48 |
| 1:L:1966:GLU:N | 1:L:1966:GLU:OE1 | 2.47 | 0.48 |
| 1:M:1821:ASP:OD1 | 1:M:1822:GLY:N | 2.46 | 0.48 |
| 1:M:2443:LYS:HG2 | 1:M:2492:ILE:HD11 | 1.96 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:M:2733:ALA:HB3 | 1:M:2740:LEU:HD11 | 1.95 | 0.48 |
| 1:N:2408:VAL:HG22 | 1:N:2473:ILE:HG22 | 1.93 | 0.48 |
| 1:N:2602:ASP:OD2 | 1:N:2604:THR:OG1 | 2.25 | 0.48 |
| 1:N:2653:PHE:HA | 1:N:2656:ARG:HH22 | 1.78 | 0.48 |
| 1:O:1148:ARG:HG3 | 1:O:1244:ARG:HB3 | 1.96 | 0.48 |
| 1:O:2586:GLU:OE2 | 1:O:2598:ILE:N | 2.45 | 0.48 |
| 1:P:79:GLN:O | 1:P:83:LYS:NZ | 2.46 | 0.48 |
| 1:P:1724:GLU:N | 1:P:1724:GLU:OE1 | 2.45 | 0.48 |
| 1:P:2614:LEU:HD11 | 1:P:2636:ARG:HH12 | 1.78 | 0.48 |
| 1:P:2620:ASN:HB3 | 1:P:2623:GLU:OE1 | 2.13 | 0.48 |
| 1:P:3078:CYS:SG | 1:P:3260:ARG:NE | 2.86 | 0.48 |
| 1:Q:1607:ASP:OD1 | 1:Q:1608:ARG:N | 2.45 | 0.48 |
| 1:Q:3067:GLN:OE1 | 1:Q:3087:LEU:HD13 | 2.11 | 0.48 |
| 1:R:869:LEU:HD23 | 1:R:925:LEU:HD11 | 1.95 | 0.48 |
| 1:R:1967:LEU:HD23 | 1:R:1967:LEU:H | 1.79 | 0.48 |
| 1:R:2511:ILE:HD12 | 1:R:2773:ASN:HB2 | 1.95 | 0.48 |
| 1:S:3089:ASN:HD21 | 1:S:3247:ILE:HD12 | 1.78 | 0.48 |
| 1:S:3217:PHE:CD1 | 1:S:3302:PRO:HB3 | 2.49 | 0.48 |
| 1:T:881:ILE:HD12 | 1:T:920:GLN:HE22 | 1.77 | 0.48 |
| 1:T:2708:HIS:O | 1:T:2712:VAL:HG13 | 2.13 | 0.48 |
| 1:T:2712:VAL:HA | 1:T:2715:GLN:CD | 2.37 | 0.48 |
| 1:T:2948:ASP:OD1 | 1:T:2948:ASP:N | 2.45 | 0.48 |
| 1:A:1663:ASN:HD21 | 1:A:1666:ASP:CG | 2.22 | 0.48 |
| 1:A:1733:VAL:HG23 | 1:A:1736:MET:HE2 | 1.94 | 0.48 |
| 1:A:2095:GLU:OE1 | 1:A:2098:HIS:N | 2.47 | 0.48 |
| 1:B:1299:HIS:HB3 | 1:B:1452:ALA:HB2 | 1.94 | 0.48 |
| 1:B:1452:ALA:HA | 1:B:1457:PHE:CD2 | 2.48 | 0.48 |
| 1:B:1492:MET:HE2 | 1:B:1492:MET:HA | 1.94 | 0.48 |
| 1:B:1748:VAL:HA | 1:B:1751:GLU:HG2 | 1.95 | 0.48 |
| 1:B:2414:GLN:HA | 1:B:2467:PHE:HA | 1.94 | 0.48 |
| 1:B:2616:ASP:OD1 | 1:B:2617:LYS:N | 2.45 | 0.48 |
| 1:B:3227:THR:OG1 | 1:B:3245:PHE:O | 2.26 | 0.48 |
| 1:C:231:LYS:HE3 | 1:C:237:TYR:CE1 | 2.48 | 0.48 |
| 1:C:1421:ASP:OD1 | 1:C:1422:PHE:N | 2.46 | 0.48 |
| 1:C:2603:TRP:NE1 | 1:C:2711:ASN:HD22 | 2.11 | 0.48 |
| 1:C:2641:GLN:HG2 | 1:C:2684:TRP:CH2 | 2.48 | 0.48 |
| 1:D:188:ILE:HD13 | 1:D:215:HIS:NE2 | 2.28 | 0.48 |
| 1:D:533:PRO:HB2 | 1:D:535:ILE:HD12 | 1.94 | 0.48 |
| 1:D:580:TYR:CG | 1:D:958:PRO:HG2 | 2.48 | 0.48 |
| 1:D:663:LYS:HB3 | 1:D:665:HIS:CE1 | 2.48 | 0.48 |
| 1:D:848:ARG:HD2 | 1:D:1123:TYR:CE2 | 2.48 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:D:958:PRO:C | 1:D:961:ASN:H | 2.21 | 0.48 |
| 1:D:1126:LEU:HD23 | 1:D:1126:LEU:H | 1.77 | 0.48 |
| 1:D:1466:ARG:O | 1:D:1470:ILE:HG12 | 2.13 | 0.48 |
| 1:D:2264:PHE:HZ | 1:D:2302:VAL:HG13 | 1.78 | 0.48 |
| 1:D:2522:VAL:HG23 | 1:D:2523:ALA:H | 1.78 | 0.48 |
| 1:D:3147:LEU:HD23 | 1:D:3150:LEU:HD12 | 1.94 | 0.48 |
| 1:E:855:THR:O | 1:E:859:VAL:HG23 | 2.14 | 0.48 |
| 1:E:881:ILE:HD12 | 1:E:884:PHE:CE2 | 2.48 | 0.48 |
| 1:F:788:GLU:CD | 1:F:791:ASP:H | 2.22 | 0.48 |
| 1:F:1048:ILE:HA | 1:F:1051:LEU:HG | 1.95 | 0.48 |
| 1:F:1840:GLN:N | 1:F:1840:GLN:OE1 | 2.45 | 0.48 |
| 1:F:2130:HIS:NE2 | 1:F:2147:CYS:SG | 2.86 | 0.48 |
| 1:F:2695:THR:HG21 | 1:F:2698:TYR:HD2 | 1.79 | 0.48 |
| 1:F:3163:ASN:ND2 | 1:F:3168:THR:OG1 | 2.47 | 0.48 |
| 1:G:24:ARG:HH12 | 1:G:125:TRP:CD1 | 2.31 | 0.48 |
| 1:G:637:PHE:HE1 | 1:G:641:HIS:CE1 | 2.31 | 0.48 |
| 1:G:754:SER:HA | 1:G:765:VAL:HG23 | 1.95 | 0.48 |
| 1:G:1723:PRO:HA | 1:G:1728:ARG:NH2 | 2.28 | 0.48 |
| 1:G:1881:PHE:CE2 | 1:G:1885:HIS:CE1 | 3.01 | 0.48 |
| 1:G:2375:LEU:HD22 | 1:G:2379:GLU:HG3 | 1.95 | 0.48 |
| 1:H:913:TRP:CD1 | 1:H:1088:LEU:HD12 | 2.49 | 0.48 |
| 1:H:1024:TYR:CD2 | 1:H:1181:PHE:HA | 2.49 | 0.48 |
| 1:H:1325:TRP:HE3 | 1:H:1496:LEU:HD21 | 1.79 | 0.48 |
| 1:H:2614:LEU:HD11 | 1:H:2636:ARG:HH12 | 1.78 | 0.48 |
| 1:I:1144:GLN:HA | 1:I:1148:ARG:NH2 | 2.29 | 0.48 |
| 1:I:1802:ILE:HD12 | 1:I:1805:GLU:HB2 | 1.95 | 0.48 |
| 1:I:2334:MET:SD | 1:I:2334:MET:N | 2.87 | 0.48 |
| 1:I:3052:LEU:O | 1:I:3055:ARG:NH2 | 2.38 | 0.48 |
| 1:J:596:GLN:NE2 | 1:J:598:ASP:H | 2.11 | 0.48 |
| 1:K:2392:ARG:HB3 | 1:K:2394:PHE:HE1 | 1.79 | 0.48 |
| 1:K:2990:LEU:HD12 | 1:K:3168:THR:HG22 | 1.96 | 0.48 |
| 1:K:3118:HIS:O | 1:K:3121:SER:OG | 2.21 | 0.48 |
| 1:L:378:LYS:NZ | 1:L:383:ASP:H | 2.10 | 0.48 |
| 1:L:737:PHE:CG | 1:L:786:LYS:HB3 | 2.49 | 0.48 |
| 1:L:812:ASP:HB3 | 1:L:818:TRP:HH2 | 1.79 | 0.48 |
| 1:L:1022:HIS:HD2 | 1:L:1026:HIS:CE1 | 2.31 | 0.48 |
| 1:L:3157:PHE:HA | 1:L:3169:ARG:HH22 | 1.79 | 0.48 |
| 1:M:2356:GLU:OE1 | 1:M:2356:GLU:N | 2.43 | 0.48 |
| 1:M:3301:THR:HG22 | 1:M:3326:LEU:HA | 1.96 | 0.48 |
| 1:N:374:GLU:OE1 | 1:N:374:GLU:N | 2.34 | 0.48 |
| 1:N:1564:ASN:HB3 | 1:N:1604:PHE:CE1 | 2.49 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:O:1756:ARG:HH12 | 1:P:2102:ARG:NE | 2.12 | 0.48 |
| 1:O:2246:ASP:OD1 | 1:O:2246:ASP:N | 2.45 | 0.48 |
| 1:O:2282:SER:H | 1:O:2285:SER:HB2 | 1.78 | 0.48 |
| 1:O:2929:LEU:HD22 | 1:O:2933:GLN:HG3 | 1.94 | 0.48 |
| 1:O:3043:GLN:HG3 | 1:O:3044:VAL:H | 1.79 | 0.48 |
| 1:P:538:LYS:NZ | 1:P:540:THR:O | 2.29 | 0.48 |
| 1:P:2645:ASP:OD1 | 1:P:2653:PHE:HB2 | 2.13 | 0.48 |
| 1:P:2675:GLU:O | 1:P:2679:ASN:ND2 | 2.46 | 0.48 |
| 1:P:2718:ILE:HD11 | 1:P:2779:LEU:HB2 | 1.95 | 0.48 |
| 1:Q:606:PHE:CZ | 1:Q:644:VAL:HG13 | 2.48 | 0.48 |
| 1:Q:718:MET:SD | 1:Q:722:GLN:HG2 | 2.53 | 0.48 |
| 1:Q:1865:LYS:NZ | 1:Q:1867:HIS:H | 2.11 | 0.48 |
| 1:Q:2190:LEU:HD21 | 1:Q:2194:PHE:HB3 | 1.94 | 0.48 |
| 1:Q:2383:GLU:O | 1:Q:2387:HIS:ND1 | 2.45 | 0.48 |
| 1:Q:2405:SER:HB3 | 1:Q:2426:PHE:HE1 | 1.77 | 0.48 |
| 1:Q:2521:THR:HG23 | 1:Q:2524:GLU:H | 1.77 | 0.48 |
| 1:R:7:ASN:HB3 | 1:R:10:LEU:HG | 1.95 | 0.48 |
| 1:R:38:LEU:HG | 1:R:73:TYR:CZ | 2.48 | 0.48 |
| 1:R:1531:ASP:OD1 | 1:R:1532:THR:N | 2.47 | 0.48 |
| 1:R:1865:LYS:O | 1:R:1868:SER:OG | 2.26 | 0.48 |
| 1:R:2714:ARG:O | 1:R:2718:ILE:HG12 | 2.14 | 0.48 |
| 1:R:2927:SER:O | 1:S:2943:LYS:NZ | 2.41 | 0.48 |
| 1:S:732:THR:HA | 1:S:836:HIS:CD2 | 2.49 | 0.48 |
| 1:S:1466:ARG:NH2 | 1:S:1534:ASN:O | 2.46 | 0.48 |
| 1:S:1775:LEU:HD11 | 1:S:1780:ASN:HD21 | 1.79 | 0.48 |
| 1:S:1802:ILE:HD12 | 1:S:1805:GLU:HB2 | 1.93 | 0.48 |
| 1:S:2156:HIS:CD2 | 1:S:2159:ARG:HH21 | 2.31 | 0.48 |
| 1:S:3072:LEU:HD23 | 1:S:3129:TRP:CD1 | 2.48 | 0.48 |
| 1:S:3179:ASP:OD1 | 1:S:3180:ALA:N | 2.46 | 0.48 |
| 1:T:1301:PHE:CG | 1:T:1302:PRO:HA | 2.48 | 0.48 |
| 1:A:399:ASN:HD21 | 1:A:401:ASN:HD21 | 1.62 | 0.48 |
| 1:A:501:ARG:NH1 | 1:A:702:TYR:HB3 | 2.29 | 0.48 |
| 1:A:559:VAL:N | 1:A:564:GLU:O | 2.45 | 0.48 |
| 1:A:950:VAL:HG12 | 1:A:968:PHE:CD2 | 2.48 | 0.48 |
| 1:A:1256:LYS:HG3 | 1:A:1258:ILE:HG22 | 1.95 | 0.48 |
| 1:A:1662:ASP:OD1 | 1:A:1662:ASP:N | 2.46 | 0.48 |
| 1:B:597:ARG:NH2 | 1:B:655:GLN:HA | 2.27 | 0.48 |
| 1:B:1849:GLN:O | 1:B:1852:ILE:HG22 | 2.13 | 0.48 |
| 1:B:2124:GLN:HG2 | 1:B:2125:ALA:N | 2.29 | 0.48 |
| 1:B:2620:ASN:HB3 | 1:B:2623:GLU:OE1 | 2.13 | 0.48 |
| 1:B:2639:ARG:HD3 | 1:B:2641:GLN:HE22 | 1.78 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:2645:ASP:HB2 | 1:B:2649:GLY:O | 2.14 | 0.48 |
| 1:B:2655:TYR:CE2 | 1:B:2659:LEU:HD11 | 2.48 | 0.48 |
| 1:B:2777:ASP:OD1 | 1:B:2777:ASP:N | 2.46 | 0.48 |
| 1:B:3225:SER:O | 1:B:3290:TYR:N | 2.47 | 0.48 |
| 1:C:953:GLU:O | 1:C:966:ASN:N | 2.30 | 0.48 |
| 1:C:1328:LEU:HD21 | 1:C:1519:VAL:HG22 | 1.95 | 0.48 |
| 1:C:1989:GLY:N | 1:C:2024:TRP:O | 2.47 | 0.48 |
| 1:C:2348:THR:HG1 | 1:C:2349:ARG:NH1 | 2.11 | 0.48 |
| 1:D:312:SER:HA | 1:D:365:TYR:O | 2.14 | 0.48 |
| 1:D:1056:THR:HA | 1:D:1059:ILE:HD12 | 1.96 | 0.48 |
| 1:D:1132:SER:O | 1:D:1135:GLN:HB3 | 2.14 | 0.48 |
| 1:D:1540:ILE:H | 1:D:1540:ILE:HD12 | 1.77 | 0.48 |
| 1:D:2235:LEU:HD12 | 1:D:2239:GLY:HA2 | 1.96 | 0.48 |
| 1:D:2425:ILE:HG21 | 1:D:2442:TYR:HE2 | 1.79 | 0.48 |
| 1:D:2603:TRP:CZ3 | 1:D:2708:HIS:HD2 | 2.31 | 0.48 |
| 1:D:2820:ASP:HB3 | 1:D:2873:ASP:OD1 | 2.13 | 0.48 |
| 1:D:3230:VAL:HG22 | 1:D:3283:PHE:HD1 | 1.78 | 0.48 |
| 1:D:3395:ARG:O | 1:D:3401:ARG:NH1 | 2.38 | 0.48 |
| 1:E:473:LEU:N | 1:E:775:LYS:HE3 | 2.28 | 0.48 |
| 1:E:1869:MET:HA | 1:E:1875:ALA:HA | 1.96 | 0.48 |
| 1:E:2248:VAL:HG13 | 1:E:2249:LEU:HD12 | 1.94 | 0.48 |
| 1:E:2405:SER:HB3 | 1:E:2426:PHE:HE1 | 1.79 | 0.48 |
| 1:E:2981:MET:SD | 1:E:2982:PRO:HD2 | 2.54 | 0.48 |
| 1:F:953:GLU:HA | 1:F:969:HIS:HB2 | 1.95 | 0.48 |
| 1:F:1521:ASP:HB3 | 1:F:1525:HIS:CD2 | 2.49 | 0.48 |
| 1:F:2574:PHE:O | 1:F:2578:HIS:ND1 | 2.45 | 0.48 |
| 1:F:3119:HIS:O | 1:F:3122:ILE:HG22 | 2.14 | 0.48 |
| 1:G:574:LEU:HD23 | 1:G:616:LEU:HG | 1.95 | 0.48 |
| 1:G:729:GLU:O | 1:G:732:THR:HG22 | 2.14 | 0.48 |
| 1:G:1081:ILE:HD13 | 1:H:2460:VAL:HG12 | 1.96 | 0.48 |
| 1:G:1350:ASP:HA | 1:G:1463:ASN:HD22 | 1.78 | 0.48 |
| 1:G:1957:THR:HG23 | 1:G:1959:GLU:HB2 | 1.95 | 0.48 |
| 1:G:1991:LYS:O | 1:G:1991:LYS:HD2 | 2.14 | 0.48 |
| 1:G:2542:ARG:HH11 | 1:G:2588:ALA:HA | 1.79 | 0.48 |
| 1:H:2191:PRO:HG2 | 1:H:2194:PHE:CD2 | 2.48 | 0.48 |
| 1:H:2819:PHE:HB3 | 1:H:2874:VAL:HG12 | 1.96 | 0.48 |
| 1:I:608:VAL:HG11 | 1:I:785:VAL:HG21 | 1.96 | 0.48 |
| 1:I:672:HIS:O | 1:I:695:ARG:NH1 | 2.38 | 0.48 |
| 1:I:2460:VAL:O | 1:J:1085:ARG:NH2 | 2.47 | 0.48 |
| 1:I:3155:GLU:HB3 | 1:I:3158:ASN:HD21 | 1.77 | 0.48 |
| 1:J:2028:ARG:CZ | 1:J:2028:ARG:HB2 | 2.43 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:J:2567:CYS:O | 1:J:2569:HIS:ND1 | 2.45 | 0.48 |
| 1:K:851:VAL:HG12 | 1:K:935:PRO:HB2 | 1.95 | 0.48 |
| 1:K:1732:CYS:C | 1:K:1734:HIS:HD1 | 2.21 | 0.48 |
| 1:K:1867:HIS:HA | 1:K:1874:TYR:CE2 | 2.49 | 0.48 |
| 1:K:2304:LYS:NZ | 1:K:2371:LYS:O | 2.37 | 0.48 |
| 1:K:2664:GLN:OE1 | 1:K:2664:GLN:N | 2.39 | 0.48 |
| 1:K:3087:LEU:O | 1:K:3090:THR:OG1 | 2.30 | 0.48 |
| 1:L:474:PRO:HB2 | 1:L:476:ARG:NH2 | 2.27 | 0.48 |
| 1:L:855:THR:O | 1:L:859:VAL:HG23 | 2.14 | 0.48 |
| 1:L:2183:TRP:CD2 | 1:L:2271:ILE:HD11 | 2.48 | 0.48 |
| 1:L:2271:ILE:HD12 | 1:L:2298:HIS:NE2 | 2.28 | 0.48 |
| 1:L:2671:GLU:HA | 1:L:2674:TYR:HB3 | 1.94 | 0.48 |
| 1:L:3047:ASP:HB2 | 1:L:3097:GLY:HA3 | 1.95 | 0.48 |
| 1:M:2797:ARG:HA | 1:M:2801:ARG:HH21 | 1.79 | 0.48 |
| 1:M:3214:TYR:CD1 | 1:M:3265:ASP:HA | 2.48 | 0.48 |
| 1:N:257:ASP:HA | 1:N:265:ARG:HD3 | 1.96 | 0.48 |
| 1:N:647:LEU:O | 1:N:650:ILE:HG22 | 2.14 | 0.48 |
| 1:N:1284:ARG:HH11 | 1:N:1284:ARG:HG2 | 1.78 | 0.48 |
| 1:N:1345:SER:OG | 1:N:1346:VAL:N | 2.46 | 0.48 |
| 1:N:1365:ALA:HA | 1:N:1378:ASN:HB3 | 1.95 | 0.48 |
| 1:N:3337:ARG:NE | 1:N:3378:ASN:OD1 | 2.42 | 0.48 |
| 1:O:1058:ARG:HA | 1:O:1123:TYR:CE1 | 2.48 | 0.48 |
| 1:O:1622:GLY:HA3 | 1:P:2786:ILE:HD13 | 1.95 | 0.48 |
| 1:O:2345:ASN:HD21 | 1:O:2347:PHE:HB3 | 1.78 | 0.48 |
| 1:O:2771:GLN:N | 1:O:3179:ASP:OD2 | 2.47 | 0.48 |
| 1:P:331:HIS:CE1 | 1:P:672:HIS:HB3 | 2.48 | 0.48 |
| 1:P:499:TRP:NE1 | 1:P:676:LYS:O | 2.47 | 0.48 |
| 1:P:938:ASP:HA | 1:P:1055:ASN:ND2 | 2.28 | 0.48 |
| 1:P:984:ASP:OD2 | 1:P:985:GLU:N | 2.47 | 0.48 |
| 1:P:1345:SER:OG | 1:P:1346:VAL:N | 2.47 | 0.48 |
| 1:P:2194:PHE:CD1 | 1:P:2212:PHE:HB3 | 2.48 | 0.48 |
| 1:P:3287:LEU:HD21 | 1:P:3299:LEU:HD21 | 1.94 | 0.48 |
| 1:Q:636:ILE:HD12 | 1:Q:636:ILE:H | 1.79 | 0.48 |
| 1:Q:2354:PRO:O | 1:Q:2357:VAL:HG22 | 2.13 | 0.48 |
| 1:Q:2508:VAL:HB | 1:Q:3138:ARG:NH2 | 2.29 | 0.48 |
| 1:R:153:VAL:HG21 | 1:R:159:THR:HA | 1.96 | 0.48 |
| 1:R:859:VAL:O | 1:R:862:LEU:HG | 2.14 | 0.48 |
| 1:S:938:ASP:HA | 1:S:1055:ASN:HD21 | 1.77 | 0.48 |
| 1:S:2037:VAL:HA | 1:S:2040:LYS:HG2 | 1.93 | 0.48 |
| 1:S:3353:GLU:OE1 | 1:S:3387:PHE:N | 2.46 | 0.48 |
| 1:T:257:ASP:HA | 1:T:265:ARG:HD3 | 1.95 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:T:869:LEU:HB3 | 1:T:928:LYS:HE3 | 1.96 | 0.48 |
| 1:T:1001:MET:HA | 1:T:1004:LEU:HD23 | 1.95 | 0.48 |
| 1:T:1085:ARG:HA | 1:T:1110:PHE:HE2 | 1.79 | 0.48 |
| 1:T:1108:VAL:HG13 | 1:T:1111:GLU:OE1 | 2.14 | 0.48 |
| 1:T:2183:TRP:CD2 | 1:T:2271:ILE:HD11 | 2.48 | 0.48 |
| 1:T:2412:VAL:HG21 | 1:T:2450:LEU:HD21 | 1.96 | 0.48 |
| 1:T:3080:PHE:N | 1:T:3081:GLU:OE1 | 2.47 | 0.48 |
| 1:T:3227:THR:OG1 | 1:T:3245:PHE:O | 2.29 | 0.48 |
| 1:A:64:ALA:HB3 | 1:A:246:LEU:HD23 | 1.96 | 0.48 |
| 1:A:75:VAL:O | 1:A:78:GLU:HG3 | 2.14 | 0.48 |
| 1:A:954:THR:HG22 | 1:A:965:PRO:HA | 1.95 | 0.48 |
| 1:A:2801:ARG:HD3 | 1:A:2803:PHE:HZ | 1.79 | 0.48 |
| 1:A:3308:PRO:HG2 | 1:A:3311:ALA:HB3 | 1.96 | 0.48 |
| 1:B:851:VAL:HG12 | 1:B:935:PRO:HB2 | 1.95 | 0.48 |
| 1:B:914:HIS:HA | 1:B:917:LEU:HG | 1.95 | 0.48 |
| 1:B:3360:LEU:HG | 1:B:3401:ARG:HD3 | 1.95 | 0.48 |
| 1:C:658:ARG:HH22 | 1:C:727:ILE:HD11 | 1.77 | 0.48 |
| 1:C:997:LYS:O | 1:C:1000:GLU:HG3 | 2.14 | 0.48 |
| 1:C:2112:ARG:NH2 | 1:C:2208:LEU:HD21 | 2.29 | 0.48 |
| 1:D:80:LYS:HA | 1:D:83:LYS:HZ3 | 1.78 | 0.48 |
| 1:D:729:GLU:O | 1:D:732:THR:HG22 | 2.14 | 0.48 |
| 1:D:956:VAL:HA | 1:D:963:PRO:HA | 1.94 | 0.48 |
| 1:D:1004:LEU:O | 1:D:1008:GLN:NE2 | 2.43 | 0.48 |
| 1:E:1596:LEU:HD12 | 1:E:1597:GLY:N | 2.28 | 0.48 |
| 1:E:1644:TYR:N | 1:H:481:ASP:OD2 | 2.47 | 0.48 |
| 1:E:1943:ASP:OD1 | 1:E:1943:ASP:N | 2.46 | 0.48 |
| 1:E:1978:LYS:NZ | 1:E:1979:SER:O | 2.36 | 0.48 |
| 1:E:2158:HIS:CE1 | 1:E:2299:HIS:HE1 | 2.31 | 0.48 |
| 1:E:2214:ARG:HH12 | 1:E:2216:TYR:HB2 | 1.79 | 0.48 |
| 1:E:2250:LEU:HA | 1:E:2253:GLU:OE1 | 2.14 | 0.48 |
| 1:F:171:GLU:HB3 | 1:F:177:PHE:HD1 | 1.79 | 0.48 |
| 1:F:719:THR:HG22 | 1:F:722:GLN:NE2 | 2.29 | 0.48 |
| 1:F:1270:ASP:OD1 | 1:F:1271:LEU:N | 2.47 | 0.48 |
| 1:F:1540:ILE:HD12 | 1:F:1540:ILE:H | 1.78 | 0.48 |
| 1:F:3266:VAL:HG21 | 1:F:3283:PHE:CE2 | 2.49 | 0.48 |
| 1:G:41:PHE:CE1 | 1:G:253:PRO:HG2 | 2.48 | 0.48 |
| 1:G:3340:PHE:CE1 | 1:G:3351:VAL:HG11 | 2.48 | 0.48 |
| 1:H:105:ARG:HA | 1:H:108:GLN:NE2 | 2.26 | 0.48 |
| 1:H:1893:ALA:O | 1:H:1896:GLN:HB2 | 2.14 | 0.48 |
| 1:H:2343:ASN:OD1 | 1:H:2344:GLU:N | 2.46 | 0.48 |
| 1:H:3124:ARG:O | 1:H:3127:GLN:HG3 | 2.13 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:H:3270:LEU:HD22 | 1:H:3275:LEU:HB2 | 1.95 | 0.48 |
| 1:H:3344:VAL:HG12 | 1:H:3346:SER:H | 1.78 | 0.48 |
| 1:I:539:GLU:N | 1:I:539:GLU:OE1 | 2.47 | 0.48 |
| 1:I:2297:THR:O | 1:I:2300:THR:OG1 | 2.28 | 0.48 |
| 1:I:3305:ILE:HA | 1:I:3315:VAL:O | 2.13 | 0.48 |
| 1:J:1108:VAL:HG13 | 1:J:1111:GLU:OE1 | 2.14 | 0.48 |
| 1:J:2718:ILE:HD11 | 1:J:2779:LEU:HB2 | 1.96 | 0.48 |
| 1:J:3183:PHE:HD2 | 1:J:3185:TYR:HE1 | 1.62 | 0.48 |
| 1:J:3213:VAL:HG22 | 1:J:3267:THR:HG23 | 1.95 | 0.48 |
| 1:K:792:ALA:O | 1:K:795:LYS:HG2 | 2.14 | 0.48 |
| 1:K:1583:GLU:HB2 | 1:N:340:SER:HB3 | 1.96 | 0.48 |
| 1:K:1638:ARG:HD2 | 1:K:1644:TYR:HE2 | 1.77 | 0.48 |
| 1:K:1710:LEU:HB3 | 1:K:1750:PHE:HE1 | 1.78 | 0.48 |
| 1:K:2376:ASN:O | 1:K:2380:LEU:HG | 2.13 | 0.48 |
| 1:K:3133:GLN:NE2 | 1:K:3138:ARG:HB3 | 2.29 | 0.48 |
| 1:L:334:ASP:OD1 | 1:L:334:ASP:N | 2.45 | 0.48 |
| 1:L:551:HIS:ND1 | 1:L:552:ASN:O | 2.43 | 0.48 |
| 1:L:634:ASP:OD1 | 1:L:636:ILE:HG12 | 2.14 | 0.48 |
| 1:L:944:THR:HA | 1:L:987:PHE:CD1 | 2.49 | 0.48 |
| 1:L:1019:GLU:HA | 1:L:1022:HIS:HE1 | 1.72 | 0.48 |
| 1:L:1599:GLU:OE2 | 1:L:1600:THR:OG1 | 2.32 | 0.48 |
| 1:L:3383:PRO:HA | 1:L:3406:ILE:HB | 1.96 | 0.48 |
| 1:M:945:ALA:HA | 1:M:987:PHE:CZ | 2.48 | 0.48 |
| 1:M:1710:LEU:HB3 | 1:M:1750:PHE:CE1 | 2.43 | 0.48 |
| 1:N:23:LEU:HD23 | 1:N:123:ASN:ND2 | 2.29 | 0.48 |
| 1:N:757:PRO:HB2 | 1:N:760:GLY:H | 1.78 | 0.48 |
| 1:N:2567:CYS:SG | 1:N:2578:HIS:NE2 | 2.86 | 0.48 |
| 1:O:436:ASP:OD1 | 1:O:436:ASP:N | 2.45 | 0.48 |
| 1:O:590:MET:HE2 | 1:O:590:MET:HA | 1.94 | 0.48 |
| 1:O:719:THR:HG21 | 1:O:847:VAL:HG21 | 1.95 | 0.48 |
| 1:O:1842:ASN:HB3 | 1:O:1845:ASP:HB2 | 1.96 | 0.48 |
| 1:O:2381:GLU:HA | 1:O:2384:ILE:HD12 | 1.96 | 0.48 |
| 1:O:2685:ILE:HG23 | 1:O:2693:MET:HE1 | 1.96 | 0.48 |
| 1:O:3086:MET:O | 1:O:3090:THR:HG23 | 2.13 | 0.48 |
| 1:O:3214:TYR:CD1 | 1:O:3265:ASP:HA | 2.47 | 0.48 |
| 1:P:1136:LEU:HA | 1:P:1139:GLU:OE2 | 2.13 | 0.48 |
| 1:Q:299:LEU:O | 1:Q:302:GLN:HG3 | 2.14 | 0.48 |
| 1:Q:585:ALA:HA | 1:Q:588:ASP:OD2 | 2.13 | 0.48 |
| 1:Q:997:LYS:O | 1:Q:1000:GLU:HG3 | 2.13 | 0.48 |
| 1:Q:1025:ILE:HD12 | 1:Q:1028:LEU:HD23 | 1.95 | 0.48 |
| 1:Q:2331:SER:HA | 1:Q:2355:LYS:NZ | 2.27 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:R:221:ARG:O | 1:R:225:ILE:HG12 | 2.13 | 0.48 |
| 1:R:1840:GLN:N | 1:R:1840:GLN:OE1 | 2.46 | 0.48 |
| 1:R:2345:ASN:O | 1:R:2349:ARG:HG2 | 2.13 | 0.48 |
| 1:R:2738:GLN:O | 1:R:2742:GLN:NE2 | 2.47 | 0.48 |
| 1:R:3124:ARG:O | 1:R:3127:GLN:HG3 | 2.13 | 0.48 |
| 1:S:2027:ASP:OD1 | 1:S:2028:ARG:N | 2.46 | 0.48 |
| 1:S:2109:ALA:HA | 1:S:2112:ARG:NH2 | 2.29 | 0.48 |
| 1:S:2570:GLY:HA2 | 1:S:2847:PHE:CE2 | 2.48 | 0.48 |
| 1:S:3284:GLN:HE22 | 1:S:3286:THR:HG23 | 1.78 | 0.48 |
| 1:T:39:ALA:HB1 | 1:T:208:TYR:CE2 | 2.49 | 0.48 |
| 1:T:1568:SER:N | 1:T:1597:GLY:O | 2.46 | 0.48 |
| 1:T:2269:ASN:HD21 | 1:T:2428:LEU:N | 2.12 | 0.48 |
| 1:A:678:PHE:O | 1:A:685:ASN:ND2 | 2.47 | 0.48 |
| 1:A:1420:CYS:HB2 | 1:A:1608:ARG:HH21 | 1.79 | 0.48 |
| 1:A:2614:LEU:HD12 | 1:A:2636:ARG:HH12 | 1.79 | 0.48 |
| 1:A:3353:GLU:HG3 | 1:A:3386:TYR:HD2 | 1.79 | 0.48 |
| 1:B:246:LEU:HA | 1:B:249:LYS:HE2 | 1.96 | 0.48 |
| 1:B:2028:ARG:HB2 | 1:B:2028:ARG:NH1 | 2.29 | 0.48 |
| 1:B:2671:GLU:H | 1:B:2671:GLU:CD | 2.18 | 0.48 |
| 1:B:3131:THR:HA | 1:B:3134:LYS:HG2 | 1.95 | 0.48 |
| 1:B:3321:LEU:O | 1:B:3395:ARG:NH2 | 2.45 | 0.48 |
| 1:C:293:ILE:H | 1:C:293:ILE:HD12 | 1.78 | 0.48 |
| 1:C:855:THR:O | 1:C:858:GLN:HG2 | 2.14 | 0.48 |
| 1:C:1865:LYS:NZ | 1:C:1867:HIS:H | 2.12 | 0.48 |
| 1:C:1943:ASP:OD1 | 1:C:1943:ASP:N | 2.47 | 0.48 |
| 1:C:1946:ASP:HB3 | 1:C:1950:HIS:HD2 | 1.78 | 0.48 |
| 1:D:960:THR:OG1 | 1:D:964:GLU:OE2 | 2.26 | 0.48 |
| 1:D:2324:ASP:OD1 | 1:D:2325:CYS:N | 2.47 | 0.48 |
| 1:D:3119:HIS:O | 1:D:3122:ILE:HG22 | 2.13 | 0.48 |
| 1:E:584:THR:HG23 | 1:E:587:PHE:H | 1.78 | 0.48 |
| 1:E:591:LEU:HD12 | 1:E:727:ILE:HD13 | 1.96 | 0.48 |
| 1:E:752:ILE:O | 1:E:808:LEU:HA | 2.14 | 0.48 |
| 1:E:1149:VAL:HG11 | 1:E:1206:LEU:HD13 | 1.96 | 0.48 |
| 1:E:2249:LEU:HD23 | 1:E:2383:GLU:CD | 2.39 | 0.48 |
| 1:E:2348:THR:HG1 | 1:E:2349:ARG:NH1 | 2.11 | 0.48 |
| 1:F:536:ALA:HB2 | 1:F:554:PHE:HD2 | 1.79 | 0.48 |
| 1:F:1367:TYR:HE2 | 1:F:1369:ASP:HB3 | 1.79 | 0.48 |
| 1:F:2132:VAL:HG13 | 1:F:2287:HIS:HD1 | 1.79 | 0.48 |
| 1:G:602:PHE:HA | 1:G:605:GLN:NE2 | 2.29 | 0.48 |
| 1:G:1219:VAL:HG23 | 1:G:1239:VAL:HG13 | 1.95 | 0.48 |
| 1:G:1223:VAL:HG13 | 1:G:1231:ILE:HB | 1.93 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:G:1424:ILE:HD11 | 1:G:1606:PHE:CD2 | 2.49 | 0.48 |
| 1:G:1733:VAL:HG23 | 1:G:1736:MET:HE2 | 1.95 | 0.48 |
| 1:G:3268:ASP:N | 1:G:3268:ASP:OD1 | 2.46 | 0.48 |
| 1:H:1270:ASP:OD1 | 1:H:1271:LEU:N | 2.46 | 0.48 |
| 1:H:3245:PHE:HB3 | 1:H:3264:TYR:HE2 | 1.79 | 0.48 |
| 1:I:855:THR:O | 1:I:859:VAL:HG23 | 2.14 | 0.48 |
| 1:I:980:ARG:NE | 1:I:1046:ASP:OD2 | 2.44 | 0.48 |
| 1:I:1684:THR:N | 1:I:1687:GLU:OE2 | 2.46 | 0.48 |
| 1:I:2338:ASN:OD1 | 1:I:2339:SER:N | 2.47 | 0.48 |
| 1:J:1540:ILE:HD12 | 1:J:1540:ILE:H | 1.79 | 0.48 |
| 1:J:1550:GLN:HA | 1:J:1553:GLN:HE22 | 1.79 | 0.48 |
| 1:J:1742:TRP:CD1 | 1:J:1920:LEU:HD12 | 2.49 | 0.48 |
| 1:J:1890:ARG:HH12 | 1:J:1959:GLU:HG3 | 1.78 | 0.48 |
| 1:K:525:TRP:NE1 | 1:K:643:ASN:HD22 | 2.11 | 0.48 |
| 1:K:675:LEU:HD11 | 1:K:696:PRO:HG3 | 1.96 | 0.48 |
| 1:K:1576:CYS:HB2 | 1:K:1632:ASP:OD1 | 2.13 | 0.48 |
| 1:L:50:LYS:NZ | 1:L:52:ASP:OD2 | 2.44 | 0.48 |
| 1:L:105:ARG:HA | 1:L:108:GLN:NE2 | 2.28 | 0.48 |
| 1:L:958:PRO:C | 1:L:961:ASN:H | 2.22 | 0.48 |
| 1:L:1788:VAL:HG12 | 1:L:1789:LEU:HD22 | 1.96 | 0.48 |
| 1:L:3324:ASN:H | 1:L:3398:GLN:HE22 | 1.60 | 0.48 |
| 1:M:887:GLN:HE21 | 1:M:889:ASN:HD21 | 1.61 | 0.48 |
| 1:M:1623:LEU:HD13 | 1:M:1631:ILE:HD11 | 1.95 | 0.48 |
| 1:M:2021:GLU:N | 1:M:2021:GLU:OE1 | 2.47 | 0.48 |
| 1:M:2124:GLN:OE1 | 1:M:2124:GLN:N | 2.36 | 0.48 |
| 1:M:3081:GLU:HA | 1:M:3084:PHE:CB | 2.44 | 0.48 |
| 1:N:506:GLN:HE22 | 1:N:687:ASN:HB3 | 1.79 | 0.48 |
| 1:N:738:VAL:HG23 | 1:N:789:ILE:HG13 | 1.96 | 0.48 |
| 1:N:1777:ALA:HB1 | 1:N:1781:GLU:HG2 | 1.96 | 0.48 |
| 1:N:2165:VAL:HG11 | 1:N:2296:PHE:CE2 | 2.48 | 0.48 |
| 1:N:2567:CYS:C | 1:N:2569:HIS:HD1 | 2.22 | 0.48 |
| 1:N:2820:ASP:HB3 | 1:N:2873:ASP:OD1 | 2.13 | 0.48 |
| 1:N:3035:TYR:H | 1:N:3044:VAL:HG22 | 1.79 | 0.48 |
| 1:O:579:GLU:HG3 | 1:O:582:ASP:CG | 2.39 | 0.48 |
| 1:O:580:TYR:CG | 1:O:958:PRO:HG2 | 2.48 | 0.48 |
| 1:O:2190:LEU:HD21 | 1:O:2194:PHE:HB3 | 1.95 | 0.48 |
| 1:O:2269:ASN:OD1 | 1:O:2428:LEU:HB2 | 2.14 | 0.48 |
| 1:O:2831:ALA:HA | 1:O:2858:VAL:HG11 | 1.94 | 0.48 |
| 1:O:3276:ASN:OD1 | 1:O:3277:ALA:N | 2.47 | 0.48 |
| 1:O:3300:ALA:HA | 1:O:3325:LYS:HE3 | 1.95 | 0.48 |
| 1:O:3353:GLU:HG3 | 1:P:3148:ARG:HH22 | 1.79 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:P:614:HIS:CD2 | 1:P:637:PHE:HE1 | 2.32 | 0.48 |
| 1:P:1694:ALA:O | 1:P:1697:SER:OG | 2.28 | 0.48 |
| 1:P:2087:LEU:HD12 | 1:P:2366:ARG:HD3 | 1.95 | 0.48 |
| 1:P:2536:GLN:HA | 1:P:2544:TYR:HB3 | 1.95 | 0.48 |
| 1:Q:731:ARG:HA | 1:Q:735:ARG:HH12 | 1.78 | 0.48 |
| 1:Q:1750:PHE:HD2 | 1:Q:1882:LEU:HD21 | 1.79 | 0.48 |
| 1:Q:2027:ASP:OD2 | 1:Q:2028:ARG:NH1 | 2.45 | 0.48 |
| 1:R:739:GLY:HA3 | 1:R:784:LEU:HB3 | 1.95 | 0.48 |
| 1:R:1294:LYS:O | 1:R:1297:SER:OG | 2.24 | 0.48 |
| 1:R:1965:ALA:HA | 1:R:1968:LEU:HG | 1.96 | 0.48 |
| 1:R:3154:LEU:HD21 | 1:R:3174:PRO:HG3 | 1.96 | 0.48 |
| 1:S:94:TRP:HB2 | 1:S:214:LEU:HD12 | 1.96 | 0.48 |
| 1:S:2090:ASN:O | 1:S:2091:ARG:HG2 | 2.13 | 0.48 |
| 1:S:3324:ASN:ND2 | 1:S:3398:GLN:O | 2.46 | 0.48 |
| 1:T:787:VAL:HG23 | 1:T:789:ILE:HD11 | 1.96 | 0.48 |
| 1:T:1840:GLN:N | 1:T:1840:GLN:OE1 | 2.47 | 0.48 |
| 1:T:1998:ILE:HD11 | 1:T:2010:ALA:HB3 | 1.95 | 0.48 |
| 1:T:2210:ASN:HD21 | 1:T:2212:PHE:HB2 | 1.79 | 0.48 |
| 1:T:2740:LEU:O | 1:T:2763:ALA:HB3 | 2.13 | 0.48 |
| 1:T:3226:ALA:HA | 1:T:3289:LYS:HA | 1.95 | 0.48 |
| 1:T:3260:ARG:HH12 | 1:T:3333:SER:HA | 1.77 | 0.48 |
| 1:A:436:ASP:HB3 | 1:A:522:TYR:CZ | 2.48 | 0.48 |
| 1:A:1100:ASP:OD2 | 1:A:1102:ILE:HG22 | 2.13 | 0.48 |
| 1:A:2849:ARG:HH11 | 1:A:2849:ARG:HA | 1.79 | 0.48 |
| 1:B:1067:GLN:HG3 | 1:B:1070:ARG:HH21 | 1.79 | 0.48 |
| 1:B:1785:ARG:HH22 | 1:B:1790:ASP:HA | 1.79 | 0.48 |
| 1:C:170:GLU:OE2 | 1:C:304:ARG:HD2 | 2.14 | 0.48 |
| 1:C:612:LEU:HB2 | 1:C:613:PRO:HD3 | 1.94 | 0.48 |
| 1:C:1763:ILE:HD11 | 1:C:1882:LEU:HB3 | 1.95 | 0.48 |
| 1:C:2696:LEU:HD21 | 1:C:2839:GLY:HA3 | 1.95 | 0.48 |
| 1:D:223:PHE:HZ | 1:D:274:PHE:HD1 | 1.61 | 0.48 |
| 1:D:474:PRO:HB2 | 1:D:476:ARG:NH2 | 2.28 | 0.48 |
| 1:D:737:PHE:N | 1:D:829:ILE:O | 2.29 | 0.48 |
| 1:E:143:ARG:HH21 | 1:E:209:ASP:CG | 2.21 | 0.48 |
| 1:E:501:ARG:NH1 | 1:E:702:TYR:HB3 | 2.29 | 0.48 |
| 1:E:2585:LEU:HG | 1:E:2589:LEU:HD23 | 1.96 | 0.48 |
| 1:E:3173:ARG:HA | 1:E:3173:ARG:HH11 | 1.78 | 0.48 |
| 1:E:3213:VAL:CG1 | 1:E:3270:LEU:HD13 | 2.44 | 0.48 |
| 1:E:3382:GLU:N | 1:E:3386:TYR:OH | 2.47 | 0.48 |
| 1:F:1716:VAL:HG23 | 1:F:1718:PRO:HD3 | 1.96 | 0.48 |
| 1:F:1895:TRP:HA | 1:F:1898:LEU:HD12 | 1.96 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:F:2645:ASP:OD1 | 1:F:2653:PHE:HB2 | 2.13 | 0.48 |
| 1:G:30:LYS:N | 1:G:30:LYS:HD2 | 2.29 | 0.48 |
| 1:G:731:ARG:HG2 | 1:G:735:ARG:HH22 | 1.79 | 0.48 |
| 1:G:736:THR:N | 1:G:790:THR:OG1 | 2.46 | 0.48 |
| 1:G:857:GLU:HG2 | 1:G:858:GLN:N | 2.29 | 0.48 |
| 1:G:881:ILE:HD11 | 1:G:920:GLN:HG2 | 1.96 | 0.48 |
| 1:H:1301:PHE:CG | 1:H:1302:PRO:HA | 2.49 | 0.48 |
| 1:H:2665:ARG:HH21 | 1:H:2726:ARG:HH21 | 1.60 | 0.48 |
| 1:H:2777:ASP:OD1 | 1:H:2777:ASP:N | 2.46 | 0.48 |
| 1:I:2409:ARG:HG3 | 1:I:2424:ALA:HB2 | 1.96 | 0.48 |
| 1:J:1058:ARG:NH1 | 1:J:1125:ASP:O | 2.47 | 0.48 |
| 1:J:2251:VAL:HG21 | 1:J:2267:THR:HG21 | 1.96 | 0.48 |
| 1:J:2757:ILE:O | 1:J:2761:ALA:HB2 | 2.14 | 0.48 |
| 1:J:3214:TYR:HB2 | 1:J:3263:LYS:HD2 | 1.96 | 0.48 |
| 1:K:1583:GLU:N | 1:N:340:SER:O | 2.46 | 0.48 |
| 1:K:2047:ASP:OD1 | 1:L:1493:ARG:NH1 | 2.47 | 0.48 |
| 1:K:2190:LEU:HD21 | 1:K:2194:PHE:CD2 | 2.46 | 0.48 |
| 1:K:2214:ARG:HH12 | 1:K:2216:TYR:HB2 | 1.78 | 0.48 |
| 1:K:2602:ASP:HA | 1:K:2711:ASN:ND2 | 2.29 | 0.48 |
| 1:K:2980:GLY:HA2 | 1:K:3258:TYR:HE1 | 1.78 | 0.48 |
| 1:K:3287:LEU:HG | 1:K:3295:LEU:HB2 | 1.95 | 0.48 |
| 1:L:196:HIS:O | 1:L:199:SER:OG | 2.25 | 0.48 |
| 1:L:325:ARG:HH21 | 1:L:391:TYR:HE2 | 1.60 | 0.48 |
| 1:L:1333:VAL:HG22 | 1:L:1458:PHE:HE1 | 1.78 | 0.48 |
| 1:L:1852:ILE:HD11 | 1:L:2013:PHE:HD2 | 1.79 | 0.48 |
| 1:L:2273:TYR:HB3 | 1:L:2426:PHE:HD1 | 1.79 | 0.48 |
| 1:L:2338:ASN:OD1 | 1:L:2339:SER:N | 2.47 | 0.48 |
| 1:M:1202:ILE:HG22 | 1:M:1205:ILE:HG22 | 1.95 | 0.48 |
| 1:M:1851:GLU:O | 1:M:1854:HIS:HB3 | 2.14 | 0.48 |
| 1:M:2849:ARG:HA | 1:M:2849:ARG:HH11 | 1.79 | 0.48 |
| 1:N:525:TRP:HD1 | 1:N:586:LEU:HD13 | 1.78 | 0.48 |
| 1:N:662:TYR:HE2 | 1:N:700:TYR:HB3 | 1.78 | 0.48 |
| 1:N:667:ALA:O | 1:N:671:THR:HG23 | 2.14 | 0.48 |
| 1:N:1772:GLN:HB2 | 1:N:1818:LEU:HD11 | 1.96 | 0.48 |
| 1:N:2432:LEU:N | 1:N:2433:GLU:OE1 | 2.47 | 0.48 |
| 1:O:255:ASP:OD1 | 1:O:255:ASP:N | 2.45 | 0.48 |
| 1:P:465:GLN:NE2 | 1:P:558:PRO:O | 2.30 | 0.48 |
| 1:Q:222:ILE:HA | 1:Q:225:ILE:HG22 | 1.95 | 0.48 |
| 1:Q:1030:GLY:HA3 | 1:Q:1038:ALA:HB2 | 1.95 | 0.48 |
| 1:Q:1152:GLY:HA3 | 1:Q:1197:LEU:HD21 | 1.96 | 0.48 |
| 1:Q:1814:LYS:HD2 | 1:Q:1860:TRP:CZ3 | 2.49 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:Q:1858:HIS:NE2 | 1:Q:1884:HIS:HE1 | 2.12 | 0.48 |
| 1:Q:2034:ILE:O | 1:Q:2038:LEU:HD23 | 2.13 | 0.48 |
| 1:Q:2088:PRO:O | 1:Q:2090:ASN:N | 2.41 | 0.48 |
| 1:R:276:TYR:O | 1:R:280:GLY:N | 2.45 | 0.48 |
| 1:R:702:TYR:N | 1:R:703:GLU:OE1 | 2.47 | 0.48 |
| 1:R:1301:PHE:CG | 1:R:1302:PRO:HA | 2.49 | 0.48 |
| 1:R:2112:ARG:HE | 1:R:2116:LYS:HZ1 | 1.60 | 0.48 |
| 1:S:742:LEU:HB2 | 1:S:781:PHE:HD2 | 1.79 | 0.48 |
| 1:S:850:ASP:OD1 | 1:S:852:SER:OG | 2.26 | 0.48 |
| 1:S:1880:ILE:HG13 | 1:S:1883:LEU:HD12 | 1.95 | 0.48 |
| 1:S:2059:ASN:ND2 | 1:S:2061:SER:OG | 2.46 | 0.48 |
| 1:T:105:ARG:O | 1:T:105:ARG:HG2 | 2.14 | 0.48 |
| 1:T:1488:ALA:HB1 | 1:T:1491:ILE:HD13 | 1.96 | 0.48 |
| 1:T:2159:ARG:O | 1:T:2162:THR:OG1 | 2.30 | 0.48 |
| 1:A:239:HIS:NE2 | 1:A:241:ASP:OD1 | 2.47 | 0.48 |
| 1:A:254:PHE:HB3 | 1:A:264:THR:HB | 1.95 | 0.48 |
| 1:A:1307:HIS:CD2 | 1:A:1602:MET:HE1 | 2.49 | 0.48 |
| 1:A:1474:LEU:HD11 | 1:A:1543:LEU:HD11 | 1.95 | 0.48 |
| 1:B:300:LEU:O | 1:B:304:ARG:HG2 | 2.13 | 0.48 |
| 1:B:337:GLN:HB2 | 1:I:1588:HIS:CE1 | 2.49 | 0.48 |
| 1:B:420:LYS:NZ | 1:B:422:SER:O | 2.32 | 0.48 |
| 1:B:705:GLU:N | 1:B:705:GLU:OE1 | 2.47 | 0.48 |
| 1:B:1055:ASN:HA | 1:B:1058:ARG:HG3 | 1.96 | 0.48 |
| 1:B:1272:SER:N | 1:B:1275:GLU:OE2 | 2.39 | 0.48 |
| 1:B:3088:HIS:HE1 | 1:B:3119:HIS:HE1 | 1.61 | 0.48 |
| 1:B:3124:ARG:HD2 | 1:B:3187:PHE:CD2 | 2.49 | 0.48 |
| 1:C:1733:VAL:HG23 | 1:C:1736:MET:HE2 | 1.96 | 0.48 |
| 1:C:1890:ARG:HB2 | 1:C:1955:TYR:CE2 | 2.49 | 0.48 |
| 1:C:2008:LYS:HZ1 | 1:C:2040:LYS:HG3 | 1.79 | 0.48 |
| 1:D:313:PHE:HB3 | 1:D:315:LEU:HD23 | 1.95 | 0.48 |
| 1:D:460:SER:HB2 | 1:D:1277:GLU:OE2 | 2.13 | 0.48 |
| 1:D:1221:TYR:OH | 1:D:1233:SER:O | 2.29 | 0.48 |
| 1:D:1802:ILE:HG22 | 1:D:1877:TYR:CD1 | 2.49 | 0.48 |
| 1:D:1888:THR:HA | 1:D:1891:ILE:HD12 | 1.96 | 0.48 |
| 1:D:2363:LEU:HB2 | 1:D:2365:PHE:CE1 | 2.49 | 0.48 |
| 1:D:2924:TYR:CD1 | 1:D:3188:ASP:HB3 | 2.48 | 0.48 |
| 1:E:436:ASP:HB3 | 1:E:522:TYR:CE2 | 2.49 | 0.48 |
| 1:E:1405:TYR:HA | 1:E:1408:ASN:HD21 | 1.79 | 0.48 |
| 1:E:1880:ILE:HG13 | 1:E:1883:LEU:HD12 | 1.95 | 0.48 |
| 1:E:2469:LEU:O | 1:E:2488:LYS:NZ | 2.43 | 0.48 |
| 1:E:2602:ASP:HA | 1:E:2711:ASN:HD21 | 1.79 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:F:937:TRP:H | 1:F:1051:LEU:HB2 | 1.78 | 0.48 |
| 1:F:958:PRO:C | 1:F:961:ASN:H | 2.22 | 0.48 |
| 1:F:1869:MET:HE2 | 1:F:1869:MET:HA | 1.95 | 0.48 |
| 1:F:2665:ARG:HE | 1:F:2726:ARG:NH2 | 2.12 | 0.48 |
| 1:F:3127:GLN:HE22 | 1:F:3190:LEU:HD22 | 1.78 | 0.48 |
| 1:G:592:LEU:HA | 1:G:595:GLU:OE1 | 2.14 | 0.48 |
| 1:G:1013:THR:HG22 | 1:G:1196:ARG:HD2 | 1.96 | 0.48 |
| 1:G:1397:GLN:H | 1:G:1400:LEU:HD12 | 1.78 | 0.48 |
| 1:G:1515:ARG:O | 1:G:1519:VAL:HG23 | 2.14 | 0.48 |
| 1:G:2666:ASP:OD1 | 1:G:2669:ASN:HB2 | 2.13 | 0.48 |
| 1:G:2972:ASP:OD1 | 1:G:2972:ASP:N | 2.47 | 0.48 |
| 1:G:3142:TYR:CE2 | 1:G:3144:ARG:HD3 | 2.49 | 0.48 |
| 1:H:87:ALA:HB3 | 1:H:89:ILE:HD12 | 1.95 | 0.48 |
| 1:H:750:LEU:HD12 | 1:H:769:ALA:HB2 | 1.95 | 0.48 |
| 1:H:812:ASP:HB3 | 1:H:818:TRP:HH2 | 1.79 | 0.48 |
| 1:H:849:SER:OG | 1:H:850:ASP:N | 2.46 | 0.48 |
| 1:H:1538:TRP:CD1 | 1:H:1542:GLN:HG3 | 2.49 | 0.48 |
| 1:I:1220:LYS:NZ | 1:I:1222:SER:HB2 | 2.29 | 0.48 |
| 1:I:1684:THR:HB | 1:I:1687:GLU:OE1 | 2.13 | 0.48 |
| 1:I:2109:ALA:HA | 1:I:2112:ARG:NH2 | 2.29 | 0.48 |
| 1:J:1677:ARG:NH2 | 1:J:1751:GLU:OE2 | 2.47 | 0.48 |
| 1:K:170:GLU:HG3 | 1:K:304:ARG:NH1 | 2.28 | 0.48 |
| 1:K:604:VAL:HG12 | 1:K:781:PHE:CD1 | 2.49 | 0.48 |
| 1:K:737:PHE:CE1 | 1:K:788:GLU:HG2 | 2.49 | 0.48 |
| 1:K:2223:TYR:CE2 | 1:N:111:ILE:HG21 | 2.49 | 0.48 |
| 1:L:60:VAL:HG23 | 1:L:63:MET:HE2 | 1.96 | 0.48 |
| 1:L:185:HIS:O | 1:L:188:ILE:HG22 | 2.14 | 0.48 |
| 1:L:224:VAL:HA | 1:L:227:GLN:OE1 | 2.12 | 0.48 |
| 1:L:799:LYS:N | 1:L:802:ASP:OD2 | 2.43 | 0.48 |
| 1:L:2513:VAL:HG21 | 1:L:2515:LYS:HZ3 | 1.79 | 0.48 |
| 1:M:441:THR:OG1 | 1:M:443:GLU:OE1 | 2.31 | 0.48 |
| 1:M:754:SER:OG | 1:M:762:SER:OG | 2.21 | 0.48 |
| 1:M:2750:ASP:HA | 1:M:2758:ARG:HD2 | 1.96 | 0.48 |
| 1:N:284:ASP:OD1 | 1:N:284:ASP:N | 2.44 | 0.48 |
| 1:N:1063:TRP:NE1 | 1:N:1067:GLN:HE22 | 2.12 | 0.48 |
| 1:N:1919:PRO:HA | 1:N:1941:PRO:HD3 | 1.95 | 0.48 |
| 1:N:1941:PRO:O | 1:N:1944:VAL:HG22 | 2.14 | 0.48 |
| 1:N:2522:VAL:O | 1:N:2526:GLU:HG2 | 2.14 | 0.48 |
| 1:N:2668:CYS:C | 1:N:2849:ARG:HH21 | 2.22 | 0.48 |
| 1:O:1865:LYS:HE3 | 1:O:1867:HIS:HB2 | 1.96 | 0.48 |
| 1:O:2696:LEU:HD21 | 1:O:2839:GLY:HA3 | 1.96 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:O:3085:GLU:HG3 | 1:O:3086:MET:HE2 | 1.96 | 0.48 |
| 1:P:253:PRO:O | 1:P:256:ARG:NH1 | 2.47 | 0.48 |
| 1:P:887:GLN:NE2 | 1:P:889:ASN:HB2 | 2.28 | 0.48 |
| 1:P:1428:ILE:HA | 1:P:1431:ASN:HD21 | 1.79 | 0.48 |
| 1:P:2880:ASN:OD1 | 2:lA:1:NAG:N2 | 2.46 | 0.48 |
| 1:P:2932:GLU:O | 1:P:2935:SER:OG | 2.26 | 0.48 |
| 1:Q:442:ASP:OD1 | 1:Q:443:GLU:N | 2.47 | 0.48 |
| 1:Q:525:TRP:CE3 | 1:Q:586:LEU:HD23 | 2.49 | 0.48 |
| 1:Q:971:GLY:H | 1:Q:978:THR:HG1 | 1.57 | 0.48 |
| 1:Q:1844:CYS:O | 1:Q:1848:VAL:HG13 | 2.13 | 0.48 |
| 1:Q:3214:TYR:HE1 | 1:Q:3267:THR:HB | 1.79 | 0.48 |
| 1:R:229:LEU:HB3 | 1:R:233:ARG:HH21 | 1.79 | 0.48 |
| 1:R:756:LYS:HD3 | 1:R:762:SER:HB2 | 1.96 | 0.48 |
| 1:R:2326:ALA:O | 1:R:2330:MET:HG2 | 2.14 | 0.48 |
| 1:R:3049:GLN:CD | 1:R:3050:PRO:HD2 | 2.39 | 0.48 |
| 1:R:3052:LEU:O | 1:R:3055:ARG:NH1 | 2.40 | 0.48 |
| 1:S:203:LEU:HD21 | 1:S:351:LEU:HB3 | 1.95 | 0.48 |
| 1:S:1223:VAL:HG13 | 1:S:1231:ILE:HB | 1.95 | 0.48 |
| 1:S:1607:ASP:OD1 | 1:S:1608:ARG:N | 2.43 | 0.48 |
| 1:S:2762:ARG:HH11 | 1:S:2762:ARG:HG3 | 1.79 | 0.48 |
| 1:S:3095:VAL:HG13 | 1:S:3103:MET:SD | 2.54 | 0.48 |
| 1:T:2112:ARG:HE | 1:T:2116:LYS:NZ | 2.11 | 0.48 |
| 1:T:2526:GLU:HA | 1:T:2529:LYS:HG2 | 1.96 | 0.48 |
| 1:A:719:THR:HG21 | 1:A:847:VAL:HG21 | 1.96 | 0.47 |
| 1:A:1166:LEU:HD22 | 1:A:1200:TYR:HD2 | 1.79 | 0.47 |
| 1:A:1645:LEU:HA | 1:D:483:ARG:HH22 | 1.79 | 0.47 |
| 1:A:2864:LEU:HD21 | 1:A:2870:TYR:CD1 | 2.49 | 0.47 |
| 1:A:2977:CYS:SG | 1:A:3106:LEU:HD11 | 2.54 | 0.47 |
| 1:B:5:ARG:HD2 | 1:B:283:TYR:CE1 | 2.48 | 0.47 |
| 1:B:48:CYS:HB2 | 1:B:58:CYS:HB2 | 1.54 | 0.47 |
| 1:B:896:ALA:HB1 | 1:B:899:LYS:HB2 | 1.96 | 0.47 |
| 1:B:1345:SER:OG | 1:B:1346:VAL:N | 2.47 | 0.47 |
| 1:B:2149:HIS:HA | 1:B:2154:PHE:CD2 | 2.48 | 0.47 |
| 1:B:3017:SER:O | 1:B:3055:ARG:NH2 | 2.48 | 0.47 |
| 1:C:129:GLU:HA | 1:C:140:SER:HA | 1.95 | 0.47 |
| 1:C:231:LYS:HE3 | 1:C:237:TYR:HE1 | 1.79 | 0.47 |
| 1:C:752:ILE:O | 1:C:808:LEU:HA | 2.13 | 0.47 |
| 1:C:1587:ASN:OD1 | 1:C:1588:HIS:N | 2.47 | 0.47 |
| 1:C:2286:LEU:HD12 | 1:C:2429:GLY:HA2 | 1.96 | 0.47 |
| 1:C:2664:GLN:NE2 | 1:C:2670:PHE:HA | 2.26 | 0.47 |
| 1:D:73:TYR:HA | 1:D:76:GLN:OE1 | 2.14 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:D:1301:PHE:CG | 1:D:1302:PRO:HA | 2.48 | 0.47 |
| 1:D:2106:SER:HB2 | 1:D:2175:THR:HG21 | 1.96 | 0.47 |
| 1:D:2616:ASP:OD1 | 1:D:2617:LYS:N | 2.46 | 0.47 |
| 1:E:287:SER:OG | 1:E:288:LEU:N | 2.47 | 0.47 |
| 1:E:636:ILE:HA | 1:E:639:LEU:HD12 | 1.94 | 0.47 |
| 1:E:1900:ARG:O | 1:E:1900:ARG:NH1 | 2.47 | 0.47 |
| 1:E:2213:ALA:O | 1:E:2226:ARG:NH2 | 2.47 | 0.47 |
| 1:E:2296:PHE:O | 1:E:2300:THR:HG23 | 2.12 | 0.47 |
| 1:E:2304:LYS:O | 1:E:2308:VAL:HG23 | 2.14 | 0.47 |
| 1:E:2460:VAL:O | 1:F:1085:ARG:NH2 | 2.46 | 0.47 |
| 1:E:2626:GLU:HG3 | 1:E:2633:LYS:HD2 | 1.95 | 0.47 |
| 1:F:562:LEU:HB3 | 1:F:564:GLU:OE1 | 2.14 | 0.47 |
| 1:F:1809:VAL:HG22 | 1:F:1811:ARG:HH12 | 1.79 | 0.47 |
| 1:F:2111:LEU:HD13 | 1:F:2212:PHE:HE1 | 1.79 | 0.47 |
| 1:G:1240:THR:HA | 1:H:2328:ASN:HD21 | 1.79 | 0.47 |
| 1:G:1388:THR:OG1 | 1:G:1390:LYS:NZ | 2.47 | 0.47 |
| 1:G:1872:LEU:HD21 | 1:G:2016:LEU:HD13 | 1.96 | 0.47 |
| 1:G:1890:ARG:HB2 | 1:G:1955:TYR:CE2 | 2.49 | 0.47 |
| 1:H:455:PHE:HB2 | 1:H:514:ARG:HH12 | 1.78 | 0.47 |
| 1:H:531:THR:OG1 | 1:H:532:VAL:N | 2.47 | 0.47 |
| 1:H:1281:SER:O | 1:H:1285:ARG:HG2 | 2.14 | 0.47 |
| 1:H:1912:ALA:O | 1:H:1916:MET:HG2 | 2.14 | 0.47 |
| 1:H:2582:VAL:HA | 1:H:2706:PHE:HE2 | 1.79 | 0.47 |
| 1:H:2784:LEU:HD12 | 1:H:2788:GLN:HB3 | 1.96 | 0.47 |
| 1:H:3119:HIS:O | 1:H:3122:ILE:HG22 | 2.14 | 0.47 |
| 1:I:657:LYS:NZ | 1:I:721:ASP:O | 2.47 | 0.47 |
| 1:I:718:MET:HE1 | 1:I:723:LEU:HA | 1.96 | 0.47 |
| 1:I:2407:GLU:HB2 | 1:I:2426:PHE:CD2 | 2.49 | 0.47 |
| 1:I:2806:PHE:O | 1:I:2850:LEU:HD12 | 2.14 | 0.47 |
| 1:I:3089:ASN:ND2 | 1:I:3247:ILE:HD12 | 2.29 | 0.47 |
| 1:I:3283:PHE:CD2 | 1:I:3302:PRO:HG3 | 2.49 | 0.47 |
| 1:I:3333:SER:OG | 1:I:3336:THR:OG1 | 2.32 | 0.47 |
| 1:J:752:ILE:HB | 1:J:809:SER:HB3 | 1.96 | 0.47 |
| 1:J:943:MET:HE1 | 1:J:945:ALA:O | 2.13 | 0.47 |
| 1:J:1048:ILE:HA | 1:J:1051:LEU:HG | 1.95 | 0.47 |
| 1:J:2124:GLN:HG2 | 1:J:2125:ALA:N | 2.28 | 0.47 |
| 1:J:2316:ARG:HG2 | 1:J:2318:LEU:HG | 1.95 | 0.47 |
| 1:K:231:LYS:HE3 | 1:K:237:TYR:CE1 | 2.49 | 0.47 |
| 1:K:1619:ARG:HD3 | 1:L:2775:GLN:HE21 | 1.78 | 0.47 |
| 1:K:2158:HIS:CE1 | 1:K:2299:HIS:HE1 | 2.32 | 0.47 |
| 1:K:3103:MET:HA | 1:K:3109:SER:HA | 1.95 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:K:3350:ASN:O | 1:K:3391:SER:N | 2.43 | 0.47 |
| 1:L:453:SER:HB3 | 1:L:553:PRO:HG3 | 1.96 | 0.47 |
| 1:L:493:MET:HE2 | 1:L:670:MET:SD | 2.54 | 0.47 |
| 1:L:1011:PHE:HA | 1:L:1063:TRP:CH2 | 2.47 | 0.47 |
| 1:L:1848:VAL:HA | 1:L:2026:PHE:CE1 | 2.49 | 0.47 |
| 1:L:1849:GLN:O | 1:L:1852:ILE:HG22 | 2.14 | 0.47 |
| 1:N:331:HIS:NE2 | 1:N:672:HIS:O | 2.45 | 0.47 |
| 1:N:725:HIS:O | 1:N:729:GLU:HG2 | 2.14 | 0.47 |
| 1:N:1531:ASP:OD1 | 1:N:1532:THR:N | 2.47 | 0.47 |
| 1:N:1742:TRP:HD1 | 1:N:1920:LEU:HD12 | 1.79 | 0.47 |
| 1:O:855:THR:O | 1:O:858:GLN:HG2 | 2.14 | 0.47 |
| 1:O:1221:TYR:OH | 1:O:1236:PHE:N | 2.40 | 0.47 |
| 1:O:1426:PHE:CZ | 1:O:1464:VAL:HG13 | 2.49 | 0.47 |
| 1:O:1956:ASP:OD1 | 1:O:1957:THR:N | 2.47 | 0.47 |
| 1:O:2232:LEU:HB2 | 1:O:2274:LEU:HD21 | 1.95 | 0.47 |
| 1:P:221:ARG:O | 1:P:225:ILE:HG12 | 2.14 | 0.47 |
| 1:P:378:LYS:NZ | 1:P:383:ASP:H | 2.12 | 0.47 |
| 1:P:1500:ASN:OD1 | 1:P:1501:ASP:N | 2.47 | 0.47 |
| 1:P:1547:LEU:O | 1:P:1550:GLN:HG3 | 2.14 | 0.47 |
| 1:P:1795:ASN:HD21 | 1:P:1797:TRP:HB2 | 1.79 | 0.47 |
| 1:P:2945:GLN:HG3 | 1:P:3035:TYR:HE1 | 1.79 | 0.47 |
| 1:P:3133:GLN:HB3 | 1:P:3138:ARG:HB2 | 1.95 | 0.47 |
| 1:Q:855:THR:O | 1:Q:858:GLN:HG2 | 2.13 | 0.47 |
| 1:Q:1301:PHE:CD1 | 1:Q:1302:PRO:HA | 2.49 | 0.47 |
| 1:R:1324:HIS:HA | 1:R:1519:VAL:HG11 | 1.95 | 0.47 |
| 1:R:2028:ARG:CZ | 1:R:2028:ARG:HB2 | 2.44 | 0.47 |
| 1:R:3122:ILE:HG13 | 1:R:3125:ILE:HD11 | 1.96 | 0.47 |
| 1:S:16:VAL:HG21 | 1:S:105:ARG:HH12 | 1.79 | 0.47 |
| 1:S:2095:GLU:OE1 | 1:S:2096:ILE:N | 2.47 | 0.47 |
| 1:T:187:HIS:HD2 | 1:T:349:PHE:HB2 | 1.78 | 0.47 |
| 1:T:1990:ILE:O | 1:T:1991:LYS:HG2 | 2.13 | 0.47 |
| 1:T:2991:LEU:HA | 1:T:2994:GLN:HE21 | 1.78 | 0.47 |
| 1:A:493:MET:SD | 1:A:670:MET:HE3 | 2.54 | 0.47 |
| 1:A:891:CYS:HB3 | 1:A:900:PHE:O | 2.13 | 0.47 |
| 1:A:1557:PHE:HB3 | 1:A:1611:LYS:HD2 | 1.97 | 0.47 |
| 1:A:3220:SER:OG | 1:A:3221:GLY:N | 2.46 | 0.47 |
| 1:B:96:TRP:CZ3 | 1:B:218:ASN:HB3 | 2.48 | 0.47 |
| 1:B:1186:ASP:H | 1:B:1189:GLU:HB2 | 1.79 | 0.47 |
| 1:B:3127:GLN:HA | 1:B:3130:GLN:HG3 | 1.96 | 0.47 |
| 1:C:613:PRO:HB2 | 1:C:640:HIS:HE1 | 1.79 | 0.47 |
| 1:C:1013:THR:HG22 | 1:C:1196:ARG:HD2 | 1.95 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:1428:ILE:HG13 | 1:C:1610:TYR:CE1 | 2.49 | 0.47 |
| 1:C:1579:THR:OG1 | 1:C:1584:ARG:NE | 2.45 | 0.47 |
| 1:C:2399:LEU:HB3 | 1:C:2436:TRP:HH2 | 1.80 | 0.47 |
| 1:C:2508:VAL:O | 1:C:2515:LYS:NZ | 2.47 | 0.47 |
| 1:C:2990:LEU:HA | 1:C:2993:VAL:HG12 | 1.96 | 0.47 |
| 1:D:166:LEU:HA | 1:D:169:LEU:HG | 1.97 | 0.47 |
| 1:D:859:VAL:O | 1:D:862:LEU:HG | 2.13 | 0.47 |
| 1:D:1011:PHE:HA | 1:D:1063:TRP:CH2 | 2.49 | 0.47 |
| 1:D:1301:PHE:CD1 | 1:D:1302:PRO:HA | 2.49 | 0.47 |
| 1:D:2552:GLY:O | 1:D:2555:GLY:N | 2.47 | 0.47 |
| 1:E:2256:ASP:OD2 | 1:E:2259:ASP:N | 2.46 | 0.47 |
| 1:F:71:ARG:O | 1:F:75:VAL:HG23 | 2.14 | 0.47 |
| 1:F:695:ARG:HE | 1:F:696:PRO:HD2 | 1.78 | 0.47 |
| 1:F:991:LYS:HB3 | 1:F:994:ARG:HE | 1.79 | 0.47 |
| 1:F:1883:LEU:O | 1:F:1886:SER:OG | 2.29 | 0.47 |
| 1:G:628:LEU:HA | 1:G:631:SER:HB3 | 1.95 | 0.47 |
| 1:G:794:ASN:OD1 | 1:G:795:LYS:N | 2.47 | 0.47 |
| 1:G:2994:GLN:OE1 | 1:G:3165:ASN:ND2 | 2.40 | 0.47 |
| 1:H:569:GLN:HB3 | 1:H:619:GLY:HA3 | 1.96 | 0.47 |
| 1:H:855:THR:O | 1:H:859:VAL:HG23 | 2.13 | 0.47 |
| 1:H:1614:ILE:HG22 | 1:H:1614:ILE:O | 2.14 | 0.47 |
| 1:H:1785:ARG:HH12 | 1:H:1790:ASP:HA | 1.79 | 0.47 |
| 1:H:2126:LEU:HD21 | 1:H:2165:VAL:HG12 | 1.95 | 0.47 |
| 1:H:2162:THR:O | 1:H:2165:VAL:HG22 | 2.15 | 0.47 |
| 1:H:2169:LEU:C | 1:H:2174:SER:HB3 | 2.38 | 0.47 |
| 1:H:2371:LYS:HD3 | 1:H:2376:ASN:HA | 1.96 | 0.47 |
| 1:H:3128:ILE:HG12 | 1:H:3190:LEU:HD13 | 1.96 | 0.47 |
| 1:I:989:LYS:HD2 | 1:I:989:LYS:HA | 1.66 | 0.47 |
| 1:I:1466:ARG:HA | 1:I:1530:TYR:CE2 | 2.49 | 0.47 |
| 1:I:1914:GLU:OE1 | 1:J:1655:LEU:HG | 2.14 | 0.47 |
| 1:I:2800:ASP:OD1 | 1:I:2801:ARG:N | 2.47 | 0.47 |
| 1:I:3304:VAL:HG23 | 1:I:3317:ILE:HB | 1.96 | 0.47 |
| 1:J:11:LEU:HD11 | 1:J:92:PRO:HG3 | 1.96 | 0.47 |
| 1:J:711:ASP:OD1 | 1:J:711:ASP:N | 2.45 | 0.47 |
| 1:J:1405:TYR:CD2 | 1:J:1406:LEU:HD22 | 2.49 | 0.47 |
| 1:J:1726:ASN:OD1 | 1:J:1727:GLN:N | 2.46 | 0.47 |
| 1:J:1840:GLN:N | 1:J:1840:GLN:OE1 | 2.47 | 0.47 |
| 1:J:1905:ASP:HB3 | 1:J:1908:GLU:HB2 | 1.96 | 0.47 |
| 1:J:2408:VAL:HG22 | 1:J:2473:ILE:HG22 | 1.95 | 0.47 |
| 1:J:3129:TRP:O | 1:J:3133:GLN:HG2 | 2.14 | 0.47 |
| 1:K:1220:LYS:NZ | 1:K:1222:SER:HB2 | 2.28 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:K:2675:GLU:OE1 | 1:K:2675:GLU:N | 2.34 | 0.47 |
| 1:L:81:LEU:HD12 | 1:L:86:LEU:HD13 | 1.96 | 0.47 |
| 1:L:227:GLN:HG3 | 1:L:237:TYR:HB2 | 1.96 | 0.47 |
| 1:L:1837:ALA:HA | 1:L:1849:GLN:HE21 | 1.78 | 0.47 |
| 1:L:2558:LYS:HD2 | 1:L:2563:THR:HA | 1.95 | 0.47 |
| 1:L:2672:VAL:HG22 | 1:L:2851:PHE:HD1 | 1.79 | 0.47 |
| 1:L:3124:ARG:HD2 | 1:L:3187:PHE:CD2 | 2.48 | 0.47 |
| 1:M:293:ILE:H | 1:M:293:ILE:HD12 | 1.79 | 0.47 |
| 1:M:750:LEU:HG | 1:M:768:LEU:O | 2.14 | 0.47 |
| 1:M:850:ASP:OD1 | 1:M:852:SER:OG | 2.32 | 0.47 |
| 1:M:954:THR:HG22 | 1:M:965:PRO:HA | 1.95 | 0.47 |
| 1:M:1495:PRO:HA | 1:M:1516:PRO:HD3 | 1.95 | 0.47 |
| 1:M:1739:PHE:HB3 | 1:M:1740:PRO:HD3 | 1.96 | 0.47 |
| 1:M:2073:VAL:HG23 | 1:N:1489:LEU:H | 1.78 | 0.47 |
| 1:M:2963:PRO:HG3 | 1:M:3039:PHE:CD2 | 2.49 | 0.47 |
| 1:M:3045:THR:N | 1:M:3101:TYR:O | 2.43 | 0.47 |
| 1:N:532:VAL:HG13 | 1:N:537:SER:HB3 | 1.96 | 0.47 |
| 1:N:673:GLU:C | 1:N:695:ARG:HH12 | 2.21 | 0.47 |
| 1:N:866:LEU:O | 1:N:869:LEU:HG | 2.14 | 0.47 |
| 1:N:3079:ASP:OD1 | 1:N:3260:ARG:NH1 | 2.47 | 0.47 |
| 1:O:1328:LEU:HD21 | 1:O:1519:VAL:HG22 | 1.95 | 0.47 |
| 1:O:3357:TYR:HB3 | 1:P:3329:LYS:HD3 | 1.96 | 0.47 |
| 1:P:914:HIS:O | 1:P:917:LEU:HG | 2.14 | 0.47 |
| 1:P:1048:ILE:HA | 1:P:1051:LEU:HG | 1.96 | 0.47 |
| 1:P:2655:TYR:CE2 | 1:P:2659:LEU:HD11 | 2.49 | 0.47 |
| 1:Q:311:ALA:HB2 | 1:Q:369:ILE:HD13 | 1.96 | 0.47 |
| 1:Q:2331:SER:HA | 1:Q:2355:LYS:HZ1 | 1.78 | 0.47 |
| 1:R:378:LYS:NZ | 1:R:383:ASP:H | 2.12 | 0.47 |
| 1:R:848:ARG:HD3 | 1:R:934:LEU:HB3 | 1.96 | 0.47 |
| 1:R:1167:GLU:HA | 1:R:1177:PRO:HA | 1.96 | 0.47 |
| 1:R:1248:GLU:HB3 | 1:R:1251:LYS:HE2 | 1.96 | 0.47 |
| 1:R:1277:GLU:HA | 1:R:1280:LYS:HG2 | 1.96 | 0.47 |
| 1:R:1365:ALA:HA | 1:R:1378:ASN:HB3 | 1.95 | 0.47 |
| 1:R:1550:GLN:HA | 1:R:1553:GLN:HE22 | 1.79 | 0.47 |
| 1:R:3183:PHE:HB2 | 1:R:3185:TYR:CE1 | 2.49 | 0.47 |
| 1:S:299:LEU:O | 1:S:302:GLN:HG3 | 2.15 | 0.47 |
| 1:S:613:PRO:HB2 | 1:S:640:HIS:NE2 | 2.29 | 0.47 |
| 1:S:1278:SER:O | 1:S:1281:SER:OG | 2.30 | 0.47 |
| 1:S:1989:GLY:N | 1:S:2024:TRP:O | 2.47 | 0.47 |
| 1:S:2111:LEU:HD12 | 1:S:2211:PRO:HG2 | 1.97 | 0.47 |
| 1:S:2266:VAL:HG21 | 1:S:2442:TYR:CD1 | 2.48 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:S:2977:CYS:SG | 1:S:3106:LEU:HD11 | 2.54 | 0.47 |
| 1:T:135:MET:SD | 1:T:137:VAL:HG22 | 2.55 | 0.47 |
| 1:T:501:ARG:NH2 | 1:T:699:ILE:O | 2.40 | 0.47 |
| 1:T:2414:GLN:HA | 1:T:2467:PHE:HA | 1.95 | 0.47 |
| 1:A:590:MET:HE2 | 1:A:590:MET:HA | 1.97 | 0.47 |
| 1:A:1579:THR:HG21 | 1:D:339:HIS:HA | 1.95 | 0.47 |
| 1:A:1956:ASP:OD1 | 1:A:1957:THR:N | 2.47 | 0.47 |
| 1:A:2059:ASN:ND2 | 1:A:2061:SER:OG | 2.47 | 0.47 |
| 1:B:178:GLU:O | 1:B:182:GLU:HG2 | 2.14 | 0.47 |
| 1:B:526:THR:HG1 | 1:B:527:ARG:NH1 | 2.11 | 0.47 |
| 1:B:1225:ASP:OD1 | 1:B:1226:LEU:N | 2.37 | 0.47 |
| 1:B:1428:ILE:HA | 1:B:1431:ASN:HD21 | 1.78 | 0.47 |
| 1:B:2269:ASN:HD21 | 1:B:2428:LEU:N | 2.11 | 0.47 |
| 1:B:2820:ASP:HB3 | 1:B:2873:ASP:OD1 | 2.15 | 0.47 |
| 1:B:3119:HIS:HA | 1:B:3122:ILE:HG22 | 1.97 | 0.47 |
| 1:C:1587:ASN:OD1 | 1:F:337:GLN:N | 2.47 | 0.47 |
| 1:C:1752:ASP:OD1 | 1:C:1753:ALA:N | 2.48 | 0.47 |
| 1:C:2232:LEU:HD13 | 1:C:2274:LEU:HD21 | 1.96 | 0.47 |
| 1:C:2714:ARG:NH2 | 1:C:2778:ASP:O | 2.46 | 0.47 |
| 1:C:3231:LYS:HE3 | 1:C:3241:ASP:HB2 | 1.95 | 0.47 |
| 1:C:3240:VAL:HG21 | 1:C:3272:LYS:HZ3 | 1.78 | 0.47 |
| 1:D:495:THR:HG22 | 1:D:495:THR:O | 2.13 | 0.47 |
| 1:D:536:ALA:HA | 1:D:552:ASN:HD21 | 1.80 | 0.47 |
| 1:D:756:LYS:HD3 | 1:D:762:SER:HB2 | 1.96 | 0.47 |
| 1:D:1677:ARG:HD2 | 1:D:1763:ILE:O | 2.13 | 0.47 |
| 1:D:2018:GLY:H | 1:D:2021:GLU:CD | 2.21 | 0.47 |
| 1:D:2574:PHE:O | 1:D:2578:HIS:ND1 | 2.39 | 0.47 |
| 1:D:2923:ARG:HE | 1:D:2924:TYR:H | 1.62 | 0.47 |
| 1:D:2954:GLU:CD | 1:D:2954:GLU:H | 2.22 | 0.47 |
| 1:E:2093:ARG:NH1 | 1:E:2177:ALA:O | 2.47 | 0.47 |
| 1:E:3071:THR:HG21 | 1:E:3087:LEU:HD11 | 1.96 | 0.47 |
| 1:F:225:ILE:O | 1:F:229:LEU:HG | 2.14 | 0.47 |
| 1:F:735:ARG:HB3 | 1:F:831:GLU:HB3 | 1.96 | 0.47 |
| 1:F:849:SER:OG | 1:F:850:ASP:N | 2.47 | 0.47 |
| 1:F:1274:GLY:O | 1:F:1277:GLU:HG3 | 2.13 | 0.47 |
| 1:G:50:LYS:HG3 | 1:G:52:ASP:H | 1.79 | 0.47 |
| 1:G:231:LYS:HE3 | 1:G:237:TYR:CE1 | 2.49 | 0.47 |
| 1:G:580:TYR:CG | 1:G:958:PRO:HG2 | 2.49 | 0.47 |
| 1:G:1687:GLU:HB2 | 1:G:1760:LEU:HD11 | 1.96 | 0.47 |
| 1:G:1858:HIS:NE2 | 1:G:1885:HIS:HE1 | 2.11 | 0.47 |
| 1:G:2091:ARG:HA | 1:G:2093:ARG:HH21 | 1.79 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:G:2353:LEU:HD22 | 1:G:2355:LYS:HZ3 | 1.79 | 0.47 |
| 1:G:2404:THR:HA | 1:G:2429:GLY:O | 2.14 | 0.47 |
| 1:G:2800:ASP:OD1 | 1:G:2801:ARG:N | 2.48 | 0.47 |
| 1:H:1978:LYS:HD2 | 1:H:2078:LYS:HZ1 | 1.79 | 0.47 |
| 1:I:293:ILE:H | 1:I:293:ILE:HD12 | 1.78 | 0.47 |
| 1:I:436:ASP:HB3 | 1:I:522:TYR:CE2 | 2.49 | 0.47 |
| 1:I:651:TRP:CZ3 | 1:I:655:GLN:HG3 | 2.50 | 0.47 |
| 1:I:1057:ASP:OD1 | 1:I:1123:TYR:OH | 2.27 | 0.47 |
| 1:I:1736:MET:HB3 | 1:I:1915:LEU:HD22 | 1.96 | 0.47 |
| 1:I:2111:LEU:HD12 | 1:I:2211:PRO:HG2 | 1.97 | 0.47 |
| 1:I:2668:CYS:HB2 | 1:I:2735:CYS:HB2 | 1.60 | 0.47 |
| 1:I:2755:ASP:OD1 | 1:I:2756:PHE:N | 2.45 | 0.47 |
| 1:I:2939:ASN:O | 1:I:2943:LYS:HE2 | 2.14 | 0.47 |
| 1:J:614:HIS:HA | 1:J:625:LEU:HG | 1.95 | 0.47 |
| 1:J:859:VAL:O | 1:J:862:LEU:HG | 2.15 | 0.47 |
| 1:J:887:GLN:NE2 | 1:J:889:ASN:HB2 | 2.29 | 0.47 |
| 1:J:1350:ASP:OD1 | 1:J:1352:THR:OG1 | 2.25 | 0.47 |
| 1:J:2558:LYS:HD2 | 1:J:2563:THR:HA | 1.96 | 0.47 |
| 1:J:2671:GLU:HA | 1:J:2674:TYR:HB3 | 1.95 | 0.47 |
| 1:K:30:LYS:N | 1:K:30:LYS:HD2 | 2.28 | 0.47 |
| 1:K:580:TYR:HE1 | 1:K:856:ARG:HD2 | 1.78 | 0.47 |
| 1:K:628:LEU:HA | 1:K:631:SER:HB3 | 1.95 | 0.47 |
| 1:K:1916:MET:N | 1:K:1916:MET:HE2 | 2.29 | 0.47 |
| 1:K:2604:THR:HA | 1:K:2654:PHE:CE2 | 2.49 | 0.47 |
| 1:K:2966:CYS:O | 1:K:2974:TYR:N | 2.42 | 0.47 |
| 1:L:337:GLN:HE21 | 1:S:1575:ILE:C | 2.21 | 0.47 |
| 1:L:2614:LEU:HD13 | 1:L:2704:ILE:HD11 | 1.97 | 0.47 |
| 1:M:2329:TYR:OH | 1:N:1238:LYS:HD3 | 2.14 | 0.47 |
| 1:N:143:ARG:NH2 | 1:N:209:ASP:OD2 | 2.47 | 0.47 |
| 1:N:197:ASP:N | 1:N:197:ASP:OD1 | 2.48 | 0.47 |
| 1:N:198:HIS:HD1 | 1:N:205:TRP:CD1 | 2.31 | 0.47 |
| 1:N:1892:TYR:O | 1:N:1896:GLN:HG2 | 2.15 | 0.47 |
| 1:O:601:ASP:HB3 | 1:O:783:ARG:HD2 | 1.96 | 0.47 |
| 1:O:1858:HIS:NE2 | 1:O:1884:HIS:HE1 | 2.12 | 0.47 |
| 1:O:2439:ASP:CG | 1:O:2440:ARG:HE | 2.22 | 0.47 |
| 1:O:2669:ASN:HA | 1:O:2672:VAL:HG12 | 1.96 | 0.47 |
| 1:P:1015:GLU:O | 1:P:1018:TYR:HB3 | 2.14 | 0.47 |
| 1:P:1167:GLU:HA | 1:P:1177:PRO:HA | 1.95 | 0.47 |
| 1:P:1557:PHE:CD2 | 1:P:1611:LYS:HB3 | 2.50 | 0.47 |
| 1:P:1777:ALA:HA | 1:P:1780:ASN:HB3 | 1.95 | 0.47 |
| 1:P:2326:ALA:HB1 | 1:P:2329:TYR:HB2 | 1.96 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:P:2628:ALA:O | 1:P:2631:ASN:ND2 | 2.47 | 0.47 |
| 1:P:3363:CYS:HB2 | 1:P:3396:CYS:HB3 | 1.87 | 0.47 |
| 1:Q:170:GLU:OE2 | 1:Q:304:ARG:HD2 | 2.14 | 0.47 |
| 1:Q:293:ILE:H | 1:Q:293:ILE:HD12 | 1.79 | 0.47 |
| 1:Q:601:ASP:O | 1:Q:604:VAL:HG22 | 2.15 | 0.47 |
| 1:Q:792:ALA:HA | 1:Q:795:LYS:HE3 | 1.95 | 0.47 |
| 1:Q:913:TRP:CD1 | 1:Q:1088:LEU:HD21 | 2.48 | 0.47 |
| 1:Q:2917:LYS:HD3 | 1:Q:2917:LYS:N | 2.28 | 0.47 |
| 1:Q:3350:ASN:O | 1:Q:3391:SER:N | 2.46 | 0.47 |
| 1:R:580:TYR:CG | 1:R:958:PRO:HG2 | 2.50 | 0.47 |
| 1:R:600:CYS:HB3 | 1:R:783:ARG:HH12 | 1.79 | 0.47 |
| 1:R:1153:PHE:HB2 | 1:R:1198:PHE:HD2 | 1.79 | 0.47 |
| 1:S:870:GLU:HA | 1:S:878:PHE:HB3 | 1.95 | 0.47 |
| 1:S:1388:THR:OG1 | 1:S:1390:LYS:NZ | 2.47 | 0.47 |
| 1:S:2157:TRP:CE3 | 1:S:2158:HIS:HD2 | 2.32 | 0.47 |
| 1:S:2878:ALA:N | 1:S:2882:THR:O | 2.44 | 0.47 |
| 1:S:3364:SER:HB2 | 1:T:3255:PRO:HG2 | 1.96 | 0.47 |
| 1:T:32:VAL:HA | 1:T:37:ASN:HD21 | 1.79 | 0.47 |
| 1:T:799:LYS:N | 1:T:802:ASP:OD2 | 2.47 | 0.47 |
| 1:T:944:THR:HA | 1:T:987:PHE:CD1 | 2.48 | 0.47 |
| 1:T:1088:LEU:HD22 | 1:T:1109:PRO:HG3 | 1.96 | 0.47 |
| 1:T:2343:ASN:OD1 | 1:T:2344:GLU:N | 2.47 | 0.47 |
| 1:T:2433:GLU:N | 1:T:2433:GLU:OE1 | 2.47 | 0.47 |
| 1:A:738:VAL:HG23 | 1:A:789:ILE:HG21 | 1.96 | 0.47 |
| 1:A:984:ASP:OD1 | 1:A:984:ASP:N | 2.47 | 0.47 |
| 1:A:2315:ARG:CZ | 1:A:2377:LEU:HB3 | 2.44 | 0.47 |
| 1:A:2465:ALA:HB2 | 1:B:1085:ARG:HD2 | 1.96 | 0.47 |
| 1:A:2796:ARG:HH22 | 1:A:2801:ARG:HE | 1.62 | 0.47 |
| 1:A:3113:PRO:HA | 1:A:3116:MET:HG3 | 1.95 | 0.47 |
| 1:B:5:ARG:HG3 | 1:B:283:TYR:HA | 1.96 | 0.47 |
| 1:B:924:ALA:O | 1:B:928:LYS:HG2 | 2.15 | 0.47 |
| 1:B:1011:PHE:HA | 1:B:1063:TRP:CH2 | 2.49 | 0.47 |
| 1:B:1223:VAL:O | 1:B:1230:LYS:NZ | 2.39 | 0.47 |
| 1:B:2898:PRO:HG2 | 1:C:2913:PRO:HB2 | 1.97 | 0.47 |
| 1:C:646:ARG:HA | 1:C:710:TYR:HE2 | 1.80 | 0.47 |
| 1:C:889:ASN:HB3 | 1:C:900:PHE:O | 2.13 | 0.47 |
| 1:C:2046:ASP:HB2 | 1:D:1493:ARG:NH1 | 2.28 | 0.47 |
| 1:D:627:THR:OG1 | 1:D:628:LEU:N | 2.48 | 0.47 |
| 1:D:1153:PHE:C | 1:D:1154:MET:HE2 | 2.38 | 0.47 |
| 1:D:1277:GLU:HA | 1:D:1280:LYS:HG2 | 1.97 | 0.47 |
| 1:D:1710:LEU:HD13 | 1:D:1750:PHE:HE1 | 1.80 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:D:1941:PRO:O | 1:D:1944:VAL:HG22 | 2.14 | 0.47 |
| 1:D:2980:GLY:HA3 | 1:D:3256:TRP:CZ3 | 2.49 | 0.47 |
| 1:E:253:PRO:O | 1:E:256:ARG:HG2 | 2.15 | 0.47 |
| 1:E:277:ARG:NH1 | 1:E:282:VAL:HG21 | 2.29 | 0.47 |
| 1:E:1301:PHE:CD1 | 1:E:1302:PRO:HA | 2.50 | 0.47 |
| 1:E:2059:ASN:ND2 | 1:E:2061:SER:OG | 2.47 | 0.47 |
| 1:E:2961:GLY:HA2 | 1:E:3106:LEU:HD23 | 1.96 | 0.47 |
| 1:E:3148:ARG:HE | 1:F:3386:TYR:HE2 | 1.62 | 0.47 |
| 1:F:554:PHE:O | 1:F:568:ARG:NH2 | 2.47 | 0.47 |
| 1:F:2995:PHE:HB3 | 1:F:3008:ILE:HD11 | 1.97 | 0.47 |
| 1:G:284:ASP:OD2 | 1:G:285:ASP:N | 2.48 | 0.47 |
| 1:H:81:LEU:HB3 | 1:H:86:LEU:HB2 | 1.96 | 0.47 |
| 1:H:327:LYS:HG3 | 1:H:343:GLU:O | 2.15 | 0.47 |
| 1:H:1080:ALA:HB1 | 1:H:1083:SER:OG | 2.14 | 0.47 |
| 1:H:2235:LEU:HD23 | 1:H:2235:LEU:H | 1.79 | 0.47 |
| 1:H:2722:LEU:O | 1:H:2726:ARG:HG2 | 2.14 | 0.47 |
| 1:H:2867:ASP:HA | 1:I:2741:ARG:CZ | 2.44 | 0.47 |
| 1:I:348:ILE:HD11 | 1:I:367:PHE:CD2 | 2.49 | 0.47 |
| 1:I:1026:HIS:HD2 | 1:I:1184:LEU:HD11 | 1.79 | 0.47 |
| 1:I:2947:ASP:OD2 | 1:I:3002:LYS:NZ | 2.46 | 0.47 |
| 1:I:3399:GLY:HA2 | 1:I:3401:ARG:HH21 | 1.79 | 0.47 |
| 1:J:1641:ASN:HD22 | 3:EA:1:NAG:H83 | 1.80 | 0.47 |
| 1:J:2271:ILE:HA | 1:J:2274:LEU:HB2 | 1.97 | 0.47 |
| 1:J:2520:LEU:HD22 | 1:J:2524:GLU:HG3 | 1.95 | 0.47 |
| 1:J:3062:ASP:OD2 | 1:J:3065:PHE:N | 2.35 | 0.47 |
| 1:K:44:GLU:N | 1:K:204:GLU:O | 2.47 | 0.47 |
| 1:K:1025:ILE:HD12 | 1:K:1028:LEU:HD23 | 1.96 | 0.47 |
| 1:K:1083:SER:O | 1:K:1086:LYS:HG2 | 2.15 | 0.47 |
| 1:K:1219:VAL:HG23 | 1:K:1239:VAL:HG13 | 1.96 | 0.47 |
| 1:K:2110:ALA:HB1 | 1:K:2172:HIS:HB3 | 1.95 | 0.47 |
| 1:K:3203:ILE:HA | 1:K:3206:ASN:HB2 | 1.96 | 0.47 |
| 1:L:408:GLY:HA3 | 1:L:669:THR:HG21 | 1.96 | 0.47 |
| 1:L:924:ALA:O | 1:L:928:LYS:HG2 | 2.14 | 0.47 |
| 1:L:1205:ILE:HD12 | 1:L:1208:LYS:HE3 | 1.97 | 0.47 |
| 1:L:1364:GLU:OE2 | 1:L:1365:ALA:N | 2.47 | 0.47 |
| 1:L:1785:ARG:HH12 | 1:L:1790:ASP:HA | 1.79 | 0.47 |
| 1:L:2343:ASN:HD22 | 1:L:2349:ARG:HH21 | 1.63 | 0.47 |
| 1:L:2379:GLU:OE2 | 1:L:2380:LEU:HD12 | 2.14 | 0.47 |
| 1:L:3373:TYR:HE2 | 1:L:3381:LEU:HD21 | 1.78 | 0.47 |
| 1:M:757:PRO:HB3 | 1:M:798:LEU:HD11 | 1.96 | 0.47 |
| 1:M:915:ARG:HD2 | 1:M:1060:TRP:HZ3 | 1.78 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:M:926:ARG:HA | 1:M:926:ARG:HD2 | 1.72 | 0.47 |
| 1:M:937:TRP:CD1 | 1:M:938:ASP:H | 2.31 | 0.47 |
| 1:M:1221:TYR:HH | 1:M:1236:PHE:H | 1.61 | 0.47 |
| 1:M:1815:ARG:HA | 1:M:1818:LEU:HG | 1.96 | 0.47 |
| 1:M:2864:LEU:HD21 | 1:M:2870:TYR:CD1 | 2.50 | 0.47 |
| 1:N:552:ASN:HD21 | 1:N:554:PHE:HB2 | 1.78 | 0.47 |
| 1:N:1726:ASN:OD1 | 1:N:1727:GLN:N | 2.47 | 0.47 |
| 1:N:1745:LEU:HD23 | 1:N:1923:PHE:HD1 | 1.80 | 0.47 |
| 1:N:1847:GLU:H | 1:N:1847:GLU:CD | 2.23 | 0.47 |
| 1:N:3114:PHE:HA | 1:N:3117:ILE:HG12 | 1.95 | 0.47 |
| 1:O:752:ILE:O | 1:O:808:LEU:HA | 2.15 | 0.47 |
| 1:O:973:VAL:HG11 | 1:O:1045:TYR:CG | 2.49 | 0.47 |
| 1:O:1301:PHE:CD1 | 1:O:1302:PRO:HA | 2.49 | 0.47 |
| 1:O:2226:ARG:O | 1:R:113:LYS:NZ | 2.43 | 0.47 |
| 1:O:2313:GLN:OE1 | 1:O:2316:ARG:NH1 | 2.48 | 0.47 |
| 1:P:938:ASP:OD1 | 1:P:1055:ASN:ND2 | 2.45 | 0.47 |
| 1:P:1011:PHE:HA | 1:P:1063:TRP:CH2 | 2.48 | 0.47 |
| 1:P:1086:LYS:HZ3 | 1:P:1087:PRO:HD2 | 1.79 | 0.47 |
| 1:P:1205:ILE:HD12 | 1:P:1208:LYS:HE3 | 1.97 | 0.47 |
| 1:P:1332:GLN:OE1 | 1:P:1505:ASN:ND2 | 2.43 | 0.47 |
| 1:P:2262:VAL:HG23 | 1:P:2438:PHE:CD1 | 2.50 | 0.47 |
| 1:P:2326:ALA:O | 1:P:2330:MET:HG2 | 2.15 | 0.47 |
| 1:P:2722:LEU:HD13 | 1:P:2726:ARG:HH21 | 1.79 | 0.47 |
| 1:Q:984:ASP:OD1 | 1:Q:984:ASP:N | 2.45 | 0.47 |
| 1:Q:1268:LEU:HD12 | 1:Q:1361:LEU:HD13 | 1.95 | 0.47 |
| 1:Q:2027:ASP:OD1 | 1:Q:2028:ARG:N | 2.48 | 0.47 |
| 1:Q:2604:THR:HA | 1:Q:2654:PHE:CE1 | 2.48 | 0.47 |
| 1:R:5:ARG:HH12 | 1:R:281:TYR:HD2 | 1.62 | 0.47 |
| 1:R:737:PHE:CG | 1:R:786:LYS:HB3 | 2.50 | 0.47 |
| 1:R:2821:LEU:HD21 | 1:R:2864:LEU:HD12 | 1.97 | 0.47 |
| 1:S:202:THR:OG1 | 1:S:204:GLU:OE1 | 2.33 | 0.47 |
| 1:S:1266:ARG:HG2 | 1:S:1531:ASP:HB3 | 1.97 | 0.47 |
| 1:S:1366:SER:HB3 | 1:S:1376:GLU:O | 2.14 | 0.47 |
| 1:S:1809:VAL:HG23 | 1:S:1868:SER:HA | 1.97 | 0.47 |
| 1:S:2639:ARG:HG2 | 1:S:2684:TRP:HZ3 | 1.77 | 0.47 |
| 1:S:2669:ASN:OD1 | 1:S:2849:ARG:NE | 2.47 | 0.47 |
| 1:T:444:GLU:HA | 1:T:447:GLU:HG2 | 1.95 | 0.47 |
| 1:T:1847:GLU:HA | 1:T:1850:PHE:HB3 | 1.95 | 0.47 |
| 1:T:1978:LYS:NZ | 1:T:1979:SER:O | 2.46 | 0.47 |
| 1:A:28:ASP:OD1 | 1:A:29:ASP:N | 2.46 | 0.47 |
| 1:A:888:PRO:HG2 | 1:A:890:TRP:CZ2 | 2.49 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:1809:VAL:HG23 | 1:A:1868:SER:HA | 1.96 | 0.47 |
| 1:A:2414:GLN:O | 1:A:2416:ASN:N | 2.47 | 0.47 |
| 1:B:1274:GLY:O | 1:B:1277:GLU:HG3 | 2.15 | 0.47 |
| 1:B:3153:PRO:HB2 | 1:B:3158:ASN:HB3 | 1.96 | 0.47 |
| 1:C:722:GLN:N | 1:C:722:GLN:OE1 | 2.46 | 0.47 |
| 1:C:750:LEU:HD21 | 1:C:767:LYS:NZ | 2.30 | 0.47 |
| 1:C:3214:TYR:CD1 | 1:C:3265:ASP:HA | 2.49 | 0.47 |
| 1:D:630:TYR:HA | 1:D:633:PHE:HD2 | 1.80 | 0.47 |
| 1:D:855:THR:O | 1:D:859:VAL:HG23 | 2.14 | 0.47 |
| 1:E:2163:LEU:HD21 | 1:E:2347:PHE:HE2 | 1.79 | 0.47 |
| 1:E:2621:PRO:HA | 1:E:2624:HIS:CE1 | 2.49 | 0.47 |
| 1:E:2849:ARG:HA | 1:E:2849:ARG:HH11 | 1.78 | 0.47 |
| 1:E:2988:HIS:HD2 | 1:E:3119:HIS:ND1 | 2.11 | 0.47 |
| 1:F:217:SER:O | 1:F:283:TYR:OH | 2.21 | 0.47 |
| 1:F:357:MET:SD | 1:F:358:PRO:HD2 | 2.54 | 0.47 |
| 1:F:689:LYS:HG3 | 1:F:690:THR:N | 2.30 | 0.47 |
| 1:F:1221:TYR:OH | 1:F:1237:GLY:N | 2.48 | 0.47 |
| 1:F:1548:LYS:HA | 1:F:1548:LYS:HD3 | 1.71 | 0.47 |
| 1:F:3287:LEU:HD21 | 1:F:3299:LEU:HD21 | 1.95 | 0.47 |
| 1:G:44:GLU:N | 1:G:204:GLU:O | 2.46 | 0.47 |
| 1:G:2105:MET:HA | 1:G:2108:LYS:HG2 | 1.97 | 0.47 |
| 1:H:57:ALA:H | 1:H:355:ASN:HB3 | 1.79 | 0.47 |
| 1:H:255:ASP:OD1 | 1:H:255:ASP:N | 2.44 | 0.47 |
| 1:H:869:LEU:HB3 | 1:H:928:LYS:HE3 | 1.96 | 0.47 |
| 1:H:2258:CYS:O | 1:H:2261:GLU:HG3 | 2.15 | 0.47 |
| 1:H:2664:GLN:HG3 | 1:H:2669:ASN:OD1 | 2.13 | 0.47 |
| 1:I:299:LEU:O | 1:I:302:GLN:HG3 | 2.15 | 0.47 |
| 1:I:436:ASP:OD1 | 1:I:436:ASP:N | 2.47 | 0.47 |
| 1:I:844:GLU:HB2 | 1:I:846:HIS:CE1 | 2.49 | 0.47 |
| 1:I:870:GLU:HA | 1:I:878:PHE:HB3 | 1.95 | 0.47 |
| 1:I:881:ILE:HA | 1:I:884:PHE:CD2 | 2.49 | 0.47 |
| 1:I:2822:CYS:HA | 1:I:2828:CYS:HB3 | 1.96 | 0.47 |
| 1:I:3089:ASN:ND2 | 1:I:3247:ILE:HA | 2.30 | 0.47 |
| 1:J:315:LEU:HB2 | 1:J:361:PHE:CE2 | 2.49 | 0.47 |
| 1:J:1152:GLY:C | 1:J:1153:PHE:HD1 | 2.21 | 0.47 |
| 1:J:1884:HIS:O | 1:J:1887:SER:OG | 2.22 | 0.47 |
| 1:J:3132:LEU:HG | 1:J:3136:ARG:NH1 | 2.29 | 0.47 |
| 1:K:674:LEU:HD22 | 1:K:695:ARG:NH2 | 2.29 | 0.47 |
| 1:K:719:THR:HG21 | 1:K:847:VAL:HG21 | 1.96 | 0.47 |
| 1:L:2343:ASN:HB3 | 1:L:2349:ARG:NH2 | 2.29 | 0.47 |
| 1:M:539:GLU:HA | 1:M:555:PHE:HB2 | 1.96 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:M:989:LYS:HA | 1:M:989:LYS:HD2 | 1.66 | 0.47 |
| 1:M:2791:GLU:O | 1:M:2794:GLU:HG3 | 2.14 | 0.47 |
| 1:N:508:GLU:HA | 1:N:511:LEU:HD12 | 1.96 | 0.47 |
| 1:N:618:GLY:HA3 | 1:N:626:SER:N | 2.29 | 0.47 |
| 1:N:1126:LEU:HD11 | 1:N:1133:ILE:HD11 | 1.95 | 0.47 |
| 1:N:1277:GLU:HA | 1:N:1280:LYS:HG2 | 1.96 | 0.47 |
| 1:N:1294:LYS:O | 1:N:1297:SER:OG | 2.23 | 0.47 |
| 1:N:1550:GLN:HA | 1:N:1553:GLN:HE22 | 1.80 | 0.47 |
| 1:N:1788:VAL:HG12 | 1:N:1789:LEU:HD22 | 1.95 | 0.47 |
| 1:N:3124:ARG:HD2 | 1:N:3187:PHE:CD2 | 2.49 | 0.47 |
| 1:N:3222:ILE:HB | 1:N:3224:VAL:HG22 | 1.96 | 0.47 |
| 1:N:3392:ASN:HB3 | 1:N:3395:ARG:HG2 | 1.95 | 0.47 |
| 1:O:1986:LEU:HB2 | 1:O:2069:PRO:HG2 | 1.96 | 0.47 |
| 1:O:2315:ARG:NH2 | 1:O:2377:LEU:HD12 | 2.30 | 0.47 |
| 1:O:3203:ILE:HA | 1:O:3206:ASN:HB2 | 1.96 | 0.47 |
| 1:P:47:MET:N | 1:P:47:MET:SD | 2.88 | 0.47 |
| 1:P:842:HIS:NE2 | 1:P:844:GLU:HB2 | 2.30 | 0.47 |
| 1:P:3334:ARG:HA | 1:P:3334:ARG:HD2 | 1.73 | 0.47 |
| 1:Q:327:LYS:HD2 | 1:Q:344:PHE:HA | 1.96 | 0.47 |
| 1:Q:414:LYS:HD2 | 1:Q:414:LYS:HA | 1.71 | 0.47 |
| 1:Q:719:THR:HG21 | 1:Q:847:VAL:HG21 | 1.96 | 0.47 |
| 1:Q:2407:GLU:HB2 | 1:Q:2426:PHE:CE2 | 2.49 | 0.47 |
| 1:R:188:ILE:HD13 | 1:R:215:HIS:NE2 | 2.30 | 0.47 |
| 1:R:409:VAL:HG13 | 1:R:666:CYS:HA | 1.97 | 0.47 |
| 1:R:502:LEU:HA | 1:R:505:VAL:HG12 | 1.97 | 0.47 |
| 1:R:866:LEU:O | 1:R:869:LEU:HG | 2.14 | 0.47 |
| 1:R:1008:GLN:N | 1:R:1008:GLN:OE1 | 2.48 | 0.47 |
| 1:R:1100:ASP:OD2 | 1:R:1103:THR:OG1 | 2.32 | 0.47 |
| 1:S:1365:ALA:HA | 1:S:1381:PHE:CZ | 2.49 | 0.47 |
| 1:S:1446:SER:OG | 1:S:1447:SER:N | 2.48 | 0.47 |
| 1:S:1628:ALA:HB1 | 1:S:1631:ILE:HD13 | 1.95 | 0.47 |
| 1:S:1684:THR:HB | 1:S:1687:GLU:OE1 | 2.13 | 0.47 |
| 1:S:1844:CYS:O | 1:S:1848:VAL:HG13 | 2.14 | 0.47 |
| 1:S:1980:ARG:HE | 1:S:1982:PHE:HZ | 1.62 | 0.47 |
| 1:T:36:GLN:NE2 | 1:T:37:ASN:OD1 | 2.47 | 0.47 |
| 1:T:673:GLU:C | 1:T:695:ARG:HH12 | 2.23 | 0.47 |
| 1:T:934:LEU:HD23 | 1:T:1054:SER:HB3 | 1.96 | 0.47 |
| 1:T:1085:ARG:HD3 | 1:T:1110:PHE:HE2 | 1.78 | 0.47 |
| 1:T:1743:HIS:CD2 | 1:T:1885:HIS:HD2 | 2.32 | 0.47 |
| 1:T:1938:TYR:CE2 | 1:T:1950:HIS:HB3 | 2.49 | 0.47 |
| 3:Z:2:NAG:H4 | 3:Z:3:BMA:H2 | 1.69 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:881:ILE:HA | 1:A:884:PHE:CD2 | 2.43 | 0.47 |
| 1:A:1111:GLU:N | 1:A:1111:GLU:OE1 | 2.47 | 0.47 |
| 1:A:1742:TRP:CD1 | 1:A:1920:LEU:HD12 | 2.43 | 0.47 |
| 1:A:1782:PRO:O | 1:A:1795:ASN:N | 2.39 | 0.47 |
| 1:A:2345:ASN:HD21 | 1:A:2347:PHE:HB3 | 1.80 | 0.47 |
| 1:A:2360:TYR:HA | 1:A:2363:LEU:HB2 | 1.96 | 0.47 |
| 1:B:460:SER:OG | 1:B:462:ASN:OD1 | 2.20 | 0.47 |
| 1:B:922:GLU:HG3 | 1:B:934:LEU:HB2 | 1.96 | 0.47 |
| 1:B:1440:ARG:HD2 | 1:I:1368:PHE:CZ | 2.49 | 0.47 |
| 1:B:1814:LYS:HE2 | 1:B:1817:ARG:HG3 | 1.95 | 0.47 |
| 1:B:1821:ASP:OD1 | 1:B:1821:ASP:N | 2.46 | 0.47 |
| 1:B:2095:GLU:CD | 1:B:2097:SER:H | 2.22 | 0.47 |
| 1:C:2581:PHE:O | 1:C:2584:THR:HG22 | 2.15 | 0.47 |
| 1:C:2724:ARG:NH1 | 1:C:2730:TYR:OH | 2.41 | 0.47 |
| 1:D:8:VAL:HA | 1:D:11:LEU:HD23 | 1.97 | 0.47 |
| 1:D:668:HIS:O | 1:D:671:THR:OG1 | 2.30 | 0.47 |
| 1:D:1351:TRP:HZ3 | 1:D:1463:ASN:HB3 | 1.78 | 0.47 |
| 1:D:1722:TYR:CE2 | 1:D:1724:GLU:HB3 | 2.50 | 0.47 |
| 1:E:1518:ASP:OD1 | 1:E:1525:HIS:ND1 | 2.28 | 0.47 |
| 1:E:2569:HIS:HA | 1:E:2574:PHE:CE2 | 2.49 | 0.47 |
| 1:F:5:ARG:HD2 | 1:F:283:TYR:CE1 | 2.50 | 0.47 |
| 1:F:592:LEU:HD11 | 1:F:737:PHE:CE1 | 2.49 | 0.47 |
| 1:F:917:LEU:O | 1:F:920:GLN:NE2 | 2.43 | 0.47 |
| 1:F:1108:VAL:HG13 | 1:F:1111:GLU:OE1 | 2.15 | 0.47 |
| 1:F:1599:GLU:OE2 | 1:F:1600:THR:OG1 | 2.32 | 0.47 |
| 1:F:2923:ARG:HD3 | 1:F:3008:ILE:C | 2.39 | 0.47 |
| 1:G:348:ILE:HD11 | 1:G:367:PHE:CD2 | 2.49 | 0.47 |
| 1:G:1539:THR:H | 1:G:1542:GLN:HE22 | 1.62 | 0.47 |
| 1:G:2399:LEU:HB3 | 1:G:2436:TRP:HH2 | 1.79 | 0.47 |
| 1:G:3103:MET:HE2 | 1:G:3115:PHE:HD1 | 1.80 | 0.47 |
| 1:H:1018:TYR:OH | 1:H:1056:THR:HB | 2.13 | 0.47 |
| 1:H:2800:ASP:OD1 | 1:H:2899:GLY:N | 2.47 | 0.47 |
| 1:H:3062:ASP:OD2 | 1:H:3065:PHE:N | 2.35 | 0.47 |
| 1:I:869:LEU:HD13 | 1:I:928:LYS:HG3 | 1.97 | 0.47 |
| 1:I:2345:ASN:O | 1:I:2349:ARG:HG2 | 2.15 | 0.47 |
| 1:J:1305:CYS:HB2 | 1:J:1312:VAL:O | 2.15 | 0.47 |
| 1:J:1848:VAL:HG12 | 1:J:2026:PHE:HD2 | 1.80 | 0.47 |
| 1:J:2213:ALA:HA | 1:J:2226:ARG:NH2 | 2.29 | 0.47 |
| 1:J:2527:SER:O | 1:J:2530:LYS:HG3 | 2.15 | 0.47 |
| 1:J:2711:ASN:O | 1:J:2714:ARG:HB3 | 2.15 | 0.47 |
| 1:K:396:THR:HG21 | 2:IA:1:NAG:HN2 | 1.79 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:K:2585:LEU:HD22 | 1:K:2706:PHE:CE2 | 2.49 | 0.47 |
| 1:L:110:PRO:HD3 | 1:S:2197:GLN:HG3 | 1.96 | 0.47 |
| 1:L:313:PHE:CE2 | 1:L:406:PRO:HB3 | 2.50 | 0.47 |
| 1:L:675:LEU:H | 1:L:695:ARG:NH2 | 2.11 | 0.47 |
| 1:L:741:HIS:HE1 | 1:L:780:ASN:HD21 | 1.63 | 0.47 |
| 1:L:1501:ASP:OD2 | 1:L:1504:GLN:N | 2.47 | 0.47 |
| 1:L:1963:ILE:HG23 | 1:L:1967:LEU:HD21 | 1.95 | 0.47 |
| 1:L:2741:ARG:NH2 | 1:M:2870:TYR:H | 2.13 | 0.47 |
| 1:M:1301:PHE:CD1 | 1:M:1302:PRO:HA | 2.50 | 0.47 |
| 1:M:1413:ALA:O | 1:M:1425:GLN:NE2 | 2.48 | 0.47 |
| 1:M:1499:PHE:HA | 1:M:1505:ASN:OD1 | 2.14 | 0.47 |
| 1:M:1652:ARG:NH1 | 1:M:1653:PRO:O | 2.47 | 0.47 |
| 1:M:3268:ASP:OD1 | 1:M:3268:ASP:N | 2.46 | 0.47 |
| 1:N:315:LEU:HB2 | 1:N:361:PHE:CE2 | 2.49 | 0.47 |
| 1:N:735:ARG:NH2 | 1:N:789:ILE:H | 2.12 | 0.47 |
| 1:N:3381:LEU:HD23 | 1:N:3386:TYR:CZ | 2.50 | 0.47 |
| 1:O:71:ARG:NE | 1:O:220:ASP:OD1 | 2.48 | 0.47 |
| 1:O:169:LEU:HD23 | 1:O:222:ILE:HD11 | 1.96 | 0.47 |
| 1:O:481:ASP:OD1 | 1:R:1644:TYR:N | 2.46 | 0.47 |
| 1:O:1731:CYS:HA | 1:O:2022:MET:HE1 | 1.97 | 0.47 |
| 1:O:3049:GLN:HG2 | 1:O:3050:PRO:HD2 | 1.97 | 0.47 |
| 1:P:795:LYS:HD3 | 1:P:796:LYS:HD3 | 1.97 | 0.47 |
| 1:P:1132:SER:O | 1:P:1135:GLN:HB3 | 2.15 | 0.47 |
| 1:P:2603:TRP:CD1 | 1:P:2654:PHE:HD2 | 2.33 | 0.47 |
| 1:P:2923:ARG:HD3 | 1:P:3008:ILE:O | 2.14 | 0.47 |
| 1:Q:197:ASP:OD1 | 1:Q:197:ASP:N | 2.46 | 0.47 |
| 1:Q:494:ALA:HA | 1:Q:603:GLU:OE1 | 2.14 | 0.47 |
| 1:Q:2525:THR:O | 1:Q:2529:LYS:HG2 | 2.14 | 0.47 |
| 1:Q:2668:CYS:HB2 | 1:Q:2735:CYS:HB2 | 1.61 | 0.47 |
| 1:Q:2755:ASP:OD1 | 1:Q:2756:PHE:N | 2.48 | 0.47 |
| 1:Q:3113:PRO:HA | 1:Q:3116:MET:HG3 | 1.97 | 0.47 |
| 1:Q:3301:THR:HG22 | 1:Q:3326:LEU:HA | 1.96 | 0.47 |
| 1:R:171:GLU:HB3 | 1:R:177:PHE:HD1 | 1.79 | 0.47 |
| 1:R:1817:ARG:HA | 1:R:1817:ARG:HD2 | 1.71 | 0.47 |
| 1:R:2693:MET:HE1 | 1:R:2702:ASP:HB3 | 1.95 | 0.47 |
| 1:R:2779:LEU:HD23 | 1:R:2779:LEU:H | 1.79 | 0.47 |
| 1:R:2954:GLU:H | 1:R:2954:GLU:CD | 2.22 | 0.47 |
| 1:S:5:ARG:HB2 | 1:S:283:TYR:HA | 1.97 | 0.47 |
| 1:S:304:ARG:CZ | 1:S:304:ARG:HA | 2.44 | 0.47 |
| 1:S:539:GLU:HG2 | 1:S:540:THR:HG23 | 1.96 | 0.47 |
| 1:S:1161:SER:N | 1:S:1185:GLY:O | 2.47 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:S:2407:GLU:OE2 | 1:S:2424:ALA:HB1 | 2.14 | 0.47 |
| 1:S:2621:PRO:HA | 1:S:2624:HIS:CE1 | 2.50 | 0.47 |
| 1:S:2800:ASP:OD1 | 1:S:2801:ARG:N | 2.46 | 0.47 |
| 1:S:2972:ASP:N | 1:S:2972:ASP:OD1 | 2.46 | 0.47 |
| 1:S:3287:LEU:HD23 | 1:S:3287:LEU:H | 1.80 | 0.47 |
| 1:T:567:SER:OG | 1:T:623:TYR:O | 2.27 | 0.47 |
| 1:T:848:ARG:HD3 | 1:T:934:LEU:HB3 | 1.96 | 0.47 |
| 1:T:991:LYS:HB3 | 1:T:994:ARG:HE | 1.78 | 0.47 |
| 1:T:2088:PRO:O | 1:T:2090:ASN:N | 2.45 | 0.47 |
| 1:T:2235:LEU:HD12 | 1:T:2239:GLY:HA2 | 1.96 | 0.47 |
| 1:T:2817:VAL:O | 1:T:2833:THR:OG1 | 2.20 | 0.47 |
| 1:A:512:LYS:HB3 | 1:A:512:LYS:HE3 | 1.77 | 0.47 |
| 1:A:525:TRP:CZ3 | 1:A:526:THR:HG22 | 2.50 | 0.47 |
| 1:A:1114:ASP:N | 1:A:1114:ASP:OD1 | 2.44 | 0.47 |
| 1:A:1122:HIS:ND1 | 1:A:1123:TYR:O | 2.47 | 0.47 |
| 1:A:1817:ARG:HG3 | 1:A:1860:TRP:CH2 | 2.50 | 0.47 |
| 1:A:2287:HIS:CD2 | 1:A:2430:GLY:HA3 | 2.50 | 0.47 |
| 1:A:2567:CYS:O | 1:A:2569:HIS:ND1 | 2.43 | 0.47 |
| 1:A:2604:THR:HG23 | 1:A:2782:HIS:NE2 | 2.29 | 0.47 |
| 1:B:72:LEU:HD11 | 1:B:254:PHE:CZ | 2.49 | 0.47 |
| 1:B:193:GLY:HA3 | 1:B:201:SER:N | 2.30 | 0.47 |
| 1:B:567:SER:OG | 1:B:623:TYR:O | 2.29 | 0.47 |
| 1:B:597:ARG:NH2 | 1:B:658:ARG:HB2 | 2.30 | 0.47 |
| 1:B:627:THR:OG1 | 1:B:628:LEU:N | 2.48 | 0.47 |
| 1:B:729:GLU:O | 1:B:732:THR:HG22 | 2.15 | 0.47 |
| 1:B:1862:GLY:HA3 | 1:B:1870:ALA:HB2 | 1.97 | 0.47 |
| 1:B:2118:GLY:HA2 | 1:B:2124:GLN:HE22 | 1.80 | 0.47 |
| 1:B:2705:PHE:CE1 | 1:B:2709:HIS:CE1 | 3.02 | 0.47 |
| 1:B:2812:LYS:HG2 | 1:B:2840:PRO:HA | 1.97 | 0.47 |
| 1:B:2930:SER:O | 1:B:2934:VAL:HG23 | 2.14 | 0.47 |
| 1:B:3088:HIS:HE1 | 1:B:3119:HIS:CE1 | 2.33 | 0.47 |
| 1:B:3147:LEU:HA | 1:B:3150:LEU:HD12 | 1.96 | 0.47 |
| 1:B:3185:TYR:HD2 | 1:B:3187:PHE:HE1 | 1.62 | 0.47 |
| 1:C:75:VAL:O | 1:C:78:GLU:HG3 | 2.14 | 0.47 |
| 1:C:1187:GLU:OE1 | 1:C:1187:GLU:N | 2.45 | 0.47 |
| 1:C:1543:LEU:O | 1:C:1547:LEU:HD23 | 2.14 | 0.47 |
| 1:C:1574:PHE:N | 1:C:1634:GLU:O | 2.36 | 0.47 |
| 1:C:1715:ALA:HB1 | 1:C:1873:HIS:HA | 1.96 | 0.47 |
| 1:C:1786:ASP:OD2 | 1:C:1789:LEU:N | 2.40 | 0.47 |
| 1:C:2085:GLN:CD | 1:C:2087:LEU:H | 2.23 | 0.47 |
| 1:C:2190:LEU:HG | 1:C:2191:PRO:HD2 | 1.96 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:2219:GLU:OE1 | 1:C:2219:GLU:N | 2.48 | 0.47 |
| 1:D:225:ILE:O | 1:D:229:LEU:HG | 2.14 | 0.47 |
| 1:D:741:HIS:HE1 | 1:D:780:ASN:HD21 | 1.62 | 0.47 |
| 1:D:752:ILE:HB | 1:D:809:SER:HB3 | 1.96 | 0.47 |
| 1:D:968:PHE:CE1 | 1:D:1047:PRO:HG2 | 2.50 | 0.47 |
| 1:D:1185:GLY:HA2 | 1:D:1189:GLU:HG3 | 1.97 | 0.47 |
| 1:D:2786:ILE:HG13 | 1:D:2787:PRO:HD3 | 1.97 | 0.47 |
| 1:E:596:GLN:C | 1:E:597:ARG:HE | 2.22 | 0.47 |
| 1:E:1084:LEU:HB3 | 1:E:1110:PHE:CE1 | 2.49 | 0.47 |
| 1:E:1085:ARG:NH2 | 1:F:2463:ALA:O | 2.31 | 0.47 |
| 1:E:1246:GLY:O | 1:E:1249:THR:OG1 | 2.26 | 0.47 |
| 1:E:1283:LEU:HD13 | 1:E:1380:PHE:HE1 | 1.79 | 0.47 |
| 1:E:1756:ARG:HH22 | 1:F:2102:ARG:NH1 | 2.12 | 0.47 |
| 1:E:1890:ARG:HB2 | 1:E:1955:TYR:CE2 | 2.49 | 0.47 |
| 1:E:2390:LYS:HB2 | 1:E:2392:ARG:HH12 | 1.80 | 0.47 |
| 1:E:2399:LEU:HB3 | 1:E:2436:TRP:CH2 | 2.50 | 0.47 |
| 1:E:2414:GLN:O | 1:E:2416:ASN:N | 2.48 | 0.47 |
| 1:E:2534:ALA:HA | 1:E:2537:GLN:HE22 | 1.79 | 0.47 |
| 1:E:3300:ALA:HA | 1:E:3325:LYS:HE3 | 1.95 | 0.47 |
| 1:F:6:LYS:HE3 | 1:F:15:GLU:CD | 2.40 | 0.47 |
| 1:F:185:HIS:ND1 | 1:F:219:VAL:HG21 | 2.29 | 0.47 |
| 1:F:228:GLU:HA | 1:F:231:LYS:HG3 | 1.97 | 0.47 |
| 1:F:427:GLN:OE1 | 1:F:427:GLN:N | 2.45 | 0.47 |
| 1:F:596:GLN:NE2 | 1:F:598:ASP:H | 2.12 | 0.47 |
| 1:F:610:HIS:HE1 | 1:F:641:HIS:CE1 | 2.33 | 0.47 |
| 1:F:1060:TRP:NE1 | 1:F:1064:GLN:HE22 | 2.12 | 0.47 |
| 1:F:1568:SER:N | 1:F:1597:GLY:O | 2.47 | 0.47 |
| 1:F:2262:VAL:HG23 | 1:F:2438:PHE:CD1 | 2.50 | 0.47 |
| 1:F:2712:VAL:O | 1:F:2715:GLN:HG2 | 2.14 | 0.47 |
| 1:F:3155:GLU:OE2 | 1:F:3158:ASN:ND2 | 2.47 | 0.47 |
| 1:G:579:GLU:HG3 | 1:G:582:ASP:CG | 2.40 | 0.47 |
| 1:G:603:GLU:O | 1:G:607:GLU:HG2 | 2.15 | 0.47 |
| 1:G:945:ALA:HA | 1:G:987:PHE:CZ | 2.49 | 0.47 |
| 1:G:1004:LEU:O | 1:G:1008:GLN:NE2 | 2.42 | 0.47 |
| 1:G:1249:THR:O | 1:G:1251:LYS:NZ | 2.28 | 0.47 |
| 1:G:1710:LEU:HB3 | 1:G:1750:PHE:CE1 | 2.49 | 0.47 |
| 1:G:2157:TRP:HE3 | 1:G:2158:HIS:HD2 | 1.61 | 0.47 |
| 1:G:2190:LEU:HG | 1:G:2191:PRO:HD2 | 1.97 | 0.47 |
| 1:G:2439:ASP:N | 1:G:2439:ASP:OD1 | 2.47 | 0.47 |
| 1:G:2569:HIS:HA | 1:G:2574:PHE:CZ | 2.50 | 0.47 |
| 1:G:2603:TRP:CZ3 | 1:G:2681:ILE:HD11 | 2.50 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:G:3165:ASN:ND2 | 1:G:3168:THR:OG1 | 2.47 | 0.47 |
| 1:G:3173:ARG:O | 1:G:3177:ILE:HG13 | 2.15 | 0.47 |
| 1:H:146:ASP:CG | 1:H:148:ARG:HG2 | 2.39 | 0.47 |
| 1:H:735:ARG:NH2 | 1:H:789:ILE:H | 2.12 | 0.47 |
| 1:H:1141:LEU:HG | 1:H:1144:GLN:HE21 | 1.79 | 0.47 |
| 1:H:1295:ILE:HG21 | 1:H:1333:VAL:HG23 | 1.96 | 0.47 |
| 1:H:1351:TRP:HZ3 | 1:H:1463:ASN:HB3 | 1.80 | 0.47 |
| 1:H:1857:ILE:HB | 1:H:1884:HIS:CE1 | 2.49 | 0.47 |
| 1:H:2105:MET:HA | 1:H:2108:LYS:HG2 | 1.97 | 0.47 |
| 1:H:2516:ASN:OD1 | 1:H:2517:ILE:N | 2.45 | 0.47 |
| 1:H:2967:PRO:O | 1:H:2973:ARG:NH1 | 2.48 | 0.47 |
| 1:I:313:PHE:HZ | 1:I:326:ILE:HD13 | 1.79 | 0.47 |
| 1:I:855:THR:O | 1:I:858:GLN:HG2 | 2.14 | 0.47 |
| 1:I:1324:HIS:HA | 1:I:1519:VAL:HG11 | 1.95 | 0.47 |
| 1:I:1577:VAL:O | 1:I:1584:ARG:NH2 | 2.48 | 0.47 |
| 1:I:1932:ASP:OD2 | 1:I:1934:ILE:HG22 | 2.15 | 0.47 |
| 1:I:1993:SER:HA | 1:I:2015:VAL:O | 2.15 | 0.47 |
| 1:I:2267:THR:O | 1:I:2271:ILE:HG12 | 2.15 | 0.47 |
| 1:I:2308:VAL:O | 1:I:2311:GLU:HG3 | 2.14 | 0.47 |
| 1:I:2378:ASP:OD1 | 1:I:2378:ASP:N | 2.46 | 0.47 |
| 1:I:2551:HIS:HB2 | 1:I:2581:PHE:CE2 | 2.50 | 0.47 |
| 1:I:3042:HIS:CD2 | 1:I:3101:TYR:HH | 2.32 | 0.47 |
| 1:J:526:THR:HG1 | 1:J:527:ARG:NH1 | 2.12 | 0.47 |
| 1:J:939:TRP:HZ3 | 1:J:1055:ASN:HB3 | 1.79 | 0.47 |
| 1:J:1195:ASP:OD1 | 1:J:1195:ASP:N | 2.47 | 0.47 |
| 1:J:1221:TYR:OH | 1:J:1233:SER:O | 2.33 | 0.47 |
| 1:J:1414:LEU:HA | 1:J:1422:PHE:HE1 | 1.79 | 0.47 |
| 1:J:2375:LEU:HB3 | 1:J:2379:GLU:OE2 | 2.13 | 0.47 |
| 1:J:3047:ASP:HB2 | 1:J:3097:GLY:HA3 | 1.96 | 0.47 |
| 1:J:3332:VAL:O | 1:J:3407:ASP:HB2 | 2.15 | 0.47 |
| 1:J:3338:VAL:HG13 | 1:J:3379:TYR:HB2 | 1.96 | 0.47 |
| 1:K:24:ARG:HH12 | 1:K:125:TRP:CD1 | 2.33 | 0.47 |
| 1:K:158:ASN:HB2 | 1:K:162:PHE:CD2 | 2.49 | 0.47 |
| 1:K:730:ARG:HG3 | 1:K:735:ARG:HH22 | 1.79 | 0.47 |
| 1:K:849:SER:HB3 | 1:K:854:LEU:HD21 | 1.95 | 0.47 |
| 1:K:889:ASN:HB3 | 1:K:900:PHE:O | 2.15 | 0.47 |
| 1:K:1223:VAL:HG13 | 1:K:1231:ILE:HB | 1.97 | 0.47 |
| 1:K:1583:GLU:OE2 | 1:N:327:LYS:NZ | 2.47 | 0.47 |
| 1:K:1638:ARG:HH12 | 1:K:1642:GLY:HA2 | 1.80 | 0.47 |
| 1:K:1731:CYS:HA | 1:K:2022:MET:HE1 | 1.95 | 0.47 |
| 1:K:1750:PHE:HD2 | 1:K:1882:LEU:HD11 | 1.80 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:K:1890:ARG:HB2 | 1:K:1955:TYR:CE2 | 2.50 | 0.47 |
| 1:K:2105:MET:HA | 1:K:2108:LYS:HG2 | 1.96 | 0.47 |
| 1:K:2663:GLU:HA | 1:K:2793:ILE:HD11 | 1.95 | 0.47 |
| 1:K:2752:ASN:OD1 | 1:K:2753:PRO:HD2 | 2.14 | 0.47 |
| 1:K:2773:ASN:HD21 | 1:K:3142:TYR:HB2 | 1.79 | 0.47 |
| 1:K:2963:PRO:HD2 | 1:K:2965:LEU:HD23 | 1.96 | 0.47 |
| 1:K:3082:VAL:HG23 | 1:K:3258:TYR:CE2 | 2.49 | 0.47 |
| 1:L:188:ILE:HD13 | 1:L:215:HIS:NE2 | 2.29 | 0.47 |
| 1:L:304:ARG:HH21 | 1:L:411:ARG:HH12 | 1.63 | 0.47 |
| 1:L:444:GLU:O | 1:L:447:GLU:HG2 | 2.14 | 0.47 |
| 1:L:471:HIS:HB3 | 1:L:632:ALA:HB1 | 1.97 | 0.47 |
| 1:L:1223:VAL:O | 1:L:1230:LYS:NZ | 2.38 | 0.47 |
| 1:L:2017:GLY:HA2 | 1:L:2021:GLU:OE2 | 2.15 | 0.47 |
| 1:L:3158:ASN:OD1 | 1:L:3159:TYR:N | 2.47 | 0.47 |
| 1:L:3296:ASP:OD1 | 1:L:3296:ASP:N | 2.46 | 0.47 |
| 1:M:408:GLY:N | 1:M:669:THR:OG1 | 2.41 | 0.47 |
| 1:M:849:SER:OG | 1:M:850:ASP:N | 2.48 | 0.47 |
| 1:M:926:ARG:NH2 | 1:M:931:GLN:O | 2.44 | 0.47 |
| 1:M:1352:THR:HG21 | 1:M:1535:PHE:HE1 | 1.79 | 0.47 |
| 1:M:1356:ARG:HB2 | 1:M:1357:GLN:OE1 | 2.15 | 0.47 |
| 1:M:1559:GLY:HA2 | 1:M:1610:TYR:O | 2.15 | 0.47 |
| 1:M:2848:ASP:OD1 | 1:M:2849:ARG:N | 2.46 | 0.47 |
| 1:M:3103:MET:HE2 | 1:M:3115:PHE:HD1 | 1.79 | 0.47 |
| 1:N:142:ALA:HB3 | 1:N:196:HIS:CE1 | 2.50 | 0.47 |
| 1:N:859:VAL:HG12 | 1:N:863:ARG:CZ | 2.45 | 0.47 |
| 1:N:1205:ILE:HD12 | 1:N:1208:LYS:HE3 | 1.97 | 0.47 |
| 1:N:1291:THR:O | 1:N:1295:ILE:HG12 | 2.15 | 0.47 |
| 1:N:1932:ASP:OD2 | 1:N:1935:THR:N | 2.31 | 0.47 |
| 1:N:2028:ARG:CZ | 1:N:2028:ARG:HB2 | 2.44 | 0.47 |
| 1:N:2126:LEU:HD11 | 1:N:2165:VAL:HG12 | 1.96 | 0.47 |
| 1:N:2997:MET:HA | 1:N:2997:MET:HE3 | 1.96 | 0.47 |
| 1:O:418:ASP:OD2 | 1:O:662:TYR:N | 2.48 | 0.47 |
| 1:O:591:LEU:HD12 | 1:O:727:ILE:HD13 | 1.97 | 0.47 |
| 1:O:598:ASP:OD1 | 1:O:599:PHE:N | 2.47 | 0.47 |
| 1:O:1111:GLU:N | 1:O:1111:GLU:OE1 | 2.48 | 0.47 |
| 1:O:1752:ASP:OD1 | 1:O:1753:ALA:N | 2.48 | 0.47 |
| 1:O:1778:PHE:HD2 | 1:O:1779:PHE:HD2 | 1.62 | 0.47 |
| 1:O:1883:LEU:O | 1:O:1886:SER:OG | 2.20 | 0.47 |
| 1:O:1890:ARG:HH21 | 1:O:1959:GLU:H | 1.62 | 0.47 |
| 1:O:2382:GLU:O | 1:O:2385:ARG:HG2 | 2.15 | 0.47 |
| 1:O:2966:CYS:O | 1:O:2974:TYR:N | 2.36 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:P:646:ARG:O | 1:P:650:ILE:HG12 | 2.15 | 0.47 |
| 1:P:738:VAL:HG23 | 1:P:789:ILE:HG13 | 1.97 | 0.47 |
| 1:P:855:THR:O | 1:P:859:VAL:HG23 | 2.14 | 0.47 |
| 1:P:1303:SER:OG | 1:P:1311:LYS:O | 2.29 | 0.47 |
| 1:P:1541:PRO:O | 1:P:1544:GLU:HG3 | 2.15 | 0.47 |
| 1:P:1626:ASP:OD1 | 1:P:1627:SER:N | 2.47 | 0.47 |
| 1:P:2242:SER:OG | 1:P:2243:VAL:N | 2.48 | 0.47 |
| 1:P:2394:PHE:HD2 | 1:P:2443:LYS:HE3 | 1.79 | 0.47 |
| 1:P:2951:ASN:ND2 | 1:P:3001:ASP:OD2 | 2.48 | 0.47 |
| 1:Q:81:LEU:HD21 | 1:Q:86:LEU:HD23 | 1.96 | 0.47 |
| 1:Q:425:ASP:OD1 | 1:Q:425:ASP:N | 2.48 | 0.47 |
| 1:Q:573:GLU:HB3 | 1:Q:616:LEU:HD13 | 1.96 | 0.47 |
| 1:Q:953:GLU:OE1 | 1:Q:969:HIS:ND1 | 2.48 | 0.47 |
| 1:Q:1246:GLY:O | 1:Q:1249:THR:OG1 | 2.26 | 0.47 |
| 1:Q:2099:LEU:HD13 | 1:Q:2103:ALA:HB3 | 1.96 | 0.47 |
| 1:Q:2614:LEU:HD12 | 1:Q:2636:ARG:HH12 | 1.80 | 0.47 |
| 1:Q:3118:HIS:O | 1:Q:3122:ILE:HG12 | 2.15 | 0.47 |
| 1:R:103:LEU:HG | 1:R:104:PRO:HD2 | 1.96 | 0.47 |
| 1:R:714:GLN:HE22 | 1:R:719:THR:HB | 1.79 | 0.47 |
| 1:R:842:HIS:NE2 | 1:R:844:GLU:HB2 | 2.29 | 0.47 |
| 1:R:1139:GLU:O | 1:R:1143:ARG:HG2 | 2.15 | 0.47 |
| 1:R:1284:ARG:NH2 | 1:R:1287:GLN:HG2 | 2.30 | 0.47 |
| 1:R:1599:GLU:OE2 | 1:R:1600:THR:OG1 | 2.32 | 0.47 |
| 1:R:1676:ILE:HG13 | 1:R:1761:VAL:HG23 | 1.97 | 0.47 |
| 1:R:2157:TRP:CD1 | 1:R:2334:MET:HE2 | 2.50 | 0.47 |
| 1:R:2368:ASP:N | 1:R:2368:ASP:OD1 | 2.47 | 0.47 |
| 1:R:3155:GLU:OE2 | 1:R:3158:ASN:ND2 | 2.40 | 0.47 |
| 1:R:3266:VAL:HG11 | 1:R:3283:PHE:HZ | 1.79 | 0.47 |
| 1:S:17:LEU:O | 1:S:20:GLU:HG3 | 2.14 | 0.47 |
| 1:S:62:GLY:HA2 | 1:S:361:PHE:HE1 | 1.79 | 0.47 |
| 1:S:590:MET:HE2 | 1:S:590:MET:HA | 1.95 | 0.47 |
| 1:S:606:PHE:CZ | 1:S:644:VAL:HG13 | 2.50 | 0.47 |
| 1:S:764:GLU:OE2 | 1:S:766:ALA:N | 2.47 | 0.47 |
| 1:S:953:GLU:O | 1:S:966:ASN:N | 2.35 | 0.47 |
| 1:S:996:THR:HG23 | 1:S:999:ALA:H | 1.80 | 0.47 |
| 1:S:1241:VAL:HG13 | 1:T:2327:VAL:HB | 1.97 | 0.47 |
| 1:S:1268:LEU:HD23 | 1:S:1268:LEU:H | 1.79 | 0.47 |
| 1:S:1325:TRP:HE1 | 1:S:1498:PRO:CG | 2.28 | 0.47 |
| 1:S:1543:LEU:HG | 1:S:1547:LEU:HD23 | 1.97 | 0.47 |
| 1:S:2330:MET:HE1 | 1:S:2354:PRO:HG2 | 1.96 | 0.47 |
| 1:S:3352:LYS:HA | 1:S:3371:ASN:O | 2.15 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:T:172:ASP:OD1 | 1:T:173:ASP:N | 2.48 | 0.47 |
| 1:T:325:ARG:HH21 | 1:T:391:TYR:HE2 | 1.62 | 0.47 |
| 1:T:848:ARG:HG2 | 1:T:933:GLY:HA3 | 1.96 | 0.47 |
| 1:T:1007:GLU:N | 1:T:1008:GLN:OE1 | 2.47 | 0.47 |
| 1:T:2028:ARG:CZ | 1:T:2028:ARG:HB2 | 2.45 | 0.47 |
| 1:T:2088:PRO:C | 1:T:2090:ASN:H | 2.22 | 0.47 |
| 1:T:2379:GLU:OE2 | 1:T:2380:LEU:HD12 | 2.14 | 0.47 |
| 1:T:2488:LYS:HD2 | 1:T:2489:PRO:HD2 | 1.95 | 0.47 |
| 1:T:2865:ARG:HG2 | 1:T:2866:PRO:HD2 | 1.95 | 0.47 |
| 1:T:3035:TYR:H | 1:T:3044:VAL:HG22 | 1.79 | 0.47 |
| 1:A:651:TRP:CZ3 | 1:A:655:GLN:HG3 | 2.49 | 0.47 |
| 1:A:938:ASP:HA | 1:A:1055:ASN:ND2 | 2.30 | 0.47 |
| 1:A:1365:ALA:HA | 1:A:1381:PHE:HZ | 1.80 | 0.47 |
| 1:A:2656:ARG:HH21 | 1:A:2659:LEU:HD12 | 1.80 | 0.47 |
| 1:A:3122:ILE:O | 1:A:3125:ILE:HG22 | 2.15 | 0.47 |
| 1:B:483:ARG:NH1 | 1:I:1646:GLU:OE1 | 2.48 | 0.47 |
| 1:B:711:ASP:OD1 | 1:B:711:ASP:N | 2.47 | 0.47 |
| 1:B:848:ARG:HB3 | 1:B:934:LEU:O | 2.14 | 0.47 |
| 1:B:958:PRO:C | 1:B:961:ASN:H | 2.23 | 0.47 |
| 1:B:2324:ASP:OD1 | 1:B:2325:CYS:N | 2.47 | 0.47 |
| 1:B:3037:ILE:HG21 | 1:B:3040:ALA:HB3 | 1.97 | 0.47 |
| 1:C:1301:PHE:CD1 | 1:C:1302:PRO:HA | 2.49 | 0.47 |
| 1:C:1559:GLY:HA2 | 1:C:1610:TYR:O | 2.15 | 0.47 |
| 1:C:2849:ARG:HA | 1:C:2849:ARG:HH11 | 1.79 | 0.47 |
| 1:D:751:VAL:HG22 | 1:D:810:ILE:HD13 | 1.97 | 0.47 |
| 1:D:1049:PHE:CG | 1:D:1053:HIS:HE1 | 2.33 | 0.47 |
| 1:D:1135:GLN:O | 1:D:1138:ARG:N | 2.48 | 0.47 |
| 1:D:1862:GLY:HA3 | 1:D:1870:ALA:HB2 | 1.97 | 0.47 |
| 1:D:2152:PRO:HD2 | 1:D:2329:TYR:CD2 | 2.50 | 0.47 |
| 1:E:230:GLN:NE2 | 1:E:235:LYS:HB2 | 2.29 | 0.47 |
| 1:E:2269:ASN:OD1 | 1:E:2428:LEU:HB2 | 2.15 | 0.47 |
| 1:E:2356:GLU:OE1 | 1:E:2356:GLU:N | 2.39 | 0.47 |
| 1:F:3:LEU:HB2 | 1:F:5:ARG:HH22 | 1.79 | 0.47 |
| 1:F:221:ARG:HB2 | 1:F:283:TYR:CD2 | 2.50 | 0.47 |
| 1:F:538:LYS:NZ | 1:F:552:ASN:HB2 | 2.25 | 0.47 |
| 1:F:988:GLU:OE2 | 1:F:996:THR:OG1 | 2.22 | 0.47 |
| 1:F:1507:PHE:CZ | 1:F:1509:LEU:HB3 | 2.49 | 0.47 |
| 1:F:2194:PHE:CD1 | 1:F:2212:PHE:HB3 | 2.46 | 0.47 |
| 1:F:2430:GLY:N | 1:F:2433:GLU:OE2 | 2.46 | 0.47 |
| 1:F:2786:ILE:H | 1:F:2786:ILE:HD12 | 1.80 | 0.47 |
| 1:F:3081:GLU:N | 1:F:3081:GLU:OE1 | 2.47 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:F:3153:PRO:HB2 | 1:F:3158:ASN:HD22 | 1.80 | 0.47 |
| 1:F:3229:ASN:H | 1:F:3286:THR:HG22 | 1.80 | 0.47 |
| 1:G:680:PHE:HB2 | 1:G:684:LEU:HD22 | 1.97 | 0.47 |
| 1:G:719:THR:H | 1:G:722:GLN:NE2 | 2.13 | 0.47 |
| 1:G:939:TRP:HA | 1:G:943:MET:HE1 | 1.96 | 0.47 |
| 1:G:2295:PHE:O | 1:G:2299:HIS:ND1 | 2.48 | 0.47 |
| 1:G:2585:LEU:HD13 | 1:G:2706:PHE:CE1 | 2.50 | 0.47 |
| 1:G:3133:GLN:OE1 | 1:G:3140:PHE:HB3 | 2.15 | 0.47 |
| 1:H:24:ARG:HA | 1:H:24:ARG:HD2 | 1.73 | 0.47 |
| 1:H:57:ALA:N | 1:H:355:ASN:O | 2.45 | 0.47 |
| 1:H:450:GLN:NE2 | 1:H:454:ARG:HH11 | 2.12 | 0.47 |
| 1:H:848:ARG:NE | 1:H:934:LEU:HG | 2.30 | 0.47 |
| 1:H:958:PRO:C | 1:H:961:ASN:H | 2.22 | 0.47 |
| 1:H:998:ILE:HA | 1:H:1001:MET:HG3 | 1.95 | 0.47 |
| 1:H:1048:ILE:HA | 1:H:1051:LEU:HG | 1.96 | 0.47 |
| 1:H:1724:GLU:HB2 | 1:J:396:THR:HA | 1.96 | 0.47 |
| 1:I:183:VAL:HG21 | 1:I:365:TYR:CE1 | 2.50 | 0.47 |
| 1:I:1331:ASP:O | 1:I:1334:GLU:HG3 | 2.15 | 0.47 |
| 1:J:105:ARG:HA | 1:J:108:GLN:NE2 | 2.29 | 0.47 |
| 1:J:454:ARG:HB2 | 1:J:514:ARG:HD3 | 1.97 | 0.47 |
| 1:J:914:HIS:O | 1:J:918:THR:HG23 | 2.15 | 0.47 |
| 1:J:1284:ARG:HH21 | 1:J:1287:GLN:HG2 | 1.80 | 0.47 |
| 1:J:1514:SER:OG | 1:J:1515:ARG:NH2 | 2.47 | 0.47 |
| 1:J:1564:ASN:HB3 | 1:J:1604:PHE:CE1 | 2.49 | 0.47 |
| 1:J:1710:LEU:HD22 | 1:J:1750:PHE:HE1 | 1.79 | 0.47 |
| 1:J:1783:ILE:HD13 | 1:J:1794:PRO:HA | 1.97 | 0.47 |
| 1:J:1898:LEU:HD21 | 1:J:1965:ALA:HB1 | 1.95 | 0.47 |
| 1:K:257:ASP:HA | 1:K:265:ARG:HE | 1.79 | 0.47 |
| 1:K:383:ASP:N | 1:K:383:ASP:OD1 | 2.48 | 0.47 |
| 1:K:579:GLU:HG3 | 1:K:582:ASP:CG | 2.39 | 0.47 |
| 1:K:680:PHE:HB2 | 1:K:684:LEU:HD22 | 1.95 | 0.47 |
| 1:K:1490:ASN:ND2 | 1:L:2049:PHE:O | 2.47 | 0.47 |
| 1:K:1991:LYS:O | 1:K:1991:LYS:HD2 | 2.15 | 0.47 |
| 1:K:2404:THR:CA | 1:K:2429:GLY:O | 2.63 | 0.47 |
| 1:K:3011:TRP:CZ3 | 1:K:3013:TRP:HB3 | 2.49 | 0.47 |
| 1:L:41:PHE:CD1 | 1:L:47:MET:HE1 | 2.50 | 0.47 |
| 1:L:437:VAL:HG21 | 1:L:533:PRO:HG3 | 1.97 | 0.47 |
| 1:L:848:ARG:HD2 | 1:L:1123:TYR:CE2 | 2.49 | 0.47 |
| 1:L:859:VAL:O | 1:L:862:LEU:HG | 2.15 | 0.47 |
| 1:L:896:ALA:HB1 | 1:L:899:LYS:HB2 | 1.97 | 0.47 |
| 1:L:1271:LEU:HB2 | 1:L:1275:GLU:HG3 | 1.96 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:L:1324:HIS:CD2 | 1:L:1324:HIS:H | 2.32 | 0.47 |
| 1:L:1345:SER:OG | 1:L:1346:VAL:N | 2.48 | 0.47 |
| 1:M:436:ASP:HB3 | 1:M:522:TYR:CE2 | 2.50 | 0.47 |
| 1:M:1220:LYS:NZ | 1:M:1222:SER:HB2 | 2.29 | 0.47 |
| 1:M:2529:LYS:HE2 | 1:M:2533:ARG:NH2 | 2.28 | 0.47 |
| 1:M:3214:TYR:HB3 | 1:M:3264:TYR:O | 2.15 | 0.47 |
| 1:N:454:ARG:NH2 | 1:N:1338:LEU:HG | 2.23 | 0.47 |
| 1:N:1802:ILE:HG22 | 1:N:1877:TYR:CD1 | 2.50 | 0.47 |
| 1:N:2513:VAL:HG21 | 1:N:2515:LYS:NZ | 2.30 | 0.47 |
| 1:N:3036:GLN:OE1 | 1:N:3042:HIS:N | 2.48 | 0.47 |
| 1:O:453:SER:OG | 3:dA:1:NAG:O7 | 2.23 | 0.47 |
| 1:O:1246:GLY:O | 1:O:1249:THR:OG1 | 2.25 | 0.47 |
| 1:O:1384:LYS:HA | 1:O:1391:VAL:HG12 | 1.95 | 0.47 |
| 1:O:2091:ARG:HH21 | 1:O:2364:ASN:HD21 | 1.62 | 0.47 |
| 1:O:2249:LEU:HD23 | 1:O:2383:GLU:CD | 2.39 | 0.47 |
| 1:P:1088:LEU:O | 1:P:1089:GLN:NE2 | 2.48 | 0.47 |
| 1:P:1141:LEU:HD11 | 1:P:1258:ILE:HD13 | 1.95 | 0.47 |
| 1:P:1963:ILE:HG23 | 1:P:1968:LEU:HD11 | 1.96 | 0.47 |
| 1:P:2488:LYS:NZ | 1:P:2489:PRO:O | 2.48 | 0.47 |
| 1:Q:954:THR:HA | 1:Q:965:PRO:HA | 1.96 | 0.47 |
| 1:Q:2538:GLN:HG3 | 1:Q:2592:GLN:HE22 | 1.78 | 0.47 |
| 1:Q:2582:VAL:O | 1:Q:2586:GLU:HG2 | 2.15 | 0.47 |
| 1:Q:2805:ASN:HB2 | 1:Q:2893:SER:HB2 | 1.97 | 0.47 |
| 1:Q:3204:ILE:HG13 | 1:Q:3205:GLU:H | 1.80 | 0.47 |
| 1:R:3106:LEU:HA | 1:R:3109:SER:HB3 | 1.96 | 0.47 |
| 1:S:77:LEU:HD13 | 1:S:213:PHE:CZ | 2.49 | 0.47 |
| 1:S:182:GLU:O | 1:S:186:ASN:ND2 | 2.48 | 0.47 |
| 1:S:718:MET:SD | 1:S:722:GLN:HG2 | 2.55 | 0.47 |
| 1:S:1275:GLU:OE1 | 1:S:1275:GLU:N | 2.36 | 0.47 |
| 1:S:2585:LEU:HG | 1:S:2589:LEU:HD23 | 1.96 | 0.47 |
| 1:T:1928:PRO:HD2 | 1:T:1929:TYR:CD2 | 2.50 | 0.47 |
| 1:T:2413:CYS:SG | 1:T:2470:ARG:NE | 2.85 | 0.47 |
| 1:T:3148:ARG:O | 1:T:3152:ARG:NH1 | 2.47 | 0.47 |
| 1:A:598:ASP:OD1 | 1:A:599:PHE:N | 2.48 | 0.47 |
| 1:A:938:ASP:HA | 1:A:1055:ASN:HD21 | 1.78 | 0.47 |
| 1:A:2959:PHE:HE1 | 1:A:3162:LYS:HE2 | 1.78 | 0.47 |
| 1:A:3317:ILE:HG12 | 1:A:3339:ARG:HB3 | 1.97 | 0.47 |
| 1:B:185:HIS:O | 1:B:188:ILE:HG22 | 2.15 | 0.47 |
| 1:B:581:GLY:H | 1:B:856:ARG:NH2 | 2.13 | 0.47 |
| 1:B:864:GLU:HA | 1:B:867:GLN:OE1 | 2.14 | 0.47 |
| 1:B:1951:PHE:O | 1:B:1952:ASN:ND2 | 2.47 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:2217:ILE:HG22 | 1:B:2219:GLU:H | 1.80 | 0.47 |
| 1:B:2392:ARG:HD2 | 1:B:2394:PHE:CE1 | 2.50 | 0.47 |
| 1:C:1152:GLY:HA3 | 1:C:1197:LEU:HD21 | 1.97 | 0.47 |
| 1:C:2315:ARG:HD3 | 1:C:2377:LEU:HD13 | 1.96 | 0.47 |
| 1:C:2601:TRP:CZ2 | 1:C:2603:TRP:HB3 | 2.49 | 0.47 |
| 1:C:2995:PHE:O | 1:C:2999:LEU:HD23 | 2.15 | 0.47 |
| 1:D:1174:PRO:HG2 | 1:D:1176:HIS:HE1 | 1.80 | 0.47 |
| 1:D:1545:GLU:HB2 | 1:D:1549:ARG:HH21 | 1.80 | 0.47 |
| 1:D:1684:THR:HG23 | 1:D:1687:GLU:H | 1.80 | 0.47 |
| 1:D:1978:LYS:NZ | 1:D:1979:SER:O | 2.45 | 0.47 |
| 1:E:409:VAL:HG13 | 1:E:666:CYS:HA | 1.95 | 0.47 |
| 1:E:639:LEU:O | 1:E:642:SER:OG | 2.30 | 0.47 |
| 1:E:850:ASP:OD1 | 1:E:852:SER:OG | 2.27 | 0.47 |
| 1:E:2797:ARG:HA | 1:E:2801:ARG:NH2 | 2.29 | 0.47 |
| 1:E:3133:GLN:NE2 | 1:E:3139:SER:O | 2.47 | 0.47 |
| 1:F:142:ALA:HB3 | 1:F:196:HIS:CG | 2.49 | 0.47 |
| 1:F:190:TYR:CD2 | 1:F:349:PHE:HD2 | 2.33 | 0.47 |
| 1:F:224:VAL:HA | 1:F:227:GLN:OE1 | 2.15 | 0.47 |
| 1:F:737:PHE:HB2 | 1:F:829:ILE:HB | 1.97 | 0.47 |
| 1:F:2393:VAL:HG11 | 1:F:2450:LEU:HD12 | 1.97 | 0.47 |
| 1:F:3164:PRO:HA | 1:F:3169:ARG:HH21 | 1.80 | 0.47 |
| 1:G:718:MET:SD | 1:G:722:GLN:HG2 | 2.55 | 0.47 |
| 1:G:1016:VAL:O | 1:G:1019:GLU:HG3 | 2.15 | 0.47 |
| 1:G:2136:CYS:HB3 | 1:G:2144:TYR:C | 2.40 | 0.47 |
| 1:G:2926:VAL:HB | 1:G:3023:LEU:HD21 | 1.97 | 0.47 |
| 1:G:3317:ILE:HA | 1:G:3339:ARG:O | 2.14 | 0.47 |
| 1:H:187:HIS:HD2 | 1:H:349:PHE:HB2 | 1.80 | 0.47 |
| 1:H:435:LYS:NZ | 1:H:439:THR:OG1 | 2.41 | 0.47 |
| 1:H:2552:GLY:O | 1:H:2555:GLY:N | 2.48 | 0.47 |
| 1:H:2978:THR:HG21 | 1:H:2983:VAL:HG13 | 1.96 | 0.47 |
| 1:H:3232:LEU:HD13 | 1:H:3269:ALA:HB3 | 1.97 | 0.47 |
| 1:I:613:PRO:HA | 1:I:616:LEU:HB3 | 1.97 | 0.47 |
| 1:I:887:GLN:HE21 | 1:I:889:ASN:HD21 | 1.61 | 0.47 |
| 1:I:1868:SER:O | 1:I:1874:TYR:HB2 | 2.15 | 0.47 |
| 1:I:2286:LEU:HD12 | 1:I:2429:GLY:HA2 | 1.97 | 0.47 |
| 1:I:2364:ASN:OD1 | 1:I:2366:ARG:NH1 | 2.27 | 0.47 |
| 1:I:2621:PRO:HA | 1:I:2624:HIS:NE2 | 2.30 | 0.47 |
| 1:J:69:TRP:O | 1:J:72:LEU:HG | 2.15 | 0.47 |
| 1:J:507:VAL:HG21 | 1:J:638:ILE:HD11 | 1.97 | 0.47 |
| 1:J:859:VAL:HG12 | 1:J:863:ARG:CZ | 2.45 | 0.47 |
| 1:J:866:LEU:O | 1:J:869:LEU:HG | 2.15 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:K:2869:VAL:HA | 1:T:2741:ARG:HH11 | 1.80 | 0.47 |
| 1:L:1772:GLN:HB2 | 1:L:1818:LEU:HD11 | 1.97 | 0.47 |
| 1:L:3127:GLN:O | 1:L:3130:GLN:HG3 | 2.15 | 0.47 |
| 1:M:171:GLU:OE2 | 1:M:173:ASP:N | 2.48 | 0.47 |
| 1:M:687:ASN:OD1 | 1:M:688:GLU:N | 2.48 | 0.47 |
| 1:M:958:PRO:HA | 1:M:961:ASN:HA | 1.97 | 0.47 |
| 1:M:1749:GLN:HE22 | 1:M:1932:ASP:HB3 | 1.79 | 0.47 |
| 1:N:531:THR:OG1 | 1:N:532:VAL:N | 2.47 | 0.47 |
| 1:N:614:HIS:HA | 1:N:625:LEU:HG | 1.96 | 0.47 |
| 1:N:1576:CYS:HB2 | 1:N:1632:ASP:OD1 | 2.14 | 0.47 |
| 1:N:2527:SER:O | 1:N:2530:LYS:HG3 | 2.14 | 0.47 |
| 1:N:2896:PHE:N | 1:O:2734:ASN:OD1 | 2.35 | 0.47 |
| 1:N:3002:LYS:HA | 1:N:3002:LYS:HD3 | 1.80 | 0.47 |
| 1:N:3122:ILE:HG13 | 1:N:3125:ILE:HD11 | 1.96 | 0.47 |
| 1:O:248:ARG:NH1 | 1:O:802:ASP:O | 2.47 | 0.47 |
| 1:O:304:ARG:HH21 | 1:O:411:ARG:NH2 | 2.13 | 0.47 |
| 1:O:724:ASP:OD1 | 1:O:725:HIS:N | 2.47 | 0.47 |
| 1:O:989:LYS:HA | 1:O:989:LYS:HD2 | 1.74 | 0.47 |
| 1:O:997:LYS:HA | 1:O:1000:GLU:OE2 | 2.15 | 0.47 |
| 1:O:1475:GLN:HB3 | 1:O:1482:ASP:HB3 | 1.96 | 0.47 |
| 1:O:2421:ARG:HH22 | 1:O:2424:ALA:HB2 | 1.80 | 0.47 |
| 1:P:5:ARG:HD2 | 1:P:283:TYR:CZ | 2.50 | 0.47 |
| 1:P:255:ASP:OD1 | 1:P:255:ASP:N | 2.47 | 0.47 |
| 1:P:522:TYR:HE2 | 1:P:524:ASP:HB2 | 1.79 | 0.47 |
| 1:P:729:GLU:O | 1:P:732:THR:HG22 | 2.15 | 0.47 |
| 1:P:1124:ASP:OD1 | 1:P:1124:ASP:N | 2.45 | 0.47 |
| 1:P:1492:MET:HB3 | 1:P:1517:ILE:HG23 | 1.96 | 0.47 |
| 1:P:3081:GLU:OE1 | 1:P:3081:GLU:N | 2.47 | 0.47 |
| 1:Q:71:ARG:HH22 | 1:Q:276:TYR:HB3 | 1.80 | 0.47 |
| 1:Q:1314:CYS:SG | 1:Q:1497:LYS:HG2 | 2.55 | 0.47 |
| 1:Q:1567:THR:HG21 | 2:oA:1:NAG:H62 | 1.97 | 0.47 |
| 1:Q:2773:ASN:HD21 | 1:Q:3142:TYR:HB2 | 1.80 | 0.47 |
| 1:Q:2961:GLY:HA2 | 1:Q:3106:LEU:HD23 | 1.95 | 0.47 |
| 1:Q:3216:GLY:HA2 | 1:Q:3262:TYR:O | 2.15 | 0.47 |
| 1:R:228:GLU:HA | 1:R:231:LYS:HG3 | 1.96 | 0.47 |
| 1:R:461:VAL:HG22 | 1:R:1277:GLU:OE2 | 2.15 | 0.47 |
| 1:R:728:ASP:HB3 | 1:R:836:HIS:CD2 | 2.49 | 0.47 |
| 1:R:1568:SER:N | 1:R:1597:GLY:O | 2.48 | 0.47 |
| 1:R:1910:ASN:OD1 | 1:R:1911:CYS:N | 2.48 | 0.47 |
| 1:R:2149:HIS:HA | 1:R:2154:PHE:CD2 | 2.43 | 0.47 |
| 1:R:2820:ASP:HB3 | 1:R:2873:ASP:OD1 | 2.15 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:T:187:HIS:CE1 | 1:T:191:LEU:HD11 | 2.50 | 0.47 |
| 1:T:188:ILE:HD13 | 1:T:215:HIS:NE2 | 2.30 | 0.47 |
| 1:T:728:ASP:HB3 | 1:T:836:HIS:CD2 | 2.50 | 0.47 |
| 1:T:740:LEU:H | 1:T:785:VAL:H | 1.63 | 0.47 |
| 1:T:1193:GLN:OE1 | 1:T:1194:TYR:N | 2.47 | 0.47 |
| 1:T:2210:ASN:ND2 | 1:T:2212:PHE:HB2 | 2.30 | 0.47 |
| 1:A:47:MET:C | 1:A:55:ARG:HH12 | 2.23 | 0.47 |
| 1:A:844:GLU:HB2 | 1:A:846:HIS:CE1 | 2.51 | 0.47 |
| 1:A:889:ASN:HB3 | 1:A:900:PHE:O | 2.15 | 0.47 |
| 1:A:973:VAL:HG11 | 1:A:1045:TYR:CG | 2.50 | 0.47 |
| 1:A:2034:ILE:O | 1:A:2038:LEU:HD23 | 2.14 | 0.47 |
| 1:A:2938:ARG:HH22 | 1:A:3030:ASN:HB2 | 1.80 | 0.47 |
| 1:A:3149:ASN:HD22 | 1:A:3152:ARG:NH2 | 2.13 | 0.47 |
| 1:B:1055:ASN:O | 1:B:1059:ILE:HG13 | 2.15 | 0.47 |
| 1:B:1420:CYS:SG | 1:B:1485:SER:OG | 2.66 | 0.47 |
| 1:B:2265:GLU:OE1 | 1:B:2268:HIS:NE2 | 2.41 | 0.47 |
| 1:B:2407:GLU:O | 1:B:2473:ILE:HA | 2.14 | 0.47 |
| 1:C:307:GLU:OE1 | 1:C:412:PRO:HA | 2.15 | 0.47 |
| 1:C:326:ILE:O | 1:C:345:ALA:HB3 | 2.15 | 0.47 |
| 1:C:1023:ASN:HD21 | 1:C:1183:ILE:HA | 1.80 | 0.47 |
| 1:C:1889:ASP:OD2 | 1:C:1955:TYR:OH | 2.32 | 0.47 |
| 1:C:2333:ALA:HB1 | 1:C:2338:ASN:HB3 | 1.97 | 0.47 |
| 1:C:2817:VAL:HG22 | 1:C:2876:ILE:HG22 | 1.96 | 0.47 |
| 1:D:74:VAL:O | 1:D:77:LEU:HB2 | 2.15 | 0.47 |
| 1:D:427:GLN:OE1 | 1:D:427:GLN:N | 2.47 | 0.47 |
| 1:D:1564:ASN:HB3 | 1:D:1604:PHE:CE1 | 2.50 | 0.47 |
| 1:D:2802:VAL:HG23 | 1:D:2855:VAL:HG23 | 1.97 | 0.47 |
| 1:E:164:MET:HE2 | 1:E:184:ALA:HA | 1.96 | 0.47 |
| 1:E:699:ILE:HG13 | 1:E:706:LEU:HD21 | 1.97 | 0.47 |
| 1:E:2064:SER:OG | 1:E:2066:SER:OG | 2.30 | 0.47 |
| 1:E:3188:ASP:OD1 | 1:E:3189:ASN:N | 2.48 | 0.47 |
| 1:E:3204:ILE:HG13 | 1:E:3205:GLU:OE1 | 2.15 | 0.47 |
| 1:F:1301:PHE:CG | 1:F:1302:PRO:HA | 2.50 | 0.47 |
| 1:F:1365:ALA:HA | 1:F:1378:ASN:HB3 | 1.96 | 0.47 |
| 1:F:1542:GLN:HA | 1:F:1545:GLU:HG2 | 1.97 | 0.47 |
| 1:F:1893:ALA:O | 1:F:1896:GLN:HB2 | 2.14 | 0.47 |
| 1:F:1946:ASP:HB3 | 1:F:1950:HIS:CD2 | 2.50 | 0.47 |
| 1:F:2326:ALA:HB1 | 1:F:2329:TYR:HB2 | 1.96 | 0.47 |
| 1:F:2556:LEU:HD11 | 1:F:2746:PRO:HG3 | 1.97 | 0.47 |
| 1:F:3398:GLN:NE2 | 1:F:3400:THR:HG1 | 2.13 | 0.47 |
| 1:G:971:GLY:H | 1:G:978:THR:HG1 | 1.61 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:G:1195:ASP:HB2 | 1:H:2441:LEU:HD21 | 1.97 | 0.47 |
| 1:G:2553:TYR:CD2 | 1:G:2554:PRO:HA | 2.49 | 0.47 |
| 1:G:2923:ARG:HG2 | 1:G:3008:ILE:O | 2.14 | 0.47 |
| 1:H:7:ASN:HB3 | 1:H:10:LEU:HD13 | 1.95 | 0.47 |
| 1:H:427:GLN:OE1 | 1:H:427:GLN:N | 2.46 | 0.47 |
| 1:H:454:ARG:HB2 | 1:H:514:ARG:NH1 | 2.30 | 0.47 |
| 1:H:636:ILE:O | 1:H:639:LEU:HG | 2.14 | 0.47 |
| 1:H:658:ARG:HH12 | 1:H:727:ILE:HD11 | 1.80 | 0.47 |
| 1:H:836:HIS:NE2 | 1:H:838:GLU:OE1 | 2.48 | 0.47 |
| 1:H:842:HIS:CE1 | 1:H:844:GLU:HB2 | 2.49 | 0.47 |
| 1:H:1108:VAL:HG13 | 1:H:1111:GLU:OE1 | 2.14 | 0.47 |
| 1:H:1132:SER:O | 1:H:1135:GLN:HB3 | 2.15 | 0.47 |
| 1:H:1847:GLU:CD | 1:H:1847:GLU:H | 2.23 | 0.47 |
| 1:H:2118:GLY:HA2 | 1:H:2124:GLN:HE22 | 1.79 | 0.47 |
| 1:H:2488:LYS:HD2 | 1:H:2489:PRO:HD2 | 1.97 | 0.47 |
| 1:H:2641:GLN:HA | 1:H:2644:SER:HG | 1.80 | 0.47 |
| 1:I:248:ARG:HH12 | 1:I:803:GLU:HA | 1.80 | 0.47 |
| 1:I:1466:ARG:HA | 1:I:1530:TYR:HE2 | 1.80 | 0.47 |
| 1:I:1507:PHE:CG | 1:I:1508:ASP:N | 2.83 | 0.47 |
| 1:I:3084:PHE:HE1 | 1:I:3125:ILE:HG23 | 1.80 | 0.47 |
| 1:J:524:ASP:HA | 1:J:643:ASN:ND2 | 2.30 | 0.47 |
| 1:J:1322:PHE:HB3 | 1:J:1323:PRO:HD3 | 1.95 | 0.47 |
| 1:J:1849:GLN:O | 1:J:1852:ILE:HG22 | 2.14 | 0.47 |
| 1:J:2130:HIS:NE2 | 1:J:2147:CYS:SG | 2.88 | 0.47 |
| 1:J:2397:PHE:CD1 | 1:J:2489:PRO:HB3 | 2.49 | 0.47 |
| 1:J:2848:ASP:OD2 | 1:J:2849:ARG:N | 2.46 | 0.47 |
| 1:J:3089:ASN:HB3 | 1:J:3248:LEU:HD13 | 1.97 | 0.47 |
| 1:K:1495:PRO:HA | 1:K:1516:PRO:HD3 | 1.96 | 0.47 |
| 1:K:2325:CYS:HA | 1:L:1242:VAL:HG13 | 1.96 | 0.47 |
| 1:K:2703:PRO:O | 1:K:2707:ILE:HG12 | 2.15 | 0.47 |
| 1:K:3082:VAL:HG23 | 1:K:3258:TYR:HE2 | 1.80 | 0.47 |
| 1:K:3191:ASN:OD1 | 1:K:3195:HIS:N | 2.48 | 0.47 |
| 1:L:1088:LEU:O | 1:L:1089:GLN:NE2 | 2.48 | 0.47 |
| 1:L:1295:ILE:HG21 | 1:L:1333:VAL:HG23 | 1.96 | 0.47 |
| 1:L:2672:VAL:HG21 | 1:L:2850:LEU:O | 2.14 | 0.47 |
| 1:L:2991:LEU:HA | 1:L:2994:GLN:HE21 | 1.80 | 0.47 |
| 1:L:3129:TRP:O | 1:L:3133:GLN:HG2 | 2.14 | 0.47 |
| 1:L:3160:GLU:CD | 1:L:3160:GLU:H | 2.22 | 0.47 |
| 1:L:3395:ARG:NE | 1:L:3400:THR:OG1 | 2.42 | 0.47 |
| 1:M:2308:VAL:O | 1:M:2311:GLU:HG3 | 2.15 | 0.47 |
| 1:N:38:LEU:HG | 1:N:73:TYR:CZ | 2.50 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:N:922:GLU:HG3 | 1:N:934:LEU:HB2 | 1.97 | 0.47 |
| 1:N:1677:ARG:HD2 | 1:N:1763:ILE:O | 2.14 | 0.47 |
| 1:N:2343:ASN:OD1 | 1:N:2344:GLU:N | 2.48 | 0.47 |
| 1:N:2394:PHE:HB2 | 1:N:2492:ILE:HB | 1.96 | 0.47 |
| 1:O:129:GLU:HA | 1:O:140:SER:HA | 1.95 | 0.47 |
| 1:O:1422:PHE:HA | 1:O:1425:GLN:NE2 | 2.30 | 0.47 |
| 1:O:1557:PHE:HB3 | 1:O:1611:LYS:HD2 | 1.96 | 0.47 |
| 1:O:1756:ARG:HH22 | 1:P:2102:ARG:NH1 | 2.14 | 0.47 |
| 1:O:2108:LYS:HE2 | 1:O:2211:PRO:HD2 | 1.97 | 0.47 |
| 1:O:2641:GLN:NE2 | 1:O:2645:ASP:OD1 | 2.46 | 0.47 |
| 1:P:526:THR:HG1 | 1:P:527:ARG:NH1 | 2.13 | 0.47 |
| 1:P:741:HIS:CE1 | 1:P:780:ASN:HD21 | 2.33 | 0.47 |
| 1:P:1281:SER:O | 1:P:1285:ARG:HG2 | 2.15 | 0.47 |
| 1:P:2407:GLU:O | 1:P:2473:ILE:HA | 2.15 | 0.47 |
| 1:P:2574:PHE:O | 1:P:2578:HIS:ND1 | 2.37 | 0.47 |
| 1:P:3071:THR:HB | 1:P:3072:LEU:HD12 | 1.97 | 0.47 |
| 1:Q:215:HIS:O | 1:Q:219:VAL:HG23 | 2.15 | 0.47 |
| 1:Q:326:ILE:O | 1:Q:345:ALA:HB3 | 2.15 | 0.47 |
| 1:Q:646:ARG:NH2 | 1:Q:714:GLN:O | 2.49 | 0.47 |
| 1:Q:1247:SER:HA | 1:Q:1250:LYS:HG2 | 1.97 | 0.47 |
| 1:Q:1420:CYS:HB2 | 1:Q:1608:ARG:NH2 | 2.30 | 0.47 |
| 1:R:729:GLU:O | 1:R:732:THR:HG22 | 2.15 | 0.47 |
| 1:R:837:GLU:N | 1:R:837:GLU:OE2 | 2.48 | 0.47 |
| 1:R:901:ALA:HB2 | 1:R:1188:TYR:HB3 | 1.95 | 0.47 |
| 1:R:914:HIS:HA | 1:R:917:LEU:HG | 1.96 | 0.47 |
| 1:R:996:THR:HG23 | 1:R:999:ALA:H | 1.80 | 0.47 |
| 1:R:1159:ARG:HG2 | 1:R:1159:ARG:O | 2.15 | 0.47 |
| 1:R:2873:ASP:OD2 | 1:R:2875:HIS:NE2 | 2.48 | 0.47 |
| 1:S:248:ARG:NH1 | 1:S:801:ASP:O | 2.47 | 0.47 |
| 1:S:583:HIS:HB3 | 1:S:587:PHE:HD2 | 1.80 | 0.47 |
| 1:S:1638:ARG:HG2 | 1:S:1644:TYR:HE1 | 1.80 | 0.47 |
| 1:S:1829:TRP:NE1 | 1:S:1833:GLN:HE22 | 2.13 | 0.47 |
| 1:S:1852:ILE:HD13 | 1:S:2030:TYR:CZ | 2.50 | 0.47 |
| 1:S:2093:ARG:HB2 | 1:S:2367:TYR:HA | 1.96 | 0.47 |
| 1:S:2163:LEU:HD21 | 1:S:2347:PHE:HE2 | 1.80 | 0.47 |
| 1:S:2348:THR:HG1 | 1:S:2349:ARG:NH1 | 2.12 | 0.47 |
| 1:S:2963:PRO:HD2 | 1:S:2965:LEU:HD23 | 1.97 | 0.47 |
| 1:S:3334:ARG:NH2 | 1:S:3406:ILE:HG23 | 2.29 | 0.47 |
| 1:S:3350:ASN:O | 1:S:3391:SER:N | 2.41 | 0.47 |
| 1:T:142:ALA:HB3 | 1:T:196:HIS:CE1 | 2.50 | 0.47 |
| 1:T:391:TYR:HE1 | 1:T:397:SER:HB2 | 1.79 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:T:3000:ARG:CZ | 1:T:3000:ARG:HA | 2.45 | 0.47 |
| 1:T:3183:PHE:HB2 | 1:T:3185:TYR:HD1 | 1.80 | 0.47 |
| 1:A:889:ASN:HB2 | 1:A:899:LYS:HB3 | 1.96 | 0.46 |
| 1:A:2508:VAL:O | 1:A:2515:LYS:NZ | 2.48 | 0.46 |
| 1:A:2941:LEU:HD22 | 1:A:3032:PHE:CD2 | 2.50 | 0.46 |
| 1:B:1087:PRO:HA | 1:B:1109:PRO:HD3 | 1.98 | 0.46 |
| 1:C:954:THR:HG22 | 1:C:965:PRO:HA | 1.97 | 0.46 |
| 1:C:1323:PRO:HG3 | 1:C:1426:PHE:CE2 | 2.50 | 0.46 |
| 1:C:2308:VAL:O | 1:C:2311:GLU:HG3 | 2.15 | 0.46 |
| 1:C:2633:LYS:HE3 | 1:C:2633:LYS:HB3 | 1.65 | 0.46 |
| 1:D:5:ARG:HD2 | 1:D:283:TYR:CZ | 2.50 | 0.46 |
| 1:D:198:HIS:HD1 | 1:D:205:TRP:CD1 | 2.32 | 0.46 |
| 1:D:442:ASP:OD1 | 1:D:443:GLU:N | 2.48 | 0.46 |
| 1:D:1294:LYS:O | 1:D:1297:SER:OG | 2.26 | 0.46 |
| 1:D:1492:MET:HA | 1:D:1516:PRO:HG2 | 1.98 | 0.46 |
| 1:D:3147:LEU:HA | 1:D:3150:LEU:HD12 | 1.97 | 0.46 |
| 1:D:3317:ILE:HA | 1:D:3339:ARG:O | 2.15 | 0.46 |
| 1:E:47:MET:C | 1:E:55:ARG:HH12 | 2.22 | 0.46 |
| 1:E:574:LEU:HD23 | 1:E:616:LEU:HG | 1.98 | 0.46 |
| 1:E:855:THR:H | 1:E:858:GLN:NE2 | 2.12 | 0.46 |
| 1:E:1315:CYS:HA | 1:E:1325:TRP:CH2 | 2.50 | 0.46 |
| 1:E:1785:ARG:NH1 | 1:E:1790:ASP:OD1 | 2.47 | 0.46 |
| 1:E:2297:THR:O | 1:E:2300:THR:OG1 | 2.28 | 0.46 |
| 1:F:421:PRO:HG3 | 1:F:662:TYR:HE1 | 1.80 | 0.46 |
| 1:F:907:MET:SD | 1:F:907:MET:N | 2.87 | 0.46 |
| 1:F:1192:TRP:HZ3 | 1:F:1194:TYR:HB2 | 1.79 | 0.46 |
| 1:F:1324:HIS:HB3 | 1:F:1519:VAL:HG21 | 1.97 | 0.46 |
| 1:F:1415:GLU:HA | 1:F:1547:LEU:HD21 | 1.97 | 0.46 |
| 1:F:1718:PRO:HG2 | 1:F:1728:ARG:HB3 | 1.97 | 0.46 |
| 1:F:2041:LYS:HE2 | 1:F:2043:LEU:HD23 | 1.95 | 0.46 |
| 1:F:2526:GLU:HA | 1:F:2529:LYS:HG2 | 1.97 | 0.46 |
| 1:F:2674:TYR:HE1 | 1:F:2715:GLN:HE21 | 1.63 | 0.46 |
| 1:F:2979:HIS:HA | 1:F:2984:PHE:CD2 | 2.49 | 0.46 |
| 1:G:1775:LEU:HD11 | 1:G:1780:ASN:HD21 | 1.80 | 0.46 |
| 1:G:1917:ARG:NH2 | 1:H:1631:ILE:H | 2.14 | 0.46 |
| 1:G:2736:ASN:O | 1:G:2739:GLU:HG3 | 2.14 | 0.46 |
| 1:H:1081:ILE:HD12 | 1:H:1081:ILE:H | 1.80 | 0.46 |
| 1:H:1772:GLN:HB2 | 1:H:1818:LEU:HD11 | 1.97 | 0.46 |
| 1:H:2093:ARG:HD2 | 1:H:2367:TYR:HE1 | 1.81 | 0.46 |
| 1:H:2665:ARG:HE | 1:H:2726:ARG:NH2 | 2.11 | 0.46 |
| 1:H:3049:GLN:H | 1:H:3052:LEU:HD13 | 1.79 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:I:236:THR:HG21 | 1:I:239:HIS:CE1 | 2.51 | 0.46 |
| 1:I:399:ASN:HD21 | 1:I:401:ASN:HD21 | 1.62 | 0.46 |
| 1:I:846:HIS:HB2 | 1:I:1121:TYR:HB2 | 1.96 | 0.46 |
| 1:I:2356:GLU:OE1 | 1:I:2356:GLU:N | 2.41 | 0.46 |
| 1:I:2941:LEU:HD22 | 1:I:3032:PHE:CD2 | 2.49 | 0.46 |
| 1:I:2966:CYS:O | 1:I:2974:TYR:N | 2.42 | 0.46 |
| 1:J:142:ALA:HB3 | 1:J:196:HIS:CE1 | 2.50 | 0.46 |
| 1:J:1714:HIS:NE2 | 1:J:1732:CYS:SG | 2.87 | 0.46 |
| 1:J:2675:GLU:O | 1:J:2679:ASN:ND2 | 2.47 | 0.46 |
| 1:J:2794:GLU:O | 1:J:2798:SER:HB3 | 2.14 | 0.46 |
| 1:K:371:LYS:HD3 | 1:K:371:LYS:HA | 1.72 | 0.46 |
| 1:K:954:THR:HG22 | 1:K:965:PRO:HA | 1.96 | 0.46 |
| 1:K:2407:GLU:OE2 | 1:K:2424:ALA:HB1 | 2.15 | 0.46 |
| 1:K:2572:ALA:HB1 | 1:K:2671:GLU:OE1 | 2.16 | 0.46 |
| 1:K:2668:CYS:HB2 | 1:K:2735:CYS:HB2 | 1.75 | 0.46 |
| 1:L:569:GLN:HB3 | 1:L:619:GLY:HA3 | 1.96 | 0.46 |
| 1:L:706:LEU:O | 1:L:707:GLU:HG3 | 2.15 | 0.46 |
| 1:L:816:LYS:HZ2 | 1:L:818:TRP:HZ2 | 1.63 | 0.46 |
| 1:L:1085:ARG:HA | 1:L:1110:PHE:CZ | 2.49 | 0.46 |
| 1:L:1990:ILE:HG22 | 1:L:1990:ILE:O | 2.16 | 0.46 |
| 1:L:2695:THR:HG21 | 1:L:2698:TYR:HD2 | 1.81 | 0.46 |
| 1:L:3287:LEU:HB3 | 1:L:3295:LEU:HB3 | 1.97 | 0.46 |
| 1:M:606:PHE:CZ | 1:M:644:VAL:HG13 | 2.50 | 0.46 |
| 1:M:998:ILE:H | 1:M:998:ILE:HD12 | 1.80 | 0.46 |
| 1:M:1187:GLU:N | 1:M:1187:GLU:OE1 | 2.46 | 0.46 |
| 1:M:1420:CYS:HB2 | 1:M:1608:ARG:NH2 | 2.30 | 0.46 |
| 1:M:1993:SER:HA | 1:M:2015:VAL:O | 2.15 | 0.46 |
| 1:M:2621:PRO:HA | 1:M:2624:HIS:NE2 | 2.30 | 0.46 |
| 1:M:3026:SER:OG | 1:M:3030:ASN:ND2 | 2.49 | 0.46 |
| 1:N:1910:ASN:OD1 | 1:N:1911:CYS:N | 2.48 | 0.46 |
| 1:N:2242:SER:OG | 1:N:2243:VAL:N | 2.46 | 0.46 |
| 1:N:2379:GLU:OE2 | 1:N:2380:LEU:HD12 | 2.15 | 0.46 |
| 1:N:2817:VAL:HG23 | 1:N:2876:ILE:HD13 | 1.97 | 0.46 |
| 1:N:3163:ASN:ND2 | 1:N:3168:THR:OG1 | 2.48 | 0.46 |
| 1:O:167:ASP:OD1 | 1:O:303:ARG:NH2 | 2.48 | 0.46 |
| 1:O:193:GLY:HA2 | 1:O:199:SER:HB2 | 1.96 | 0.46 |
| 1:O:473:LEU:N | 1:O:775:LYS:HE3 | 2.30 | 0.46 |
| 1:O:2812:LYS:HE3 | 1:O:2840:PRO:HA | 1.95 | 0.46 |
| 1:O:2812:LYS:NZ | 1:O:2842:GLU:O | 2.42 | 0.46 |
| 1:O:3211:ASP:HB2 | 1:O:3309:ALA:HB2 | 1.97 | 0.46 |
| 1:P:1266:ARG:HB3 | 1:P:1531:ASP:HB3 | 1.97 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:P:1852:ILE:HD11 | 1:P:2013:PHE:HD2 | 1.80 | 0.46 |
| 1:P:2313:GLN:NE2 | 1:P:2318:LEU:O | 2.40 | 0.46 |
| 1:P:2430:GLY:N | 1:P:2433:GLU:OE2 | 2.44 | 0.46 |
| 1:P:2786:ILE:H | 1:P:2786:ILE:HD12 | 1.79 | 0.46 |
| 1:P:2822:CYS:HB2 | 1:P:2871:HIS:NE2 | 2.30 | 0.46 |
| 1:P:3139:SER:OG | 1:P:3142:TYR:HB3 | 2.15 | 0.46 |
| 1:P:3154:LEU:O | 1:P:3158:ASN:N | 2.48 | 0.46 |
| 1:Q:581:GLY:H | 1:Q:856:ARG:NH2 | 2.13 | 0.46 |
| 1:Q:939:TRP:HZ3 | 1:Q:1055:ASN:HB3 | 1.79 | 0.46 |
| 1:Q:1405:TYR:HA | 1:Q:1408:ASN:HD21 | 1.78 | 0.46 |
| 1:Q:1583:GLU:HB2 | 1:T:340:SER:HB3 | 1.97 | 0.46 |
| 1:Q:2583:VAL:HG21 | 1:Q:2772:PHE:HB3 | 1.97 | 0.46 |
| 1:Q:2814:SER:N | 1:Q:2838:GLY:O | 2.48 | 0.46 |
| 1:R:608:VAL:HG21 | 1:R:785:VAL:HG21 | 1.96 | 0.46 |
| 1:R:1775:LEU:HD11 | 1:R:1779:PHE:HE1 | 1.80 | 0.46 |
| 1:R:2399:LEU:HD22 | 1:R:2438:PHE:HE2 | 1.79 | 0.46 |
| 1:S:755:ILE:HD11 | 1:S:763:TYR:HD2 | 1.80 | 0.46 |
| 1:S:885:HIS:HD2 | 1:S:913:TRP:CZ3 | 2.34 | 0.46 |
| 1:S:1405:TYR:CD2 | 1:S:1406:LEU:HD22 | 2.50 | 0.46 |
| 1:S:1936:LYS:HE2 | 1:S:1936:LYS:HB2 | 1.79 | 0.46 |
| 1:S:2214:ARG:HH22 | 1:S:2216:TYR:HD1 | 1.63 | 0.46 |
| 1:S:2414:GLN:O | 1:S:2416:ASN:N | 2.47 | 0.46 |
| 1:S:2668:CYS:HB2 | 1:S:2735:CYS:HB2 | 1.43 | 0.46 |
| 1:S:2773:ASN:HD21 | 1:S:3142:TYR:HB2 | 1.80 | 0.46 |
| 1:S:2822:CYS:HA | 1:S:2828:CYS:HB3 | 1.98 | 0.46 |
| 1:T:1014:PHE:N | 1:T:1015:GLU:OE1 | 2.42 | 0.46 |
| 1:T:1847:GLU:O | 1:T:1851:GLU:HG2 | 2.15 | 0.46 |
| 1:T:2045:VAL:HG13 | 1:T:2046:ASP:OD1 | 2.15 | 0.46 |
| 1:T:2848:ASP:OD1 | 1:T:2849:ARG:N | 2.48 | 0.46 |
| 1:T:3119:HIS:O | 1:T:3122:ILE:HG22 | 2.15 | 0.46 |
| 1:A:1246:GLY:O | 1:A:1249:THR:OG1 | 2.26 | 0.46 |
| 1:A:2941:LEU:HD22 | 1:A:3032:PHE:CE2 | 2.51 | 0.46 |
| 1:A:3081:GLU:HA | 1:A:3084:PHE:HB3 | 1.97 | 0.46 |
| 1:B:2055:LEU:HB2 | 1:B:2063:LEU:HB2 | 1.95 | 0.46 |
| 1:B:3036:GLN:OE1 | 1:B:3042:HIS:N | 2.48 | 0.46 |
| 1:B:3088:HIS:CD2 | 1:B:3092:HIS:HD2 | 2.32 | 0.46 |
| 1:C:973:VAL:HB | 1:C:974:GLU:OE1 | 2.16 | 0.46 |
| 1:C:1247:SER:HA | 1:C:1250:LYS:HG2 | 1.97 | 0.46 |
| 1:C:1315:CYS:HA | 1:C:1325:TRP:CH2 | 2.50 | 0.46 |
| 1:C:1646:GLU:OE1 | 1:C:1646:GLU:N | 2.38 | 0.46 |
| 1:C:1956:ASP:OD1 | 1:C:1957:THR:N | 2.48 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:2509:SER:HB3 | 1:C:3138:ARG:HH12 | 1.80 | 0.46 |
| 1:C:2579:ARG:HG3 | 1:C:2713:ASP:OD1 | 2.14 | 0.46 |
| 1:C:3219:LEU:HD21 | 1:C:3247:ILE:HD13 | 1.95 | 0.46 |
| 1:D:450:GLN:NE2 | 1:D:454:ARG:HH11 | 2.13 | 0.46 |
| 1:D:542:VAL:HA | 1:D:549:SER:HA | 1.96 | 0.46 |
| 1:D:1452:ALA:HA | 1:D:1457:PHE:CG | 2.51 | 0.46 |
| 1:D:1869:MET:HE2 | 1:D:1869:MET:HA | 1.97 | 0.46 |
| 1:D:2326:ALA:O | 1:D:2330:MET:HG2 | 2.14 | 0.46 |
| 1:D:2412:VAL:HG21 | 1:D:2450:LEU:HD21 | 1.97 | 0.46 |
| 1:D:2527:SER:O | 1:D:2530:LYS:HG3 | 2.15 | 0.46 |
| 1:E:278:GLN:OE1 | 1:E:278:GLN:N | 2.43 | 0.46 |
| 1:E:850:ASP:O | 1:E:853:SER:OG | 2.32 | 0.46 |
| 1:E:954:THR:HA | 1:E:965:PRO:HA | 1.98 | 0.46 |
| 1:E:1111:GLU:N | 1:E:1111:GLU:OE1 | 2.48 | 0.46 |
| 1:E:1328:LEU:HD21 | 1:E:1519:VAL:HG22 | 1.97 | 0.46 |
| 1:E:1919:PRO:HG3 | 1:E:1940:LYS:HZ1 | 1.79 | 0.46 |
| 1:E:2963:PRO:HD2 | 1:E:2965:LEU:HD23 | 1.98 | 0.46 |
| 1:G:326:ILE:O | 1:G:345:ALA:HB3 | 2.15 | 0.46 |
| 1:G:914:HIS:NE2 | 1:G:1053:HIS:HE1 | 2.13 | 0.46 |
| 1:G:1876:SER:HA | 1:G:1881:PHE:CD1 | 2.50 | 0.46 |
| 1:G:2112:ARG:HH11 | 1:G:2211:PRO:HG3 | 1.81 | 0.46 |
| 1:G:2585:LEU:HD22 | 1:G:2706:PHE:CE1 | 2.48 | 0.46 |
| 1:G:2668:CYS:HB2 | 1:G:2735:CYS:HB2 | 1.69 | 0.46 |
| 1:H:31:THR:O | 1:H:36:GLN:NE2 | 2.35 | 0.46 |
| 1:H:38:LEU:HD21 | 1:H:213:PHE:CZ | 2.51 | 0.46 |
| 1:H:2355:LYS:HA | 1:H:2358:PHE:HE1 | 1.79 | 0.46 |
| 1:I:947:PRO:HB2 | 1:I:949:ILE:HG22 | 1.97 | 0.46 |
| 1:I:1977:GLU:O | 1:I:2078:LYS:NZ | 2.42 | 0.46 |
| 1:I:2797:ARG:HA | 1:I:2801:ARG:HH12 | 1.79 | 0.46 |
| 1:J:1857:ILE:HB | 1:J:1884:HIS:CE1 | 2.50 | 0.46 |
| 1:K:580:TYR:CG | 1:K:958:PRO:HG2 | 2.51 | 0.46 |
| 1:K:950:VAL:HG12 | 1:K:968:PHE:CD2 | 2.50 | 0.46 |
| 1:K:1830:LEU:HG | 1:K:1834:PHE:CE2 | 2.47 | 0.46 |
| 1:K:3074:GLU:O | 1:K:3136:ARG:NH2 | 2.45 | 0.46 |
| 1:L:657:LYS:NZ | 1:L:721:ASP:HA | 2.30 | 0.46 |
| 1:L:1542:GLN:HA | 1:L:1545:GLU:OE2 | 2.15 | 0.46 |
| 1:L:1550:GLN:HA | 1:L:1553:GLN:HE22 | 1.80 | 0.46 |
| 1:L:2183:TRP:CG | 1:L:2271:ILE:HD11 | 2.50 | 0.46 |
| 1:L:2377:LEU:HA | 1:L:2380:LEU:HB2 | 1.96 | 0.46 |
| 1:L:2421:ARG:CZ | 1:L:2423:GLY:HA2 | 2.45 | 0.46 |
| 1:L:2944:LEU:HA | 1:L:3002:LYS:HE2 | 1.97 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:L:3124:ARG:O | 1:L:3127:GLN:HG3 | 2.14 | 0.46 |
| 1:M:278:GLN:OE1 | 1:M:278:GLN:N | 2.37 | 0.46 |
| 1:M:926:ARG:HH12 | 1:M:931:GLN:C | 2.22 | 0.46 |
| 1:M:1835:LEU:HA | 1:M:1838:LEU:HD12 | 1.97 | 0.46 |
| 1:M:2542:ARG:NE | 1:M:2588:ALA:O | 2.48 | 0.46 |
| 1:N:130:ILE:O | 1:N:138:HIS:HA | 2.15 | 0.46 |
| 1:N:160:GLN:NE2 | 1:N:161:LEU:HG | 2.27 | 0.46 |
| 1:N:1857:ILE:HB | 1:N:1884:HIS:CE1 | 2.50 | 0.46 |
| 1:N:2622:PHE:O | 1:N:2636:ARG:NH2 | 2.48 | 0.46 |
| 1:N:2675:GLU:O | 1:N:2679:ASN:ND2 | 2.48 | 0.46 |
| 1:N:2798:SER:OG | 1:N:2799:GLU:OE1 | 2.32 | 0.46 |
| 1:O:635:PRO:O | 1:O:638:ILE:HG12 | 2.15 | 0.46 |
| 1:O:866:LEU:HD23 | 1:O:967:PRO:HB2 | 1.96 | 0.46 |
| 1:O:1741:GLN:N | 1:O:1741:GLN:OE1 | 2.49 | 0.46 |
| 1:O:2297:THR:O | 1:O:2300:THR:OG1 | 2.28 | 0.46 |
| 1:O:3389:VAL:HG22 | 1:O:3401:ARG:HG2 | 1.96 | 0.46 |
| 1:P:71:ARG:O | 1:P:75:VAL:HG23 | 2.15 | 0.46 |
| 1:P:300:LEU:O | 1:P:304:ARG:HG2 | 2.15 | 0.46 |
| 1:P:567:SER:OG | 1:P:623:TYR:O | 2.28 | 0.46 |
| 1:P:974:GLU:OE2 | 1:P:1035:TYR:OH | 2.33 | 0.46 |
| 1:P:1372:SER:O | 1:P:1374:THR:OG1 | 2.32 | 0.46 |
| 1:P:1748:VAL:HA | 1:P:1751:GLU:HG2 | 1.96 | 0.46 |
| 1:P:2948:ASP:OD1 | 1:P:2948:ASP:N | 2.48 | 0.46 |
| 1:P:3020:LEU:HD11 | 1:P:3025:THR:HB | 1.97 | 0.46 |
| 1:P:3036:GLN:OE1 | 1:P:3042:HIS:N | 2.48 | 0.46 |
| 1:Q:674:LEU:HD22 | 1:Q:695:ARG:NH2 | 2.30 | 0.46 |
| 1:Q:866:LEU:HD22 | 1:Q:968:PHE:HE1 | 1.80 | 0.46 |
| 1:Q:950:VAL:HG12 | 1:Q:968:PHE:CD2 | 2.50 | 0.46 |
| 1:Q:1307:HIS:HB3 | 1:Q:1312:VAL:HG11 | 1.98 | 0.46 |
| 1:Q:1956:ASP:OD1 | 1:Q:1957:THR:N | 2.48 | 0.46 |
| 1:Q:2224:THR:HB | 1:Q:2226:ARG:NH1 | 2.25 | 0.46 |
| 1:Q:2624:HIS:HB2 | 1:Q:2633:LYS:HZ1 | 1.80 | 0.46 |
| 1:Q:2654:PHE:HA | 1:Q:2657:GLN:NE2 | 2.30 | 0.46 |
| 1:Q:2668:CYS:O | 1:Q:2671:GLU:HG3 | 2.15 | 0.46 |
| 1:Q:2849:ARG:HA | 1:Q:2849:ARG:HH11 | 1.79 | 0.46 |
| 1:R:6:LYS:HD2 | 1:R:11:LEU:HD13 | 1.97 | 0.46 |
| 1:R:887:GLN:NE2 | 1:R:889:ASN:HB2 | 2.30 | 0.46 |
| 1:R:1694:ALA:O | 1:R:1697:SER:OG | 2.29 | 0.46 |
| 1:R:2204:LYS:HB2 | 1:R:2204:LYS:HE2 | 1.70 | 0.46 |
| 1:R:2769:TYR:HB2 | 1:R:2774:TYR:CE1 | 2.50 | 0.46 |
| 1:S:193:GLY:HA3 | 1:S:201:SER:N | 2.30 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:S:938:ASP:HA | 1:S:1055:ASN:ND2 | 2.31 | 0.46 |
| 1:S:1494:GLN:HE21 | 1:S:1500:ASN:HD21 | 1.63 | 0.46 |
| 1:S:1596:LEU:HD12 | 1:S:1597:GLY:N | 2.30 | 0.46 |
| 1:S:2604:THR:HA | 1:S:2654:PHE:HE1 | 1.80 | 0.46 |
| 1:S:2980:GLY:HA2 | 1:S:3258:TYR:CE1 | 2.47 | 0.46 |
| 1:T:695:ARG:HH21 | 1:T:696:PRO:HD2 | 1.81 | 0.46 |
| 1:T:1284:ARG:NH2 | 1:T:1379:PRO:HB3 | 2.30 | 0.46 |
| 1:T:1380:PHE:HA | 1:T:1455:PRO:HG3 | 1.97 | 0.46 |
| 1:T:1854:HIS:O | 1:T:1884:HIS:HE1 | 1.97 | 0.46 |
| 1:T:2616:ASP:HB3 | 1:T:2620:ASN:HD22 | 1.80 | 0.46 |
| 1:T:2655:TYR:O | 1:T:2659:LEU:HD23 | 2.14 | 0.46 |
| 1:T:2718:ILE:HD11 | 1:T:2779:LEU:HB2 | 1.97 | 0.46 |
| 1:T:3017:SER:O | 1:T:3055:ARG:NH2 | 2.27 | 0.46 |
| 1:T:3043:GLN:N | 1:T:3043:GLN:OE1 | 2.48 | 0.46 |
| 1:A:608:VAL:HG11 | 1:A:785:VAL:HG21 | 1.97 | 0.46 |
| 1:A:2311:GLU:OE1 | 1:A:2377:LEU:HD21 | 2.15 | 0.46 |
| 1:A:2668:CYS:HB2 | 1:A:2735:CYS:HB2 | 1.65 | 0.46 |
| 1:A:2724:ARG:NH1 | 1:A:2730:TYR:OH | 2.38 | 0.46 |
| 1:B:229:LEU:HB3 | 1:B:233:ARG:NH2 | 2.30 | 0.46 |
| 1:B:244:VAL:HG23 | 1:B:248:ARG:HE | 1.81 | 0.46 |
| 1:B:842:HIS:NE2 | 1:B:844:GLU:HB2 | 2.31 | 0.46 |
| 1:B:869:LEU:HB3 | 1:B:928:LYS:HE3 | 1.98 | 0.46 |
| 1:B:998:ILE:HA | 1:B:1001:MET:HG3 | 1.96 | 0.46 |
| 1:B:1626:ASP:OD1 | 1:B:1627:SER:N | 2.48 | 0.46 |
| 1:B:1990:ILE:HG22 | 3:b:2:NAG:H81 | 1.96 | 0.46 |
| 1:B:3008:ILE:HD13 | 1:B:3116:MET:HB3 | 1.97 | 0.46 |
| 1:C:559:VAL:HG13 | 1:C:633:PHE:CE2 | 2.50 | 0.46 |
| 1:C:1137:GLN:O | 1:C:1141:LEU:HD23 | 2.15 | 0.46 |
| 1:C:2602:ASP:HA | 1:C:2711:ASN:HD21 | 1.81 | 0.46 |
| 1:C:2604:THR:HG23 | 1:C:2782:HIS:NE2 | 2.31 | 0.46 |
| 1:D:543:ASP:HB3 | 1:D:546:SER:HB3 | 1.96 | 0.46 |
| 1:D:740:LEU:HB2 | 1:D:785:VAL:HB | 1.97 | 0.46 |
| 1:D:1985:PHE:O | 1:D:2029:LEU:HD12 | 2.15 | 0.46 |
| 1:D:2001:CYS:HB2 | 1:D:2050:THR:OG1 | 2.16 | 0.46 |
| 1:E:764:GLU:OE2 | 1:E:766:ALA:N | 2.48 | 0.46 |
| 1:E:1144:GLN:HA | 1:E:1148:ARG:HH22 | 1.81 | 0.46 |
| 1:E:2034:ILE:O | 1:E:2038:LEU:HD23 | 2.15 | 0.46 |
| 1:E:2364:ASN:OD1 | 1:E:2366:ARG:NH2 | 2.48 | 0.46 |
| 1:E:2399:LEU:HB3 | 1:E:2436:TRP:HH2 | 1.79 | 0.46 |
| 1:E:2521:THR:O | 1:E:2525:THR:OG1 | 2.28 | 0.46 |
| 1:E:2668:CYS:HB2 | 1:E:2735:CYS:HB2 | 1.63 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:E:2794:GLU:HA | 1:E:2797:ARG:HG3 | 1.96 | 0.46 |
| 1:E:3207:LEU:O | 1:E:3212:ARG:NH1 | 2.48 | 0.46 |
| 1:E:3276:ASN:OD1 | 1:E:3277:ALA:N | 2.48 | 0.46 |
| 1:F:533:PRO:HB2 | 1:F:535:ILE:HD12 | 1.96 | 0.46 |
| 1:F:543:ASP:HB3 | 1:F:546:SER:HB3 | 1.97 | 0.46 |
| 1:F:744:ASN:HB3 | 1:F:779:TRP:NE1 | 2.30 | 0.46 |
| 1:F:842:HIS:NE2 | 1:F:844:GLU:HB2 | 2.30 | 0.46 |
| 1:F:905:HIS:HA | 1:F:910:PHE:CD2 | 2.49 | 0.46 |
| 1:F:3106:LEU:HA | 1:F:3109:SER:HB3 | 1.97 | 0.46 |
| 1:G:525:TRP:CD1 | 1:G:643:ASN:HD22 | 2.33 | 0.46 |
| 1:G:597:ARG:HD3 | 1:G:658:ARG:CZ | 2.45 | 0.46 |
| 1:G:1722:TYR:CD2 | 1:G:1724:GLU:HB3 | 2.51 | 0.46 |
| 1:G:2306:TRP:CD1 | 1:G:2310:GLN:HE22 | 2.34 | 0.46 |
| 1:G:2475:ALA:HB2 | 1:G:2481:LEU:HD11 | 1.95 | 0.46 |
| 1:G:2676:VAL:HG11 | 1:G:2851:PHE:CZ | 2.50 | 0.46 |
| 1:G:2762:ARG:HB2 | 1:G:2765:ASP:OD1 | 2.15 | 0.46 |
| 1:G:3015:ARG:NH1 | 1:G:3016:PRO:O | 2.49 | 0.46 |
| 1:G:3122:ILE:O | 1:G:3125:ILE:HG22 | 2.15 | 0.46 |
| 1:H:246:LEU:HA | 1:H:249:LYS:HE2 | 1.98 | 0.46 |
| 1:H:2152:PRO:HD2 | 1:H:2329:TYR:HD2 | 1.79 | 0.46 |
| 1:H:2623:GLU:OE1 | 1:H:2623:GLU:N | 2.48 | 0.46 |
| 1:H:2816:ASP:OD1 | 1:H:2817:VAL:N | 2.47 | 0.46 |
| 1:I:957:ASN:HD21 | 1:I:959:GLU:HB3 | 1.80 | 0.46 |
| 1:J:735:ARG:HE | 1:J:736:THR:H | 1.62 | 0.46 |
| 1:J:1356:ARG:NH1 | 1:J:1356:ARG:HA | 2.30 | 0.46 |
| 1:J:1683:LEU:O | 1:J:1688:ARG:NH1 | 2.48 | 0.46 |
| 1:J:2273:TYR:HE1 | 1:J:2476:VAL:HG12 | 1.80 | 0.46 |
| 1:J:2945:GLN:HG3 | 1:J:3035:TYR:HE1 | 1.80 | 0.46 |
| 1:J:3183:PHE:HB2 | 1:J:3185:TYR:CD1 | 2.51 | 0.46 |
| 1:K:164:MET:HE1 | 1:K:187:HIS:CE1 | 2.49 | 0.46 |
| 1:K:204:GLU:OE2 | 1:K:354:ALA:N | 2.49 | 0.46 |
| 1:K:444:GLU:HB3 | 1:K:518:PHE:HZ | 1.80 | 0.46 |
| 1:K:1475:GLN:HB3 | 1:K:1482:ASP:HB3 | 1.97 | 0.46 |
| 1:K:2018:GLY:N | 1:K:2021:GLU:OE2 | 2.48 | 0.46 |
| 1:K:3214:TYR:CD1 | 1:K:3265:ASP:HA | 2.44 | 0.46 |
| 1:K:3305:ILE:HA | 1:K:3315:VAL:O | 2.16 | 0.46 |
| 1:K:3329:LYS:HE3 | 1:L:3357:TYR:HD2 | 1.79 | 0.46 |
| 1:L:2149:HIS:HA | 1:L:2154:PHE:CD2 | 2.46 | 0.46 |
| 1:L:2375:LEU:HD22 | 1:L:2379:GLU:HG2 | 1.98 | 0.46 |
| 1:M:913:TRP:CD1 | 1:M:1088:LEU:HD21 | 2.50 | 0.46 |
| 1:M:1405:TYR:HA | 1:M:1408:ASN:HD21 | 1.81 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:M:1494:GLN:NE2 | 1:M:1495:PRO:O | 2.49 | 0.46 |
| 1:M:1847:GLU:HA | 1:M:1850:PHE:HB3 | 1.97 | 0.46 |
| 1:M:2414:GLN:HE21 | 1:M:2453:LEU:HD22 | 1.81 | 0.46 |
| 1:M:3227:THR:OG1 | 1:M:3245:PHE:O | 2.16 | 0.46 |
| 1:N:554:PHE:O | 1:N:568:ARG:NH2 | 2.49 | 0.46 |
| 1:N:705:GLU:N | 1:N:705:GLU:OE1 | 2.49 | 0.46 |
| 1:N:1753:ALA:O | 1:N:1757:ARG:HG2 | 2.15 | 0.46 |
| 1:O:3095:VAL:HG13 | 1:O:3103:MET:SD | 2.54 | 0.46 |
| 1:P:588:ASP:HA | 1:P:591:LEU:HD12 | 1.98 | 0.46 |
| 1:P:756:LYS:HD3 | 1:P:762:SER:HB2 | 1.98 | 0.46 |
| 1:P:1100:ASP:OD2 | 1:P:1103:THR:OG1 | 2.27 | 0.46 |
| 1:P:1849:GLN:O | 1:P:1852:ILE:HG22 | 2.16 | 0.46 |
| 1:P:3058:GLN:NE2 | 1:P:3268:ASP:OD2 | 2.49 | 0.46 |
| 1:P:3211:ASP:OD1 | 1:P:3309:ALA:N | 2.49 | 0.46 |
| 1:Q:348:ILE:HD11 | 1:Q:367:PHE:CD1 | 2.50 | 0.46 |
| 1:Q:1064:GLN:HE21 | 1:Q:1115:TYR:HE1 | 1.63 | 0.46 |
| 1:Q:1525:HIS:C | 1:Q:1526:PHE:HD1 | 2.22 | 0.46 |
| 1:Q:2986:HIS:HD2 | 1:Q:3177:ILE:HG21 | 1.81 | 0.46 |
| 1:R:81:LEU:HD12 | 1:R:86:LEU:HD13 | 1.96 | 0.46 |
| 1:R:254:PHE:HD2 | 1:R:264:THR:HB | 1.80 | 0.46 |
| 1:R:1345:SER:OG | 1:R:1346:VAL:N | 2.48 | 0.46 |
| 1:R:1560:PHE:CZ | 1:R:1573:LEU:HD11 | 2.45 | 0.46 |
| 1:R:2376:ASN:ND2 | 1:R:2378:ASP:HB2 | 2.30 | 0.46 |
| 1:S:222:ILE:O | 1:S:225:ILE:HG22 | 2.16 | 0.46 |
| 1:S:348:ILE:HD11 | 1:S:367:PHE:CD1 | 2.50 | 0.46 |
| 1:S:1405:TYR:HA | 1:S:1408:ASN:HD21 | 1.80 | 0.46 |
| 1:S:1693:LEU:O | 1:S:1696:GLN:HG3 | 2.16 | 0.46 |
| 1:S:1811:ARG:HH22 | 1:S:1880:ILE:HB | 1.80 | 0.46 |
| 1:S:1811:ARG:HH12 | 1:S:1880:ILE:HD12 | 1.80 | 0.46 |
| 1:S:2990:LEU:HB3 | 1:S:3157:PHE:CE2 | 2.50 | 0.46 |
| 1:S:3382:GLU:N | 1:S:3386:TYR:OH | 2.49 | 0.46 |
| 1:T:930:PHE:CZ | 1:T:932:ASP:HB2 | 2.50 | 0.46 |
| 1:T:1295:ILE:HG21 | 1:T:1333:VAL:HG23 | 1.97 | 0.46 |
| 1:T:1772:GLN:HB2 | 1:T:1818:LEU:HD11 | 1.97 | 0.46 |
| 1:T:2513:VAL:HG11 | 1:T:2515:LYS:HZ3 | 1.80 | 0.46 |
| 1:T:2602:ASP:HA | 1:T:2711:ASN:ND2 | 2.30 | 0.46 |
| 1:T:3163:ASN:ND2 | 1:T:3168:THR:OG1 | 2.48 | 0.46 |
| 1:A:647:LEU:HA | 1:A:650:ILE:HG12 | 1.97 | 0.46 |
| 1:A:926:ARG:NH1 | 1:A:931:GLN:O | 2.43 | 0.46 |
| 1:A:1646:GLU:OE1 | 1:D:483:ARG:NH2 | 2.48 | 0.46 |
| 1:A:1749:GLN:HE22 | 1:A:1932:ASP:HB3 | 1.79 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:2780:ASN:OD1 | 1:A:2784:LEU:N | 2.49 | 0.46 |
| 1:B:71:ARG:NH1 | 1:B:273:LEU:O | 2.38 | 0.46 |
| 1:B:412:PRO:HG3 | 1:B:665:HIS:CD2 | 2.51 | 0.46 |
| 1:B:441:THR:HB | 1:B:444:GLU:OE1 | 2.16 | 0.46 |
| 1:B:525:TRP:HB2 | 1:B:586:LEU:HD13 | 1.97 | 0.46 |
| 1:B:1192:TRP:HZ3 | 1:B:1194:TYR:HB2 | 1.80 | 0.46 |
| 1:C:442:ASP:OD1 | 1:C:443:GLU:N | 2.48 | 0.46 |
| 1:C:1079:CYS:O | 1:D:2492:ILE:HD13 | 2.16 | 0.46 |
| 1:C:2538:GLN:NE2 | 1:C:2592:GLN:HE22 | 2.13 | 0.46 |
| 1:D:69:TRP:O | 1:D:72:LEU:HG | 2.15 | 0.46 |
| 1:D:80:LYS:HZ1 | 1:D:261:ILE:HG13 | 1.80 | 0.46 |
| 1:D:728:ASP:HB3 | 1:D:836:HIS:CD2 | 2.50 | 0.46 |
| 1:D:750:LEU:HD12 | 1:D:768:LEU:O | 2.15 | 0.46 |
| 1:D:837:GLU:N | 1:D:837:GLU:OE2 | 2.49 | 0.46 |
| 1:D:1654:SER:OG | 1:D:1655:LEU:N | 2.48 | 0.46 |
| 1:E:442:ASP:N | 1:E:442:ASP:OD1 | 2.48 | 0.46 |
| 1:E:1677:ARG:C | 1:E:1678:LYS:HD3 | 2.41 | 0.46 |
| 1:E:2266:VAL:HG21 | 1:E:2442:TYR:CD1 | 2.51 | 0.46 |
| 1:E:2941:LEU:HA | 1:E:2944:LEU:HG | 1.98 | 0.46 |
| 1:E:3211:ASP:OD1 | 1:E:3212:ARG:N | 2.47 | 0.46 |
| 1:F:602:PHE:O | 1:F:606:PHE:HB2 | 2.16 | 0.46 |
| 1:F:753:LEU:HB3 | 1:F:766:ALA:HB3 | 1.97 | 0.46 |
| 1:F:1351:TRP:HZ3 | 1:F:1463:ASN:HB3 | 1.81 | 0.46 |
| 1:F:2243:VAL:HG23 | 1:F:2244:LEU:HD12 | 1.95 | 0.46 |
| 1:F:3395:ARG:C | 1:F:3401:ARG:HH12 | 2.24 | 0.46 |
| 1:G:169:LEU:HD12 | 1:G:300:LEU:HD21 | 1.98 | 0.46 |
| 1:G:811:LYS:HD2 | 1:G:815:GLY:HA2 | 1.97 | 0.46 |
| 1:G:811:LYS:HE2 | 1:G:811:LYS:HB2 | 1.79 | 0.46 |
| 1:G:866:LEU:HD13 | 1:G:968:PHE:CE1 | 2.44 | 0.46 |
| 1:G:1485:SER:HB3 | 1:G:1492:MET:HE2 | 1.97 | 0.46 |
| 1:G:1513:TYR:HB3 | 1:G:1518:ASP:OD2 | 2.15 | 0.46 |
| 1:G:1721:PRO:HD3 | 1:G:1729:TYR:CE2 | 2.51 | 0.46 |
| 1:G:1865:LYS:NZ | 1:G:1867:HIS:H | 2.14 | 0.46 |
| 1:G:2257:TYR:OH | 1:G:2306:TRP:HZ2 | 1.99 | 0.46 |
| 1:G:2266:VAL:HG21 | 1:G:2442:TYR:CD1 | 2.51 | 0.46 |
| 1:G:2648:ARG:HD2 | 1:G:2656:ARG:HH22 | 1.80 | 0.46 |
| 1:G:2960:HIS:HA | 1:G:2987:TRP:HH2 | 1.80 | 0.46 |
| 1:G:3046:ARG:NH2 | 1:G:3112:ASP:OD2 | 2.47 | 0.46 |
| 1:H:524:ASP:HA | 1:H:643:ASN:ND2 | 2.30 | 0.46 |
| 1:H:655:GLN:HG2 | 1:H:662:TYR:HB3 | 1.97 | 0.46 |
| 1:H:1023:ASN:ND2 | 1:H:1184:LEU:HB2 | 2.30 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:H:2469:LEU:HD23 | 1:H:2491:ILE:HD11 | 1.96 | 0.46 |
| 1:I:231:LYS:HE3 | 1:I:237:TYR:CE1 | 2.50 | 0.46 |
| 1:I:914:HIS:CE1 | 1:I:1053:HIS:HE1 | 2.32 | 0.46 |
| 1:I:1415:GLU:HB3 | 1:I:1547:LEU:HD12 | 1.98 | 0.46 |
| 1:I:2287:HIS:CD2 | 1:I:2430:GLY:HA3 | 2.50 | 0.46 |
| 1:I:3231:LYS:HB2 | 1:I:3284:GLN:HG3 | 1.98 | 0.46 |
| 1:J:38:LEU:HB3 | 1:J:73:TYR:OH | 2.15 | 0.46 |
| 1:J:480:PRO:O | 1:J:485:ARG:NH1 | 2.48 | 0.46 |
| 1:K:1016:VAL:O | 1:K:1019:GLU:HG3 | 2.14 | 0.46 |
| 1:K:1284:ARG:HE | 1:K:1379:PRO:HG3 | 1.80 | 0.46 |
| 1:L:148:ARG:NH2 | 1:L:151:GLN:OE1 | 2.48 | 0.46 |
| 1:L:1324:HIS:HA | 1:L:1519:VAL:HG11 | 1.98 | 0.46 |
| 1:M:2624:HIS:HB2 | 1:M:2633:LYS:HZ1 | 1.79 | 0.46 |
| 1:N:408:GLY:HA3 | 1:N:669:THR:HG21 | 1.98 | 0.46 |
| 1:N:1134:PRO:O | 1:N:1138:ARG:NE | 2.33 | 0.46 |
| 1:N:1910:ASN:O | 1:N:1913:LEU:HG | 2.15 | 0.46 |
| 1:N:2736:ASN:OD1 | 1:O:2893:SER:OG | 2.26 | 0.46 |
| 1:N:3234:PRO:HG2 | 1:N:3237:GLY:HA3 | 1.97 | 0.46 |
| 1:N:3374:ASP:HB3 | 1:N:3377:VAL:HG21 | 1.97 | 0.46 |
| 1:O:1474:LEU:HD11 | 1:O:1543:LEU:HD11 | 1.97 | 0.46 |
| 1:O:2183:TRP:O | 1:O:2242:SER:OG | 2.23 | 0.46 |
| 1:P:56:VAL:HB | 1:P:355:ASN:O | 2.15 | 0.46 |
| 1:P:111:ILE:HG23 | 1:P:122:LYS:HB2 | 1.96 | 0.46 |
| 1:P:507:VAL:HG21 | 1:P:638:ILE:HD11 | 1.96 | 0.46 |
| 1:P:958:PRO:C | 1:P:961:ASN:H | 2.23 | 0.46 |
| 1:P:1223:VAL:HG13 | 1:P:1231:ILE:HB | 1.98 | 0.46 |
| 1:P:1274:GLY:O | 1:P:1277:GLU:HG3 | 2.15 | 0.46 |
| 1:Q:1350:ASP:OD2 | 1:Q:1352:THR:OG1 | 2.33 | 0.46 |
| 1:Q:2048:ALA:HA | 1:R:1493:ARG:NE | 2.30 | 0.46 |
| 1:R:738:VAL:HG23 | 1:R:789:ILE:HG13 | 1.97 | 0.46 |
| 1:R:2132:VAL:HG13 | 1:R:2287:HIS:HD1 | 1.79 | 0.46 |
| 1:R:2137:PRO:HD2 | 1:R:2143:LYS:HE2 | 1.97 | 0.46 |
| 1:S:612:LEU:HD21 | 1:S:768:LEU:HD12 | 1.98 | 0.46 |
| 1:S:1100:ASP:OD2 | 1:S:1102:ILE:HG22 | 2.16 | 0.46 |
| 1:T:63:MET:HE1 | 1:T:65:THR:HB | 1.98 | 0.46 |
| 1:T:788:GLU:CD | 1:T:791:ASP:H | 2.23 | 0.46 |
| 1:T:1842:ASN:OD1 | 1:T:1843:TYR:N | 2.48 | 0.46 |
| 1:A:304:ARG:HH21 | 1:A:411:ARG:CZ | 2.29 | 0.46 |
| 1:A:980:ARG:NE | 1:A:1046:ASP:OD2 | 2.35 | 0.46 |
| 1:A:1301:PHE:CD1 | 1:A:1302:PRO:HA | 2.50 | 0.46 |
| 1:A:1390:LYS:HD2 | 1:A:1443:TYR:CE2 | 2.50 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:1506:GLU:OE1 | 1:A:1507:PHE:HB2 | 2.14 | 0.46 |
| 1:A:2581:PHE:O | 1:A:2584:THR:HG22 | 2.15 | 0.46 |
| 1:A:3263:LYS:HD2 | 1:A:3305:ILE:HD11 | 1.98 | 0.46 |
| 1:A:3287:LEU:HD23 | 1:A:3287:LEU:H | 1.81 | 0.46 |
| 1:B:69:TRP:O | 1:B:72:LEU:HG | 2.16 | 0.46 |
| 1:B:866:LEU:O | 1:B:869:LEU:HG | 2.14 | 0.46 |
| 1:B:2469:LEU:HD11 | 1:B:2489:PRO:HG2 | 1.96 | 0.46 |
| 1:C:1356:ARG:HB2 | 1:C:1357:GLN:OE1 | 2.16 | 0.46 |
| 1:C:2080:ARG:HB3 | 1:C:2314:LYS:HZ1 | 1.79 | 0.46 |
| 1:C:2553:TYR:CD2 | 1:C:2554:PRO:HA | 2.51 | 0.46 |
| 1:D:1276:VAL:O | 1:D:1279:LEU:HG | 2.15 | 0.46 |
| 1:D:1324:HIS:CD2 | 1:D:1324:HIS:H | 2.33 | 0.46 |
| 1:D:1550:GLN:HA | 1:D:1553:GLN:HE22 | 1.79 | 0.46 |
| 1:D:1995:HIS:ND1 | 1:D:2013:PHE:O | 2.47 | 0.46 |
| 1:E:77:LEU:HD22 | 1:E:213:PHE:CZ | 2.51 | 0.46 |
| 1:E:1424:ILE:O | 1:E:1428:ILE:HG12 | 2.15 | 0.46 |
| 1:E:1452:ALA:HA | 1:E:1457:PHE:CG | 2.51 | 0.46 |
| 1:E:1896:GLN:NE2 | 1:E:1906:PRO:O | 2.33 | 0.46 |
| 1:E:1903:GLY:HA3 | 1:F:1667:GLN:HB2 | 1.96 | 0.46 |
| 1:E:2382:GLU:O | 1:E:2385:ARG:HG2 | 2.15 | 0.46 |
| 1:E:2581:PHE:HE1 | 1:E:2706:PHE:HZ | 1.62 | 0.46 |
| 1:E:3315:VAL:HG23 | 1:E:3337:ARG:HG3 | 1.97 | 0.46 |
| 1:F:1772:GLN:HB2 | 1:F:1818:LEU:HD11 | 1.96 | 0.46 |
| 1:G:1732:CYS:C | 1:G:1734:HIS:HD1 | 2.19 | 0.46 |
| 1:G:2404:THR:CA | 1:G:2429:GLY:O | 2.63 | 0.46 |
| 1:H:687:ASN:HB3 | 1:H:690:THR:OG1 | 2.16 | 0.46 |
| 1:H:984:ASP:OD2 | 1:H:985:GLU:N | 2.48 | 0.46 |
| 1:H:2109:ALA:HA | 1:H:2112:ARG:HG2 | 1.98 | 0.46 |
| 1:H:2754:ASN:HD22 | 1:H:2757:ILE:HG12 | 1.81 | 0.46 |
| 1:H:2930:SER:HA | 1:I:2943:LYS:HD2 | 1.97 | 0.46 |
| 1:I:953:GLU:HB2 | 1:I:969:HIS:CD2 | 2.50 | 0.46 |
| 1:I:998:ILE:H | 1:I:998:ILE:HD12 | 1.80 | 0.46 |
| 1:I:1720:CYS:HB2 | 1:I:1731:CYS:HB3 | 1.77 | 0.46 |
| 1:I:2258:CYS:HA | 1:I:2261:GLU:HG2 | 1.97 | 0.46 |
| 1:I:2517:ILE:HD13 | 1:I:2611:PRO:HB3 | 1.98 | 0.46 |
| 1:I:2960:HIS:HE1 | 1:I:3119:HIS:HE1 | 1.64 | 0.46 |
| 1:J:474:PRO:HG2 | 1:J:476:ARG:HH22 | 1.81 | 0.46 |
| 1:J:1802:ILE:HD11 | 1:J:1805:GLU:HB2 | 1.96 | 0.46 |
| 1:J:2413:CYS:HA | 1:J:2419:CYS:HB3 | 1.98 | 0.46 |
| 1:J:3124:ARG:HD2 | 1:J:3187:PHE:CD2 | 2.51 | 0.46 |
| 1:K:197:ASP:OD1 | 1:K:197:ASP:N | 2.48 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:K:284:ASP:OD1 | 1:K:285:ASP:N | 2.49 | 0.46 |
| 1:K:441:THR:OG1 | 1:K:444:GLU:OE1 | 2.33 | 0.46 |
| 1:K:735:ARG:HD3 | 1:K:737:PHE:HZ | 1.80 | 0.46 |
| 1:K:1749:GLN:HE22 | 1:K:1932:ASP:HB3 | 1.80 | 0.46 |
| 1:K:2101:ALA:O | 1:K:2104:THR:OG1 | 2.24 | 0.46 |
| 1:K:2805:ASN:N | 1:K:2893:SER:O | 2.42 | 0.46 |
| 1:L:1350:ASP:HA | 1:L:1463:ASN:HD21 | 1.80 | 0.46 |
| 1:L:1433:LEU:HA | 1:L:1436:LEU:HB2 | 1.98 | 0.46 |
| 1:L:2637:SER:HB3 | 1:L:2686:GLY:O | 2.15 | 0.46 |
| 1:L:2676:VAL:HA | 1:L:2679:ASN:HD21 | 1.81 | 0.46 |
| 1:L:2718:ILE:HD11 | 1:L:2779:LEU:HB2 | 1.96 | 0.46 |
| 1:L:3332:VAL:HB | 1:L:3336:THR:HB | 1.97 | 0.46 |
| 1:M:861:SER:OG | 1:M:929:GLY:O | 2.34 | 0.46 |
| 1:M:1773:ASN:OD1 | 1:M:1774:SER:N | 2.47 | 0.46 |
| 1:M:2112:ARG:NH2 | 1:M:2208:LEU:HD21 | 2.30 | 0.46 |
| 1:M:2190:LEU:HD21 | 1:M:2194:PHE:HB3 | 1.97 | 0.46 |
| 1:M:2196:GLU:OE2 | 1:M:2210:ASN:HB2 | 2.15 | 0.46 |
| 1:M:2533:ARG:CZ | 1:M:2621:PRO:HD3 | 2.44 | 0.46 |
| 1:M:3350:ASN:O | 1:M:3391:SER:N | 2.45 | 0.46 |
| 1:N:567:SER:OG | 1:N:623:TYR:O | 2.30 | 0.46 |
| 1:N:1284:ARG:HH21 | 1:N:1287:GLN:HG2 | 1.80 | 0.46 |
| 1:N:1362:ILE:HG22 | 1:N:1380:PHE:HB3 | 1.98 | 0.46 |
| 1:N:1539:THR:HG22 | 1:N:1542:GLN:NE2 | 2.30 | 0.46 |
| 1:N:1743:HIS:HD2 | 1:N:1885:HIS:CD2 | 2.33 | 0.46 |
| 1:O:584:THR:HG23 | 1:O:587:PHE:H | 1.79 | 0.46 |
| 1:O:750:LEU:HG | 1:O:768:LEU:O | 2.16 | 0.46 |
| 1:O:980:ARG:NE | 1:O:1046:ASP:OD2 | 2.35 | 0.46 |
| 1:O:1161:SER:OG | 1:O:1185:GLY:N | 2.27 | 0.46 |
| 1:O:1539:THR:H | 1:O:1542:GLN:HE22 | 1.63 | 0.46 |
| 1:O:1732:CYS:C | 1:O:1734:HIS:HD1 | 2.19 | 0.46 |
| 1:O:2159:ARG:HH22 | 1:O:2360:TYR:HD2 | 1.64 | 0.46 |
| 1:O:3019:ALA:HA | 1:O:3053:TYR:CZ | 2.50 | 0.46 |
| 1:P:812:ASP:HB3 | 1:P:818:TRP:HH2 | 1.80 | 0.46 |
| 1:P:1351:TRP:HZ3 | 1:P:1463:ASN:HB3 | 1.80 | 0.46 |
| 1:P:3218:VAL:HA | 1:P:3258:TYR:CD2 | 2.50 | 0.46 |
| 1:Q:277:ARG:HG3 | 1:Q:278:GLN:N | 2.31 | 0.46 |
| 1:Q:332:ASP:OD1 | 1:Q:332:ASP:N | 2.49 | 0.46 |
| 1:Q:2155:PRO:HB2 | 1:Q:2306:TRP:CZ3 | 2.51 | 0.46 |
| 1:Q:2988:HIS:HD2 | 1:Q:3119:HIS:CD2 | 2.34 | 0.46 |
| 1:Q:3287:LEU:HD23 | 1:Q:3287:LEU:H | 1.81 | 0.46 |
| 1:Q:3334:ARG:HH21 | 1:Q:3406:ILE:HG23 | 1.80 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:R:81:LEU:HA | 1:R:84:LYS:HB2 | 1.97 | 0.46 |
| 1:R:314:THR:HG21 | 1:R:782:ASP:HB3 | 1.97 | 0.46 |
| 1:R:2658:ILE:HD11 | 1:R:2677:THR:HG21 | 1.96 | 0.46 |
| 1:R:3360:LEU:HD11 | 1:R:3401:ARG:HB3 | 1.97 | 0.46 |
| 1:S:148:ARG:O | 1:S:151:GLN:NE2 | 2.39 | 0.46 |
| 1:S:1159:ARG:HA | 1:S:1186:ASP:O | 2.16 | 0.46 |
| 1:T:6:LYS:NZ | 1:T:15:GLU:HG2 | 2.31 | 0.46 |
| 1:T:1497:LYS:HE3 | 1:T:1497:LYS:HB3 | 1.85 | 0.46 |
| 1:T:1802:ILE:HG22 | 1:T:1877:TYR:CD1 | 2.50 | 0.46 |
| 1:T:2837:LEU:HD12 | 1:T:2838:GLY:H | 1.81 | 0.46 |
| 1:T:3203:ILE:HG22 | 1:T:3207:LEU:HD23 | 1.97 | 0.46 |
| 1:A:197:ASP:OD1 | 1:A:197:ASP:N | 2.48 | 0.46 |
| 1:A:663:LYS:HG2 | 1:A:700:TYR:CE2 | 2.51 | 0.46 |
| 1:A:3041:GLN:HE21 | 1:J:3053:TYR:HE2 | 1.63 | 0.46 |
| 1:B:220:ASP:OD2 | 1:B:281:TYR:OH | 2.30 | 0.46 |
| 1:B:756:LYS:HD3 | 1:B:762:SER:HB2 | 1.98 | 0.46 |
| 1:B:860:GLN:O | 1:B:860:GLN:NE2 | 2.48 | 0.46 |
| 1:B:1266:ARG:HB3 | 1:B:1531:ASP:HB3 | 1.98 | 0.46 |
| 1:B:2922:VAL:HA | 1:B:3186:ASN:O | 2.16 | 0.46 |
| 1:C:436:ASP:HB3 | 1:C:522:TYR:CZ | 2.51 | 0.46 |
| 1:C:2229:GLN:HB2 | 1:C:2274:LEU:HD12 | 1.98 | 0.46 |
| 1:C:2392:ARG:HB3 | 1:C:2394:PHE:HE1 | 1.80 | 0.46 |
| 1:C:2676:VAL:HG21 | 1:C:2851:PHE:CZ | 2.51 | 0.46 |
| 1:C:3308:PRO:HG2 | 1:C:3311:ALA:HB3 | 1.98 | 0.46 |
| 1:D:501:ARG:NH2 | 1:D:648:TRP:HB3 | 2.31 | 0.46 |
| 1:D:594:LEU:HA | 1:D:602:PHE:CE2 | 2.41 | 0.46 |
| 1:D:2604:THR:OG1 | 1:D:2782:HIS:NE2 | 2.47 | 0.46 |
| 1:D:2674:TYR:CE1 | 1:D:2712:VAL:HG22 | 2.51 | 0.46 |
| 1:D:2925:GLU:HA | 1:D:3010:TYR:O | 2.16 | 0.46 |
| 1:E:915:ARG:HH21 | 1:E:1115:TYR:CB | 2.29 | 0.46 |
| 1:E:1316:VAL:HG11 | 1:E:1321:VAL:HG13 | 1.97 | 0.46 |
| 1:E:2085:GLN:HG3 | 1:E:2087:LEU:HD22 | 1.97 | 0.46 |
| 1:E:3144:ARG:HH21 | 1:E:3147:LEU:HD21 | 1.79 | 0.46 |
| 1:E:3357:TYR:HA | 1:E:3360:LEU:HD23 | 1.97 | 0.46 |
| 1:F:428:SER:OG | 1:F:429:ALA:N | 2.48 | 0.46 |
| 1:F:1011:PHE:HA | 1:F:1063:TRP:CH2 | 2.46 | 0.46 |
| 1:F:1205:ILE:HD12 | 1:F:1208:LYS:HE3 | 1.97 | 0.46 |
| 1:F:2004:GLU:OE1 | 1:F:2004:GLU:N | 2.45 | 0.46 |
| 1:F:2375:LEU:HD22 | 1:F:2379:GLU:HG2 | 1.98 | 0.46 |
| 1:G:475:ALA:HB3 | 1:G:485:ARG:HB3 | 1.97 | 0.46 |
| 1:G:1268:LEU:HD12 | 1:G:1361:LEU:HD13 | 1.97 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:G:1446:SER:OG | 1:G:1447:SER:N | 2.48 | 0.46 |
| 1:G:1788:VAL:HG12 | 1:G:1789:LEU:HD22 | 1.96 | 0.46 |
| 1:G:1916:MET:HE2 | 1:G:1916:MET:N | 2.30 | 0.46 |
| 1:G:2181:TRP:H | 1:G:2297:THR:HG22 | 1.81 | 0.46 |
| 1:G:2214:ARG:HH11 | 1:J:111:ILE:HG13 | 1.81 | 0.46 |
| 1:G:3308:PRO:HG2 | 1:G:3311:ALA:HB3 | 1.97 | 0.46 |
| 1:H:1193:GLN:OE1 | 1:H:1194:TYR:N | 2.47 | 0.46 |
| 1:H:1777:ALA:HB1 | 1:H:1781:GLU:HG3 | 1.97 | 0.46 |
| 1:I:64:ALA:O | 1:I:174:TYR:OH | 2.34 | 0.46 |
| 1:I:913:TRP:HD1 | 1:I:1088:LEU:HD23 | 1.81 | 0.46 |
| 1:I:2802:VAL:H | 1:I:2856:THR:HG22 | 1.79 | 0.46 |
| 1:I:3173:ARG:O | 1:I:3177:ILE:HG13 | 2.15 | 0.46 |
| 1:J:1742:TRP:HD1 | 1:J:1920:LEU:HD12 | 1.81 | 0.46 |
| 1:J:2008:LYS:HD3 | 1:J:2041:LYS:HZ2 | 1.81 | 0.46 |
| 1:J:2111:LEU:HD13 | 1:J:2212:PHE:HE1 | 1.79 | 0.46 |
| 1:J:2978:THR:HG21 | 1:J:2983:VAL:HG13 | 1.98 | 0.46 |
| 1:J:3122:ILE:HG13 | 1:J:3125:ILE:HD11 | 1.98 | 0.46 |
| 1:K:914:HIS:CE1 | 1:K:1053:HIS:HE1 | 2.33 | 0.46 |
| 1:K:1646:GLU:OE1 | 1:K:1646:GLU:N | 2.48 | 0.46 |
| 1:K:2027:ASP:HA | 1:L:1651:ARG:HH12 | 1.80 | 0.46 |
| 1:K:2517:ILE:HD11 | 1:K:2601:TRP:CD1 | 2.49 | 0.46 |
| 1:K:3055:ARG:HH12 | 1:K:3064:LEU:HD22 | 1.80 | 0.46 |
| 1:K:3072:LEU:HA | 1:K:3080:PHE:HE1 | 1.81 | 0.46 |
| 1:L:597:ARG:NH2 | 1:L:655:GLN:HA | 2.31 | 0.46 |
| 1:L:848:ARG:HD3 | 1:L:934:LEU:HB3 | 1.98 | 0.46 |
| 1:L:1364:GLU:O | 1:L:1378:ASN:ND2 | 2.36 | 0.46 |
| 1:L:1842:ASN:OD1 | 1:L:1843:TYR:N | 2.49 | 0.46 |
| 1:L:2552:GLY:O | 1:L:2555:GLY:N | 2.49 | 0.46 |
| 1:M:2297:THR:O | 1:M:2300:THR:OG1 | 2.27 | 0.46 |
| 1:M:2668:CYS:HB2 | 1:M:2735:CYS:HB2 | 1.73 | 0.46 |
| 1:M:2673:GLN:HE22 | 1:M:2852:GLN:N | 2.11 | 0.46 |
| 1:M:2814:SER:OG | 1:M:2838:GLY:O | 2.33 | 0.46 |
| 1:M:2821:LEU:O | 1:M:2828:CYS:HB2 | 2.16 | 0.46 |
| 1:N:459:THR:HG23 | 1:N:1285:ARG:HH12 | 1.80 | 0.46 |
| 1:N:600:CYS:HB3 | 1:N:783:ARG:HH12 | 1.80 | 0.46 |
| 1:N:816:LYS:HZ2 | 1:N:818:TRP:HZ2 | 1.62 | 0.46 |
| 1:N:980:ARG:NH2 | 1:N:1046:ASP:OD1 | 2.49 | 0.46 |
| 1:N:1040:LEU:HD11 | 1:N:1184:LEU:HG | 1.96 | 0.46 |
| 1:N:1223:VAL:HG13 | 1:N:1231:ILE:HB | 1.97 | 0.46 |
| 1:N:1444:SER:O | 1:N:1451:SER:OG | 2.32 | 0.46 |
| 1:N:3132:LEU:HG | 1:N:3136:ARG:NH1 | 2.30 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:O:913:TRP:HD1 | 1:O:1088:LEU:HD23 | 1.81 | 0.46 |
| 1:O:1575:ILE:O | 1:R:337:GLN:NE2 | 2.49 | 0.46 |
| 1:P:460:SER:HB2 | 1:P:1277:GLU:OE2 | 2.15 | 0.46 |
| 1:P:1384:LYS:HB3 | 1:P:1391:VAL:HG12 | 1.97 | 0.46 |
| 1:Q:1544:GLU:OE1 | 1:Q:1544:GLU:N | 2.38 | 0.46 |
| 1:Q:1890:ARG:NH2 | 1:Q:1959:GLU:O | 2.44 | 0.46 |
| 1:Q:3043:GLN:HG3 | 1:Q:3044:VAL:H | 1.81 | 0.46 |
| 1:S:399:ASN:HD21 | 1:S:401:ASN:HD21 | 1.62 | 0.46 |
| 1:S:1399:GLU:N | 1:S:1399:GLU:OE1 | 2.49 | 0.46 |
| 1:S:1651:ARG:NE | 1:T:2025:SER:OG | 2.44 | 0.46 |
| 1:S:2008:LYS:HE2 | 1:S:2041:LYS:HA | 1.96 | 0.46 |
| 1:S:2114:LEU:HD13 | 1:S:2172:HIS:HE1 | 1.81 | 0.46 |
| 1:S:2517:ILE:HD13 | 1:S:2601:TRP:HD1 | 1.80 | 0.46 |
| 1:S:2586:GLU:OE2 | 1:S:2598:ILE:N | 2.46 | 0.46 |
| 1:T:41:PHE:CD1 | 1:T:47:MET:HE1 | 2.51 | 0.46 |
| 1:T:225:ILE:O | 1:T:229:LEU:HG | 2.15 | 0.46 |
| 1:T:635:PRO:O | 1:T:638:ILE:HG22 | 2.16 | 0.46 |
| 1:T:806:VAL:HG11 | 1:T:825:HIS:O | 2.16 | 0.46 |
| 1:T:1936:LYS:HE3 | 1:T:1936:LYS:HB2 | 1.80 | 0.46 |
| 1:T:2538:GLN:HE22 | 1:T:2542:ARG:HB2 | 1.81 | 0.46 |
| 1:T:3158:ASN:ND2 | 1:T:3172:SER:OG | 2.46 | 0.46 |
| 1:T:3270:LEU:HD11 | 1:T:3281:PHE:CZ | 2.50 | 0.46 |
| 3:m:1:NAG:O3 | 3:m:2:NAG:O6 | 2.32 | 0.46 |
| 1:A:718:MET:SD | 1:A:722:GLN:HG2 | 2.55 | 0.46 |
| 1:A:1212:GLU:CD | 1:A:1214:ASN:H | 2.24 | 0.46 |
| 1:A:1356:ARG:NH1 | 1:A:1402:ASN:OD1 | 2.49 | 0.46 |
| 1:A:2232:LEU:HB2 | 1:A:2274:LEU:HD21 | 1.96 | 0.46 |
| 1:B:454:ARG:NH2 | 1:B:1338:LEU:O | 2.49 | 0.46 |
| 1:B:1075:ASN:HB2 | 1:B:1113:PHE:HB3 | 1.97 | 0.46 |
| 1:B:1677:ARG:HD2 | 1:B:1763:ILE:O | 2.16 | 0.46 |
| 1:B:1695:LEU:HG | 1:B:1796:PRO:HB2 | 1.97 | 0.46 |
| 1:B:2343:ASN:CG | 1:B:2349:ARG:HH12 | 2.24 | 0.46 |
| 1:C:579:GLU:HG3 | 1:C:582:ASP:CG | 2.41 | 0.46 |
| 1:C:738:VAL:HG23 | 1:C:789:ILE:HG21 | 1.98 | 0.46 |
| 1:C:2394:PHE:HD2 | 1:C:2443:LYS:HG2 | 1.81 | 0.46 |
| 1:C:2614:LEU:HD12 | 1:C:2636:ARG:HH12 | 1.80 | 0.46 |
| 1:C:2750:ASP:HA | 1:C:2758:ARG:HH11 | 1.81 | 0.46 |
| 1:D:5:ARG:HB2 | 1:D:284:ASP:OD1 | 2.15 | 0.46 |
| 1:D:103:LEU:HB2 | 1:D:150:PHE:HZ | 1.81 | 0.46 |
| 1:D:378:LYS:NZ | 1:D:383:ASP:H | 2.13 | 0.46 |
| 1:D:569:GLN:HB3 | 1:D:619:GLY:HA3 | 1.97 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:D:924:ALA:O | 1:D:928:LYS:HG2 | 2.16 | 0.46 |
| 1:D:1280:LYS:O | 1:D:1284:ARG:HG2 | 2.16 | 0.46 |
| 1:D:2141:ALA:HB3 | 1:D:2143:LYS:HZ3 | 1.80 | 0.46 |
| 1:D:2149:HIS:HA | 1:D:2154:PHE:CD2 | 2.46 | 0.46 |
| 1:D:2551:HIS:HB2 | 1:D:2700:ALA:HB2 | 1.96 | 0.46 |
| 1:D:2582:VAL:HA | 1:D:2706:PHE:HE2 | 1.80 | 0.46 |
| 1:D:3023:LEU:O | 1:D:3030:ASN:ND2 | 2.49 | 0.46 |
| 1:E:449:ARG:HD3 | 1:E:541:TYR:CZ | 2.50 | 0.46 |
| 1:E:937:TRP:CD1 | 1:E:938:ASP:H | 2.34 | 0.46 |
| 1:E:996:THR:HG23 | 1:E:999:ALA:H | 1.79 | 0.46 |
| 1:E:1986:LEU:HB2 | 1:E:2069:PRO:HG2 | 1.98 | 0.46 |
| 1:E:2155:PRO:HB2 | 1:E:2159:ARG:NH2 | 2.30 | 0.46 |
| 1:E:2967:PRO:HD3 | 1:E:2974:TYR:CE2 | 2.51 | 0.46 |
| 1:E:3065:PHE:HA | 1:E:3068:THR:HG22 | 1.98 | 0.46 |
| 1:F:32:VAL:HA | 1:F:37:ASN:HD21 | 1.80 | 0.46 |
| 1:F:1714:HIS:NE2 | 1:F:1732:CYS:SG | 2.88 | 0.46 |
| 1:F:2376:ASN:O | 1:F:2379:GLU:HG3 | 2.16 | 0.46 |
| 1:F:2637:SER:HB3 | 1:F:2686:GLY:O | 2.16 | 0.46 |
| 1:F:3088:HIS:CE1 | 1:F:3119:HIS:CE1 | 3.03 | 0.46 |
| 1:G:606:PHE:CZ | 1:G:644:VAL:HG13 | 2.51 | 0.46 |
| 1:G:958:PRO:HA | 1:G:961:ASN:HA | 1.97 | 0.46 |
| 1:G:1284:ARG:NH2 | 1:G:1377:SER:O | 2.48 | 0.46 |
| 1:G:1301:PHE:CG | 1:G:1302:PRO:HA | 2.51 | 0.46 |
| 1:G:1867:HIS:HA | 1:G:1874:TYR:CD2 | 2.50 | 0.46 |
| 1:G:1868:SER:O | 1:G:1874:TYR:HB2 | 2.15 | 0.46 |
| 1:G:2152:PRO:HA | 1:G:2261:GLU:OE1 | 2.16 | 0.46 |
| 1:H:1324:HIS:CD2 | 1:H:1324:HIS:H | 2.34 | 0.46 |
| 1:H:1550:GLN:HA | 1:H:1553:GLN:HE22 | 1.80 | 0.46 |
| 1:H:1568:SER:N | 1:H:1597:GLY:O | 2.49 | 0.46 |
| 1:H:2368:ASP:OD1 | 1:H:2368:ASP:N | 2.48 | 0.46 |
| 1:H:2408:VAL:HG22 | 1:H:2473:ILE:HG22 | 1.97 | 0.46 |
| 1:I:750:LEU:HG | 1:I:768:LEU:O | 2.16 | 0.46 |
| 1:I:939:TRP:CD1 | 1:I:998:ILE:HG21 | 2.51 | 0.46 |
| 1:I:2073:VAL:HG23 | 1:J:1489:LEU:H | 1.80 | 0.46 |
| 1:I:2531:ALA:O | 1:I:2535:VAL:HG23 | 2.14 | 0.46 |
| 1:I:3350:ASN:HD22 | 1:I:3372:SER:HB3 | 1.80 | 0.46 |
| 1:J:449:ARG:HH21 | 1:J:535:ILE:HA | 1.80 | 0.46 |
| 1:J:1264:ILE:HD11 | 1:J:1531:ASP:HA | 1.97 | 0.46 |
| 1:J:1277:GLU:HA | 1:J:1280:LYS:HG2 | 1.98 | 0.46 |
| 1:J:1345:SER:OG | 1:J:1346:VAL:N | 2.49 | 0.46 |
| 1:J:1607:ASP:C | 1:J:1608:ARG:HD2 | 2.40 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:J:1785:ARG:NH1 | 1:J:1786:ASP:O | 2.49 | 0.46 |
| 1:J:3147:LEU:HA | 1:J:3150:LEU:HD12 | 1.98 | 0.46 |
| 1:K:2163:LEU:HD22 | 1:K:2363:LEU:HD12 | 1.97 | 0.46 |
| 1:K:3173:ARG:O | 1:K:3177:ILE:HG13 | 2.15 | 0.46 |
| 1:L:836:HIS:NE2 | 1:L:838:GLU:OE1 | 2.48 | 0.46 |
| 1:L:1150:PHE:HB3 | 1:L:1199:GLN:OE1 | 2.16 | 0.46 |
| 1:L:1221:TYR:OH | 1:L:1237:GLY:N | 2.49 | 0.46 |
| 1:L:2654:PHE:CD1 | 1:L:2677:THR:HG23 | 2.50 | 0.46 |
| 1:L:3319:PRO:HB2 | 1:L:3343:PRO:HD3 | 1.96 | 0.46 |
| 1:M:1204:ASP:OD1 | 1:M:1205:ILE:N | 2.48 | 0.46 |
| 1:M:2034:ILE:O | 1:M:2038:LEU:HD23 | 2.16 | 0.46 |
| 1:M:2328:ASN:HD21 | 1:N:1240:THR:HA | 1.81 | 0.46 |
| 1:M:2508:VAL:HG21 | 1:M:3137:HIS:HB3 | 1.97 | 0.46 |
| 1:M:2811:PHE:HE2 | 1:M:2836:VAL:HG11 | 1.80 | 0.46 |
| 1:M:3019:ALA:HA | 1:M:3053:TYR:CZ | 2.51 | 0.46 |
| 1:M:3173:ARG:HB2 | 1:M:3176:GLN:HG3 | 1.97 | 0.46 |
| 1:N:5:ARG:HG3 | 1:N:283:TYR:HA | 1.98 | 0.46 |
| 1:N:69:TRP:O | 1:N:72:LEU:HG | 2.14 | 0.46 |
| 1:N:740:LEU:H | 1:N:785:VAL:H | 1.64 | 0.46 |
| 1:N:896:ALA:HB1 | 1:N:899:LYS:HB2 | 1.98 | 0.46 |
| 1:N:1324:HIS:HA | 1:N:1519:VAL:HG11 | 1.98 | 0.46 |
| 1:N:2559:ASP:OD2 | 1:N:2559:ASP:N | 2.48 | 0.46 |
| 1:N:2978:THR:HG21 | 1:N:2983:VAL:HG13 | 1.98 | 0.46 |
| 1:N:3214:TYR:CD1 | 1:N:3265:ASP:HA | 2.51 | 0.46 |
| 1:O:1159:ARG:HA | 1:O:1186:ASP:O | 2.16 | 0.46 |
| 1:O:1585:ASN:ND2 | 1:R:338:SER:OG | 2.49 | 0.46 |
| 1:O:1817:ARG:HG3 | 1:O:1860:TRP:CH2 | 2.51 | 0.46 |
| 1:O:3131:THR:HA | 1:O:3134:LYS:HD3 | 1.96 | 0.46 |
| 1:P:758:LYS:HD3 | 1:P:803:GLU:HB3 | 1.98 | 0.46 |
| 1:P:3037:ILE:HG21 | 1:P:3040:ALA:HB3 | 1.98 | 0.46 |
| 1:Q:47:MET:SD | 1:Q:47:MET:N | 2.89 | 0.46 |
| 1:Q:755:ILE:HG23 | 1:Q:765:VAL:HG21 | 1.98 | 0.46 |
| 1:Q:1186:ASP:OD2 | 1:Q:1188:TYR:N | 2.48 | 0.46 |
| 1:Q:2392:ARG:HB3 | 1:Q:2394:PHE:HE1 | 1.80 | 0.46 |
| 1:Q:3133:GLN:NE2 | 1:Q:3138:ARG:O | 2.49 | 0.46 |
| 1:R:1539:THR:HG22 | 1:R:1542:GLN:NE2 | 2.31 | 0.46 |
| 1:R:1802:ILE:HG22 | 1:R:1877:TYR:CD1 | 2.50 | 0.46 |
| 1:R:2088:PRO:C | 1:R:2090:ASN:H | 2.24 | 0.46 |
| 1:R:2235:LEU:HD12 | 1:R:2239:GLY:HA2 | 1.97 | 0.46 |
| 1:R:2623:GLU:N | 1:R:2623:GLU:OE1 | 2.49 | 0.46 |
| 1:R:2671:GLU:H | 1:R:2671:GLU:CD | 2.23 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:R:2798:SER:OG | 1:R:2799:GLU:OE1 | 2.31 | 0.46 |
| 1:R:2919:LYS:HB3 | 1:R:2920:ASP:H | 1.58 | 0.46 |
| 1:S:2393:VAL:H | 1:S:2447:THR:HG22 | 1.80 | 0.46 |
| 1:S:3337:ARG:NE | 1:S:3378:ASN:HB2 | 2.30 | 0.46 |
| 1:T:1539:THR:HG22 | 1:T:1542:GLN:NE2 | 2.30 | 0.46 |
| 1:T:1827:ASP:HA | 1:T:1831:TRP:CD1 | 2.50 | 0.46 |
| 1:T:2001:CYS:HB2 | 1:T:2050:THR:OG1 | 2.15 | 0.46 |
| 1:T:2130:HIS:NE2 | 1:T:2147:CYS:SG | 2.89 | 0.46 |
| 1:T:3183:PHE:HB2 | 1:T:3185:TYR:CD1 | 2.51 | 0.46 |
| 1:A:250:LYS:HD2 | 1:A:268:SER:HB3 | 1.97 | 0.46 |
| 1:A:2551:HIS:HB2 | 1:A:2581:PHE:HE1 | 1.80 | 0.46 |
| 1:A:3350:ASN:O | 1:A:3391:SER:N | 2.47 | 0.46 |
| 1:B:225:ILE:O | 1:B:229:LEU:HG | 2.15 | 0.46 |
| 1:B:960:THR:OG1 | 1:B:964:GLU:OE2 | 2.30 | 0.46 |
| 1:B:1281:SER:O | 1:B:1285:ARG:HG2 | 2.16 | 0.46 |
| 1:B:1299:HIS:CD2 | 1:B:1457:PHE:HZ | 2.33 | 0.46 |
| 1:B:2303:ASP:OD2 | 1:B:2367:TYR:OH | 2.34 | 0.46 |
| 1:C:754:SER:HA | 1:C:765:VAL:HG23 | 1.97 | 0.46 |
| 1:D:452:LEU:HD23 | 1:D:554:PHE:CE1 | 2.51 | 0.46 |
| 1:D:503:PHE:HA | 1:D:678:PHE:CE1 | 2.49 | 0.46 |
| 1:D:705:GLU:HG2 | 1:D:706:LEU:HD22 | 1.98 | 0.46 |
| 1:D:1350:ASP:OD1 | 1:D:1352:THR:OG1 | 2.29 | 0.46 |
| 1:D:2656:ARG:HG3 | 1:D:2796:ARG:HH21 | 1.80 | 0.46 |
| 1:E:848:ARG:HG2 | 1:E:933:GLY:HA3 | 1.98 | 0.46 |
| 1:E:958:PRO:HA | 1:E:961:ASN:HA | 1.98 | 0.46 |
| 1:E:1588:HIS:HB2 | 1:H:337:GLN:CD | 2.41 | 0.46 |
| 1:E:1596:LEU:HD12 | 1:E:1597:GLY:H | 1.81 | 0.46 |
| 1:E:1852:ILE:HD13 | 1:E:2030:TYR:CZ | 2.50 | 0.46 |
| 1:E:2328:ASN:HD21 | 1:F:1240:THR:HA | 1.80 | 0.46 |
| 1:E:2392:ARG:HE | 1:E:2447:THR:HG21 | 1.81 | 0.46 |
| 1:E:2719:TRP:NE1 | 1:E:2723:GLN:HE22 | 2.14 | 0.46 |
| 1:E:3330:VAL:HB | 1:E:3404:ILE:HD12 | 1.98 | 0.46 |
| 1:E:3350:ASN:O | 1:E:3391:SER:N | 2.48 | 0.46 |
| 1:F:325:ARG:HH21 | 1:F:391:TYR:HE2 | 1.61 | 0.46 |
| 1:F:567:SER:OG | 1:F:623:TYR:O | 2.25 | 0.46 |
| 1:F:571:GLN:NE2 | 1:F:616:LEU:O | 2.34 | 0.46 |
| 1:F:1303:SER:OG | 1:F:1311:LYS:O | 2.30 | 0.46 |
| 1:F:1706:GLY:O | 1:F:1710:LEU:HG | 2.15 | 0.46 |
| 1:F:2538:GLN:HE22 | 1:F:2542:ARG:HB2 | 1.81 | 0.46 |
| 1:F:2839:GLY:O | 1:F:2842:GLU:HG2 | 2.15 | 0.46 |
| 1:G:304:ARG:HB3 | 1:G:414:LYS:NZ | 2.30 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:G:2155:PRO:HB2 | 1:G:2306:TRP:CZ3 | 2.51 | 0.46 |
| 1:G:2414:GLN:O | 1:G:2416:ASN:N | 2.46 | 0.46 |
| 1:G:2696:LEU:O | 1:G:2699:SER:OG | 2.32 | 0.46 |
| 1:G:3260:ARG:HH21 | 1:G:3261:VAL:HG12 | 1.80 | 0.46 |
| 1:H:598:ASP:O | 1:H:602:PHE:HB2 | 2.15 | 0.46 |
| 1:H:705:GLU:HG2 | 1:H:706:LEU:HD22 | 1.98 | 0.46 |
| 1:H:914:HIS:O | 1:H:917:LEU:HG | 2.15 | 0.46 |
| 1:H:1087:PRO:HA | 1:H:1109:PRO:HD3 | 1.97 | 0.46 |
| 1:H:1204:ASP:OD1 | 1:H:1204:ASP:N | 2.49 | 0.46 |
| 1:H:1542:GLN:HA | 1:H:1545:GLU:OE2 | 2.16 | 0.46 |
| 1:H:2616:ASP:HB3 | 1:H:2620:ASN:HD22 | 1.81 | 0.46 |
| 1:I:2525:THR:O | 1:I:2529:LYS:HG2 | 2.16 | 0.46 |
| 1:I:2654:PHE:HA | 1:I:2657:GLN:CD | 2.41 | 0.46 |
| 1:I:3086:MET:HG2 | 1:I:3262:TYR:CE1 | 2.51 | 0.46 |
| 1:I:3334:ARG:NH2 | 1:I:3406:ILE:HG23 | 2.24 | 0.46 |
| 1:J:225:ILE:O | 1:J:229:LEU:HG | 2.16 | 0.46 |
| 1:J:229:LEU:HB3 | 1:J:233:ARG:HH21 | 1.80 | 0.46 |
| 1:J:1040:LEU:HD11 | 1:J:1184:LEU:HG | 1.97 | 0.46 |
| 1:J:1405:TYR:HD2 | 1:J:1406:LEU:HD22 | 1.80 | 0.46 |
| 1:J:2448:ASP:OD1 | 1:J:2449:THR:N | 2.49 | 0.46 |
| 1:J:2559:ASP:N | 1:J:2559:ASP:OD2 | 2.48 | 0.46 |
| 1:J:2923:ARG:HH11 | 1:J:3007:GLY:C | 2.24 | 0.46 |
| 1:J:3037:ILE:HG21 | 1:J:3040:ALA:HB3 | 1.97 | 0.46 |
| 1:K:405:ARG:HH12 | 1:K:670:MET:HE1 | 1.80 | 0.46 |
| 1:K:475:ALA:HB3 | 1:K:485:ARG:HB3 | 1.98 | 0.46 |
| 1:K:635:PRO:O | 1:K:638:ILE:HG12 | 2.16 | 0.46 |
| 1:K:1260:ALA:H | 1:K:1529:HIS:HE1 | 1.63 | 0.46 |
| 1:K:1461:HIS:HA | 1:K:1464:VAL:HB | 1.97 | 0.46 |
| 1:K:1738:THR:HG22 | 1:K:1916:MET:HE1 | 1.97 | 0.46 |
| 1:K:1868:SER:O | 1:K:1874:TYR:HB2 | 2.16 | 0.46 |
| 1:K:2672:VAL:HG21 | 1:K:2849:ARG:HB2 | 1.98 | 0.46 |
| 1:K:2981:MET:HG3 | 1:K:2983:VAL:HG22 | 1.97 | 0.46 |
| 1:L:38:LEU:O | 1:L:73:TYR:OH | 2.33 | 0.46 |
| 1:L:1557:PHE:HD2 | 1:L:1611:LYS:HD3 | 1.80 | 0.46 |
| 1:L:2967:PRO:O | 1:L:2973:ARG:NH1 | 2.49 | 0.46 |
| 1:L:3020:LEU:HD13 | 1:L:3024:LEU:HB2 | 1.98 | 0.46 |
| 1:L:3144:ARG:HA | 1:L:3147:LEU:HG | 1.98 | 0.46 |
| 1:M:409:VAL:HG13 | 1:M:666:CYS:HA | 1.97 | 0.46 |
| 1:M:2037:VAL:HA | 1:M:2040:LYS:HG2 | 1.98 | 0.46 |
| 1:M:2216:TYR:HD1 | 1:M:2223:TYR:HB3 | 1.81 | 0.46 |
| 1:M:2231:GLU:O | 1:M:2234:LYS:HG2 | 2.15 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:M:2315:ARG:HD3 | 1:M:2377:LEU:HD13 | 1.97 | 0.46 |
| 1:M:3082:VAL:HG11 | 1:M:3260:ARG:HG2 | 1.97 | 0.46 |
| 1:N:744:ASN:ND2 | 1:N:778:PRO:HA | 2.31 | 0.46 |
| 1:N:2786:ILE:HG13 | 1:N:2787:PRO:HD3 | 1.97 | 0.46 |
| 1:O:66:PHE:HZ | 1:O:185:HIS:CE1 | 2.34 | 0.46 |
| 1:O:1424:ILE:HG12 | 1:O:1606:PHE:CD2 | 2.50 | 0.46 |
| 1:O:1619:ARG:HD2 | 1:P:2775:GLN:NE2 | 2.31 | 0.46 |
| 1:O:2515:LYS:HG2 | 1:O:2777:ASP:HB3 | 1.97 | 0.46 |
| 1:O:2963:PRO:HD2 | 1:O:2965:LEU:HD23 | 1.98 | 0.46 |
| 1:O:3044:VAL:HG13 | 1:O:3102:SER:HA | 1.97 | 0.46 |
| 1:P:1108:VAL:HG13 | 1:P:1111:GLU:OE1 | 2.15 | 0.46 |
| 1:P:1192:TRP:HZ3 | 1:P:1194:TYR:HB2 | 1.80 | 0.46 |
| 1:P:1607:ASP:OD2 | 1:P:1608:ARG:NH1 | 2.49 | 0.46 |
| 1:P:1914:GLU:HG2 | 1:P:1915:LEU:N | 2.29 | 0.46 |
| 1:P:2210:ASN:HD21 | 1:P:2212:PHE:HB2 | 1.80 | 0.46 |
| 1:Q:71:ARG:NH2 | 1:Q:276:TYR:HB3 | 2.31 | 0.46 |
| 1:Q:1008:GLN:OE1 | 1:Q:1008:GLN:N | 2.43 | 0.46 |
| 1:Q:1351:TRP:NE1 | 1:Q:1460:HIS:HD2 | 2.14 | 0.46 |
| 1:Q:1899:GLN:HE22 | 1:Q:1905:ASP:C | 2.22 | 0.46 |
| 1:Q:2234:LYS:HG3 | 1:Q:2243:VAL:HG11 | 1.97 | 0.46 |
| 1:Q:3353:GLU:HG3 | 1:Q:3386:TYR:HD2 | 1.81 | 0.46 |
| 1:R:612:LEU:HD21 | 1:R:768:LEU:HD13 | 1.98 | 0.46 |
| 1:R:1011:PHE:HA | 1:R:1063:TRP:CH2 | 2.50 | 0.46 |
| 1:R:1985:PHE:O | 1:R:2029:LEU:HD12 | 2.15 | 0.46 |
| 1:R:3096:GLY:HA3 | 1:R:3104:SER:HB3 | 1.98 | 0.46 |
| 1:S:341:HIS:NE2 | 1:S:343:GLU:OE2 | 2.49 | 0.46 |
| 1:S:2099:LEU:HD21 | 1:S:2179:PRO:HG3 | 1.98 | 0.46 |
| 1:S:2199:PHE:CE1 | 1:S:2208:LEU:HB3 | 2.51 | 0.46 |
| 1:S:2773:ASN:CG | 1:S:3141:ASN:HB2 | 2.41 | 0.46 |
| 1:T:453:SER:HB3 | 1:T:553:PRO:HG3 | 1.97 | 0.46 |
| 1:T:2163:LEU:HD12 | 1:T:2365:PHE:CE1 | 2.51 | 0.46 |
| 1:T:2695:THR:OG1 | 1:T:2697:GLU:OE1 | 2.34 | 0.46 |
| 1:T:2777:ASP:OD1 | 1:T:2777:ASP:N | 2.40 | 0.46 |
| 1:T:2786:ILE:H | 1:T:2786:ILE:HD12 | 1.81 | 0.46 |
| 1:T:2993:VAL:O | 1:T:2997:MET:HG2 | 2.16 | 0.46 |
| 1:A:953:GLU:HG3 | 1:A:954:THR:HG23 | 1.98 | 0.46 |
| 1:A:3389:VAL:HG22 | 1:A:3401:ARG:HG2 | 1.98 | 0.46 |
| 1:B:52:ASP:OD1 | 1:B:53:GLY:N | 2.48 | 0.46 |
| 1:B:408:GLY:HA3 | 1:B:669:THR:HG21 | 1.98 | 0.46 |
| 1:B:479:ARG:NH2 | 1:B:481:ASP:O | 2.49 | 0.46 |
| 1:B:1165:THR:N | 1:B:1222:SER:O | 2.38 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:2262:VAL:HG23 | 1:B:2438:PHE:CD1 | 2.51 | 0.46 |
| 1:B:2786:ILE:H | 1:B:2786:ILE:HD12 | 1.81 | 0.46 |
| 1:B:3142:TYR:CZ | 1:B:3144:ARG:HB3 | 2.51 | 0.46 |
| 1:C:2155:PRO:HB2 | 1:C:2306:TRP:CZ3 | 2.50 | 0.46 |
| 1:C:3304:VAL:HG23 | 1:C:3317:ILE:HB | 1.98 | 0.46 |
| 1:D:65:THR:HG21 | 1:D:251:LEU:HD21 | 1.98 | 0.46 |
| 1:D:472:GLY:HA3 | 1:D:629:HIS:HA | 1.98 | 0.46 |
| 1:D:757:PRO:HB2 | 1:D:760:GLY:H | 1.80 | 0.46 |
| 1:D:905:HIS:H | 1:D:907:MET:HE1 | 1.81 | 0.46 |
| 1:D:1362:ILE:HG22 | 1:D:1380:PHE:HB3 | 1.98 | 0.46 |
| 1:D:1539:THR:HG22 | 1:D:1542:GLN:NE2 | 2.31 | 0.46 |
| 1:D:2287:HIS:CE1 | 1:D:2432:LEU:HB2 | 2.51 | 0.46 |
| 1:E:1317:HIS:CD2 | 1:E:1322:PHE:HE1 | 2.34 | 0.46 |
| 1:E:1506:GLU:O | 1:E:1507:PHE:HD1 | 1.99 | 0.46 |
| 1:E:1622:GLY:HA3 | 1:F:2786:ILE:HD13 | 1.97 | 0.46 |
| 1:E:2586:GLU:OE2 | 1:E:2598:ILE:N | 2.47 | 0.46 |
| 1:E:2997:MET:SD | 1:E:3000:ARG:NH1 | 2.89 | 0.46 |
| 1:F:80:LYS:NZ | 1:F:261:ILE:HG13 | 2.31 | 0.46 |
| 1:F:257:ASP:HA | 1:F:265:ARG:HD3 | 1.98 | 0.46 |
| 1:F:461:VAL:HG22 | 1:F:1277:GLU:CD | 2.41 | 0.46 |
| 1:F:950:VAL:HA | 1:F:968:PHE:HB3 | 1.97 | 0.46 |
| 1:F:1325:TRP:HE3 | 1:F:1496:LEU:HD21 | 1.81 | 0.46 |
| 1:F:1802:ILE:HG22 | 1:F:1877:TYR:CD1 | 2.51 | 0.46 |
| 1:F:2511:ILE:HD12 | 1:F:2773:ASN:HB2 | 1.97 | 0.46 |
| 1:F:2790:GLU:HG2 | 1:F:2791:GLU:N | 2.31 | 0.46 |
| 1:G:612:LEU:HB2 | 1:G:613:PRO:HD3 | 1.98 | 0.46 |
| 1:G:1331:ASP:O | 1:G:1334:GLU:HG3 | 2.16 | 0.46 |
| 1:G:1482:ASP:OD1 | 1:G:1483:ASP:N | 2.48 | 0.46 |
| 1:G:1786:ASP:OD1 | 1:G:1789:LEU:N | 2.31 | 0.46 |
| 1:G:2669:ASN:OD1 | 1:G:2849:ARG:NE | 2.45 | 0.46 |
| 1:G:3089:ASN:ND2 | 1:G:3247:ILE:HD12 | 2.31 | 0.46 |
| 1:H:103:LEU:HD23 | 1:H:108:GLN:HB3 | 1.98 | 0.46 |
| 1:H:455:PHE:HA | 1:H:514:ARG:HH22 | 1.80 | 0.46 |
| 1:H:503:PHE:HB2 | 1:H:678:PHE:HE1 | 1.80 | 0.46 |
| 1:H:1009:THR:HA | 1:H:1070:ARG:HH22 | 1.81 | 0.46 |
| 1:H:1051:LEU:HD12 | 1:H:1052:HIS:N | 2.31 | 0.46 |
| 1:H:1677:ARG:HD3 | 1:H:1677:ARG:HA | 1.78 | 0.46 |
| 1:H:2313:GLN:HA | 1:H:2316:ARG:NH1 | 2.31 | 0.46 |
| 1:H:2397:PHE:CD1 | 1:H:2489:PRO:HB3 | 2.50 | 0.46 |
| 1:H:2527:SER:O | 1:H:2530:LYS:HG3 | 2.16 | 0.46 |
| 1:H:2672:VAL:HG22 | 1:H:2851:PHE:HD1 | 1.81 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:H:3392:ASN:OD1 | 1:H:3395:ARG:N | 2.46 | 0.46 |
| 1:I:275:SER:HB3 | 1:I:278:GLN:HE22 | 1.81 | 0.46 |
| 1:I:597:ARG:O | 1:I:655:GLN:NE2 | 2.37 | 0.46 |
| 1:I:903:CYS:C | 1:I:905:HIS:HD1 | 2.22 | 0.46 |
| 1:I:1571:VAL:O | 1:I:1592:SER:HB2 | 2.16 | 0.46 |
| 1:I:1721:PRO:HD3 | 1:I:1729:TYR:CE2 | 2.51 | 0.46 |
| 1:I:2216:TYR:HD1 | 1:I:2223:TYR:HB3 | 1.81 | 0.46 |
| 1:J:509:ASP:OD1 | 1:J:509:ASP:N | 2.47 | 0.46 |
| 1:J:1026:HIS:CE1 | 1:J:1053:HIS:HE1 | 2.33 | 0.46 |
| 1:J:1041:ARG:NH2 | 1:J:1188:TYR:OH | 2.36 | 0.46 |
| 1:J:1087:PRO:HA | 1:J:1109:PRO:HD3 | 1.98 | 0.46 |
| 1:J:2287:HIS:CE1 | 1:J:2432:LEU:HB2 | 2.51 | 0.46 |
| 1:J:2645:ASP:OD2 | 1:J:2656:ARG:NH2 | 2.41 | 0.46 |
| 1:K:539:GLU:HA | 1:K:555:PHE:HB2 | 1.98 | 0.46 |
| 1:K:1865:LYS:NZ | 1:K:1867:HIS:HB2 | 2.31 | 0.46 |
| 1:K:2034:ILE:HB | 1:K:2038:LEU:HD23 | 1.96 | 0.46 |
| 1:K:3144:ARG:HA | 1:K:3147:LEU:HD21 | 1.97 | 0.46 |
| 1:L:313:PHE:CD2 | 1:L:406:PRO:HB3 | 2.51 | 0.46 |
| 1:L:441:THR:HB | 1:L:444:GLU:OE1 | 2.16 | 0.46 |
| 1:L:705:GLU:N | 1:L:705:GLU:OE1 | 2.48 | 0.46 |
| 1:L:914:HIS:O | 1:L:917:LEU:HG | 2.16 | 0.46 |
| 1:L:940:THR:HG21 | 1:L:1128:PHE:HE1 | 1.80 | 0.46 |
| 1:L:1359:PRO:HG2 | 1:L:1362:ILE:HG12 | 1.97 | 0.46 |
| 1:L:3190:LEU:HD13 | 1:L:3197:VAL:HG12 | 1.97 | 0.46 |
| 1:L:3320:LEU:N | 1:L:3341:HIS:O | 2.48 | 0.46 |
| 1:M:509:ASP:HA | 1:M:512:LYS:HZ2 | 1.79 | 0.46 |
| 1:M:1084:LEU:HD23 | 1:M:1110:PHE:HE1 | 1.81 | 0.46 |
| 1:M:2315:ARG:CZ | 1:M:2377:LEU:HB3 | 2.45 | 0.46 |
| 1:M:2569:HIS:HA | 1:M:2574:PHE:CE2 | 2.51 | 0.46 |
| 1:M:2980:GLY:HA2 | 1:M:3258:TYR:CE1 | 2.51 | 0.46 |
| 1:N:31:THR:O | 1:N:36:GLN:NE2 | 2.34 | 0.46 |
| 1:N:737:PHE:N | 1:N:829:ILE:O | 2.37 | 0.46 |
| 1:N:947:PRO:HB2 | 1:N:950:VAL:HG22 | 1.97 | 0.46 |
| 1:N:998:ILE:HA | 1:N:1001:MET:HG3 | 1.98 | 0.46 |
| 1:N:1108:VAL:HG13 | 1:N:1111:GLU:OE1 | 2.16 | 0.46 |
| 1:N:1193:GLN:OE1 | 1:N:1194:TYR:N | 2.48 | 0.46 |
| 1:N:1542:GLN:HA | 1:N:1545:GLU:OE2 | 2.15 | 0.46 |
| 1:N:2602:ASP:HA | 1:N:2711:ASN:ND2 | 2.31 | 0.46 |
| 1:N:3120:SER:O | 1:N:3124:ARG:HG2 | 2.16 | 0.46 |
| 1:O:197:ASP:OD1 | 1:O:197:ASP:N | 2.49 | 0.46 |
| 1:O:514:ARG:NH1 | 1:O:1343:ALA:HA | 2.27 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:O:870:GLU:HA | 1:O:878:PHE:HB3 | 1.98 | 0.46 |
| 1:O:949:ILE:HG23 | 1:O:950:VAL:HG13 | 1.98 | 0.46 |
| 1:O:1991:LYS:O | 1:O:1991:LYS:HD2 | 2.16 | 0.46 |
| 1:O:2407:GLU:OE2 | 1:O:2424:ALA:HB1 | 2.15 | 0.46 |
| 1:O:2414:GLN:O | 1:O:2416:ASN:N | 2.47 | 0.46 |
| 1:O:2713:ASP:OD2 | 1:O:2776:TYR:OH | 2.32 | 0.46 |
| 1:P:221:ARG:HH12 | 1:P:285:ASP:HB3 | 1.80 | 0.46 |
| 1:P:727:ILE:HG22 | 1:P:730:ARG:HH21 | 1.80 | 0.46 |
| 1:P:1720:CYS:SG | 1:P:1731:CYS:N | 2.89 | 0.46 |
| 1:P:2637:SER:HB3 | 1:P:2686:GLY:O | 2.16 | 0.46 |
| 1:P:2671:GLU:OE1 | 1:P:2671:GLU:N | 2.38 | 0.46 |
| 1:Q:758:LYS:HZ1 | 1:Q:805:ASP:CG | 2.24 | 0.46 |
| 1:Q:2085:GLN:CD | 1:Q:2087:LEU:H | 2.23 | 0.46 |
| 1:R:5:ARG:HB3 | 1:R:93:TYR:HD1 | 1.81 | 0.46 |
| 1:R:11:LEU:HD21 | 1:R:92:PRO:HB3 | 1.97 | 0.46 |
| 1:R:673:GLU:C | 1:R:695:ARG:HH12 | 2.24 | 0.46 |
| 1:R:788:GLU:OE2 | 1:R:791:ASP:N | 2.38 | 0.46 |
| 1:R:914:HIS:O | 1:R:918:THR:HG23 | 2.16 | 0.46 |
| 1:R:1012:CYS:SG | 1:R:1196:ARG:NH1 | 2.88 | 0.46 |
| 1:S:639:LEU:O | 1:S:642:SER:OG | 2.27 | 0.46 |
| 1:S:714:GLN:OE1 | 1:S:718:MET:N | 2.49 | 0.46 |
| 1:S:887:GLN:HE21 | 1:S:889:ASN:HD21 | 1.62 | 0.46 |
| 1:S:1567:THR:HG21 | 2:yA:1:NAG:H62 | 1.96 | 0.46 |
| 1:S:3227:THR:OG1 | 1:S:3245:PHE:O | 2.23 | 0.46 |
| 1:T:220:ASP:O | 1:T:224:VAL:HG13 | 2.16 | 0.46 |
| 1:T:444:GLU:HA | 1:T:447:GLU:OE1 | 2.16 | 0.46 |
| 1:T:605:GLN:HE22 | 1:T:786:LYS:H | 1.63 | 0.46 |
| 1:A:2585:LEU:HD22 | 1:A:2706:PHE:CD2 | 2.50 | 0.46 |
| 1:A:2791:GLU:O | 1:A:2794:GLU:HG3 | 2.16 | 0.46 |
| 1:A:3024:LEU:HD12 | 1:A:3025:THR:HG23 | 1.98 | 0.46 |
| 1:B:69:TRP:CD1 | 1:B:251:LEU:HD22 | 2.50 | 0.46 |
| 1:B:171:GLU:HB3 | 1:B:177:PHE:HD1 | 1.81 | 0.46 |
| 1:B:224:VAL:HA | 1:B:227:GLN:OE1 | 2.15 | 0.46 |
| 1:B:524:ASP:HA | 1:B:643:ASN:ND2 | 2.31 | 0.46 |
| 1:B:859:VAL:O | 1:B:862:LEU:HG | 2.16 | 0.46 |
| 1:B:938:ASP:OD1 | 1:B:1055:ASN:ND2 | 2.49 | 0.46 |
| 1:B:953:GLU:HA | 1:B:969:HIS:HB2 | 1.98 | 0.46 |
| 1:B:1088:LEU:HD22 | 1:B:1109:PRO:HG3 | 1.97 | 0.46 |
| 1:B:1286:MET:HB3 | 1:B:1340:ARG:HG3 | 1.98 | 0.46 |
| 1:C:453:SER:OG | 3:f:1:NAG:N2 | 2.34 | 0.46 |
| 1:C:986:LEU:HD12 | 1:C:1028:LEU:HG | 1.98 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:3197:VAL:O | 1:C:3201:ASN:ND2 | 2.49 | 0.46 |
| 1:D:331:HIS:CE1 | 1:D:672:HIS:HB3 | 2.50 | 0.46 |
| 1:D:501:ARG:NE | 1:D:645:ASP:OD2 | 2.49 | 0.46 |
| 1:D:673:GLU:C | 1:D:695:ARG:HH12 | 2.24 | 0.46 |
| 1:D:920:GLN:HB3 | 1:D:1103:THR:HG21 | 1.98 | 0.46 |
| 1:D:1019:GLU:HG3 | 1:D:1023:ASN:ND2 | 2.31 | 0.46 |
| 1:D:1284:ARG:HG2 | 1:D:1284:ARG:HH11 | 1.81 | 0.46 |
| 1:D:2967:PRO:O | 1:D:2973:ARG:NH1 | 2.49 | 0.46 |
| 1:D:3037:ILE:HG21 | 1:D:3040:ALA:HB3 | 1.98 | 0.46 |
| 1:E:1025:ILE:HG21 | 1:E:1052:HIS:NE2 | 2.31 | 0.46 |
| 1:E:1317:HIS:HA | 1:E:1322:PHE:CD1 | 2.50 | 0.46 |
| 1:E:1325:TRP:HE1 | 1:E:1498:PRO:HG3 | 1.81 | 0.46 |
| 1:E:2806:PHE:CE1 | 1:E:2892:PRO:HB3 | 2.51 | 0.46 |
| 1:F:220:ASP:O | 1:F:224:VAL:HG13 | 2.16 | 0.46 |
| 1:F:524:ASP:HA | 1:F:643:ASN:ND2 | 2.31 | 0.46 |
| 1:F:885:HIS:HD1 | 1:F:1044:ALA:HB2 | 1.81 | 0.46 |
| 1:F:938:ASP:OD2 | 1:F:940:THR:OG1 | 2.33 | 0.46 |
| 1:F:1356:ARG:HH21 | 1:F:1402:ASN:H | 1.62 | 0.46 |
| 1:F:1720:CYS:SG | 1:F:1731:CYS:N | 2.89 | 0.46 |
| 1:F:2622:PHE:HA | 1:F:2703:PRO:HG2 | 1.98 | 0.46 |
| 1:F:3043:GLN:N | 1:F:3043:GLN:OE1 | 2.49 | 0.46 |
| 1:G:222:ILE:O | 1:G:225:ILE:HG22 | 2.16 | 0.46 |
| 1:G:1171:PRO:HD3 | 1:G:1217:TYR:HA | 1.98 | 0.46 |
| 1:G:2061:SER:HB3 | 3:1:1:NAG:H82 | 1.96 | 0.46 |
| 1:G:2407:GLU:HB2 | 1:G:2426:PHE:CE2 | 2.51 | 0.46 |
| 1:G:3255:PRO:HD2 | 1:H:3366:PRO:HB3 | 1.97 | 0.46 |
| 1:H:529:GLY:HA2 | 1:H:575:SER:HA | 1.97 | 0.46 |
| 1:H:1332:GLN:OE1 | 1:H:1505:ASN:ND2 | 2.45 | 0.46 |
| 1:H:1849:GLN:O | 1:H:1852:ILE:HG22 | 2.16 | 0.46 |
| 1:H:3319:PRO:HA | 1:H:3341:HIS:HB3 | 1.98 | 0.46 |
| 1:H:3319:PRO:HB2 | 1:H:3343:PRO:HD3 | 1.98 | 0.46 |
| 1:I:627:THR:HA | 1:I:771:LEU:HD11 | 1.97 | 0.46 |
| 1:I:1114:ASP:N | 1:I:1114:ASP:OD1 | 2.47 | 0.46 |
| 1:I:1433:LEU:HD21 | 1:I:1460:HIS:NE2 | 2.30 | 0.46 |
| 1:I:2201:ASP:OD1 | 1:I:2202:ALA:N | 2.49 | 0.46 |
| 1:I:2465:ALA:HB2 | 1:J:1085:ARG:HD2 | 1.98 | 0.46 |
| 1:I:2964:LYS:HD3 | 1:I:3252:GLY:HA3 | 1.97 | 0.46 |
| 1:J:460:SER:HB2 | 1:J:1277:GLU:OE2 | 2.16 | 0.46 |
| 1:J:625:LEU:HD22 | 1:J:636:ILE:HD12 | 1.98 | 0.46 |
| 1:J:1493:ARG:HD3 | 1:J:1493:ARG:H | 1.80 | 0.46 |
| 1:J:2238:ASP:OD1 | 1:J:2240:LYS:N | 2.45 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:J:2377:LEU:HA | 1:J:2380:LEU:HB2 | 1.98 | 0.46 |
| 1:J:2666:ASP:HB3 | 1:J:2669:ASN:OD1 | 2.16 | 0.46 |
| 1:J:2972:ASP:OD1 | 1:J:2972:ASP:N | 2.49 | 0.46 |
| 1:J:3036:GLN:OE1 | 1:J:3042:HIS:N | 2.49 | 0.46 |
| 1:K:1079:CYS:O | 1:L:2492:ILE:HD13 | 2.16 | 0.46 |
| 1:K:1247:SER:HA | 1:K:1250:LYS:HG2 | 1.98 | 0.46 |
| 1:K:1301:PHE:CD1 | 1:K:1302:PRO:HA | 2.51 | 0.46 |
| 1:K:1969:LEU:HA | 1:K:1972:ILE:HG12 | 1.97 | 0.46 |
| 1:K:2037:VAL:HA | 1:K:2040:LYS:HG2 | 1.97 | 0.46 |
| 1:L:69:TRP:O | 1:L:72:LEU:HG | 2.16 | 0.46 |
| 1:L:187:HIS:CE1 | 1:L:191:LEU:HD11 | 2.51 | 0.46 |
| 1:L:197:ASP:OD1 | 1:L:197:ASP:N | 2.49 | 0.46 |
| 1:L:1351:TRP:HZ3 | 1:L:1463:ASN:HB3 | 1.81 | 0.46 |
| 1:L:1941:PRO:O | 1:L:1944:VAL:HG22 | 2.16 | 0.46 |
| 1:L:2182:ASP:OD1 | 1:L:2185:LEU:N | 2.43 | 0.46 |
| 1:L:2526:GLU:HA | 1:L:2529:LYS:HG2 | 1.97 | 0.46 |
| 1:L:3023:LEU:O | 1:L:3030:ASN:ND2 | 2.49 | 0.46 |
| 1:M:193:GLY:HA3 | 1:M:201:SER:H | 1.81 | 0.46 |
| 1:M:494:ALA:HA | 1:M:603:GLU:OE1 | 2.16 | 0.46 |
| 1:M:577:LYS:HD3 | 1:M:577:LYS:HA | 1.77 | 0.46 |
| 1:M:1247:SER:HA | 1:M:1250:LYS:HG2 | 1.98 | 0.46 |
| 1:M:1315:CYS:HA | 1:M:1325:TRP:CH2 | 2.51 | 0.46 |
| 1:M:1993:SER:HB2 | 1:M:2017:GLY:H | 1.81 | 0.46 |
| 1:M:2549:ALA:HB1 | 1:M:2554:PRO:HD2 | 1.98 | 0.46 |
| 1:M:2673:GLN:HA | 1:M:2673:GLN:OE1 | 2.15 | 0.46 |
| 1:M:2912:ASP:OD1 | 1:M:2912:ASP:N | 2.48 | 0.46 |
| 1:N:187:HIS:CE1 | 1:N:191:LEU:HD11 | 2.51 | 0.46 |
| 1:N:1058:ARG:HG2 | 1:N:1123:TYR:CE2 | 2.51 | 0.46 |
| 1:N:1802:ILE:HG22 | 1:N:1877:TYR:CG | 2.51 | 0.46 |
| 1:O:1365:ALA:HA | 1:O:1381:PHE:HZ | 1.79 | 0.46 |
| 1:O:1896:GLN:NE2 | 1:O:1906:PRO:O | 2.35 | 0.46 |
| 1:O:2091:ARG:HA | 1:O:2093:ARG:HH21 | 1.81 | 0.46 |
| 1:O:2867:ASP:OD1 | 1:O:2867:ASP:N | 2.44 | 0.46 |
| 1:O:3289:LYS:HB3 | 1:O:3295:LEU:HD11 | 1.98 | 0.46 |
| 1:P:160:GLN:NE2 | 1:P:161:LEU:HG | 2.30 | 0.46 |
| 1:P:524:ASP:HA | 1:P:643:ASN:ND2 | 2.31 | 0.46 |
| 1:P:924:ALA:O | 1:P:928:LYS:HG2 | 2.16 | 0.46 |
| 1:P:1159:ARG:O | 1:P:1159:ARG:HD2 | 2.16 | 0.46 |
| 1:P:2979:HIS:HA | 1:P:2984:PHE:CD2 | 2.46 | 0.46 |
| 1:Q:2407:GLU:HB3 | 1:Q:2474:ILE:HB | 1.97 | 0.46 |
| 1:R:198:HIS:HD1 | 1:R:205:TRP:CD1 | 2.34 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:R:695:ARG:HG3 | 1:R:697:THR:HG23 | 1.98 | 0.46 |
| 1:R:750:LEU:HD12 | 1:R:768:LEU:O | 2.16 | 0.46 |
| 1:R:795:LYS:HD3 | 1:R:796:LYS:HD3 | 1.96 | 0.46 |
| 1:R:1115:TYR:O | 1:R:1120:GLN:N | 2.40 | 0.46 |
| 1:R:1223:VAL:HG13 | 1:R:1231:ILE:HB | 1.98 | 0.46 |
| 1:R:1452:ALA:HA | 1:R:1457:PHE:CD2 | 2.50 | 0.46 |
| 1:R:2162:THR:O | 1:R:2165:VAL:HG22 | 2.15 | 0.46 |
| 1:S:527:ARG:HG2 | 1:S:528:PRO:HD2 | 1.98 | 0.46 |
| 1:S:754:SER:HA | 1:S:765:VAL:HG23 | 1.98 | 0.46 |
| 1:S:1374:THR:HG22 | 1:S:1375:GLU:N | 2.31 | 0.46 |
| 1:S:2078:LYS:HB3 | 1:S:2080:ARG:HH22 | 1.81 | 0.46 |
| 1:S:2967:PRO:HD3 | 1:S:2974:TYR:CE2 | 2.51 | 0.46 |
| 1:S:3011:TRP:CZ3 | 1:S:3013:TRP:HB3 | 2.50 | 0.46 |
| 1:S:3173:ARG:HB2 | 1:S:3176:GLN:HE21 | 1.80 | 0.46 |
| 1:T:947:PRO:HB2 | 1:T:950:VAL:HG22 | 1.98 | 0.46 |
| 1:T:1124:ASP:OD1 | 1:T:1124:ASP:N | 2.48 | 0.46 |
| 1:T:1415:GLU:OE2 | 1:T:1551:ARG:HG2 | 2.16 | 0.46 |
| 1:T:2378:ASP:O | 1:T:2381:GLU:HG2 | 2.15 | 0.46 |
| 1:T:3037:ILE:HG21 | 1:T:3040:ALA:HB3 | 1.98 | 0.46 |
| 1:T:3350:ASN:OD1 | 1:T:3372:SER:HB3 | 2.16 | 0.46 |
| 3:zA:1:NAG:H62 | 3:zA:2:NAG:H82 | 1.98 | 0.46 |
| 1:A:594:LEU:O | 1:A:597:ARG:NH2 | 2.48 | 0.45 |
| 1:A:1588:HIS:O | 1:D:337:GLN:NE2 | 2.49 | 0.45 |
| 1:A:1993:SER:HB2 | 1:A:2017:GLY:H | 1.81 | 0.45 |
| 1:A:2752:ASN:OD1 | 1:A:2753:PRO:HD2 | 2.16 | 0.45 |
| 1:A:2963:PRO:HD2 | 1:A:2965:LEU:HD23 | 1.98 | 0.45 |
| 1:A:3289:LYS:HB3 | 1:A:3295:LEU:HD21 | 1.98 | 0.45 |
| 1:B:245:GLU:CD | 1:B:245:GLU:H | 2.24 | 0.45 |
| 1:B:378:LYS:NZ | 1:B:383:ASP:H | 2.14 | 0.45 |
| 1:B:460:SER:HB2 | 1:B:1277:GLU:OE2 | 2.16 | 0.45 |
| 1:B:2647:GLU:OE2 | 1:B:2656:ARG:NH2 | 2.29 | 0.45 |
| 1:B:2866:PRO:O | 1:B:2870:TYR:OH | 2.26 | 0.45 |
| 1:C:436:ASP:OD1 | 1:C:436:ASP:N | 2.47 | 0.45 |
| 1:C:1111:GLU:N | 1:C:1111:GLU:OE1 | 2.48 | 0.45 |
| 1:C:1350:ASP:OD1 | 1:C:1352:THR:N | 2.43 | 0.45 |
| 1:C:1919:PRO:HG3 | 1:C:1940:LYS:HZ1 | 1.80 | 0.45 |
| 1:C:3072:LEU:HA | 1:C:3080:PHE:CE1 | 2.50 | 0.45 |
| 1:D:471:HIS:ND1 | 1:D:471:HIS:O | 2.49 | 0.45 |
| 1:D:610:HIS:O | 1:D:613:PRO:HD2 | 2.17 | 0.45 |
| 1:D:635:PRO:O | 1:D:638:ILE:HG22 | 2.15 | 0.45 |
| 1:D:2530:LYS:HB2 | 1:D:2533:ARG:HH22 | 1.81 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:D:3127:GLN:O | 1:D:3130:GLN:HG3 | 2.15 | 0.45 |
| 1:E:891:CYS:HB3 | 1:E:900:PHE:O | 2.17 | 0.45 |
| 1:E:1967:LEU:HD13 | 1:E:2086:GLU:OE1 | 2.16 | 0.45 |
| 1:E:1991:LYS:O | 1:E:1991:LYS:HD2 | 2.16 | 0.45 |
| 1:F:81:LEU:HD12 | 1:F:86:LEU:HD13 | 1.98 | 0.45 |
| 1:F:479:ARG:NH2 | 1:F:481:ASP:O | 2.49 | 0.45 |
| 1:F:1947:TYR:CE1 | 1:F:1948:LYS:HG3 | 2.50 | 0.45 |
| 1:F:2095:GLU:CD | 1:F:2097:SER:H | 2.23 | 0.45 |
| 1:F:2448:ASP:OD1 | 1:F:2449:THR:N | 2.49 | 0.45 |
| 1:F:2487:SER:OG | 1:F:2488:LYS:N | 2.49 | 0.45 |
| 1:F:3138:ARG:HA | 1:F:3138:ARG:HD3 | 1.76 | 0.45 |
| 1:G:1093:GLN:HB2 | 1:G:1097:ILE:HG21 | 1.97 | 0.45 |
| 1:G:1273:GLU:OE1 | 1:G:1273:GLU:N | 2.39 | 0.45 |
| 1:G:1365:ALA:HA | 1:G:1381:PHE:CE2 | 2.51 | 0.45 |
| 1:G:1405:TYR:HA | 1:G:1408:ASN:HD21 | 1.81 | 0.45 |
| 1:G:1855:ASN:HD21 | 1:G:2015:VAL:HA | 1.80 | 0.45 |
| 1:H:69:TRP:CD1 | 1:H:251:LEU:HD22 | 2.51 | 0.45 |
| 1:H:3032:PHE:O | 1:H:3046:ARG:NH1 | 2.49 | 0.45 |
| 1:H:3151:TYR:HA | 1:H:3173:ARG:HH21 | 1.81 | 0.45 |
| 1:I:1244:ARG:HD3 | 1:I:1245:PRO:HD2 | 1.98 | 0.45 |
| 1:I:1698:LEU:HD13 | 1:I:1757:ARG:HD2 | 1.98 | 0.45 |
| 1:I:1737:ALA:HA | 1:I:1847:GLU:OE1 | 2.15 | 0.45 |
| 1:J:1488:ALA:O | 1:J:1492:MET:HE3 | 2.15 | 0.45 |
| 1:J:1910:ASN:OD1 | 1:J:1911:CYS:N | 2.49 | 0.45 |
| 1:J:2137:PRO:HD2 | 1:J:2143:LYS:HE2 | 1.97 | 0.45 |
| 1:J:3020:LEU:HD13 | 1:J:3024:LEU:HB2 | 1.97 | 0.45 |
| 1:K:750:LEU:HD21 | 1:K:767:LYS:NZ | 2.31 | 0.45 |
| 1:K:1195:ASP:OD1 | 1:K:1196:ARG:HG2 | 2.16 | 0.45 |
| 1:K:1195:ASP:OD1 | 1:K:1196:ARG:N | 2.49 | 0.45 |
| 1:K:1900:ARG:HD3 | 1:K:1906:PRO:HB3 | 1.97 | 0.45 |
| 1:K:2034:ILE:O | 1:K:2038:LEU:HD23 | 2.16 | 0.45 |
| 1:K:2784:LEU:HG | 1:K:2788:GLN:HB3 | 1.98 | 0.45 |
| 1:K:3046:ARG:NH2 | 1:K:3112:ASP:OD2 | 2.49 | 0.45 |
| 1:L:507:VAL:HG21 | 1:L:638:ILE:HD11 | 1.99 | 0.45 |
| 1:L:980:ARG:NH2 | 1:L:1046:ASP:OD1 | 2.50 | 0.45 |
| 1:L:2521:THR:HG22 | 1:L:2524:GLU:CD | 2.41 | 0.45 |
| 1:L:2602:ASP:HA | 1:L:2711:ASN:ND2 | 2.30 | 0.45 |
| 1:L:2617:LYS:HD2 | 1:L:2617:LYS:HA | 1.69 | 0.45 |
| 1:M:1397:GLN:HG2 | 1:M:1436:LEU:HD22 | 1.98 | 0.45 |
| 1:M:1670:LYS:HA | 1:M:1670:LYS:HD2 | 1.70 | 0.45 |
| 1:M:1858:HIS:CE1 | 1:M:1884:HIS:HE2 | 2.34 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:M:1899:GLN:OE1 | 1:M:1904:HIS:HB2 | 2.16 | 0.45 |
| 1:M:2713:ASP:OD2 | 1:M:2776:TYR:OH | 2.27 | 0.45 |
| 1:M:3088:HIS:HD2 | 1:M:3122:ILE:HG13 | 1.80 | 0.45 |
| 1:N:2345:ASN:O | 1:N:2349:ARG:HG2 | 2.16 | 0.45 |
| 1:N:2397:PHE:CD1 | 1:N:2489:PRO:HB3 | 2.50 | 0.45 |
| 1:N:2552:GLY:O | 1:N:2555:GLY:N | 2.49 | 0.45 |
| 1:O:972:LEU:HD23 | 1:O:977:LYS:HB3 | 1.98 | 0.45 |
| 1:O:2553:TYR:HB2 | 1:O:2697:GLU:HB3 | 1.98 | 0.45 |
| 1:O:3086:MET:HE3 | 1:O:3258:TYR:CE1 | 2.51 | 0.45 |
| 1:P:408:GLY:HA3 | 1:P:669:THR:HG21 | 1.98 | 0.45 |
| 1:P:1116:GLU:O | 1:P:1120:GLN:HB3 | 2.16 | 0.45 |
| 1:P:1702:SER:O | 1:P:1702:SER:OG | 2.33 | 0.45 |
| 1:P:2191:PRO:HG2 | 1:P:2194:PHE:CD2 | 2.50 | 0.45 |
| 1:P:2371:LYS:HB3 | 1:P:2371:LYS:HE3 | 1.85 | 0.45 |
| 1:P:3049:GLN:CD | 1:P:3050:PRO:HD2 | 2.41 | 0.45 |
| 1:Q:307:GLU:OE2 | 1:Q:413:ALA:N | 2.44 | 0.45 |
| 1:Q:1350:ASP:HA | 1:Q:1463:ASN:ND2 | 2.30 | 0.45 |
| 1:Q:2159:ARG:HH22 | 1:Q:2360:TYR:HB3 | 1.81 | 0.45 |
| 1:Q:2693:MET:SD | 1:Q:2699:SER:HB2 | 2.56 | 0.45 |
| 1:R:79:GLN:O | 1:R:83:LYS:NZ | 2.49 | 0.45 |
| 1:R:1324:HIS:HB3 | 1:R:1519:VAL:HG21 | 1.98 | 0.45 |
| 1:R:2311:GLU:OE1 | 1:R:2315:ARG:NH1 | 2.48 | 0.45 |
| 1:R:2666:ASP:HB3 | 1:R:2669:ASN:OD1 | 2.16 | 0.45 |
| 1:R:2809:GLN:HE22 | 1:R:2846:HIS:HA | 1.80 | 0.45 |
| 1:S:890:TRP:HD1 | 1:S:894:PRO:HB3 | 1.81 | 0.45 |
| 1:S:913:TRP:CD1 | 1:S:1088:LEU:HD21 | 2.50 | 0.45 |
| 1:S:1299:HIS:ND1 | 1:S:1299:HIS:O | 2.49 | 0.45 |
| 1:S:1420:CYS:HB2 | 1:S:1608:ARG:NH2 | 2.31 | 0.45 |
| 1:S:1632:ASP:OD1 | 1:T:1917:ARG:NH1 | 2.49 | 0.45 |
| 1:S:3131:THR:HA | 1:S:3134:LYS:HG2 | 1.98 | 0.45 |
| 1:T:1881:PHE:O | 1:T:1885:HIS:ND1 | 2.47 | 0.45 |
| 1:T:1893:ALA:O | 1:T:1896:GLN:HB2 | 2.16 | 0.45 |
| 1:T:1965:ALA:HA | 1:T:1968:LEU:HB3 | 1.98 | 0.45 |
| 1:T:2752:ASN:HD21 | 1:T:2757:ILE:HG13 | 1.80 | 0.45 |
| 1:A:508:GLU:CD | 1:A:520:ILE:H | 2.24 | 0.45 |
| 1:A:674:LEU:HD22 | 1:A:695:ARG:NH2 | 2.31 | 0.45 |
| 1:A:1715:ALA:HB1 | 1:A:1873:HIS:HA | 1.97 | 0.45 |
| 1:A:2806:PHE:O | 1:A:2850:LEU:HD12 | 2.16 | 0.45 |
| 1:A:3304:VAL:HG23 | 1:A:3317:ILE:HB | 1.98 | 0.45 |
| 1:A:3358:THR:H | 1:B:3329:LYS:HE3 | 1.80 | 0.45 |
| 1:B:80:LYS:HA | 1:B:83:LYS:HZ3 | 1.80 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:196:HIS:CE1 | 1:B:198:HIS:HB2 | 2.51 | 0.45 |
| 1:B:253:PRO:O | 1:B:256:ARG:NH1 | 2.49 | 0.45 |
| 1:B:357:MET:HE3 | 1:B:358:PRO:HD2 | 1.97 | 0.45 |
| 1:B:1624:LYS:HD2 | 1:B:1624:LYS:HA | 1.79 | 0.45 |
| 1:B:2488:LYS:HD2 | 1:B:2489:PRO:HD2 | 1.98 | 0.45 |
| 1:B:3320:LEU:N | 1:B:3341:HIS:O | 2.49 | 0.45 |
| 1:C:255:ASP:N | 1:C:255:ASP:OD1 | 2.46 | 0.45 |
| 1:C:1081:ILE:HD12 | 1:D:2461:PHE:CD1 | 2.52 | 0.45 |
| 1:C:1815:ARG:HA | 1:C:1818:LEU:HG | 1.97 | 0.45 |
| 1:C:3196:SER:O | 1:C:3200:ILE:HD12 | 2.16 | 0.45 |
| 1:D:866:LEU:O | 1:D:869:LEU:HG | 2.16 | 0.45 |
| 1:D:1345:SER:OG | 1:D:1346:VAL:N | 2.50 | 0.45 |
| 1:D:2273:TYR:CE2 | 1:D:2407:GLU:HB2 | 2.50 | 0.45 |
| 1:D:2655:TYR:HD1 | 1:D:2659:LEU:HD23 | 1.81 | 0.45 |
| 1:D:2720:GLN:HE22 | 1:D:2730:TYR:HD2 | 1.64 | 0.45 |
| 1:D:3227:THR:HB | 1:D:3246:TYR:CD2 | 2.51 | 0.45 |
| 1:E:38:LEU:HA | 1:E:38:LEU:HD12 | 1.76 | 0.45 |
| 1:E:376:LEU:HB3 | 1:E:378:LYS:HZ1 | 1.80 | 0.45 |
| 1:E:391:TYR:HA | 1:E:397:SER:HA | 1.98 | 0.45 |
| 1:E:483:ARG:HD2 | 1:E:484:VAL:N | 2.32 | 0.45 |
| 1:E:583:HIS:HB3 | 1:E:587:PHE:HD2 | 1.81 | 0.45 |
| 1:E:657:LYS:NZ | 1:E:720:ILE:O | 2.39 | 0.45 |
| 1:E:1083:SER:O | 1:E:1086:LYS:NZ | 2.49 | 0.45 |
| 1:E:1434:HIS:NE2 | 1:E:1460:HIS:HD2 | 2.15 | 0.45 |
| 1:E:1989:GLY:N | 1:E:2024:TRP:O | 2.49 | 0.45 |
| 1:E:2331:SER:HA | 1:E:2355:LYS:HZ1 | 1.81 | 0.45 |
| 1:F:229:LEU:HB3 | 1:F:233:ARG:NH2 | 2.32 | 0.45 |
| 1:F:729:GLU:O | 1:F:732:THR:HG22 | 2.17 | 0.45 |
| 1:F:2088:PRO:C | 1:F:2090:ASN:H | 2.24 | 0.45 |
| 1:F:3037:ILE:HG21 | 1:F:3040:ALA:HB3 | 1.99 | 0.45 |
| 1:G:220:ASP:OD2 | 1:G:283:TYR:OH | 2.27 | 0.45 |
| 1:G:332:ASP:OD1 | 1:G:332:ASP:N | 2.46 | 0.45 |
| 1:G:342:CYS:H | 1:J:1581:ASN:ND2 | 2.14 | 0.45 |
| 1:G:674:LEU:HD22 | 1:G:695:ARG:NH2 | 2.31 | 0.45 |
| 1:G:704:HIS:HB3 | 1:G:705:GLU:OE1 | 2.17 | 0.45 |
| 1:G:847:VAL:HA | 1:G:1122:HIS:O | 2.17 | 0.45 |
| 1:G:938:ASP:HA | 1:G:1055:ASN:ND2 | 2.31 | 0.45 |
| 1:G:1168:VAL:N | 1:G:1178:GLU:OE1 | 2.50 | 0.45 |
| 1:G:1624:LYS:HD3 | 1:G:1624:LYS:HA | 1.80 | 0.45 |
| 1:G:1732:CYS:HA | 1:G:1742:TRP:CZ3 | 2.52 | 0.45 |
| 1:G:2581:PHE:O | 1:G:2584:THR:HG22 | 2.16 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:G:3103:MET:HA | 1:G:3109:SER:HA | 1.98 | 0.45 |
| 1:G:3287:LEU:HG | 1:G:3295:LEU:HB2 | 1.98 | 0.45 |
| 1:H:1425:GLN:HA | 1:H:1610:TYR:HE1 | 1.81 | 0.45 |
| 1:H:1941:PRO:O | 1:H:1944:VAL:HG22 | 2.16 | 0.45 |
| 1:H:2387:HIS:C | 1:H:2392:ARG:HH21 | 2.24 | 0.45 |
| 1:H:3020:LEU:HD13 | 1:H:3024:LEU:HB2 | 1.99 | 0.45 |
| 1:I:222:ILE:O | 1:I:225:ILE:HG22 | 2.16 | 0.45 |
| 1:I:539:GLU:HA | 1:I:555:PHE:HB2 | 1.97 | 0.45 |
| 1:I:1212:GLU:CD | 1:I:1214:ASN:H | 2.25 | 0.45 |
| 1:I:2158:HIS:O | 1:I:2162:THR:HG23 | 2.15 | 0.45 |
| 1:I:2403:GLY:HA2 | 1:I:2433:GLU:HG2 | 1.99 | 0.45 |
| 1:I:2407:GLU:OE2 | 1:I:2424:ALA:HB1 | 2.15 | 0.45 |
| 1:J:453:SER:HB3 | 1:J:553:PRO:HG3 | 1.98 | 0.45 |
| 1:J:599:PHE:HD2 | 1:J:600:CYS:SG | 2.39 | 0.45 |
| 1:J:753:LEU:HD23 | 1:J:766:ALA:HB3 | 1.99 | 0.45 |
| 1:J:860:GLN:NE2 | 1:J:860:GLN:O | 2.50 | 0.45 |
| 1:J:1531:ASP:OD1 | 1:J:1532:THR:N | 2.49 | 0.45 |
| 1:J:1795:ASN:HD21 | 1:J:1797:TRP:HB2 | 1.82 | 0.45 |
| 1:J:1979:SER:N | 1:J:2078:LYS:HZ1 | 2.13 | 0.45 |
| 1:J:2159:ARG:O | 1:J:2162:THR:OG1 | 2.33 | 0.45 |
| 1:K:657:LYS:NZ | 1:K:720:ILE:O | 2.40 | 0.45 |
| 1:K:1365:ALA:HA | 1:K:1381:PHE:HZ | 1.82 | 0.45 |
| 1:K:2091:ARG:HA | 1:K:2093:ARG:HH21 | 1.82 | 0.45 |
| 1:K:2604:THR:HG23 | 1:K:2782:HIS:NE2 | 2.31 | 0.45 |
| 1:L:947:PRO:HB2 | 1:L:950:VAL:HG22 | 1.97 | 0.45 |
| 1:L:1005:ALA:HB2 | 1:L:1017:GLN:HG3 | 1.98 | 0.45 |
| 1:L:1193:GLN:OE1 | 1:L:1194:TYR:N | 2.49 | 0.45 |
| 1:L:2371:LYS:HD2 | 1:L:2375:LEU:C | 2.41 | 0.45 |
| 1:L:2708:HIS:O | 1:L:2712:VAL:HG13 | 2.16 | 0.45 |
| 1:L:2754:ASN:ND2 | 1:L:2757:ILE:HG12 | 2.31 | 0.45 |
| 1:M:718:MET:SD | 1:M:722:GLN:HG2 | 2.56 | 0.45 |
| 1:M:1212:GLU:CD | 1:M:1214:ASN:H | 2.24 | 0.45 |
| 1:M:1709:ALA:O | 1:M:1712:SER:OG | 2.32 | 0.45 |
| 1:M:2392:ARG:HE | 1:M:2447:THR:HG21 | 1.81 | 0.45 |
| 1:M:2414:GLN:O | 1:M:2416:ASN:N | 2.47 | 0.45 |
| 1:M:3231:LYS:HB2 | 1:M:3284:GLN:HE21 | 1.80 | 0.45 |
| 1:M:3287:LEU:HD23 | 1:M:3287:LEU:H | 1.81 | 0.45 |
| 1:N:321:SER:OG | 1:N:352:GLY:N | 2.47 | 0.45 |
| 1:N:695:ARG:HH21 | 1:N:696:PRO:HD2 | 1.80 | 0.45 |
| 1:N:1827:ASP:HA | 1:N:1831:TRP:HD1 | 1.81 | 0.45 |
| 1:N:2780:ASN:OD1 | 1:N:2780:ASN:N | 2.50 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:O:64:ALA:HB1 | 1:O:174:TYR:HE2 | 1.81 | 0.45 |
| 1:O:1220:LYS:NZ | 1:O:1222:SER:HB2 | 2.31 | 0.45 |
| 1:O:2567:CYS:HA | 1:O:2577:TRP:CE2 | 2.51 | 0.45 |
| 1:O:3155:GLU:HB3 | 1:O:3158:ASN:HD21 | 1.82 | 0.45 |
| 1:P:1135:GLN:HA | 1:P:1138:ARG:CZ | 2.46 | 0.45 |
| 1:P:1289:ASP:OD1 | 1:P:1289:ASP:N | 2.48 | 0.45 |
| 1:P:1726:ASN:OD1 | 1:P:1727:GLN:N | 2.49 | 0.45 |
| 1:Q:2972:ASP:OD1 | 1:Q:2972:ASP:N | 2.49 | 0.45 |
| 1:R:11:LEU:HD11 | 1:R:92:PRO:HG3 | 1.97 | 0.45 |
| 1:R:146:ASP:HB3 | 1:R:149:LEU:HD13 | 1.98 | 0.45 |
| 1:R:618:GLY:HA3 | 1:R:626:SER:N | 2.30 | 0.45 |
| 1:R:1966:GLU:N | 1:R:1966:GLU:OE1 | 2.49 | 0.45 |
| 1:R:2602:ASP:OD2 | 1:R:2604:THR:OG1 | 2.33 | 0.45 |
| 1:R:2660:LEU:HD11 | 1:R:2803:PHE:HZ | 1.81 | 0.45 |
| 1:S:71:ARG:HA | 1:S:74:VAL:HG12 | 1.99 | 0.45 |
| 1:S:1114:ASP:OD1 | 1:S:1114:ASP:N | 2.47 | 0.45 |
| 1:S:1775:LEU:HD12 | 1:S:1779:PHE:HE1 | 1.80 | 0.45 |
| 1:T:5:ARG:HB3 | 1:T:93:TYR:HD2 | 1.81 | 0.45 |
| 1:T:1159:ARG:O | 1:T:1159:ARG:HD2 | 2.16 | 0.45 |
| 1:T:1358:LEU:O | 1:T:1363:ASN:ND2 | 2.49 | 0.45 |
| 1:T:2876:ILE:HB | 1:T:2884:LEU:HB2 | 1.98 | 0.45 |
| 1:T:3304:VAL:HG23 | 1:T:3317:ILE:HB | 1.97 | 0.45 |
| 3:r:1:NAG:H62 | 3:r:2:NAG:H82 | 1.99 | 0.45 |
| 1:A:313:PHE:HZ | 1:A:326:ILE:HD13 | 1.81 | 0.45 |
| 1:A:1385:ILE:H | 1:A:1385:ILE:HD12 | 1.82 | 0.45 |
| 1:A:1890:ARG:NH2 | 1:A:1959:GLU:O | 2.49 | 0.45 |
| 1:A:2154:PHE:HB3 | 1:A:2155:PRO:HD3 | 1.99 | 0.45 |
| 1:A:2159:ARG:HD2 | 1:A:2306:TRP:CE3 | 2.52 | 0.45 |
| 1:A:2191:PRO:O | 1:A:2195:THR:HG23 | 2.16 | 0.45 |
| 1:A:2696:LEU:O | 1:A:2699:SER:OG | 2.27 | 0.45 |
| 1:B:176:HIS:HA | 1:B:179:VAL:HG12 | 1.97 | 0.45 |
| 1:B:608:VAL:HG21 | 1:B:785:VAL:HG21 | 1.98 | 0.45 |
| 1:B:968:PHE:CD1 | 1:B:1047:PRO:HG2 | 2.52 | 0.45 |
| 1:B:1153:PHE:O | 1:B:1154:MET:HE2 | 2.16 | 0.45 |
| 1:B:2664:GLN:HB2 | 1:B:2669:ASN:HD21 | 1.81 | 0.45 |
| 1:B:2978:THR:HG21 | 1:B:2983:VAL:HG13 | 1.99 | 0.45 |
| 1:C:1278:SER:O | 1:C:1281:SER:OG | 2.26 | 0.45 |
| 1:C:2918:THR:O | 1:C:2920:ASP:N | 2.47 | 0.45 |
| 1:C:3129:TRP:CD1 | 1:C:3129:TRP:C | 2.95 | 0.45 |
| 1:D:281:TYR:HE2 | 1:D:283:TYR:HE1 | 1.64 | 0.45 |
| 1:D:1709:ALA:O | 1:D:1712:SER:OG | 2.22 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:D:1881:PHE:O | 1:D:1885:HIS:ND1 | 2.43 | 0.45 |
| 1:D:2368:ASP:OD1 | 1:D:2368:ASP:N | 2.49 | 0.45 |
| 1:D:3035:TYR:H | 1:D:3044:VAL:HG22 | 1.81 | 0.45 |
| 1:E:13:ASP:OD1 | 1:E:14:GLN:N | 2.49 | 0.45 |
| 1:E:299:LEU:O | 1:E:302:GLN:HG3 | 2.15 | 0.45 |
| 1:E:580:TYR:HE1 | 1:E:856:ARG:HD2 | 1.81 | 0.45 |
| 1:E:920:GLN:HE22 | 1:E:1100:ASP:HB3 | 1.81 | 0.45 |
| 1:E:1195:ASP:HB2 | 1:F:2441:LEU:HD21 | 1.97 | 0.45 |
| 1:E:1284:ARG:NE | 1:E:1379:PRO:HG3 | 2.24 | 0.45 |
| 1:E:1365:ALA:HA | 1:E:1381:PHE:CZ | 2.51 | 0.45 |
| 1:E:2217:ILE:HG13 | 1:E:2219:GLU:HG3 | 1.97 | 0.45 |
| 1:E:2941:LEU:HD23 | 1:E:3031:PRO:HG2 | 1.98 | 0.45 |
| 1:F:2980:GLY:HA3 | 1:F:3256:TRP:CZ3 | 2.51 | 0.45 |
| 1:F:3322:GLU:OE1 | 1:F:3322:GLU:N | 2.46 | 0.45 |
| 1:G:221:ARG:NH2 | 1:G:287:SER:O | 2.49 | 0.45 |
| 1:G:225:ILE:O | 1:G:228:GLU:HG3 | 2.16 | 0.45 |
| 1:G:635:PRO:O | 1:G:638:ILE:HG12 | 2.17 | 0.45 |
| 1:G:878:PHE:HA | 1:G:881:ILE:HG22 | 1.98 | 0.45 |
| 1:G:891:CYS:HB3 | 1:G:900:PHE:O | 2.17 | 0.45 |
| 1:G:996:THR:HG23 | 1:G:999:ALA:H | 1.80 | 0.45 |
| 1:G:1350:ASP:HA | 1:G:1463:ASN:ND2 | 2.31 | 0.45 |
| 1:G:1775:LEU:HD12 | 1:G:1779:PHE:HE1 | 1.82 | 0.45 |
| 1:G:2407:GLU:OE2 | 1:G:2424:ALA:HB1 | 2.15 | 0.45 |
| 1:G:3089:ASN:HD21 | 1:G:3248:LEU:N | 2.12 | 0.45 |
| 1:G:3113:PRO:HA | 1:G:3116:MET:HG3 | 1.97 | 0.45 |
| 1:G:3118:HIS:O | 1:G:3121:SER:OG | 2.26 | 0.45 |
| 1:H:618:GLY:HA3 | 1:H:626:SER:N | 2.31 | 0.45 |
| 1:H:1221:TYR:OH | 1:H:1237:GLY:N | 2.50 | 0.45 |
| 1:H:1564:ASN:ND2 | 1:H:1601:GLU:OE2 | 2.50 | 0.45 |
| 1:I:276:TYR:HA | 1:I:279:LEU:HD23 | 1.97 | 0.45 |
| 1:I:579:GLU:HG3 | 1:I:582:ASP:CG | 2.41 | 0.45 |
| 1:I:1189:GLU:N | 1:I:1189:GLU:OE1 | 2.49 | 0.45 |
| 1:I:1801:ASP:OD1 | 1:I:1802:ILE:N | 2.48 | 0.45 |
| 1:I:2534:ALA:HA | 1:I:2537:GLN:HE22 | 1.81 | 0.45 |
| 1:I:2686:GLY:HA2 | 1:I:2693:MET:HG3 | 1.99 | 0.45 |
| 1:J:52:ASP:OD1 | 1:J:53:GLY:N | 2.49 | 0.45 |
| 1:J:57:ALA:HB2 | 1:J:355:ASN:HB2 | 1.98 | 0.45 |
| 1:J:596:GLN:CD | 1:J:598:ASP:H | 2.25 | 0.45 |
| 1:J:739:GLY:HA3 | 1:J:784:LEU:HB3 | 1.97 | 0.45 |
| 1:J:980:ARG:NH2 | 1:J:1046:ASP:OD1 | 2.50 | 0.45 |
| 1:J:1223:VAL:HG13 | 1:J:1231:ILE:HB | 1.98 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:J:1821:ASP:OD1 | 1:J:1822:GLY:N | 2.49 | 0.45 |
| 1:J:2923:ARG:HD3 | 1:J:3008:ILE:C | 2.41 | 0.45 |
| 1:K:945:ALA:HA | 1:K:987:PHE:CZ | 2.52 | 0.45 |
| 1:K:1246:GLY:O | 1:K:1249:THR:OG1 | 2.28 | 0.45 |
| 1:K:1433:LEU:HA | 1:K:1436:LEU:HB2 | 1.99 | 0.45 |
| 1:K:1489:LEU:HD11 | 1:L:2075:TYR:HB2 | 1.98 | 0.45 |
| 1:K:1817:ARG:HG3 | 1:K:1860:TRP:CH2 | 2.52 | 0.45 |
| 1:K:2626:GLU:HB3 | 1:K:2633:LYS:HD2 | 1.97 | 0.45 |
| 1:L:310:LEU:HD13 | 1:L:366:HIS:HB3 | 1.98 | 0.45 |
| 1:L:524:ASP:HA | 1:L:643:ASN:ND2 | 2.31 | 0.45 |
| 1:L:1521:ASP:HB3 | 1:L:1525:HIS:CD2 | 2.51 | 0.45 |
| 1:L:1538:TRP:CD1 | 1:L:1542:GLN:HG3 | 2.51 | 0.45 |
| 1:L:1783:ILE:HD13 | 1:L:1794:PRO:HA | 1.98 | 0.45 |
| 1:L:2088:PRO:C | 1:L:2090:ASN:H | 2.23 | 0.45 |
| 1:L:2805:ASN:HD21 | 1:L:2850:LEU:HB3 | 1.81 | 0.45 |
| 1:L:3037:ILE:HG21 | 1:L:3040:ALA:HB3 | 1.98 | 0.45 |
| 1:M:613:PRO:HA | 1:M:616:LEU:HB3 | 1.97 | 0.45 |
| 1:M:953:GLU:HB2 | 1:M:969:HIS:CD2 | 2.51 | 0.45 |
| 1:M:1747:THR:O | 1:M:1751:GLU:HG2 | 2.16 | 0.45 |
| 1:M:2354:PRO:O | 1:M:2357:VAL:HG22 | 2.16 | 0.45 |
| 1:N:327:LYS:HD2 | 1:N:342:CYS:HB3 | 1.98 | 0.45 |
| 1:N:465:GLN:NE2 | 1:N:558:PRO:O | 2.29 | 0.45 |
| 1:N:503:PHE:HA | 1:N:678:PHE:HE2 | 1.81 | 0.45 |
| 1:N:524:ASP:OD2 | 1:N:527:ARG:HG2 | 2.16 | 0.45 |
| 1:N:542:VAL:HA | 1:N:549:SER:HA | 1.97 | 0.45 |
| 1:N:676:LYS:HD3 | 1:N:680:PHE:CE2 | 2.51 | 0.45 |
| 1:N:1363:ASN:OD1 | 1:N:1364:GLU:N | 2.47 | 0.45 |
| 1:N:1714:HIS:NE2 | 1:N:1732:CYS:SG | 2.89 | 0.45 |
| 1:N:2028:ARG:HB2 | 1:N:2028:ARG:NH1 | 2.32 | 0.45 |
| 1:N:2313:GLN:OE1 | 1:N:2318:LEU:HB2 | 2.16 | 0.45 |
| 1:O:50:LYS:HG2 | 1:O:52:ASP:H | 1.81 | 0.45 |
| 1:O:326:ILE:O | 1:O:345:ALA:HB3 | 2.16 | 0.45 |
| 1:O:442:ASP:OD1 | 1:O:442:ASP:N | 2.50 | 0.45 |
| 1:O:524:ASP:OD2 | 1:O:646:ARG:NH2 | 2.49 | 0.45 |
| 1:O:689:LYS:HD3 | 1:O:689:LYS:HA | 1.69 | 0.45 |
| 1:O:1385:ILE:HD12 | 1:O:1385:ILE:H | 1.81 | 0.45 |
| 1:O:2533:ARG:HH12 | 1:O:2619:ASP:HB2 | 1.81 | 0.45 |
| 1:P:197:ASP:OD1 | 1:P:197:ASP:N | 2.48 | 0.45 |
| 1:P:533:PRO:HB2 | 1:P:535:ILE:HD12 | 1.97 | 0.45 |
| 1:P:1433:LEU:HA | 1:P:1436:LEU:HB2 | 1.99 | 0.45 |
| 1:P:2095:GLU:CD | 1:P:2097:SER:H | 2.24 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:P:2269:ASN:HD21 | 1:P:2428:LEU:N | 2.15 | 0.45 |
| 1:P:2839:GLY:N | 1:P:2842:GLU:OE1 | 2.49 | 0.45 |
| 1:P:3396:CYS:HA | 1:P:3401:ARG:NH1 | 2.31 | 0.45 |
| 1:Q:240:ALA:HB2 | 1:Q:247:PHE:CE2 | 2.52 | 0.45 |
| 1:Q:539:GLU:HA | 1:Q:555:PHE:HB2 | 1.98 | 0.45 |
| 1:Q:2048:ALA:HA | 1:R:1493:ARG:CZ | 2.47 | 0.45 |
| 1:Q:2190:LEU:HD21 | 1:Q:2194:PHE:HD2 | 1.81 | 0.45 |
| 1:R:524:ASP:HA | 1:R:643:ASN:ND2 | 2.31 | 0.45 |
| 1:R:1724:GLU:N | 1:R:1724:GLU:OE1 | 2.50 | 0.45 |
| 1:R:2111:LEU:HD13 | 1:R:2212:PHE:CE1 | 2.51 | 0.45 |
| 1:S:80:LYS:O | 1:S:83:LYS:HG2 | 2.17 | 0.45 |
| 1:S:304:ARG:HH21 | 1:S:411:ARG:CZ | 2.29 | 0.45 |
| 1:S:2052:LYS:HA | 1:S:2052:LYS:HD2 | 1.61 | 0.45 |
| 1:S:2158:HIS:O | 1:S:2162:THR:HG23 | 2.16 | 0.45 |
| 1:S:2335:GLN:NE2 | 1:S:2336:PRO:HB3 | 2.31 | 0.45 |
| 1:S:2848:ASP:OD1 | 1:S:2849:ARG:N | 2.48 | 0.45 |
| 1:S:3033:SER:O | 1:S:3046:ARG:NH2 | 2.49 | 0.45 |
| 1:T:597:ARG:NH2 | 1:T:658:ARG:HB2 | 2.32 | 0.45 |
| 1:T:1291:THR:HA | 1:T:1294:LYS:HG2 | 1.98 | 0.45 |
| 1:T:1305:CYS:HB2 | 1:T:1312:VAL:O | 2.15 | 0.45 |
| 1:T:1465:ASP:OD2 | 1:T:1530:TYR:OH | 2.33 | 0.45 |
| 1:T:1560:PHE:O | 1:T:1609:LEU:HD12 | 2.17 | 0.45 |
| 1:T:1890:ARG:NH1 | 1:T:1959:GLU:O | 2.49 | 0.45 |
| 1:T:1999:LYS:HG2 | 1:T:2007:CYS:HB3 | 1.97 | 0.45 |
| 1:T:2972:ASP:OD1 | 1:T:2972:ASP:N | 2.49 | 0.45 |
| 1:A:730:ARG:HG3 | 1:A:735:ARG:NH2 | 2.29 | 0.45 |
| 1:A:734:ASP:HB3 | 1:A:833:GLY:H | 1.80 | 0.45 |
| 1:A:1919:PRO:O | 1:A:1921:LYS:NZ | 2.38 | 0.45 |
| 1:A:3047:ASP:HB2 | 1:A:3097:GLY:HA3 | 1.99 | 0.45 |
| 1:A:3082:VAL:HG23 | 1:A:3258:TYR:CE2 | 2.50 | 0.45 |
| 1:B:284:ASP:OD1 | 1:B:284:ASP:N | 2.46 | 0.45 |
| 1:B:635:PRO:O | 1:B:638:ILE:HG22 | 2.17 | 0.45 |
| 1:B:759:ASP:OD1 | 1:B:759:ASP:N | 2.45 | 0.45 |
| 1:B:848:ARG:O | 1:B:1124:ASP:N | 2.45 | 0.45 |
| 1:B:947:PRO:HB2 | 1:B:950:VAL:HG22 | 1.98 | 0.45 |
| 1:C:1149:VAL:HG13 | 1:C:1202:ILE:HB | 1.99 | 0.45 |
| 1:C:2398:LEU:HB2 | 1:C:2441:LEU:HD22 | 1.98 | 0.45 |
| 1:C:2446:ILE:HD11 | 1:C:2491:ILE:HD11 | 1.99 | 0.45 |
| 1:C:2641:GLN:NE2 | 1:C:2645:ASP:OD1 | 2.49 | 0.45 |
| 1:C:3118:HIS:O | 1:C:3122:ILE:HG12 | 2.16 | 0.45 |
| 1:D:2376:ASN:OD1 | 1:D:2377:LEU:N | 2.50 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:D:2602:ASP:OD2 | 1:D:2604:THR:OG1 | 2.31 | 0.45 |
| 1:D:2754:ASN:HD22 | 1:D:2757:ILE:HG12 | 1.81 | 0.45 |
| 1:D:3036:GLN:OE1 | 1:D:3042:HIS:N | 2.49 | 0.45 |
| 1:E:435:LYS:NZ | 1:E:1127:GLU:HG3 | 2.30 | 0.45 |
| 1:E:1143:ARG:HG3 | 1:E:1148:ARG:HH21 | 1.81 | 0.45 |
| 1:E:1741:GLN:N | 1:E:1741:GLN:OE1 | 2.50 | 0.45 |
| 1:E:2375:LEU:HB3 | 1:E:2379:GLU:OE2 | 2.16 | 0.45 |
| 1:E:3287:LEU:HD23 | 1:E:3287:LEU:H | 1.81 | 0.45 |
| 1:F:281:TYR:CE2 | 1:F:283:TYR:HE1 | 2.35 | 0.45 |
| 1:F:461:VAL:HG12 | 1:F:1371:ARG:HB2 | 1.99 | 0.45 |
| 1:F:627:THR:HG21 | 1:F:630:TYR:HD2 | 1.81 | 0.45 |
| 1:F:914:HIS:HA | 1:F:917:LEU:HG | 1.98 | 0.45 |
| 1:F:1010:ASP:OD1 | 1:F:1011:PHE:N | 2.49 | 0.45 |
| 1:F:1568:SER:OG | 1:F:1597:GLY:O | 2.31 | 0.45 |
| 1:F:1777:ALA:HA | 1:F:1780:ASN:HB3 | 1.99 | 0.45 |
| 1:F:1967:LEU:HD23 | 1:F:1967:LEU:H | 1.82 | 0.45 |
| 1:F:2326:ALA:O | 1:F:2330:MET:HG2 | 2.17 | 0.45 |
| 1:F:2822:CYS:HB2 | 1:F:2871:HIS:NE2 | 2.32 | 0.45 |
| 1:F:3018:LYS:HE2 | 1:G:3038:LYS:HG3 | 1.98 | 0.45 |
| 1:F:3126:TRP:CZ3 | 1:F:3130:GLN:HG2 | 2.52 | 0.45 |
| 1:G:299:LEU:O | 1:G:302:GLN:HG3 | 2.16 | 0.45 |
| 1:G:1084:LEU:HG | 1:G:1110:PHE:CE1 | 2.52 | 0.45 |
| 1:G:1269:GLN:NE2 | 1:G:1270:ASP:OD2 | 2.49 | 0.45 |
| 1:G:1687:GLU:HA | 1:G:1760:LEU:HD21 | 1.98 | 0.45 |
| 1:G:1896:GLN:NE2 | 1:G:1906:PRO:O | 2.40 | 0.45 |
| 1:G:2742:GLN:HG2 | 1:G:2743:PRO:HD2 | 1.98 | 0.45 |
| 1:G:2981:MET:HG2 | 1:G:2983:VAL:HG22 | 1.97 | 0.45 |
| 1:G:3086:MET:HE2 | 1:G:3086:MET:HA | 1.97 | 0.45 |
| 1:G:3118:HIS:O | 1:G:3122:ILE:HG12 | 2.16 | 0.45 |
| 1:G:3304:VAL:HG23 | 1:G:3317:ILE:HB | 1.98 | 0.45 |
| 1:H:245:GLU:CD | 1:H:245:GLU:H | 2.25 | 0.45 |
| 1:H:1327:ARG:NE | 1:H:1465:ASP:OD1 | 2.50 | 0.45 |
| 1:H:1350:ASP:HA | 1:H:1463:ASN:ND2 | 2.32 | 0.45 |
| 1:H:2304:LYS:HE2 | 1:H:2367:TYR:CG | 2.51 | 0.45 |
| 1:H:2648:ARG:HG3 | 1:H:2656:ARG:HD2 | 1.98 | 0.45 |
| 1:I:489:CYS:O | 1:I:491:HIS:ND1 | 2.49 | 0.45 |
| 1:I:687:ASN:OD1 | 1:I:688:GLU:N | 2.49 | 0.45 |
| 1:I:1278:SER:O | 1:I:1281:SER:OG | 2.30 | 0.45 |
| 1:I:1405:TYR:HA | 1:I:1408:ASN:HD21 | 1.81 | 0.45 |
| 1:J:420:LYS:NZ | 1:J:422:SER:OG | 2.45 | 0.45 |
| 1:J:543:ASP:OD2 | 1:J:546:SER:N | 2.39 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:J:998:ILE:HA | 1:J:1001:MET:HG3 | 1.98 | 0.45 |
| 1:J:1280:LYS:O | 1:J:1284:ARG:HG2 | 2.17 | 0.45 |
| 1:J:2252:LEU:HD23 | 1:J:2309:TRP:HD1 | 1.82 | 0.45 |
| 1:J:3303:VAL:HG13 | 1:J:3305:ILE:HD11 | 1.98 | 0.45 |
| 1:K:603:GLU:O | 1:K:607:GLU:HG2 | 2.16 | 0.45 |
| 1:K:1989:GLY:HA2 | 1:K:2024:TRP:NE1 | 2.32 | 0.45 |
| 1:K:2334:MET:N | 1:K:2334:MET:SD | 2.89 | 0.45 |
| 1:K:2585:LEU:HD13 | 1:K:2706:PHE:CE2 | 2.51 | 0.45 |
| 1:K:2916:THR:C | 1:K:2918:THR:H | 2.25 | 0.45 |
| 1:K:2938:ARG:HD3 | 1:K:3032:PHE:HE2 | 1.81 | 0.45 |
| 1:L:696:PRO:HA | 1:L:699:ILE:HD13 | 1.97 | 0.45 |
| 1:L:2712:VAL:O | 1:L:2715:GLN:HG2 | 2.16 | 0.45 |
| 1:L:3332:VAL:HG22 | 1:L:3406:ILE:HA | 1.98 | 0.45 |
| 1:M:193:GLY:HA3 | 1:M:201:SER:N | 2.32 | 0.45 |
| 1:M:326:ILE:HG23 | 1:M:345:ALA:HB3 | 1.98 | 0.45 |
| 1:M:1732:CYS:HA | 1:M:1742:TRP:CH2 | 2.52 | 0.45 |
| 1:M:2439:ASP:OD1 | 1:M:2439:ASP:N | 2.50 | 0.45 |
| 1:M:2495:PRO:HB2 | 1:M:2500:ARG:HD2 | 1.97 | 0.45 |
| 1:M:2963:PRO:HD2 | 1:M:2965:LEU:HD23 | 1.97 | 0.45 |
| 1:M:3087:LEU:O | 1:M:3090:THR:OG1 | 2.32 | 0.45 |
| 1:N:365:TYR:CE2 | 1:N:367:PHE:HB2 | 2.52 | 0.45 |
| 1:N:930:PHE:CE2 | 1:N:932:ASP:HB2 | 2.51 | 0.45 |
| 1:N:1143:ARG:O | 1:N:1148:ARG:NH1 | 2.32 | 0.45 |
| 1:N:1276:VAL:HG12 | 1:N:1280:LYS:HE3 | 1.98 | 0.45 |
| 1:N:1718:PRO:HG2 | 1:N:1728:ARG:HB3 | 1.98 | 0.45 |
| 1:N:1923:PHE:O | 1:N:1930:ASN:ND2 | 2.49 | 0.45 |
| 1:N:2671:GLU:N | 1:N:2671:GLU:OE1 | 2.49 | 0.45 |
| 1:N:2695:THR:HG21 | 1:N:2698:TYR:HD2 | 1.82 | 0.45 |
| 1:O:559:VAL:HG22 | 1:O:633:PHE:CD2 | 2.51 | 0.45 |
| 1:O:2029:LEU:HD23 | 1:O:2029:LEU:H | 1.82 | 0.45 |
| 1:O:2407:GLU:HB2 | 1:O:2426:PHE:CE2 | 2.51 | 0.45 |
| 1:O:2679:ASN:HD21 | 1:O:2836:VAL:C | 2.25 | 0.45 |
| 1:O:2960:HIS:CE1 | 1:O:3115:PHE:HE2 | 2.35 | 0.45 |
| 1:P:148:ARG:HA | 1:P:151:GLN:HG2 | 1.97 | 0.45 |
| 1:P:542:VAL:HA | 1:P:549:SER:HA | 1.98 | 0.45 |
| 1:P:654:LEU:HD13 | 1:P:723:LEU:HD11 | 1.98 | 0.45 |
| 1:P:925:LEU:HD22 | 1:P:928:LYS:NZ | 2.30 | 0.45 |
| 1:P:998:ILE:HA | 1:P:1001:MET:HG3 | 1.98 | 0.45 |
| 1:P:1286:MET:HB3 | 1:P:1340:ARG:HG3 | 1.97 | 0.45 |
| 1:P:1376:GLU:OE2 | 1:P:1377:SER:N | 2.50 | 0.45 |
| 1:P:1672:GLU:HG3 | 1:P:1673:ARG:HG2 | 1.97 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:P:1967:LEU:HD23 | 1:P:1967:LEU:H | 1.81 | 0.45 |
| 1:P:2149:HIS:HA | 1:P:2154:PHE:CD2 | 2.48 | 0.45 |
| 1:P:3245:PHE:HB3 | 1:P:3264:TYR:HE2 | 1.81 | 0.45 |
| 1:Q:193:GLY:HA2 | 1:Q:199:SER:HB2 | 1.98 | 0.45 |
| 1:Q:461:VAL:HA | 1:Q:1371:ARG:HD3 | 1.98 | 0.45 |
| 1:Q:1818:LEU:HA | 1:Q:1860:TRP:HE1 | 1.81 | 0.45 |
| 1:Q:2542:ARG:HA | 1:Q:2542:ARG:HD3 | 1.82 | 0.45 |
| 1:Q:3013:TRP:H | 1:Q:3013:TRP:CD1 | 2.34 | 0.45 |
| 1:Q:3086:MET:HE3 | 1:Q:3258:TYR:CE1 | 2.52 | 0.45 |
| 1:R:8:VAL:HG11 | 1:R:94:TRP:HB2 | 1.98 | 0.45 |
| 1:R:496:PHE:HB3 | 1:R:497:PRO:HD3 | 1.98 | 0.45 |
| 1:R:725:HIS:O | 1:R:729:GLU:HG2 | 2.17 | 0.45 |
| 1:R:920:GLN:HA | 1:R:923:ASN:HD21 | 1.82 | 0.45 |
| 1:R:1284:ARG:HH21 | 1:R:1287:GLN:HG2 | 1.82 | 0.45 |
| 1:R:1839:GLU:HA | 1:R:1902:ARG:HH22 | 1.81 | 0.45 |
| 1:R:1857:ILE:HB | 1:R:1884:HIS:CE1 | 2.51 | 0.45 |
| 1:R:1928:PRO:HD2 | 1:R:1929:TYR:CD2 | 2.52 | 0.45 |
| 1:R:2574:PHE:O | 1:R:2578:HIS:ND1 | 2.40 | 0.45 |
| 1:R:2921:VAL:HG11 | 1:R:3000:ARG:NH2 | 2.29 | 0.45 |
| 1:R:2988:HIS:O | 1:R:2992:THR:HG23 | 2.17 | 0.45 |
| 1:S:284:ASP:OD1 | 1:S:285:ASP:N | 2.49 | 0.45 |
| 1:S:2500:ARG:NH1 | 1:S:2502:GLU:HG3 | 2.31 | 0.45 |
| 1:S:2604:THR:HA | 1:S:2654:PHE:CE1 | 2.52 | 0.45 |
| 1:S:3100:THR:HA | 1:S:3290:TYR:CE2 | 2.51 | 0.45 |
| 1:T:222:ILE:HA | 1:T:225:ILE:HG12 | 1.97 | 0.45 |
| 1:T:255:ASP:OD1 | 1:T:255:ASP:N | 2.49 | 0.45 |
| 1:T:995:LEU:HD13 | 1:T:999:ALA:HB3 | 1.98 | 0.45 |
| 1:T:2287:HIS:CE1 | 1:T:2432:LEU:HB2 | 2.51 | 0.45 |
| 1:T:2724:ARG:HG3 | 1:T:2730:TYR:CD2 | 2.51 | 0.45 |
| 3:4A:1:NAG:H4 | 3:4A:2:NAG:C7 | 2.47 | 0.45 |
| 1:A:299:LEU:O | 1:A:302:GLN:HG3 | 2.17 | 0.45 |
| 1:A:418:ASP:OD2 | 1:A:662:TYR:N | 2.50 | 0.45 |
| 1:A:1025:ILE:HD12 | 1:A:1028:LEU:HD23 | 1.98 | 0.45 |
| 1:A:1315:CYS:HA | 1:A:1325:TRP:CH2 | 2.52 | 0.45 |
| 1:A:1539:THR:H | 1:A:1542:GLN:HE22 | 1.64 | 0.45 |
| 1:A:2091:ARG:HA | 1:A:2093:ARG:HH21 | 1.82 | 0.45 |
| 1:A:2199:PHE:CZ | 1:A:2208:LEU:HD23 | 2.50 | 0.45 |
| 1:A:2246:ASP:OD1 | 1:A:2247:GLU:N | 2.49 | 0.45 |
| 1:A:3085:GLU:HG3 | 1:A:3086:MET:HE2 | 1.99 | 0.45 |
| 1:B:1284:ARG:NH2 | 1:B:1287:GLN:HG2 | 2.31 | 0.45 |
| 1:C:651:TRP:CZ3 | 1:C:655:GLN:HG3 | 2.51 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:1405:TYR:HA | 1:C:1408:ASN:HD21 | 1.82 | 0.45 |
| 1:C:1649:VAL:HG13 | 1:C:1650:LEU:HD23 | 1.99 | 0.45 |
| 1:C:1815:ARG:HD3 | 1:C:1818:LEU:HD21 | 1.99 | 0.45 |
| 1:C:2345:ASN:O | 1:C:2349:ARG:NH1 | 2.50 | 0.45 |
| 1:C:2360:TYR:HA | 1:C:2363:LEU:HB2 | 1.99 | 0.45 |
| 1:C:3089:ASN:ND2 | 1:C:3248:LEU:H | 2.14 | 0.45 |
| 1:C:3358:THR:H | 1:D:3329:LYS:HE3 | 1.81 | 0.45 |
| 1:D:172:ASP:OD1 | 1:D:173:ASP:N | 2.49 | 0.45 |
| 1:D:220:ASP:O | 1:D:224:VAL:HG13 | 2.16 | 0.45 |
| 1:D:712:ASN:HD22 | 1:D:714:GLN:HB2 | 1.81 | 0.45 |
| 1:D:1098:ASN:O | 1:D:1104:ARG:NH1 | 2.48 | 0.45 |
| 1:D:1420:CYS:SG | 1:D:1485:SER:OG | 2.70 | 0.45 |
| 1:D:1880:ILE:HD12 | 1:D:1880:ILE:H | 1.82 | 0.45 |
| 1:D:2798:SER:OG | 1:D:2799:GLU:OE1 | 2.31 | 0.45 |
| 1:E:844:GLU:HB2 | 1:E:846:HIS:CE1 | 2.52 | 0.45 |
| 1:E:1399:GLU:N | 1:E:1399:GLU:OE1 | 2.49 | 0.45 |
| 1:E:1407:LEU:O | 1:E:1411:LEU:HD13 | 2.16 | 0.45 |
| 1:E:1506:GLU:O | 1:E:1507:PHE:CD1 | 2.70 | 0.45 |
| 1:E:3216:GLY:HA2 | 1:E:3262:TYR:O | 2.17 | 0.45 |
| 1:F:2397:PHE:CD1 | 1:F:2489:PRO:HB3 | 2.52 | 0.45 |
| 1:F:2653:PHE:HA | 1:F:2656:ARG:NH2 | 2.31 | 0.45 |
| 1:F:3266:VAL:HG11 | 1:F:3283:PHE:CZ | 2.51 | 0.45 |
| 1:G:1301:PHE:CD1 | 1:G:1302:PRO:HA | 2.51 | 0.45 |
| 1:G:1388:THR:HG23 | 1:G:1390:LYS:H | 1.80 | 0.45 |
| 1:G:2966:CYS:O | 1:G:2974:TYR:N | 2.44 | 0.45 |
| 1:H:310:LEU:HD13 | 1:H:366:HIS:HB3 | 1.98 | 0.45 |
| 1:H:452:LEU:HD23 | 1:H:554:PHE:CE1 | 2.51 | 0.45 |
| 1:H:588:ASP:HA | 1:H:591:LEU:HD12 | 1.99 | 0.45 |
| 1:H:2254:GLN:HE21 | 1:H:2260:PHE:HA | 1.82 | 0.45 |
| 1:I:257:ASP:O | 1:I:265:ARG:NH2 | 2.39 | 0.45 |
| 1:I:612:LEU:HD21 | 1:I:768:LEU:HA | 1.99 | 0.45 |
| 1:I:636:ILE:H | 1:I:636:ILE:HD12 | 1.82 | 0.45 |
| 1:I:1385:ILE:H | 1:I:1385:ILE:HD12 | 1.81 | 0.45 |
| 1:I:2115:GLN:HE22 | 1:I:2211:PRO:HB2 | 1.81 | 0.45 |
| 1:I:2404:THR:OG1 | 1:I:2405:SER:N | 2.49 | 0.45 |
| 1:I:2673:GLN:HA | 1:I:2673:GLN:OE1 | 2.16 | 0.45 |
| 1:I:2791:GLU:O | 1:I:2794:GLU:HG3 | 2.17 | 0.45 |
| 1:J:378:LYS:NZ | 1:J:383:ASP:O | 2.48 | 0.45 |
| 1:J:758:LYS:HD3 | 1:J:803:GLU:HB3 | 1.97 | 0.45 |
| 1:J:842:HIS:NE2 | 1:J:844:GLU:HB2 | 2.32 | 0.45 |
| 1:J:1542:GLN:HA | 1:J:1545:GLU:OE2 | 2.16 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:K:225:ILE:O | 1:K:228:GLU:HG3 | 2.16 | 0.45 |
| 1:K:2915:PRO:HA | 1:K:2917:LYS:HZ2 | 1.81 | 0.45 |
| 1:K:3165:ASN:ND2 | 1:K:3168:THR:H | 2.15 | 0.45 |
| 1:L:480:PRO:O | 1:L:485:ARG:NH1 | 2.44 | 0.45 |
| 1:L:1324:HIS:HB3 | 1:L:1519:VAL:HG21 | 1.98 | 0.45 |
| 1:L:1928:PRO:HD2 | 1:L:1929:TYR:CD2 | 2.52 | 0.45 |
| 1:M:734:ASP:OD1 | 1:M:833:GLY:N | 2.33 | 0.45 |
| 1:M:3083:GLN:O | 1:M:3087:LEU:HG | 2.17 | 0.45 |
| 1:M:3329:LYS:HE2 | 1:M:3403:GLN:HE22 | 1.82 | 0.45 |
| 1:N:80:LYS:NZ | 1:N:261:ILE:HG13 | 2.32 | 0.45 |
| 1:N:1165:THR:O | 1:N:1222:SER:N | 2.49 | 0.45 |
| 1:N:1284:ARG:NH2 | 1:N:1287:GLN:HG2 | 2.32 | 0.45 |
| 1:N:1641:ASN:HD22 | 3:YA:1:NAG:H83 | 1.81 | 0.45 |
| 1:N:2802:VAL:HG23 | 1:N:2855:VAL:HG23 | 1.98 | 0.45 |
| 1:N:2923:ARG:HD3 | 1:N:3008:ILE:C | 2.41 | 0.45 |
| 1:N:2945:GLN:HG3 | 1:N:3035:TYR:HE1 | 1.80 | 0.45 |
| 1:N:3126:TRP:CZ3 | 1:N:3130:GLN:HG2 | 2.51 | 0.45 |
| 1:O:81:LEU:HD21 | 1:O:86:LEU:HD23 | 1.98 | 0.45 |
| 1:O:176:HIS:CD2 | 1:O:363:LEU:HD21 | 2.51 | 0.45 |
| 1:O:699:ILE:HG13 | 1:O:706:LEU:HD21 | 1.98 | 0.45 |
| 1:O:749:ALA:HA | 1:O:812:ASP:HA | 1.99 | 0.45 |
| 1:O:914:HIS:NE2 | 1:O:1053:HIS:HE1 | 2.15 | 0.45 |
| 1:O:3128:ILE:HG22 | 1:O:3190:LEU:HD22 | 1.99 | 0.45 |
| 1:O:3212:ARG:O | 1:O:3306:SER:OG | 2.28 | 0.45 |
| 1:P:220:ASP:O | 1:P:224:VAL:HG13 | 2.17 | 0.45 |
| 1:P:221:ARG:NH1 | 1:P:285:ASP:HB3 | 2.32 | 0.45 |
| 1:P:251:LEU:HD11 | 1:P:270:ALA:HB2 | 1.99 | 0.45 |
| 1:P:1193:GLN:OE1 | 1:P:1194:TYR:N | 2.49 | 0.45 |
| 1:P:1299:HIS:CD2 | 1:P:1457:PHE:HZ | 2.34 | 0.45 |
| 1:P:1893:ALA:O | 1:P:1897:GLU:OE1 | 2.35 | 0.45 |
| 1:P:1928:PRO:HD2 | 1:P:1929:TYR:CD2 | 2.52 | 0.45 |
| 1:P:1946:ASP:HB3 | 1:P:1950:HIS:CD2 | 2.52 | 0.45 |
| 1:P:2720:GLN:NE2 | 1:P:2730:TYR:HB2 | 2.31 | 0.45 |
| 1:P:3398:GLN:NE2 | 1:P:3400:THR:HG1 | 2.15 | 0.45 |
| 1:Q:63:MET:HB3 | 1:Q:246:LEU:HD21 | 1.99 | 0.45 |
| 1:Q:1328:LEU:HD21 | 1:Q:1519:VAL:HG22 | 1.97 | 0.45 |
| 1:Q:1756:ARG:HH21 | 1:R:2176:VAL:HG13 | 1.81 | 0.45 |
| 1:Q:1852:ILE:HD11 | 1:Q:2013:PHE:HB2 | 1.98 | 0.45 |
| 1:R:479:ARG:NH2 | 1:R:482:ALA:HA | 2.32 | 0.45 |
| 1:R:973:VAL:HG11 | 1:R:1042:TYR:HD1 | 1.82 | 0.45 |
| 1:R:3037:ILE:HG21 | 1:R:3040:ALA:HB3 | 1.98 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:R:3270:LEU:HD11 | 1:R:3281:PHE:CZ | 2.52 | 0.45 |
| 1:S:409:VAL:HG13 | 1:S:666:CYS:HA | 1.97 | 0.45 |
| 1:S:980:ARG:NE | 1:S:1046:ASP:OD2 | 2.41 | 0.45 |
| 1:S:1025:ILE:HG21 | 1:S:1052:HIS:CE1 | 2.51 | 0.45 |
| 1:S:3067:GLN:OE1 | 1:S:3087:LEU:HD13 | 2.17 | 0.45 |
| 1:T:246:LEU:HA | 1:T:249:LYS:HE2 | 1.98 | 0.45 |
| 1:T:428:SER:OG | 1:T:429:ALA:N | 2.49 | 0.45 |
| 1:T:2194:PHE:CD1 | 1:T:2212:PHE:HB3 | 2.51 | 0.45 |
| 1:T:2376:ASN:O | 1:T:2379:GLU:HG3 | 2.17 | 0.45 |
| 1:T:3078:CYS:SG | 1:T:3260:ARG:NE | 2.86 | 0.45 |
| 1:A:434:ARG:HD2 | 1:A:710:TYR:HE1 | 1.81 | 0.45 |
| 1:A:1345:SER:OG | 1:A:1346:VAL:N | 2.48 | 0.45 |
| 1:A:2633:LYS:HE3 | 1:A:2633:LYS:HB3 | 1.82 | 0.45 |
| 1:B:74:VAL:HA | 1:B:77:LEU:HD23 | 1.98 | 0.45 |
| 1:B:477:CYS:HB2 | 1:B:478:PRO:HA | 1.98 | 0.45 |
| 1:B:806:VAL:HG11 | 1:B:825:HIS:O | 2.16 | 0.45 |
| 1:B:1148:ARG:HD2 | 1:B:1244:ARG:HH21 | 1.82 | 0.45 |
| 1:B:1547:LEU:O | 1:B:1550:GLN:HG3 | 2.17 | 0.45 |
| 1:B:1678:LYS:NZ | 1:B:1683:LEU:HA | 2.32 | 0.45 |
| 1:B:2652:SER:O | 1:B:2656:ARG:NH1 | 2.50 | 0.45 |
| 1:B:3155:GLU:OE2 | 1:B:3158:ASN:ND2 | 2.38 | 0.45 |
| 1:B:3266:VAL:HG11 | 1:B:3283:PHE:CZ | 2.51 | 0.45 |
| 1:C:229:LEU:HD11 | 1:C:297:TYR:HD1 | 1.82 | 0.45 |
| 1:C:1338:LEU:HD21 | 1:C:1345:SER:HA | 1.99 | 0.45 |
| 1:C:2614:LEU:O | 1:C:2617:LYS:NZ | 2.48 | 0.45 |
| 1:C:2814:SER:N | 1:C:2838:GLY:O | 2.50 | 0.45 |
| 1:C:3254:MET:HE2 | 1:C:3254:MET:HB2 | 1.83 | 0.45 |
| 1:C:3329:LYS:HB2 | 1:C:3403:GLN:OE1 | 2.16 | 0.45 |
| 1:D:597:ARG:HD3 | 1:D:658:ARG:HH11 | 1.81 | 0.45 |
| 1:D:699:ILE:HD12 | 1:D:699:ILE:H | 1.82 | 0.45 |
| 1:D:1018:TYR:CE1 | 1:D:1056:THR:HB | 2.51 | 0.45 |
| 1:D:1772:GLN:HB2 | 1:D:1818:LEU:HD21 | 1.99 | 0.45 |
| 1:D:1878:ASP:OD2 | 1:D:1880:ILE:HB | 2.17 | 0.45 |
| 1:D:2516:ASN:OD1 | 1:D:2517:ILE:N | 2.48 | 0.45 |
| 1:D:2667:TYR:HA | 1:D:2719:TRP:HH2 | 1.82 | 0.45 |
| 1:E:1687:GLU:OE1 | 1:E:1687:GLU:N | 2.48 | 0.45 |
| 1:E:2216:TYR:CD1 | 1:E:2223:TYR:HB3 | 2.52 | 0.45 |
| 1:E:2217:ILE:HD13 | 1:E:2291:TYR:CE1 | 2.51 | 0.45 |
| 1:E:2938:ARG:HD3 | 1:E:3032:PHE:CE2 | 2.51 | 0.45 |
| 1:E:3100:THR:HA | 1:E:3290:TYR:HE2 | 1.80 | 0.45 |
| 1:E:3259:GLU:OE1 | 1:E:3259:GLU:N | 2.43 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:F:460:SER:HB2 | 1:F:1277:GLU:OE2 | 2.16 | 0.45 |
| 1:F:507:VAL:HG21 | 1:F:638:ILE:HD11 | 1.99 | 0.45 |
| 1:F:695:ARG:HH21 | 1:F:696:PRO:HD2 | 1.82 | 0.45 |
| 1:F:801:ASP:OD1 | 1:F:801:ASP:N | 2.46 | 0.45 |
| 1:F:999:ALA:HA | 1:F:1002:VAL:HG22 | 1.98 | 0.45 |
| 1:F:1359:PRO:HG2 | 1:F:1362:ILE:HG12 | 1.99 | 0.45 |
| 1:F:2111:LEU:HD13 | 1:F:2212:PHE:CE1 | 2.52 | 0.45 |
| 1:F:2292:ASP:OD1 | 1:F:2294:ILE:HG12 | 2.16 | 0.45 |
| 1:F:2865:ARG:HD3 | 1:F:2867:ASP:H | 1.81 | 0.45 |
| 1:G:63:MET:SD | 1:G:63:MET:N | 2.90 | 0.45 |
| 1:G:755:ILE:HG23 | 1:G:765:VAL:HG21 | 1.99 | 0.45 |
| 1:G:950:VAL:HG11 | 1:G:1048:ILE:HG22 | 1.97 | 0.45 |
| 1:G:2798:SER:O | 1:G:2900:LYS:N | 2.49 | 0.45 |
| 1:H:1448:LEU:HD21 | 1:H:1596:LEU:HG | 1.98 | 0.45 |
| 1:H:1576:CYS:HB2 | 1:H:1632:ASP:OD2 | 2.16 | 0.45 |
| 1:H:1607:ASP:OD2 | 1:H:1608:ARG:NH1 | 2.50 | 0.45 |
| 1:H:2149:HIS:CD2 | 1:H:2154:PHE:HE2 | 2.34 | 0.45 |
| 1:H:2788:GLN:OE1 | 1:H:2788:GLN:N | 2.50 | 0.45 |
| 1:I:230:GLN:NE2 | 1:I:235:LYS:HB2 | 2.31 | 0.45 |
| 1:I:583:HIS:HB3 | 1:I:587:PHE:HD2 | 1.82 | 0.45 |
| 1:I:1980:ARG:HE | 1:I:1982:PHE:HZ | 1.65 | 0.45 |
| 1:I:2059:ASN:ND2 | 1:I:2061:SER:OG | 2.50 | 0.45 |
| 1:I:2112:ARG:HH11 | 1:I:2211:PRO:HG3 | 1.81 | 0.45 |
| 1:I:3008:ILE:HD11 | 1:I:3117:ILE:HG22 | 1.99 | 0.45 |
| 1:I:3251:ASP:N | 1:I:3251:ASP:OD1 | 2.49 | 0.45 |
| 1:J:44:GLU:N | 1:J:204:GLU:OE1 | 2.49 | 0.45 |
| 1:J:1084:LEU:HB3 | 1:J:1110:PHE:HE2 | 1.81 | 0.45 |
| 1:J:2582:VAL:HA | 1:J:2706:PHE:HE2 | 1.82 | 0.45 |
| 1:J:3396:CYS:HA | 1:J:3401:ARG:HH22 | 1.82 | 0.45 |
| 1:K:326:ILE:O | 1:K:345:ALA:HB3 | 2.16 | 0.45 |
| 1:K:953:GLU:OE1 | 1:K:969:HIS:ND1 | 2.50 | 0.45 |
| 1:K:1854:HIS:HE1 | 1:K:1885:HIS:CE1 | 2.35 | 0.45 |
| 1:K:2674:TYR:HE1 | 1:K:2712:VAL:HG22 | 1.81 | 0.45 |
| 1:K:3340:PHE:O | 1:K:3376:ASP:N | 2.41 | 0.45 |
| 1:K:3351:VAL:HG21 | 1:K:3388:PHE:HB3 | 1.99 | 0.45 |
| 1:K:3407:ASP:OD1 | 1:K:3407:ASP:N | 2.46 | 0.45 |
| 1:L:231:LYS:HB3 | 1:L:237:TYR:CE2 | 2.50 | 0.45 |
| 1:L:1009:THR:HG22 | 1:L:1070:ARG:NH1 | 2.30 | 0.45 |
| 1:L:2471:TYR:OH | 1:L:2483:PRO:O | 2.35 | 0.45 |
| 1:L:3232:LEU:HD23 | 1:L:3234:PRO:HD3 | 1.98 | 0.45 |
| 1:M:585:ALA:HA | 1:M:588:ASP:OD2 | 2.17 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:M:1801:ASP:OD1 | 1:M:1802:ILE:N | 2.49 | 0.45 |
| 1:M:1871:HIS:CD2 | 1:M:1873:HIS:H | 2.33 | 0.45 |
| 1:M:2090:ASN:O | 1:M:2091:ARG:HD3 | 2.16 | 0.45 |
| 1:M:2266:VAL:HG21 | 1:M:2442:TYR:CD1 | 2.52 | 0.45 |
| 1:M:2961:GLY:HA2 | 1:M:3106:LEU:HD23 | 1.97 | 0.45 |
| 1:M:3329:LYS:HE2 | 1:M:3403:GLN:NE2 | 2.32 | 0.45 |
| 1:N:188:ILE:HA | 1:N:191:LEU:HB2 | 1.97 | 0.45 |
| 1:N:842:HIS:NE2 | 1:N:844:GLU:HB2 | 2.31 | 0.45 |
| 1:O:9:ASP:OD1 | 1:O:9:ASP:N | 2.48 | 0.45 |
| 1:O:309:ALA:H | 1:O:370:SER:HG | 1.64 | 0.45 |
| 1:O:330:ASP:OD1 | 1:O:331:HIS:N | 2.50 | 0.45 |
| 1:O:1588:HIS:HB2 | 1:R:337:GLN:CD | 2.42 | 0.45 |
| 1:O:1739:PHE:HB3 | 1:O:1740:PRO:HD3 | 1.98 | 0.45 |
| 1:O:1974:LYS:NZ | 1:O:2361:GLN:HB3 | 2.32 | 0.45 |
| 1:O:2378:ASP:N | 1:O:2378:ASP:OD1 | 2.49 | 0.45 |
| 1:O:2718:ILE:HD13 | 1:O:2779:LEU:HB3 | 1.97 | 0.45 |
| 1:P:297:TYR:O | 1:P:301:GLU:OE1 | 2.35 | 0.45 |
| 1:P:705:GLU:N | 1:P:705:GLU:OE1 | 2.50 | 0.45 |
| 1:P:3183:PHE:HB2 | 1:P:3185:TYR:CE1 | 2.51 | 0.45 |
| 1:Q:891:CYS:HB3 | 1:Q:900:PHE:O | 2.17 | 0.45 |
| 1:Q:1195:ASP:OD1 | 1:Q:1196:ARG:N | 2.49 | 0.45 |
| 1:Q:2021:GLU:OE1 | 1:Q:2021:GLU:N | 2.41 | 0.45 |
| 1:R:197:ASP:OD1 | 1:R:197:ASP:N | 2.49 | 0.45 |
| 1:R:1219:VAL:HB | 1:R:1239:VAL:HG21 | 1.97 | 0.45 |
| 1:R:2576:GLN:OE1 | 1:R:2576:GLN:N | 2.47 | 0.45 |
| 1:R:2784:LEU:HD12 | 1:R:2788:GLN:HB3 | 1.98 | 0.45 |
| 1:R:3374:ASP:N | 1:R:3379:TYR:OH | 2.38 | 0.45 |
| 1:S:1152:GLY:HA3 | 1:S:1197:LEU:HD21 | 1.99 | 0.45 |
| 1:S:1742:TRP:HD1 | 1:S:1920:LEU:HD12 | 1.82 | 0.45 |
| 1:S:2369:ASP:OD1 | 1:S:2369:ASP:N | 2.49 | 0.45 |
| 1:S:3055:ARG:HH12 | 1:S:3064:LEU:HD12 | 1.79 | 0.45 |
| 1:T:281:TYR:CD2 | 1:T:283:TYR:HE1 | 2.34 | 0.45 |
| 1:T:711:ASP:N | 1:T:711:ASP:OD1 | 2.49 | 0.45 |
| 1:T:1015:GLU:O | 1:T:1019:GLU:HG2 | 2.16 | 0.45 |
| 1:T:3103:MET:HE3 | 1:T:3114:PHE:HD2 | 1.80 | 0.45 |
| 1:A:202:THR:OG1 | 1:A:204:GLU:OE1 | 2.35 | 0.45 |
| 1:A:1751:GLU:OE2 | 1:A:1763:ILE:N | 2.49 | 0.45 |
| 1:A:1991:LYS:HD2 | 1:A:1991:LYS:O | 2.16 | 0.45 |
| 1:A:2091:ARG:HH21 | 1:A:2364:ASN:HD21 | 1.65 | 0.45 |
| 1:A:2568:HIS:HB2 | 1:A:2573:SER:OG | 2.17 | 0.45 |
| 1:A:3037:ILE:HG12 | 1:A:3040:ALA:H | 1.82 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:3289:LYS:HB3 | 1:A:3295:LEU:HD11 | 1.99 | 0.45 |
| 1:A:3395:ARG:HD3 | 1:A:3400:THR:HB | 1.98 | 0.45 |
| 1:B:845:LEU:O | 1:B:926:ARG:NH1 | 2.49 | 0.45 |
| 1:B:1094:THR:OG1 | 1:B:1096:THR:OG1 | 2.35 | 0.45 |
| 1:B:1425:GLN:O | 1:B:1429:VAL:HG22 | 2.17 | 0.45 |
| 1:B:1884:HIS:O | 1:B:1887:SER:OG | 2.24 | 0.45 |
| 1:B:2636:ARG:HH21 | 1:B:2702:ASP:CG | 2.24 | 0.45 |
| 1:B:3303:VAL:HG13 | 1:B:3305:ILE:HD11 | 1.98 | 0.45 |
| 1:C:2000:VAL:O | 1:C:2041:LYS:NZ | 2.47 | 0.45 |
| 1:C:2287:HIS:CD2 | 1:C:2430:GLY:HA3 | 2.52 | 0.45 |
| 1:C:2392:ARG:HE | 1:C:2447:THR:HG21 | 1.82 | 0.45 |
| 1:C:2743:PRO:HA | 1:C:2762:ARG:NE | 2.32 | 0.45 |
| 1:C:2926:VAL:HG12 | 1:C:3009:PRO:HB2 | 1.99 | 0.45 |
| 1:C:3133:GLN:NE2 | 1:C:3138:ARG:HB3 | 2.32 | 0.45 |
| 1:D:128:GLY:N | 1:D:141:THR:OG1 | 2.50 | 0.45 |
| 1:D:1839:GLU:OE2 | 1:D:1840:GLN:NE2 | 2.49 | 0.45 |
| 1:D:2312:LEU:O | 1:D:2316:ARG:NH1 | 2.49 | 0.45 |
| 1:D:2944:LEU:HA | 1:D:3002:LYS:HE2 | 1.98 | 0.45 |
| 1:D:3227:THR:OG1 | 1:D:3245:PHE:O | 2.28 | 0.45 |
| 1:E:348:ILE:HD11 | 1:E:367:PHE:CD2 | 2.52 | 0.45 |
| 1:E:441:THR:OG1 | 1:E:444:GLU:OE1 | 2.30 | 0.45 |
| 1:E:719:THR:HG21 | 1:E:847:VAL:HG21 | 1.99 | 0.45 |
| 1:E:1867:HIS:HA | 1:E:1874:TYR:CD2 | 2.52 | 0.45 |
| 1:E:2407:GLU:HB2 | 1:E:2426:PHE:CE2 | 2.52 | 0.45 |
| 1:E:2407:GLU:OE2 | 1:E:2424:ALA:HB1 | 2.16 | 0.45 |
| 1:E:2986:HIS:O | 1:E:2990:LEU:HD23 | 2.16 | 0.45 |
| 1:F:454:ARG:HH21 | 1:F:1339:ALA:HA | 1.82 | 0.45 |
| 1:F:592:LEU:HD11 | 1:F:737:PHE:HE1 | 1.81 | 0.45 |
| 1:F:938:ASP:CG | 1:F:1055:ASN:HD21 | 2.25 | 0.45 |
| 1:F:1257:ASN:CG | 1:F:1258:ILE:H | 2.24 | 0.45 |
| 1:F:1963:ILE:HD11 | 1:F:1967:LEU:HD11 | 1.99 | 0.45 |
| 1:F:2001:CYS:HB2 | 1:F:2050:THR:OG1 | 2.16 | 0.45 |
| 1:F:2523:ALA:O | 1:F:2526:GLU:HG3 | 2.16 | 0.45 |
| 1:F:2960:HIS:HA | 1:F:2977:CYS:HB3 | 1.98 | 0.45 |
| 1:G:131:ASN:HA | 1:G:138:HIS:HA | 1.99 | 0.45 |
| 1:G:392:SER:OG | 1:G:393:VAL:N | 2.48 | 0.45 |
| 1:G:601:ASP:O | 1:G:604:VAL:HG22 | 2.17 | 0.45 |
| 1:G:1317:HIS:HA | 1:G:1322:PHE:CD1 | 2.51 | 0.45 |
| 1:G:1574:PHE:HB2 | 1:G:1634:GLU:HB3 | 1.99 | 0.45 |
| 1:G:1674:ARG:HD3 | 1:G:1954:GLU:HG2 | 1.98 | 0.45 |
| 1:H:461:VAL:H | 1:H:1277:GLU:CD | 2.25 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:H:1248:GLU:HB3 | 1:H:1251:LYS:HE3 | 1.99 | 0.45 |
| 1:H:1274:GLY:O | 1:H:1277:GLU:HG3 | 2.17 | 0.45 |
| 1:H:2001:CYS:HB2 | 1:H:2050:THR:OG1 | 2.17 | 0.45 |
| 1:H:2004:GLU:OE1 | 1:H:2004:GLU:N | 2.46 | 0.45 |
| 1:H:2494:LYS:HD3 | 1:H:2494:LYS:HA | 1.77 | 0.45 |
| 1:H:2559:ASP:N | 1:H:2559:ASP:OD2 | 2.47 | 0.45 |
| 1:I:602:PHE:HA | 1:I:605:GLN:NE2 | 2.31 | 0.45 |
| 1:I:704:HIS:HB3 | 1:I:705:GLU:OE1 | 2.16 | 0.45 |
| 1:I:758:LYS:HD3 | 1:I:758:LYS:HA | 1.78 | 0.45 |
| 1:I:1362:ILE:HB | 1:I:1394:ARG:HH22 | 1.82 | 0.45 |
| 1:I:2567:CYS:O | 1:I:2569:HIS:ND1 | 2.46 | 0.45 |
| 1:I:3055:ARG:HH12 | 1:I:3064:LEU:HD12 | 1.81 | 0.45 |
| 1:J:1254:ILE:HG23 | 1:J:1256:LYS:H | 1.81 | 0.45 |
| 1:J:1486:ASP:OD1 | 1:J:1486:ASP:N | 2.46 | 0.45 |
| 1:J:1963:ILE:HD11 | 1:J:1967:LEU:HD11 | 1.98 | 0.45 |
| 1:J:1999:LYS:NZ | 1:J:2009:ASP:OD1 | 2.50 | 0.45 |
| 1:J:2577:TRP:C | 1:J:2577:TRP:CD1 | 2.94 | 0.45 |
| 1:J:2823:ASP:N | 1:J:2823:ASP:OD1 | 2.46 | 0.45 |
| 1:J:3082:VAL:O | 1:J:3086:MET:HG2 | 2.16 | 0.45 |
| 1:K:98:LYS:HG2 | 1:K:99:PRO:HD2 | 1.98 | 0.45 |
| 1:K:580:TYR:CE1 | 1:K:856:ARG:HD2 | 2.51 | 0.45 |
| 1:K:866:LEU:HD13 | 1:K:968:PHE:CE1 | 2.45 | 0.45 |
| 1:K:1575:ILE:HD11 | 1:K:1590:ALA:HB2 | 1.98 | 0.45 |
| 1:K:1742:TRP:CD1 | 1:K:1920:LEU:HD12 | 2.51 | 0.45 |
| 1:K:2376:ASN:N | 1:K:2379:GLU:OE2 | 2.49 | 0.45 |
| 1:K:2777:ASP:O | 1:K:3137:HIS:NE2 | 2.50 | 0.45 |
| 1:L:427:GLN:OE1 | 1:L:427:GLN:N | 2.46 | 0.45 |
| 1:L:554:PHE:O | 1:L:568:ARG:NH2 | 2.50 | 0.45 |
| 1:L:1166:LEU:HB3 | 1:L:1179:GLY:O | 2.17 | 0.45 |
| 1:L:1421:ASP:O | 1:L:1424:ILE:HG22 | 2.17 | 0.45 |
| 1:L:1694:ALA:O | 1:L:1697:SER:OG | 2.31 | 0.45 |
| 1:L:2985:PRO:HB2 | 1:L:2989:ARG:NH2 | 2.31 | 0.45 |
| 1:M:71:ARG:NH1 | 1:M:273:LEU:O | 2.50 | 0.45 |
| 1:M:197:ASP:OD1 | 1:M:198:HIS:N | 2.49 | 0.45 |
| 1:M:284:ASP:OD1 | 1:M:285:ASP:N | 2.49 | 0.45 |
| 1:M:307:GLU:OE1 | 1:M:412:PRO:HA | 2.17 | 0.45 |
| 1:M:983:ARG:HD3 | 1:M:1031:GLY:HA2 | 1.98 | 0.45 |
| 1:M:1506:GLU:O | 1:M:1507:PHE:CD1 | 2.70 | 0.45 |
| 1:M:1587:ASN:OD1 | 1:P:337:GLN:N | 2.49 | 0.45 |
| 1:M:2029:LEU:HD23 | 1:M:2029:LEU:H | 1.80 | 0.45 |
| 1:M:2108:LYS:O | 1:M:2112:ARG:NH1 | 2.50 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:N:1011:PHE:HA | 1:N:1063:TRP:HH2 | 1.82 | 0.45 |
| 1:N:1262:SER:OG | 1:N:1263:HIS:N | 2.50 | 0.45 |
| 1:N:3103:MET:HA | 1:N:3109:SER:HA | 1.98 | 0.45 |
| 1:O:104:PRO:HA | 1:O:105:ARG:NH1 | 2.32 | 0.45 |
| 1:O:444:GLU:HB3 | 1:O:518:PHE:HZ | 1.81 | 0.45 |
| 1:O:884:PHE:CE1 | 1:O:1090:PRO:HG2 | 2.52 | 0.45 |
| 1:O:1079:CYS:O | 1:P:2492:ILE:HD13 | 2.17 | 0.45 |
| 1:O:2047:ASP:O | 1:P:1493:ARG:NH2 | 2.43 | 0.45 |
| 1:O:2535:VAL:HG22 | 1:O:2592:GLN:NE2 | 2.31 | 0.45 |
| 1:O:2602:ASP:HA | 1:O:2711:ASN:ND2 | 2.31 | 0.45 |
| 1:O:2986:HIS:O | 1:O:2990:LEU:HD23 | 2.17 | 0.45 |
| 1:P:225:ILE:O | 1:P:229:LEU:HG | 2.17 | 0.45 |
| 1:P:1018:TYR:OH | 1:P:1056:THR:HB | 2.17 | 0.45 |
| 1:P:2001:CYS:HB2 | 1:P:2050:THR:OG1 | 2.17 | 0.45 |
| 1:P:3010:TYR:OH | 1:P:3188:ASP:OD1 | 2.35 | 0.45 |
| 1:P:3088:HIS:CE1 | 1:P:3119:HIS:CE1 | 3.04 | 0.45 |
| 1:Q:313:PHE:HZ | 1:Q:326:ILE:HD13 | 1.82 | 0.45 |
| 1:Q:678:PHE:O | 1:Q:685:ASN:ND2 | 2.49 | 0.45 |
| 1:Q:1013:THR:O | 1:Q:1016:VAL:HG12 | 2.17 | 0.45 |
| 1:Q:1811:ARG:NH2 | 1:Q:1880:ILE:HB | 2.32 | 0.45 |
| 1:Q:1993:SER:HB2 | 1:Q:2017:GLY:H | 1.82 | 0.45 |
| 1:Q:2026:PHE:O | 1:R:1651:ARG:NH1 | 2.50 | 0.45 |
| 1:R:459:THR:HG23 | 1:R:1285:ARG:HH12 | 1.82 | 0.45 |
| 1:R:953:GLU:HA | 1:R:969:HIS:HB2 | 1.98 | 0.45 |
| 1:R:1821:ASP:OD1 | 1:R:1822:GLY:N | 2.49 | 0.45 |
| 1:R:1892:TYR:O | 1:R:1896:GLN:HG2 | 2.17 | 0.45 |
| 1:R:2088:PRO:O | 1:R:2090:ASN:N | 2.47 | 0.45 |
| 1:R:2412:VAL:H | 1:R:2422:ALA:HB2 | 1.81 | 0.45 |
| 1:R:3173:ARG:HB2 | 1:R:3176:GLN:OE1 | 2.16 | 0.45 |
| 1:S:601:ASP:OD1 | 1:S:602:PHE:N | 2.49 | 0.45 |
| 1:S:958:PRO:HA | 1:S:961:ASN:HA | 1.98 | 0.45 |
| 1:S:1221:TYR:OH | 1:S:1236:PHE:N | 2.38 | 0.45 |
| 1:S:1555:ARG:HE | 1:S:1557:PHE:HZ | 1.63 | 0.45 |
| 1:S:2021:GLU:OE1 | 1:S:2021:GLU:N | 2.40 | 0.45 |
| 1:S:2849:ARG:HH11 | 1:S:2849:ARG:HA | 1.81 | 0.45 |
| 1:T:30:LYS:HD3 | 1:T:30:LYS:HA | 1.81 | 0.45 |
| 1:T:69:TRP:O | 1:T:72:LEU:HG | 2.16 | 0.45 |
| 1:T:627:THR:HG21 | 1:T:630:TYR:HD2 | 1.81 | 0.45 |
| 1:T:1085:ARG:HD3 | 1:T:1110:PHE:CE2 | 2.52 | 0.45 |
| 1:T:1359:PRO:HG2 | 1:T:1362:ILE:HG12 | 1.98 | 0.45 |
| 1:T:2095:GLU:CD | 1:T:2097:SER:H | 2.24 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:T:2217:ILE:HG22 | 1:T:2219:GLU:H | 1.80 | 0.45 |
| 1:T:3160:GLU:CD | 1:T:3160:GLU:H | 2.25 | 0.45 |
| 1:T:3357:TYR:CE1 | 1:T:3360:LEU:HD22 | 2.52 | 0.45 |
| 3:hA:2:NAG:H4 | 3:hA:3:BMA:H2 | 1.69 | 0.45 |
| 1:A:1820:ASP:HB2 | 1:A:1828:ASN:HD21 | 1.81 | 0.45 |
| 1:A:3231:LYS:HB2 | 1:A:3284:GLN:HG3 | 1.98 | 0.45 |
| 1:B:112:PHE:HB3 | 1:B:121:GLN:O | 2.16 | 0.45 |
| 1:B:1283:LEU:HG | 1:B:1284:ARG:HH22 | 1.82 | 0.45 |
| 1:B:1376:GLU:OE2 | 1:B:1377:SER:N | 2.49 | 0.45 |
| 1:B:1416:GLN:HE21 | 1:B:1422:PHE:HA | 1.81 | 0.45 |
| 1:B:1433:LEU:HD21 | 1:B:1460:HIS:NE2 | 2.32 | 0.45 |
| 1:B:1963:ILE:HD11 | 1:B:1967:LEU:HD11 | 1.98 | 0.45 |
| 1:C:939:TRP:HA | 1:C:943:MET:HE1 | 1.98 | 0.45 |
| 1:C:2460:VAL:O | 1:D:1085:ARG:NH2 | 2.50 | 0.45 |
| 1:C:3228:ALA:O | 1:C:3245:PHE:N | 2.46 | 0.45 |
| 1:D:81:LEU:HB3 | 1:D:86:LEU:HB2 | 1.98 | 0.45 |
| 1:D:2413:CYS:SG | 1:D:2470:ARG:NE | 2.88 | 0.45 |
| 1:D:2610:LEU:HG | 1:D:2614:LEU:HD23 | 1.98 | 0.45 |
| 1:E:170:GLU:OE2 | 1:E:304:ARG:HD2 | 2.17 | 0.45 |
| 1:E:1159:ARG:HA | 1:E:1186:ASP:O | 2.16 | 0.45 |
| 1:E:1865:LYS:HZ1 | 1:E:1867:HIS:HB2 | 1.82 | 0.45 |
| 1:E:2059:ASN:OD1 | 1:E:2061:SER:N | 2.49 | 0.45 |
| 1:E:2802:VAL:H | 1:E:2856:THR:HG22 | 1.82 | 0.45 |
| 1:E:3325:LYS:HD2 | 1:E:3325:LYS:HA | 1.81 | 0.45 |
| 1:F:47:MET:HA | 1:F:55:ARG:HE | 1.81 | 0.45 |
| 1:F:606:PHE:HA | 1:F:609:VAL:HG22 | 1.98 | 0.45 |
| 1:F:1315:CYS:O | 1:F:1317:HIS:ND1 | 2.45 | 0.45 |
| 1:F:1857:ILE:HB | 1:F:1884:HIS:CE1 | 2.52 | 0.45 |
| 1:F:3350:ASN:OD1 | 1:F:3372:SER:HB3 | 2.16 | 0.45 |
| 1:G:35:TYR:OH | 1:G:208:TYR:O | 2.33 | 0.45 |
| 1:G:240:ALA:HB2 | 1:G:247:PHE:CE2 | 2.52 | 0.45 |
| 1:G:441:THR:OG1 | 1:G:444:GLU:OE1 | 2.34 | 0.45 |
| 1:G:442:ASP:OD1 | 1:G:442:ASP:N | 2.50 | 0.45 |
| 1:G:738:VAL:HG23 | 1:G:789:ILE:HG21 | 1.99 | 0.45 |
| 1:G:1532:THR:OG1 | 1:G:1534:ASN:OD1 | 2.27 | 0.45 |
| 1:G:1662:ASP:N | 1:G:1662:ASP:OD1 | 2.50 | 0.45 |
| 1:G:1723:PRO:O | 1:G:1728:ARG:NH1 | 2.50 | 0.45 |
| 1:G:2667:TYR:O | 1:G:2671:GLU:HG3 | 2.16 | 0.45 |
| 1:H:845:LEU:HD21 | 1:H:932:ASP:HA | 1.98 | 0.45 |
| 1:H:872:ASP:HB3 | 1:H:877:GLY:HA2 | 1.98 | 0.45 |
| 1:H:1356:ARG:HH22 | 1:H:1402:ASN:ND2 | 2.15 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:H:1433:LEU:HD21 | 1:H:1460:HIS:NE2 | 2.32 | 0.45 |
| 1:H:2660:LEU:HD21 | 1:H:2803:PHE:HE1 | 1.82 | 0.45 |
| 1:H:2695:THR:OG1 | 1:H:2696:LEU:N | 2.50 | 0.45 |
| 1:I:24:ARG:HH12 | 1:I:125:TRP:CD1 | 2.35 | 0.45 |
| 1:I:502:LEU:HD23 | 1:I:502:LEU:HA | 1.82 | 0.45 |
| 1:I:891:CYS:HB3 | 1:I:900:PHE:O | 2.16 | 0.45 |
| 1:I:1446:SER:OG | 1:I:1447:SER:N | 2.50 | 0.45 |
| 1:I:2929:LEU:HD22 | 1:I:2933:GLN:HG3 | 1.98 | 0.45 |
| 1:I:3160:GLU:HG2 | 1:I:3169:ARG:HH22 | 1.81 | 0.45 |
| 1:J:1063:TRP:NE1 | 1:J:1067:GLN:HE22 | 2.14 | 0.45 |
| 1:J:1276:VAL:O | 1:J:1279:LEU:HG | 2.17 | 0.45 |
| 1:J:1281:SER:O | 1:J:1285:ARG:HG2 | 2.17 | 0.45 |
| 1:J:1351:TRP:HZ3 | 1:J:1463:ASN:HB3 | 1.82 | 0.45 |
| 1:J:2088:PRO:C | 1:J:2090:ASN:H | 2.24 | 0.45 |
| 1:J:2113:ASP:HA | 1:J:2116:LYS:HE3 | 1.99 | 0.45 |
| 1:J:2959:PHE:O | 1:J:2976:CYS:HB2 | 2.16 | 0.45 |
| 1:J:3128:ILE:HD11 | 1:J:3190:LEU:HD22 | 1.99 | 0.45 |
| 1:J:3163:ASN:ND2 | 1:J:3168:THR:OG1 | 2.49 | 0.45 |
| 1:K:230:GLN:NE2 | 1:K:235:LYS:HB2 | 2.31 | 0.45 |
| 1:K:2580:LEU:HA | 1:K:2583:VAL:HG12 | 1.97 | 0.45 |
| 1:K:2587:ARG:NH1 | 1:K:2753:PRO:HG2 | 2.30 | 0.45 |
| 1:L:181:PHE:CZ | 1:L:219:VAL:HG13 | 2.52 | 0.45 |
| 1:L:970:HIS:HD2 | 1:L:972:LEU:HG | 1.82 | 0.45 |
| 1:L:1368:PHE:CG | 1:S:1440:ARG:HD2 | 2.52 | 0.45 |
| 1:L:1679:SER:OG | 1:L:1680:VAL:N | 2.49 | 0.45 |
| 1:L:1710:LEU:HD13 | 1:L:1750:PHE:CE1 | 2.51 | 0.45 |
| 1:L:2695:THR:OG1 | 1:L:2696:LEU:N | 2.50 | 0.45 |
| 1:L:3122:ILE:HG13 | 1:L:3125:ILE:HD11 | 1.99 | 0.45 |
| 1:M:484:VAL:O | 1:M:485:ARG:NH1 | 2.46 | 0.45 |
| 1:M:636:ILE:HD12 | 1:M:636:ILE:H | 1.81 | 0.45 |
| 1:M:646:ARG:O | 1:M:650:ILE:HG23 | 2.16 | 0.45 |
| 1:M:1278:SER:O | 1:M:1281:SER:OG | 2.26 | 0.45 |
| 1:M:1865:LYS:NZ | 1:M:1867:HIS:HB2 | 2.30 | 0.45 |
| 1:M:2246:ASP:N | 1:M:2246:ASP:OD1 | 2.49 | 0.45 |
| 1:M:2533:ARG:HA | 1:M:2536:GLN:OE1 | 2.17 | 0.45 |
| 1:M:3211:ASP:OD1 | 1:M:3212:ARG:N | 2.49 | 0.45 |
| 1:N:581:GLY:H | 1:N:856:ARG:HH22 | 1.63 | 0.45 |
| 1:N:837:GLU:OE1 | 1:N:837:GLU:N | 2.50 | 0.45 |
| 1:N:914:HIS:HA | 1:N:917:LEU:HG | 1.97 | 0.45 |
| 1:N:1167:GLU:HA | 1:N:1177:PRO:HA | 1.99 | 0.45 |
| 1:N:1364:GLU:OE2 | 1:N:1365:ALA:N | 2.50 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:O:601:ASP:OD1 | 1:O:602:PHE:N | 2.50 | 0.45 |
| 1:O:1278:SER:O | 1:O:1281:SER:OG | 2.30 | 0.45 |
| 1:O:1433:LEU:HA | 1:O:1436:LEU:HB2 | 1.97 | 0.45 |
| 1:P:13:ASP:O | 1:P:17:LEU:HD23 | 2.16 | 0.45 |
| 1:P:618:GLY:HA3 | 1:P:626:SER:N | 2.30 | 0.45 |
| 1:P:728:ASP:HB3 | 1:P:836:HIS:CD2 | 2.51 | 0.45 |
| 1:P:1280:LYS:O | 1:P:1284:ARG:HG2 | 2.17 | 0.45 |
| 1:P:1421:ASP:O | 1:P:1424:ILE:HG22 | 2.16 | 0.45 |
| 1:P:1457:PHE:CE1 | 1:P:1461:HIS:HE1 | 2.35 | 0.45 |
| 1:P:1483:ASP:OD1 | 1:P:1484:LYS:N | 2.50 | 0.45 |
| 1:P:1556:LEU:HB2 | 1:P:1625:LEU:HD11 | 1.99 | 0.45 |
| 1:Q:255:ASP:OD1 | 1:Q:255:ASP:N | 2.47 | 0.45 |
| 1:Q:650:ILE:HG22 | 1:Q:713:LEU:HD12 | 1.98 | 0.45 |
| 1:Q:1366:SER:HB3 | 1:Q:1377:SER:HA | 1.99 | 0.45 |
| 1:Q:2200:TYR:OH | 1:Q:2205:ASP:OD1 | 2.29 | 0.45 |
| 1:Q:2762:ARG:HD3 | 1:Q:2762:ARG:HA | 1.68 | 0.45 |
| 1:Q:2800:ASP:OD1 | 1:Q:2801:ARG:N | 2.49 | 0.45 |
| 1:Q:3396:CYS:HA | 1:Q:3401:ARG:CZ | 2.47 | 0.45 |
| 1:R:752:ILE:HB | 1:R:809:SER:HB3 | 1.97 | 0.45 |
| 1:R:1457:PHE:CE1 | 1:R:1461:HIS:HE1 | 2.35 | 0.45 |
| 1:R:2524:GLU:HG3 | 1:R:2595:ARG:HG2 | 1.98 | 0.45 |
| 1:R:2695:THR:HG21 | 1:R:2698:TYR:CD2 | 2.51 | 0.45 |
| 1:R:2795:LYS:HE2 | 1:R:2795:LYS:HB2 | 1.72 | 0.45 |
| 1:R:3351:VAL:HG23 | 1:R:3390:SER:HA | 1.97 | 0.45 |
| 1:R:3395:ARG:O | 1:R:3401:ARG:NH1 | 2.42 | 0.45 |
| 1:S:849:SER:OG | 1:S:850:ASP:N | 2.49 | 0.45 |
| 1:S:3165:ASN:ND2 | 1:S:3168:THR:H | 2.15 | 0.45 |
| 1:T:1539:THR:HG22 | 1:T:1542:GLN:CD | 2.41 | 0.45 |
| 1:T:1557:PHE:HD2 | 1:T:1611:LYS:HD2 | 1.82 | 0.45 |
| 1:T:1633:LEU:HD11 | 1:T:1653:PRO:HG2 | 1.98 | 0.45 |
| 1:A:508:GLU:C | 1:A:512:LYS:HZ2 | 2.25 | 0.45 |
| 1:A:589:GLY:HA2 | 1:A:592:LEU:HG | 1.98 | 0.45 |
| 1:A:939:TRP:HA | 1:A:943:MET:HE1 | 1.99 | 0.45 |
| 1:A:1221:TYR:OH | 1:A:1236:PHE:N | 2.38 | 0.45 |
| 1:A:1741:GLN:OE1 | 1:A:1741:GLN:N | 2.50 | 0.45 |
| 1:A:2156:HIS:HB3 | 1:A:2357:VAL:HG21 | 1.99 | 0.45 |
| 1:A:2542:ARG:HH22 | 1:A:2591:LEU:HD12 | 1.82 | 0.45 |
| 1:A:2604:THR:HA | 1:A:2654:PHE:HE1 | 1.81 | 0.45 |
| 1:B:244:VAL:HA | 1:B:247:PHE:HD2 | 1.81 | 0.45 |
| 1:B:1132:SER:O | 1:B:1135:GLN:HB3 | 2.17 | 0.45 |
| 1:B:1433:LEU:HD21 | 1:B:1460:HIS:CE1 | 2.52 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:1492:MET:O | 1:B:1516:PRO:HG2 | 2.16 | 0.45 |
| 1:B:2610:LEU:HG | 1:B:2614:LEU:HD23 | 1.98 | 0.45 |
| 1:C:1322:PHE:HD2 | 1:C:1426:PHE:CE2 | 2.34 | 0.45 |
| 1:C:2090:ASN:O | 1:C:2091:ARG:HG2 | 2.17 | 0.45 |
| 1:C:2229:GLN:HB3 | 1:C:2231:GLU:OE1 | 2.17 | 0.45 |
| 1:C:2279:GLN:HG2 | 1:C:2281:TYR:H | 1.80 | 0.45 |
| 1:C:2407:GLU:OE2 | 1:C:2424:ALA:HB1 | 2.17 | 0.45 |
| 1:C:2603:TRP:H | 1:C:2711:ASN:HD21 | 1.64 | 0.45 |
| 1:C:3389:VAL:HG22 | 1:C:3401:ARG:HG2 | 1.99 | 0.45 |
| 1:D:371:LYS:HD3 | 1:D:371:LYS:C | 2.42 | 0.45 |
| 1:D:994:ARG:HH21 | 1:D:995:LEU:HB2 | 1.82 | 0.45 |
| 1:D:1011:PHE:HA | 1:D:1063:TRP:HH2 | 1.81 | 0.45 |
| 1:D:1814:LYS:HB3 | 1:D:1816:ASN:OD1 | 2.17 | 0.45 |
| 1:D:1847:GLU:CD | 1:D:1847:GLU:H | 2.24 | 0.45 |
| 1:D:2086:GLU:HA | 1:D:2366:ARG:HH12 | 1.82 | 0.45 |
| 1:D:2718:ILE:CD1 | 1:D:2779:LEU:HB2 | 2.47 | 0.45 |
| 1:D:3198:SER:HA | 1:D:3201:ASN:ND2 | 2.32 | 0.45 |
| 1:E:1731:CYS:HA | 1:E:2022:MET:HE1 | 1.99 | 0.45 |
| 1:E:2056:ARG:HH22 | 1:E:2060:GLY:HA2 | 1.82 | 0.45 |
| 1:E:2111:LEU:HD12 | 1:E:2211:PRO:HG2 | 1.98 | 0.45 |
| 1:E:2473:ILE:HD12 | 1:E:2483:PRO:HA | 1.99 | 0.45 |
| 1:E:3100:THR:HA | 1:E:3290:TYR:CE2 | 2.52 | 0.45 |
| 1:F:103:LEU:HG | 1:F:104:PRO:HD2 | 1.98 | 0.45 |
| 1:F:255:ASP:N | 1:F:255:ASP:OD1 | 2.48 | 0.45 |
| 1:F:469:GLU:OE1 | 1:F:469:GLU:N | 2.50 | 0.45 |
| 1:F:735:ARG:HH22 | 1:F:788:GLU:CD | 2.24 | 0.45 |
| 1:F:981:SER:HB3 | 1:F:1031:GLY:HA3 | 1.99 | 0.45 |
| 1:F:2045:VAL:HG13 | 1:F:2046:ASP:OD1 | 2.17 | 0.45 |
| 1:F:2541:PRO:HB3 | 1:F:2753:PRO:HB3 | 1.99 | 0.45 |
| 1:G:12:THR:OG1 | 1:G:15:GLU:OE2 | 2.21 | 0.45 |
| 1:G:164:MET:HE1 | 1:G:187:HIS:CE1 | 2.51 | 0.45 |
| 1:G:181:PHE:CE1 | 1:G:219:VAL:HG13 | 2.52 | 0.45 |
| 1:G:1475:GLN:HB3 | 1:G:1482:ASP:HB3 | 1.97 | 0.45 |
| 1:G:1979:SER:OG | 1:G:2078:LYS:N | 2.50 | 0.45 |
| 1:G:2190:LEU:HD21 | 1:G:2194:PHE:CD2 | 2.52 | 0.45 |
| 1:G:2371:LYS:HA | 1:G:2371:LYS:HD2 | 1.77 | 0.45 |
| 1:G:2465:ALA:HB2 | 1:H:1085:ARG:HD2 | 1.98 | 0.45 |
| 1:H:251:LEU:HD23 | 1:H:251:LEU:HA | 1.87 | 0.45 |
| 1:H:471:HIS:HB3 | 1:H:632:ALA:HB1 | 1.99 | 0.45 |
| 1:H:1036:SER:O | 1:H:1042:TYR:HB2 | 2.16 | 0.45 |
| 1:H:1135:GLN:O | 1:H:1138:ARG:N | 2.50 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:H:1415:GLU:OE2 | 1:H:1555:ARG:NH2 | 2.50 | 0.45 |
| 1:H:1990:ILE:HG22 | 1:H:1990:ILE:O | 2.17 | 0.45 |
| 1:I:77:LEU:HD13 | 1:I:213:PHE:CE1 | 2.52 | 0.45 |
| 1:I:651:TRP:CH2 | 1:I:655:GLN:HG3 | 2.52 | 0.45 |
| 1:I:938:ASP:HA | 1:I:1055:ASN:ND2 | 2.32 | 0.45 |
| 1:I:1263:HIS:HB2 | 1:I:1528:TYR:HB2 | 1.99 | 0.45 |
| 1:I:1991:LYS:O | 1:I:1991:LYS:HD2 | 2.17 | 0.45 |
| 1:I:2621:PRO:HD2 | 1:I:2622:PHE:CD1 | 2.48 | 0.45 |
| 1:I:2855:VAL:O | 1:I:2855:VAL:HG12 | 2.17 | 0.45 |
| 1:I:3366:PRO:HB3 | 1:J:3254:MET:HB2 | 1.99 | 0.45 |
| 1:J:477:CYS:HA | 1:J:479:ARG:N | 2.32 | 0.45 |
| 1:J:1222:SER:HA | 1:J:1233:SER:HB3 | 1.99 | 0.45 |
| 1:J:1350:ASP:HA | 1:J:1463:ASN:ND2 | 2.31 | 0.45 |
| 1:J:1720:CYS:SG | 1:J:1731:CYS:N | 2.89 | 0.45 |
| 1:J:2754:ASN:HD22 | 1:J:2757:ILE:HG12 | 1.82 | 0.45 |
| 1:J:3182:LYS:HG3 | 1:J:3183:PHE:CE1 | 2.52 | 0.45 |
| 1:K:133:ASP:OD1 | 1:K:134:SER:N | 2.50 | 0.45 |
| 1:K:1489:LEU:HA | 1:K:1492:MET:HG2 | 1.99 | 0.45 |
| 1:K:1832:LYS:O | 1:K:1835:LEU:HG | 2.17 | 0.45 |
| 1:L:1869:MET:HE1 | 1:L:1881:PHE:HB2 | 1.98 | 0.45 |
| 1:L:2088:PRO:O | 1:L:2090:ASN:N | 2.44 | 0.45 |
| 1:L:2930:SER:O | 1:L:2934:VAL:HG23 | 2.17 | 0.45 |
| 1:M:719:THR:HG21 | 1:M:847:VAL:HG21 | 1.99 | 0.45 |
| 1:M:1489:LEU:HD11 | 1:N:2075:TYR:HB2 | 1.98 | 0.45 |
| 1:M:1834:PHE:CE1 | 1:M:1853:ALA:HB1 | 2.52 | 0.45 |
| 1:M:2250:LEU:HA | 1:M:2253:GLU:OE1 | 2.17 | 0.45 |
| 1:M:2348:THR:OG1 | 1:M:2349:ARG:NH1 | 2.50 | 0.45 |
| 1:M:2602:ASP:HA | 1:M:2711:ASN:HD21 | 1.82 | 0.45 |
| 1:M:2900:LYS:HB3 | 1:M:2900:LYS:HE3 | 1.81 | 0.45 |
| 1:N:1238:LYS:NZ | 1:N:1239:VAL:O | 2.50 | 0.45 |
| 1:N:1528:TYR:HE1 | 1:N:1530:TYR:HE1 | 1.64 | 0.45 |
| 1:N:1985:PHE:O | 1:N:2029:LEU:HD12 | 2.17 | 0.45 |
| 1:N:2266:VAL:HG21 | 1:N:2442:TYR:CZ | 2.52 | 0.45 |
| 1:N:3076:ASN:ND2 | 1:N:3079:ASP:OD2 | 2.33 | 0.45 |
| 1:N:3340:PHE:CE2 | 1:N:3351:VAL:HG11 | 2.51 | 0.45 |
| 1:N:3389:VAL:HG23 | 1:N:3401:ARG:HH21 | 1.81 | 0.45 |
| 1:O:449:ARG:CZ | 1:O:552:ASN:HD21 | 2.29 | 0.45 |
| 1:O:953:GLU:HB2 | 1:O:969:HIS:CD2 | 2.52 | 0.45 |
| 1:O:954:THR:HA | 1:O:965:PRO:HA | 1.99 | 0.45 |
| 1:O:2114:LEU:HD13 | 1:O:2172:HIS:CE1 | 2.52 | 0.45 |
| 1:O:2977:CYS:HA | 1:O:2987:TRP:CH2 | 2.52 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:O:3351:VAL:O | 1:O:3372:SER:HA | 2.16 | 0.45 |
| 1:P:788:GLU:CD | 1:P:791:ASP:H | 2.24 | 0.45 |
| 1:P:1521:ASP:HB3 | 1:P:1525:HIS:CD2 | 2.52 | 0.45 |
| 1:P:2695:THR:HG21 | 1:P:2698:TYR:HD2 | 1.81 | 0.45 |
| 1:Q:248:ARG:NH1 | 1:Q:803:GLU:HA | 2.32 | 0.45 |
| 1:Q:687:ASN:OD1 | 1:Q:688:GLU:N | 2.50 | 0.45 |
| 1:Q:1033:GLU:O | 1:Q:1036:SER:OG | 2.21 | 0.45 |
| 1:Q:1428:ILE:HG21 | 1:Q:1610:TYR:CZ | 2.51 | 0.45 |
| 1:Q:1817:ARG:HG3 | 1:Q:1860:TRP:CH2 | 2.52 | 0.45 |
| 1:R:458:ASP:HB2 | 1:R:1341:GLY:HA3 | 1.99 | 0.45 |
| 1:R:1777:ALA:HA | 1:R:1780:ASN:HB3 | 1.98 | 0.45 |
| 1:R:1999:LYS:NZ | 1:R:2009:ASP:OD1 | 2.50 | 0.45 |
| 1:R:2741:ARG:HH12 | 1:S:2870:TYR:N | 2.14 | 0.45 |
| 1:S:193:GLY:HA2 | 1:S:199:SER:HB2 | 1.99 | 0.45 |
| 1:S:469:GLU:OE1 | 1:S:474:PRO:HD2 | 2.16 | 0.45 |
| 1:S:866:LEU:HD22 | 1:S:968:PHE:CE1 | 2.52 | 0.45 |
| 1:S:1033:GLU:OE2 | 1:S:1035:TYR:N | 2.35 | 0.45 |
| 1:S:1268:LEU:HD12 | 1:S:1361:LEU:HD13 | 1.98 | 0.45 |
| 1:S:1366:SER:HB2 | 1:S:1375:GLU:OE2 | 2.17 | 0.45 |
| 1:S:2190:LEU:HD21 | 1:S:2194:PHE:HB3 | 1.98 | 0.45 |
| 1:S:2583:VAL:HG21 | 1:S:2772:PHE:HB3 | 1.99 | 0.45 |
| 1:S:3173:ARG:HB2 | 1:S:3176:GLN:HG3 | 1.99 | 0.45 |
| 1:T:427:GLN:OE1 | 1:T:427:GLN:N | 2.46 | 0.45 |
| 1:T:639:LEU:O | 1:T:642:SER:OG | 2.22 | 0.45 |
| 1:T:845:LEU:O | 1:T:926:ARG:NH1 | 2.50 | 0.45 |
| 1:T:2695:THR:OG1 | 1:T:2696:LEU:N | 2.50 | 0.45 |
| 1:T:2714:ARG:O | 1:T:2718:ILE:HG12 | 2.17 | 0.45 |
| 1:A:2148:LEU:HB3 | 1:A:2151:VAL:HG11 | 1.99 | 0.45 |
| 1:A:2827:HIS:ND1 | 1:A:2827:HIS:O | 2.50 | 0.45 |
| 1:A:3174:PRO:HA | 1:A:3177:ILE:HG12 | 1.98 | 0.45 |
| 1:B:542:VAL:HA | 1:B:549:SER:HA | 1.98 | 0.45 |
| 1:B:674:LEU:HD12 | 1:B:695:ARG:NH2 | 2.32 | 0.45 |
| 1:B:872:ASP:HB3 | 1:B:877:GLY:HA2 | 1.99 | 0.45 |
| 1:B:1036:SER:O | 1:B:1042:TYR:HB2 | 2.17 | 0.45 |
| 1:B:1720:CYS:SG | 1:B:1731:CYS:N | 2.90 | 0.45 |
| 1:B:2377:LEU:HA | 1:B:2380:LEU:HD12 | 1.98 | 0.45 |
| 1:B:2666:ASP:HB3 | 1:B:2669:ASN:OD1 | 2.16 | 0.45 |
| 1:C:47:MET:SD | 1:C:47:MET:N | 2.90 | 0.45 |
| 1:C:193:GLY:HA2 | 1:C:199:SER:HB2 | 1.98 | 0.45 |
| 1:C:604:VAL:HG12 | 1:C:781:PHE:CD1 | 2.52 | 0.45 |
| 1:C:2356:GLU:OE1 | 1:C:2356:GLU:N | 2.42 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:2676:VAL:HG21 | 1:C:2851:PHE:CE1 | 2.52 | 0.45 |
| 1:D:23:LEU:HD12 | 1:D:26:LEU:HD11 | 1.98 | 0.45 |
| 1:D:571:GLN:NE2 | 1:D:616:LEU:O | 2.28 | 0.45 |
| 1:D:706:LEU:HB3 | 1:D:708:TYR:CD1 | 2.51 | 0.45 |
| 1:D:1009:THR:HA | 1:D:1070:ARG:NH2 | 2.32 | 0.45 |
| 1:D:1049:PHE:CG | 1:D:1053:HIS:CE1 | 3.05 | 0.45 |
| 1:D:1788:VAL:HG12 | 1:D:1789:LEU:HD22 | 1.99 | 0.45 |
| 1:D:1854:HIS:HE1 | 1:D:1885:HIS:NE2 | 2.14 | 0.45 |
| 1:D:3295:LEU:HG | 1:D:3297:ALA:H | 1.81 | 0.45 |
| 1:E:408:GLY:HA3 | 1:E:669:THR:HG23 | 1.99 | 0.45 |
| 1:E:585:ALA:HA | 1:E:588:ASP:OD2 | 2.17 | 0.45 |
| 1:E:597:ARG:HH12 | 1:E:654:LEU:HD21 | 1.82 | 0.45 |
| 1:E:647:LEU:HA | 1:E:650:ILE:HG12 | 1.97 | 0.45 |
| 1:E:742:LEU:HB2 | 1:E:781:PHE:HD2 | 1.81 | 0.45 |
| 1:E:1221:TYR:OH | 1:E:1236:PHE:N | 2.44 | 0.45 |
| 1:E:3048:VAL:HG13 | 1:E:3052:LEU:HD12 | 1.99 | 0.45 |
| 1:F:444:GLU:HA | 1:F:447:GLU:CD | 2.41 | 0.45 |
| 1:F:444:GLU:O | 1:F:447:GLU:HG2 | 2.16 | 0.45 |
| 1:F:568:ARG:NH1 | 1:F:634:ASP:OD1 | 2.50 | 0.45 |
| 1:F:859:VAL:HG12 | 1:F:863:ARG:CZ | 2.47 | 0.45 |
| 1:F:1017:GLN:HA | 1:F:1020:ILE:HG12 | 1.99 | 0.45 |
| 1:F:1299:HIS:ND1 | 1:F:1299:HIS:O | 2.50 | 0.45 |
| 1:F:1367:TYR:CE2 | 1:F:1369:ASP:HB3 | 2.52 | 0.45 |
| 1:F:1827:ASP:HA | 1:F:1831:TRP:CD1 | 2.52 | 0.45 |
| 1:F:2416:ASN:OD1 | 1:F:2417:GLY:N | 2.50 | 0.45 |
| 1:F:3071:THR:HG23 | 1:F:3083:GLN:HG3 | 1.97 | 0.45 |
| 1:G:1328:LEU:HD21 | 1:G:1519:VAL:HG22 | 1.99 | 0.45 |
| 1:G:1588:HIS:HB2 | 1:J:337:GLN:HE22 | 1.82 | 0.45 |
| 1:G:2108:LYS:O | 1:G:2112:ARG:NH1 | 2.50 | 0.45 |
| 1:G:2392:ARG:HB3 | 1:G:2394:PHE:CE1 | 2.51 | 0.45 |
| 1:G:2987:TRP:HE3 | 1:G:2988:HIS:CE1 | 2.35 | 0.45 |
| 1:H:543:ASP:OD2 | 1:H:546:SER:N | 2.35 | 0.45 |
| 1:H:968:PHE:CD1 | 1:H:1047:PRO:HG2 | 2.51 | 0.45 |
| 1:H:1283:LEU:HA | 1:H:1286:MET:HG3 | 1.99 | 0.45 |
| 1:H:2369:ASP:OD1 | 1:H:2369:ASP:N | 2.50 | 0.45 |
| 1:H:2754:ASN:ND2 | 1:H:2757:ILE:HG12 | 2.32 | 0.45 |
| 1:I:758:LYS:HG2 | 1:I:803:GLU:OE1 | 2.17 | 0.45 |
| 1:I:1157:GLY:HA3 | 1:I:1159:ARG:HH12 | 1.82 | 0.45 |
| 1:I:1356:ARG:HB2 | 1:I:1357:GLN:OE1 | 2.16 | 0.45 |
| 1:I:1827:ASP:OD1 | 1:I:1827:ASP:N | 2.49 | 0.45 |
| 1:J:220:ASP:O | 1:J:224:VAL:HG13 | 2.16 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:J:295:GLN:O | 1:J:299:LEU:HD23 | 2.17 | 0.45 |
| 1:J:461:VAL:HG22 | 1:J:1277:GLU:OE2 | 2.17 | 0.45 |
| 1:J:1009:THR:O | 1:J:1072:LEU:HD21 | 2.17 | 0.45 |
| 1:J:2227:ASP:HB3 | 1:J:2277:GLY:HA3 | 1.99 | 0.45 |
| 1:J:2954:GLU:H | 1:J:2954:GLU:CD | 2.25 | 0.45 |
| 1:K:202:THR:OG1 | 1:K:204:GLU:OE1 | 2.35 | 0.45 |
| 1:K:304:ARG:HB3 | 1:K:414:LYS:HE3 | 1.98 | 0.45 |
| 1:K:729:GLU:O | 1:K:732:THR:HG22 | 2.17 | 0.45 |
| 1:K:755:ILE:HG23 | 1:K:765:VAL:HG21 | 1.99 | 0.45 |
| 1:K:1362:ILE:CD1 | 1:K:1380:PHE:HB3 | 2.47 | 0.45 |
| 1:K:1588:HIS:CE1 | 1:N:337:GLN:HB2 | 2.51 | 0.45 |
| 1:K:1739:PHE:HB3 | 1:K:1740:PRO:HD3 | 1.98 | 0.45 |
| 1:K:2229:GLN:HB3 | 1:K:2274:LEU:HD12 | 1.98 | 0.45 |
| 1:K:3061:LEU:HD23 | 1:K:3066:TYR:HD1 | 1.82 | 0.45 |
| 1:L:509:ASP:OD1 | 1:L:509:ASP:N | 2.48 | 0.45 |
| 1:L:2777:ASP:OD1 | 1:L:2777:ASP:N | 2.43 | 0.45 |
| 1:L:3334:ARG:HA | 1:L:3334:ARG:HD2 | 1.82 | 0.45 |
| 1:M:1093:GLN:HB2 | 1:M:1097:ILE:HG21 | 1.98 | 0.45 |
| 1:M:1133:ILE:O | 1:M:1136:LEU:HG | 2.17 | 0.45 |
| 1:M:1852:ILE:HD13 | 1:M:2030:TYR:CZ | 2.52 | 0.45 |
| 1:M:2633:LYS:HB3 | 1:M:2633:LYS:HE3 | 1.68 | 0.45 |
| 1:M:3203:ILE:HA | 1:M:3206:ASN:HB2 | 1.99 | 0.45 |
| 1:N:795:LYS:HD3 | 1:N:796:LYS:HD3 | 1.98 | 0.45 |
| 1:N:1356:ARG:NH1 | 1:N:1356:ARG:HA | 2.31 | 0.45 |
| 1:N:1956:ASP:OD1 | 1:N:1957:THR:N | 2.50 | 0.45 |
| 1:N:2392:ARG:HD2 | 1:N:2394:PHE:CZ | 2.51 | 0.45 |
| 1:N:2572:ALA:HB2 | 1:N:2736:ASN:HD22 | 1.82 | 0.45 |
| 1:N:3227:THR:HB | 1:N:3246:TYR:CD2 | 2.52 | 0.45 |
| 1:O:6:LYS:NZ | 1:O:89:ILE:HG12 | 2.32 | 0.45 |
| 1:O:663:LYS:HG2 | 1:O:700:TYR:CE2 | 2.52 | 0.45 |
| 1:O:674:LEU:HD22 | 1:O:695:ARG:NH2 | 2.31 | 0.45 |
| 1:O:849:SER:HB3 | 1:O:854:LEU:HD21 | 1.98 | 0.45 |
| 1:O:875:ILE:HG13 | 1:O:1099:PRO:HD3 | 1.99 | 0.45 |
| 1:O:2446:ILE:HD11 | 1:O:2491:ILE:HD11 | 1.99 | 0.45 |
| 1:O:2712:VAL:HA | 1:O:2715:GLN:HG2 | 1.98 | 0.45 |
| 1:O:2796:ARG:CZ | 1:O:2801:ARG:HH21 | 2.30 | 0.45 |
| 1:O:2930:SER:H | 1:O:2933:GLN:NE2 | 2.15 | 0.45 |
| 1:O:3068:THR:HA | 1:O:3087:LEU:HD21 | 1.99 | 0.45 |
| 1:P:1772:GLN:HB2 | 1:P:1818:LEU:HD21 | 1.99 | 0.45 |
| 1:P:2343:ASN:CG | 1:P:2349:ARG:HH12 | 2.24 | 0.45 |
| 1:P:3080:PHE:HA | 1:P:3083:GLN:HE22 | 1.82 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:P:3131:THR:HA | 1:P:3134:LYS:HG2 | 1.99 | 0.45 |
| 1:Q:307:GLU:OE1 | 1:Q:412:PRO:HA | 2.17 | 0.45 |
| 1:Q:884:PHE:CE1 | 1:Q:1090:PRO:HG2 | 2.52 | 0.45 |
| 1:Q:1032:ASN:HA | 1:Q:1226:LEU:HD12 | 1.98 | 0.45 |
| 1:Q:1079:CYS:O | 1:R:2492:ILE:HD13 | 2.17 | 0.45 |
| 1:Q:1756:ARG:HH12 | 1:R:2175:THR:HB | 1.81 | 0.45 |
| 1:Q:2130:HIS:O | 1:Q:2130:HIS:ND1 | 2.43 | 0.45 |
| 1:Q:2153:THR:HA | 1:Q:2156:HIS:ND1 | 2.32 | 0.45 |
| 1:Q:3082:VAL:HG23 | 1:Q:3258:TYR:CE1 | 2.52 | 0.45 |
| 1:R:69:TRP:O | 1:R:72:LEU:HG | 2.16 | 0.45 |
| 1:R:1276:VAL:O | 1:R:1279:LEU:HG | 2.17 | 0.45 |
| 1:R:2674:TYR:CE1 | 1:R:2712:VAL:HG22 | 2.52 | 0.45 |
| 1:R:2805:ASN:HB3 | 1:R:2893:SER:OG | 2.17 | 0.45 |
| 1:R:2861:GLN:OE1 | 1:R:2862:MET:HG3 | 2.15 | 0.45 |
| 1:S:888:PRO:HG2 | 1:S:890:TRP:CH2 | 2.52 | 0.45 |
| 1:S:1356:ARG:HB2 | 1:S:1357:GLN:OE1 | 2.17 | 0.45 |
| 1:S:1832:LYS:O | 1:S:1835:LEU:HG | 2.16 | 0.45 |
| 1:S:2250:LEU:HA | 1:S:2253:GLU:OE1 | 2.17 | 0.45 |
| 1:S:2404:THR:OG1 | 1:S:2405:SER:N | 2.50 | 0.45 |
| 1:S:2855:VAL:HG12 | 1:S:2855:VAL:O | 2.17 | 0.45 |
| 1:S:2997:MET:HE2 | 1:S:2997:MET:HB2 | 1.86 | 0.45 |
| 1:T:559:VAL:N | 1:T:564:GLU:O | 2.45 | 0.45 |
| 1:T:1267:ASN:HB3 | 1:T:1348:TYR:CZ | 2.52 | 0.45 |
| 1:T:1777:ALA:HA | 1:T:1780:ASN:HB3 | 1.99 | 0.45 |
| 1:T:2614:LEU:HD13 | 1:T:2704:ILE:HD11 | 1.98 | 0.45 |
| 1:T:2623:GLU:N | 1:T:2623:GLU:OE1 | 2.50 | 0.45 |
| 1:T:2664:GLN:OE1 | 1:T:2664:GLN:N | 2.45 | 0.45 |
| 1:T:2739:GLU:HA | 1:T:2742:GLN:OE1 | 2.17 | 0.45 |
| 1:T:3218:VAL:C | 1:T:3219:LEU:HD12 | 2.42 | 0.45 |
| 1:T:3232:LEU:HD23 | 1:T:3234:PRO:HD3 | 1.99 | 0.45 |
| 1:T:3289:LYS:HG2 | 1:T:3290:TYR:H | 1.82 | 0.45 |
| 1:A:635:PRO:O | 1:A:638:ILE:HG12 | 2.16 | 0.44 |
| 1:A:1433:LEU:HD21 | 1:A:1460:HIS:HE1 | 1.81 | 0.44 |
| 1:A:3082:VAL:O | 1:A:3086:MET:HG2 | 2.17 | 0.44 |
| 1:A:3133:GLN:OE1 | 1:A:3140:PHE:HB3 | 2.17 | 0.44 |
| 1:A:3144:ARG:HA | 1:A:3147:LEU:HD21 | 1.99 | 0.44 |
| 1:B:705:GLU:HG2 | 1:B:706:LEU:HD22 | 1.99 | 0.44 |
| 1:B:816:LYS:HZ2 | 1:B:818:TRP:HZ2 | 1.63 | 0.44 |
| 1:B:1093:GLN:N | 1:B:1093:GLN:OE1 | 2.50 | 0.44 |
| 1:B:1135:GLN:O | 1:B:1138:ARG:HG2 | 2.16 | 0.44 |
| 1:B:1153:PHE:HZ | 1:B:1166:LEU:HD22 | 1.82 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:2004:GLU:OE1 | 1:B:2004:GLU:N | 2.46 | 0.44 |
| 1:B:2213:ALA:HA | 1:B:2226:ARG:NH2 | 2.33 | 0.44 |
| 1:B:2343:ASN:OD1 | 1:B:2344:GLU:N | 2.50 | 0.44 |
| 1:B:2661:ALA:HA | 1:B:2664:GLN:HE22 | 1.81 | 0.44 |
| 1:B:3148:ARG:HD3 | 1:B:3152:ARG:HH22 | 1.83 | 0.44 |
| 1:B:3324:ASN:H | 1:B:3398:GLN:HE22 | 1.64 | 0.44 |
| 1:C:28:ASP:OD1 | 1:C:29:ASP:N | 2.51 | 0.44 |
| 1:C:513:SER:HG | 1:C:514:ARG:HH11 | 1.61 | 0.44 |
| 1:C:854:LEU:HB3 | 1:C:858:GLN:HG3 | 1.99 | 0.44 |
| 1:C:866:LEU:HD22 | 1:C:968:PHE:HE1 | 1.82 | 0.44 |
| 1:C:1383:VAL:H | 1:C:1392:THR:HG22 | 1.82 | 0.44 |
| 1:C:2112:ARG:HH11 | 1:C:2211:PRO:HG3 | 1.81 | 0.44 |
| 1:C:2570:GLY:HA2 | 1:C:2847:PHE:CE1 | 2.52 | 0.44 |
| 1:C:2864:LEU:HD11 | 1:C:2870:TYR:HB3 | 1.99 | 0.44 |
| 1:C:2930:SER:H | 1:C:2933:GLN:CD | 2.25 | 0.44 |
| 1:C:3091:ILE:O | 1:C:3095:VAL:HG12 | 2.17 | 0.44 |
| 1:D:54:LYS:NZ | 1:D:355:ASN:OD1 | 2.41 | 0.44 |
| 1:D:859:VAL:HG12 | 1:D:863:ARG:CZ | 2.46 | 0.44 |
| 1:D:1501:ASP:OD2 | 1:D:1504:GLN:N | 2.51 | 0.44 |
| 1:D:2777:ASP:N | 1:D:2777:ASP:OD1 | 2.49 | 0.44 |
| 1:D:2988:HIS:HD2 | 1:D:3119:HIS:CD2 | 2.35 | 0.44 |
| 1:E:278:GLN:HG2 | 1:E:279:LEU:HD22 | 1.99 | 0.44 |
| 1:E:1284:ARG:NH2 | 1:E:1376:GLU:OE1 | 2.49 | 0.44 |
| 1:E:1993:SER:HA | 1:E:2016:LEU:HA | 1.99 | 0.44 |
| 1:E:2404:THR:OG1 | 1:E:2405:SER:N | 2.49 | 0.44 |
| 1:E:3089:ASN:HD21 | 1:E:3247:ILE:HD12 | 1.82 | 0.44 |
| 1:E:3352:LYS:HA | 1:E:3371:ASN:O | 2.17 | 0.44 |
| 1:F:1193:GLN:OE1 | 1:F:1194:TYR:N | 2.50 | 0.44 |
| 1:F:1363:ASN:OD1 | 1:F:1364:GLU:N | 2.50 | 0.44 |
| 1:F:2527:SER:O | 1:F:2530:LYS:HG3 | 2.18 | 0.44 |
| 1:G:75:VAL:O | 1:G:78:GLU:HG3 | 2.17 | 0.44 |
| 1:G:636:ILE:H | 1:G:636:ILE:HD12 | 1.82 | 0.44 |
| 1:G:1352:THR:HG21 | 1:G:1535:PHE:HE2 | 1.82 | 0.44 |
| 1:G:1917:ARG:HH22 | 1:H:1631:ILE:H | 1.64 | 0.44 |
| 1:G:1958:LEU:H | 1:G:1958:LEU:HD12 | 1.80 | 0.44 |
| 1:G:2051:VAL:HB | 1:G:2071:PRO:HG2 | 1.99 | 0.44 |
| 1:G:2674:TYR:OH | 1:G:2712:VAL:O | 2.31 | 0.44 |
| 1:G:2900:LYS:HE3 | 1:G:2900:LYS:HB3 | 1.75 | 0.44 |
| 1:H:68:GLN:HA | 1:H:71:ARG:HG2 | 1.98 | 0.44 |
| 1:H:735:ARG:CZ | 1:H:788:GLU:HG2 | 2.48 | 0.44 |
| 1:H:2088:PRO:C | 1:H:2090:ASN:H | 2.24 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:H:2551:HIS:HB2 | 1:H:2700:ALA:HB2 | 1.98 | 0.44 |
| 1:H:2754:ASN:OD1 | 1:H:2755:ASP:N | 2.51 | 0.44 |
| 1:H:3017:SER:O | 1:H:3055:ARG:NH2 | 2.46 | 0.44 |
| 1:H:3312:ASP:OD1 | 1:H:3312:ASP:N | 2.49 | 0.44 |
| 1:I:915:ARG:HD2 | 1:I:1060:TRP:HZ3 | 1.81 | 0.44 |
| 1:I:1008:GLN:OE1 | 1:I:1008:GLN:N | 2.39 | 0.44 |
| 1:I:1204:ASP:OD1 | 1:I:1205:ILE:N | 2.48 | 0.44 |
| 1:I:2622:PHE:CD2 | 1:I:2703:PRO:HB2 | 2.52 | 0.44 |
| 1:I:3065:PHE:HA | 1:I:3068:THR:HG22 | 1.98 | 0.44 |
| 1:I:3216:GLY:HA2 | 1:I:3262:TYR:O | 2.17 | 0.44 |
| 1:J:357:MET:SD | 1:J:358:PRO:HD2 | 2.58 | 0.44 |
| 1:J:1827:ASP:HA | 1:J:1831:TRP:HD1 | 1.79 | 0.44 |
| 1:K:5:ARG:HH12 | 1:K:78:GLU:CD | 2.25 | 0.44 |
| 1:K:104:PRO:HG2 | 1:K:107:VAL:HG22 | 1.99 | 0.44 |
| 1:K:525:TRP:CD1 | 1:K:643:ASN:HD22 | 2.36 | 0.44 |
| 1:K:738:VAL:HG23 | 1:K:789:ILE:HG21 | 1.99 | 0.44 |
| 1:K:754:SER:HA | 1:K:765:VAL:HG23 | 1.99 | 0.44 |
| 1:K:773:GLY:O | 1:K:776:GLU:HG2 | 2.17 | 0.44 |
| 1:K:973:VAL:HG11 | 1:K:1045:TYR:CG | 2.52 | 0.44 |
| 1:K:1405:TYR:HA | 1:K:1408:ASN:HD21 | 1.81 | 0.44 |
| 1:K:1635:ILE:O | 1:K:1647:SER:OG | 2.34 | 0.44 |
| 1:K:1979:SER:OG | 1:K:2078:LYS:N | 2.49 | 0.44 |
| 1:K:1993:SER:O | 1:K:2058:LEU:HD22 | 2.17 | 0.44 |
| 1:K:2095:GLU:CD | 1:K:2097:SER:H | 2.23 | 0.44 |
| 1:K:2287:HIS:CD2 | 1:K:2430:GLY:HA3 | 2.52 | 0.44 |
| 1:K:3084:PHE:HE2 | 1:K:3126:TRP:HD1 | 1.64 | 0.44 |
| 1:K:3197:VAL:O | 1:K:3201:ASN:ND2 | 2.51 | 0.44 |
| 1:K:3317:ILE:HA | 1:K:3339:ARG:O | 2.16 | 0.44 |
| 1:L:461:VAL:HG12 | 1:L:1371:ARG:HB2 | 1.99 | 0.44 |
| 1:L:531:THR:OG1 | 1:L:532:VAL:N | 2.50 | 0.44 |
| 1:L:718:MET:HA | 1:L:722:GLN:HE21 | 1.81 | 0.44 |
| 1:L:1131:PHE:HB3 | 1:L:1136:LEU:CD2 | 2.48 | 0.44 |
| 1:L:3190:LEU:HD13 | 1:L:3197:VAL:H | 1.81 | 0.44 |
| 1:L:3270:LEU:HD12 | 1:L:3275:LEU:HB2 | 1.98 | 0.44 |
| 1:M:1840:GLN:HG2 | 1:M:1845:ASP:OD2 | 2.17 | 0.44 |
| 1:M:1966:GLU:H | 1:M:1966:GLU:CD | 2.25 | 0.44 |
| 1:M:2226:ARG:NH1 | 1:M:2292:ASP:OD2 | 2.50 | 0.44 |
| 1:M:2822:CYS:HA | 1:M:2828:CYS:HB3 | 1.99 | 0.44 |
| 1:M:2966:CYS:O | 1:M:2974:TYR:N | 2.39 | 0.44 |
| 1:N:719:THR:HG22 | 1:N:722:GLN:HB2 | 1.99 | 0.44 |
| 1:N:974:GLU:OE2 | 1:N:1035:TYR:OH | 2.32 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:N:3360:LEU:HD11 | 1:N:3401:ARG:HB3 | 1.99 | 0.44 |
| 1:O:215:HIS:O | 1:O:219:VAL:HG23 | 2.17 | 0.44 |
| 1:O:2157:TRP:HD1 | 1:O:2334:MET:HG2 | 1.82 | 0.44 |
| 1:O:2626:GLU:OE2 | 1:O:2626:GLU:N | 2.50 | 0.44 |
| 1:O:2848:ASP:OD1 | 1:O:2849:ARG:N | 2.50 | 0.44 |
| 1:O:3317:ILE:HA | 1:O:3339:ARG:O | 2.16 | 0.44 |
| 1:P:69:TRP:HD1 | 1:P:251:LEU:HD22 | 1.82 | 0.44 |
| 1:P:270:ALA:HA | 1:P:273:LEU:HD12 | 2.00 | 0.44 |
| 1:P:859:VAL:O | 1:P:862:LEU:HG | 2.18 | 0.44 |
| 1:P:1040:LEU:HD21 | 1:P:1184:LEU:HD11 | 1.98 | 0.44 |
| 1:P:1108:VAL:HA | 1:P:1109:PRO:HD3 | 1.84 | 0.44 |
| 1:P:1990:ILE:O | 1:P:1991:LYS:HG2 | 2.16 | 0.44 |
| 1:P:2752:ASN:HD21 | 1:P:2757:ILE:HG13 | 1.82 | 0.44 |
| 1:P:3219:LEU:HB2 | 1:P:3258:TYR:CZ | 2.52 | 0.44 |
| 1:Q:376:LEU:HB3 | 1:Q:378:LYS:HZ1 | 1.80 | 0.44 |
| 1:Q:1555:ARG:HE | 1:Q:1557:PHE:HZ | 1.64 | 0.44 |
| 1:Q:2603:TRP:CZ3 | 1:Q:2681:ILE:HD11 | 2.52 | 0.44 |
| 1:R:848:ARG:HB3 | 1:R:934:LEU:O | 2.17 | 0.44 |
| 1:R:1004:LEU:O | 1:R:1008:GLN:NE2 | 2.38 | 0.44 |
| 1:R:1284:ARG:HG2 | 1:R:1284:ARG:HH11 | 1.81 | 0.44 |
| 1:R:1338:LEU:HA | 1:R:1342:SER:OG | 2.18 | 0.44 |
| 1:R:2409:ARG:HD3 | 1:R:2421:ARG:NH1 | 2.32 | 0.44 |
| 1:R:3124:ARG:HD2 | 1:R:3187:PHE:CD2 | 2.52 | 0.44 |
| 1:R:3270:LEU:HD22 | 1:R:3275:LEU:HB2 | 2.00 | 0.44 |
| 1:S:636:ILE:HA | 1:S:639:LEU:HD12 | 1.98 | 0.44 |
| 1:S:1174:PRO:HG2 | 1:S:1176:HIS:CE1 | 2.52 | 0.44 |
| 1:S:1428:ILE:HG21 | 1:S:1610:TYR:CZ | 2.52 | 0.44 |
| 1:S:1584:ARG:NH2 | 1:S:1585:ASN:O | 2.34 | 0.44 |
| 1:S:2531:ALA:O | 1:S:2535:VAL:HG23 | 2.16 | 0.44 |
| 1:S:2941:LEU:HD23 | 1:S:3031:PRO:HG2 | 1.98 | 0.44 |
| 1:T:60:VAL:HG21 | 1:T:63:MET:HE3 | 1.99 | 0.44 |
| 1:T:790:THR:HA | 1:T:793:LEU:HD12 | 1.99 | 0.44 |
| 1:T:1008:GLN:OE1 | 1:T:1008:GLN:N | 2.50 | 0.44 |
| 1:T:1607:ASP:OD2 | 1:T:1608:ARG:NH1 | 2.50 | 0.44 |
| 1:T:2664:GLN:HB3 | 1:T:2669:ASN:ND2 | 2.32 | 0.44 |
| 1:T:2800:ASP:OD1 | 1:T:2899:GLY:N | 2.50 | 0.44 |
| 1:T:3008:ILE:HG21 | 1:T:3116:MET:HB3 | 1.98 | 0.44 |
| 1:T:3124:ARG:HD2 | 1:T:3187:PHE:CD2 | 2.52 | 0.44 |
| 1:T:3287:LEU:HD21 | 1:T:3299:LEU:HD21 | 1.99 | 0.44 |
| 1:T:3296:ASP:OD1 | 1:T:3296:ASP:N | 2.49 | 0.44 |
| 1:A:151:GLN:N | 1:A:151:GLN:OE1 | 2.50 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:473:LEU:N | 1:A:775:LYS:HE3 | 2.32 | 0.44 |
| 1:A:602:PHE:HA | 1:A:605:GLN:NE2 | 2.31 | 0.44 |
| 1:A:675:LEU:HD11 | 1:A:696:PRO:HG3 | 1.99 | 0.44 |
| 1:A:1161:SER:N | 1:A:1185:GLY:O | 2.50 | 0.44 |
| 1:A:1334:GLU:HG3 | 1:A:1346:VAL:HG12 | 1.99 | 0.44 |
| 1:A:1705:THR:OG1 | 1:A:1931:LEU:HD21 | 2.18 | 0.44 |
| 1:A:2262:VAL:HG23 | 1:A:2438:PHE:CD1 | 2.52 | 0.44 |
| 1:A:2570:GLY:H | 1:A:2574:PHE:HE2 | 1.65 | 0.44 |
| 1:A:2990:LEU:HA | 1:A:2993:VAL:HG12 | 1.99 | 0.44 |
| 1:B:1267:ASN:HB3 | 1:B:1348:TYR:CZ | 2.53 | 0.44 |
| 1:B:1350:ASP:HA | 1:B:1463:ASN:ND2 | 2.32 | 0.44 |
| 1:B:2045:VAL:HG13 | 1:B:2046:ASP:OD1 | 2.17 | 0.44 |
| 1:B:2987:TRP:CD1 | 1:B:3154:LEU:HD12 | 2.52 | 0.44 |
| 1:B:3131:THR:HG23 | 1:B:3134:LYS:HE2 | 1.98 | 0.44 |
| 1:B:3350:ASN:ND2 | 1:B:3369:ASP:OD1 | 2.51 | 0.44 |
| 1:C:884:PHE:CE1 | 1:C:1090:PRO:HG2 | 2.52 | 0.44 |
| 1:C:2095:GLU:OE1 | 1:C:2098:HIS:ND1 | 2.50 | 0.44 |
| 1:C:2737:ILE:H | 1:C:2737:ILE:HD12 | 1.81 | 0.44 |
| 1:C:2797:ARG:HA | 1:C:2801:ARG:HH22 | 1.82 | 0.44 |
| 1:C:2939:ASN:O | 1:C:2943:LYS:HD3 | 2.17 | 0.44 |
| 1:C:3208:ARG:HA | 1:C:3212:ARG:HH12 | 1.83 | 0.44 |
| 1:C:3333:SER:OG | 1:C:3336:THR:OG1 | 2.33 | 0.44 |
| 1:D:435:LYS:HG2 | 1:D:436:ASP:N | 2.31 | 0.44 |
| 1:D:454:ARG:C | 1:D:514:ARG:HH12 | 2.25 | 0.44 |
| 1:D:1728:ARG:NH2 | 4:F:3501:NAG:O7 | 2.51 | 0.44 |
| 1:D:2152:PRO:HA | 1:D:2261:GLU:CD | 2.43 | 0.44 |
| 1:E:889:ASN:HB3 | 1:E:900:PHE:O | 2.18 | 0.44 |
| 1:E:1607:ASP:OD1 | 1:E:1608:ARG:N | 2.49 | 0.44 |
| 1:E:2195:THR:O | 1:E:2197:GLN:NE2 | 2.42 | 0.44 |
| 1:E:3086:MET:O | 1:E:3090:THR:HG23 | 2.16 | 0.44 |
| 1:E:3205:GLU:HA | 1:E:3208:ARG:HB2 | 1.99 | 0.44 |
| 1:F:230:GLN:NE2 | 1:F:236:THR:O | 2.51 | 0.44 |
| 1:F:995:LEU:HD13 | 1:F:999:ALA:HB3 | 1.99 | 0.44 |
| 1:F:1085:ARG:HA | 1:F:1110:PHE:HE2 | 1.83 | 0.44 |
| 1:F:1167:GLU:HA | 1:F:1177:PRO:HA | 1.99 | 0.44 |
| 1:F:1750:PHE:CD2 | 1:F:1882:LEU:HD11 | 2.53 | 0.44 |
| 1:F:2318:LEU:HG | 1:F:2319:PRO:HD2 | 1.98 | 0.44 |
| 1:F:2695:THR:HG21 | 1:F:2698:TYR:CD2 | 2.52 | 0.44 |
| 1:F:2802:VAL:HG23 | 1:F:2855:VAL:HG23 | 1.99 | 0.44 |
| 1:G:483:ARG:HD2 | 1:G:483:ARG:C | 2.42 | 0.44 |
| 1:G:501:ARG:NH1 | 1:G:648:TRP:HZ3 | 2.15 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:G:1046:ASP:OD1 | 1:G:1048:ILE:HG12 | 2.17 | 0.44 |
| 1:G:2584:THR:HG21 | 1:G:2747:PHE:HE2 | 1.82 | 0.44 |
| 1:G:2986:HIS:HB3 | 1:G:3177:ILE:HG21 | 1.99 | 0.44 |
| 1:H:69:TRP:O | 1:H:72:LEU:HG | 2.16 | 0.44 |
| 1:H:938:ASP:CG | 1:H:1055:ASN:HD21 | 2.26 | 0.44 |
| 1:H:1067:GLN:HG3 | 1:H:1070:ARG:HH21 | 1.83 | 0.44 |
| 1:H:1928:PRO:HD2 | 1:H:1929:TYR:CD2 | 2.52 | 0.44 |
| 1:H:2092:VAL:HG22 | 1:H:2366:ARG:HE | 1.82 | 0.44 |
| 1:H:3141:ASN:HA | 1:H:3178:PHE:CD1 | 2.52 | 0.44 |
| 1:H:3203:ILE:HG22 | 1:H:3207:LEU:HD23 | 2.00 | 0.44 |
| 1:I:310:LEU:HD23 | 1:I:366:HIS:HB3 | 1.99 | 0.44 |
| 1:I:2354:PRO:O | 1:I:2357:VAL:HG22 | 2.17 | 0.44 |
| 1:I:3204:ILE:HG13 | 1:I:3205:GLU:H | 1.81 | 0.44 |
| 1:J:188:ILE:HA | 1:J:191:LEU:HB2 | 1.99 | 0.44 |
| 1:J:310:LEU:HD13 | 1:J:366:HIS:HB3 | 1.98 | 0.44 |
| 1:J:312:SER:HB3 | 1:J:407:VAL:HG13 | 1.99 | 0.44 |
| 1:J:487:ALA:HB2 | 1:J:775:LYS:HB3 | 1.99 | 0.44 |
| 1:J:667:ALA:O | 1:J:671:THR:HG23 | 2.18 | 0.44 |
| 1:J:968:PHE:CD1 | 1:J:1047:PRO:HG2 | 2.52 | 0.44 |
| 1:J:1080:ALA:HB1 | 1:J:1083:SER:OG | 2.17 | 0.44 |
| 1:J:1321:VAL:HA | 1:J:1324:HIS:CD2 | 2.52 | 0.44 |
| 1:J:1364:GLU:OE2 | 1:J:1365:ALA:N | 2.50 | 0.44 |
| 1:J:1430:HIS:HE1 | 1:J:1461:HIS:NE2 | 2.16 | 0.44 |
| 1:J:2183:TRP:CD1 | 1:J:2183:TRP:H | 2.35 | 0.44 |
| 1:J:2958:SER:HB3 | 1:J:2963:PRO:HD3 | 1.99 | 0.44 |
| 1:J:3146:ALA:O | 1:J:3150:LEU:HG | 2.18 | 0.44 |
| 1:K:41:PHE:CE1 | 1:K:253:PRO:HG2 | 2.52 | 0.44 |
| 1:K:483:ARG:HD2 | 1:K:484:VAL:N | 2.33 | 0.44 |
| 1:K:1775:LEU:HD12 | 1:K:1779:PHE:CE2 | 2.52 | 0.44 |
| 1:K:1996:VAL:HG22 | 1:K:2055:LEU:HD13 | 1.99 | 0.44 |
| 1:K:2266:VAL:HG21 | 1:K:2442:TYR:CD1 | 2.52 | 0.44 |
| 1:K:3173:ARG:HA | 1:K:3173:ARG:HD2 | 1.79 | 0.44 |
| 1:K:3333:SER:OG | 1:K:3336:THR:OG1 | 2.27 | 0.44 |
| 1:L:196:HIS:HE1 | 1:L:198:HIS:HB2 | 1.82 | 0.44 |
| 1:L:676:LYS:HG3 | 1:L:680:PHE:CE1 | 2.52 | 0.44 |
| 1:L:1722:TYR:CE2 | 1:L:1724:GLU:HB2 | 2.51 | 0.44 |
| 1:L:2109:ALA:HA | 1:L:2112:ARG:HG2 | 1.98 | 0.44 |
| 1:L:2262:VAL:HG23 | 1:L:2438:PHE:CD1 | 2.52 | 0.44 |
| 1:L:2806:PHE:HE2 | 1:L:2834:PHE:HE1 | 1.64 | 0.44 |
| 1:L:3357:TYR:CE1 | 1:L:3360:LEU:HD22 | 2.52 | 0.44 |
| 1:M:674:LEU:HD22 | 1:M:695:ARG:NH2 | 2.33 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:M:1114:ASP:OD1 | 1:M:1114:ASP:N | 2.43 | 0.44 |
| 1:M:1991:LYS:O | 1:M:1991:LYS:HD2 | 2.17 | 0.44 |
| 1:N:200:LEU:HD21 | 1:N:209:ASP:HB3 | 1.99 | 0.44 |
| 1:N:245:GLU:CD | 1:N:245:GLU:H | 2.25 | 0.44 |
| 1:N:673:GLU:C | 1:N:695:ARG:HH22 | 2.20 | 0.44 |
| 1:N:750:LEU:HD12 | 1:N:768:LEU:O | 2.17 | 0.44 |
| 1:N:756:LYS:HD3 | 1:N:762:SER:HB2 | 1.99 | 0.44 |
| 1:N:2792:ALA:O | 1:N:2796:ARG:HG2 | 2.17 | 0.44 |
| 1:N:2939:ASN:HB3 | 1:N:2943:LYS:HZ1 | 1.80 | 0.44 |
| 1:N:3350:ASN:OD1 | 1:N:3372:SER:HB3 | 2.17 | 0.44 |
| 1:O:183:VAL:HG21 | 1:O:365:TYR:CE1 | 2.52 | 0.44 |
| 1:O:1025:ILE:HD12 | 1:O:1028:LEU:HD23 | 1.98 | 0.44 |
| 1:O:1025:ILE:O | 1:O:1029:VAL:HG12 | 2.17 | 0.44 |
| 1:O:2158:HIS:O | 1:O:2162:THR:HG23 | 2.17 | 0.44 |
| 1:O:2754:ASN:OD1 | 1:O:2755:ASP:N | 2.47 | 0.44 |
| 1:O:3157:PHE:O | 1:O:3163:ASN:ND2 | 2.49 | 0.44 |
| 1:P:365:TYR:CE2 | 1:P:367:PHE:HB2 | 2.52 | 0.44 |
| 1:P:773:GLY:N | 1:P:776:GLU:OE1 | 2.39 | 0.44 |
| 1:P:1666:ASP:O | 1:P:1668:THR:HG23 | 2.17 | 0.44 |
| 1:P:2252:LEU:HD23 | 1:P:2309:TRP:HD1 | 1.82 | 0.44 |
| 1:P:2660:LEU:HD11 | 1:P:2803:PHE:HZ | 1.82 | 0.44 |
| 1:P:2695:THR:OG1 | 1:P:2696:LEU:N | 2.51 | 0.44 |
| 1:Q:580:TYR:CG | 1:Q:958:PRO:HG2 | 2.52 | 0.44 |
| 1:Q:1756:ARG:NH2 | 1:R:2175:THR:HB | 2.29 | 0.44 |
| 1:Q:2509:SER:N | 1:Q:3138:ARG:HH22 | 2.15 | 0.44 |
| 1:Q:3002:LYS:HD3 | 1:Q:3002:LYS:HA | 1.69 | 0.44 |
| 1:R:371:LYS:C | 1:R:371:LYS:HD3 | 2.42 | 0.44 |
| 1:R:461:VAL:H | 1:R:1277:GLU:CD | 2.24 | 0.44 |
| 1:R:587:PHE:O | 1:R:591:LEU:HG | 2.17 | 0.44 |
| 1:R:668:HIS:O | 1:R:671:THR:OG1 | 2.36 | 0.44 |
| 1:R:958:PRO:C | 1:R:961:ASN:H | 2.25 | 0.44 |
| 1:R:996:THR:O | 1:R:999:ALA:N | 2.51 | 0.44 |
| 1:R:1051:LEU:HD12 | 1:R:1052:HIS:N | 2.32 | 0.44 |
| 1:R:1056:THR:HA | 1:R:1059:ILE:HD12 | 1.99 | 0.44 |
| 1:R:1571:VAL:HB | 1:R:1637:ILE:HG22 | 1.99 | 0.44 |
| 1:R:2316:ARG:HD3 | 1:R:2316:ARG:H | 1.82 | 0.44 |
| 1:S:950:VAL:HG12 | 1:S:968:PHE:CD2 | 2.52 | 0.44 |
| 1:S:1828:ASN:ND2 | 1:S:1830:LEU:HB3 | 2.32 | 0.44 |
| 1:S:1903:GLY:HA3 | 1:T:1667:GLN:HB2 | 2.00 | 0.44 |
| 1:S:2806:PHE:CE1 | 1:S:2892:PRO:HB3 | 2.52 | 0.44 |
| 1:T:1041:ARG:HD2 | 1:T:1042:TYR:CZ | 2.52 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:T:1327:ARG:NE | 1:T:1528:TYR:OH | 2.45 | 0.44 |
| 1:T:1849:GLN:O | 1:T:1852:ILE:HG22 | 2.17 | 0.44 |
| 1:T:2165:VAL:HG11 | 1:T:2296:PHE:CE2 | 2.52 | 0.44 |
| 1:T:2182:ASP:HA | 1:T:2301:PHE:CE2 | 2.52 | 0.44 |
| 1:T:3117:ILE:O | 1:T:3120:SER:OG | 2.27 | 0.44 |
| 1:T:3124:ARG:O | 1:T:3127:GLN:HG3 | 2.17 | 0.44 |
| 1:A:471:HIS:HB3 | 1:A:632:ALA:HB2 | 2.00 | 0.44 |
| 1:A:612:LEU:HD21 | 1:A:768:LEU:HA | 1.99 | 0.44 |
| 1:A:1137:GLN:O | 1:A:1140:ILE:HG22 | 2.17 | 0.44 |
| 1:A:1428:ILE:HG21 | 1:A:1610:TYR:CZ | 2.52 | 0.44 |
| 1:A:2271:ILE:HA | 1:A:2274:LEU:HB3 | 1.99 | 0.44 |
| 1:A:2356:GLU:OE1 | 1:A:2356:GLU:N | 2.48 | 0.44 |
| 1:A:2378:ASP:OD1 | 1:A:2378:ASP:N | 2.46 | 0.44 |
| 1:A:2626:GLU:OE2 | 1:A:2633:LYS:NZ | 2.44 | 0.44 |
| 1:A:2726:ARG:HB3 | 1:A:2728:LEU:HD23 | 2.00 | 0.44 |
| 1:B:409:VAL:HG13 | 1:B:666:CYS:HA | 1.98 | 0.44 |
| 1:B:428:SER:OG | 1:B:429:ALA:N | 2.50 | 0.44 |
| 1:B:1385:ILE:HD11 | 1:B:1450:TYR:HB3 | 1.98 | 0.44 |
| 1:B:2376:ASN:O | 1:B:2379:GLU:HG3 | 2.17 | 0.44 |
| 1:B:3049:GLN:CD | 1:B:3050:PRO:HD2 | 2.43 | 0.44 |
| 1:C:608:VAL:HG11 | 1:C:785:VAL:HG21 | 1.99 | 0.44 |
| 1:C:1910:ASN:ND2 | 1:D:1657:PHE:O | 2.50 | 0.44 |
| 1:C:2857:SER:C | 1:C:2861:GLN:HE21 | 2.25 | 0.44 |
| 1:D:1100:ASP:OD2 | 1:D:1103:THR:OG1 | 2.25 | 0.44 |
| 1:D:1325:TRP:HD1 | 1:D:1326:HIS:CE1 | 2.35 | 0.44 |
| 1:D:1367:TYR:CE2 | 1:D:1369:ASP:HB3 | 2.53 | 0.44 |
| 1:D:1435:SER:HA | 1:D:1446:SER:OG | 2.17 | 0.44 |
| 1:D:2183:TRP:CD2 | 1:D:2271:ILE:HD11 | 2.52 | 0.44 |
| 1:D:2693:MET:HE1 | 1:D:2702:ASP:HB3 | 2.00 | 0.44 |
| 1:D:2987:TRP:CD1 | 1:D:3154:LEU:HD12 | 2.52 | 0.44 |
| 1:D:3019:ALA:HB3 | 1:E:3038:LYS:HE3 | 1.99 | 0.44 |
| 1:D:3032:PHE:HA | 1:D:3113:PRO:HG2 | 1.99 | 0.44 |
| 1:E:964:GLU:HB2 | 1:E:965:PRO:HD2 | 1.99 | 0.44 |
| 1:E:1446:SER:OG | 1:E:1447:SER:N | 2.51 | 0.44 |
| 1:E:2287:HIS:CD2 | 1:E:2430:GLY:HA3 | 2.52 | 0.44 |
| 1:E:2580:LEU:HA | 1:E:2580:LEU:HD23 | 1.78 | 0.44 |
| 1:E:2786:ILE:HD13 | 1:E:2789:LEU:HD21 | 1.99 | 0.44 |
| 1:E:2878:ALA:HB3 | 1:E:2882:THR:HG22 | 2.00 | 0.44 |
| 1:F:80:LYS:HZ1 | 1:F:261:ILE:HG13 | 1.82 | 0.44 |
| 1:F:472:GLY:HA3 | 1:F:629:HIS:HA | 1.98 | 0.44 |
| 1:F:480:PRO:HD3 | 1:F:680:PHE:CZ | 2.53 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:F:702:TYR:N | 1:F:703:GLU:OE1 | 2.51 | 0.44 |
| 1:F:1162:ALA:HB3 | 1:F:1183:ILE:HD11 | 2.00 | 0.44 |
| 1:F:1847:GLU:O | 1:F:1851:GLU:HG2 | 2.17 | 0.44 |
| 1:F:3217:PHE:HB2 | 1:F:3262:TYR:HB3 | 1.98 | 0.44 |
| 1:F:3228:ALA:HB3 | 1:F:3245:PHE:CE1 | 2.51 | 0.44 |
| 1:G:1588:HIS:HB2 | 1:J:337:GLN:NE2 | 2.32 | 0.44 |
| 1:G:2164:GLN:HE22 | 1:G:2348:THR:HG21 | 1.83 | 0.44 |
| 1:G:3065:PHE:O | 1:G:3068:THR:HG22 | 2.18 | 0.44 |
| 1:H:1869:MET:HE1 | 1:H:1881:PHE:HB2 | 1.98 | 0.44 |
| 1:I:523:TRP:CD1 | 1:I:533:PRO:HG3 | 2.52 | 0.44 |
| 1:I:647:LEU:HA | 1:I:650:ILE:HG12 | 1.98 | 0.44 |
| 1:I:1168:VAL:N | 1:I:1178:GLU:OE1 | 2.50 | 0.44 |
| 1:I:1322:PHE:HB3 | 1:I:1323:PRO:HD3 | 1.99 | 0.44 |
| 1:I:2544:TYR:OH | 1:I:2701:TYR:O | 2.35 | 0.44 |
| 1:I:2770:ASP:OD1 | 1:I:2770:ASP:N | 2.50 | 0.44 |
| 1:I:3074:GLU:HG3 | 1:I:3076:ASN:H | 1.82 | 0.44 |
| 1:J:1415:GLU:OE1 | 1:J:1551:ARG:HG2 | 2.17 | 0.44 |
| 1:J:1500:ASN:OD1 | 1:J:1500:ASN:N | 2.50 | 0.44 |
| 1:J:1998:ILE:HD11 | 1:J:2010:ALA:HB3 | 1.99 | 0.44 |
| 1:J:2316:ARG:HD3 | 1:J:2316:ARG:H | 1.82 | 0.44 |
| 1:J:3149:ASN:HA | 1:J:3152:ARG:HD3 | 1.98 | 0.44 |
| 1:K:182:GLU:O | 1:K:186:ASN:ND2 | 2.51 | 0.44 |
| 1:L:24:ARG:HA | 1:L:24:ARG:HD2 | 1.69 | 0.44 |
| 1:L:112:PHE:HB3 | 1:L:121:GLN:O | 2.18 | 0.44 |
| 1:L:160:GLN:O | 1:L:163:GLU:HG3 | 2.18 | 0.44 |
| 1:L:252:GLU:OE1 | 1:L:256:ARG:NH2 | 2.50 | 0.44 |
| 1:L:1362:ILE:HD13 | 1:L:1456:LEU:HD11 | 1.99 | 0.44 |
| 1:L:2748:ASN:OD1 | 1:L:2748:ASN:N | 2.50 | 0.44 |
| 1:L:3081:GLU:N | 1:L:3081:GLU:OE1 | 2.50 | 0.44 |
| 1:L:3110:ALA:HA | 1:L:3115:PHE:CD2 | 2.53 | 0.44 |
| 1:M:483:ARG:C | 1:M:483:ARG:HD2 | 2.43 | 0.44 |
| 1:M:678:PHE:O | 1:M:685:ASN:ND2 | 2.50 | 0.44 |
| 1:M:939:TRP:NE1 | 1:M:998:ILE:HG21 | 2.32 | 0.44 |
| 1:M:2129:PHE:HE1 | 1:M:2342:LEU:HD13 | 1.81 | 0.44 |
| 1:M:2376:ASN:N | 1:M:2379:GLU:OE2 | 2.43 | 0.44 |
| 1:M:2621:PRO:HD2 | 1:M:2622:PHE:HD1 | 1.83 | 0.44 |
| 1:M:2941:LEU:HD22 | 1:M:3032:PHE:CE1 | 2.52 | 0.44 |
| 1:N:185:HIS:ND1 | 1:N:219:VAL:HG21 | 2.32 | 0.44 |
| 1:N:192:VAL:HG13 | 1:N:200:LEU:HB2 | 2.00 | 0.44 |
| 1:N:741:HIS:HE1 | 1:N:780:ASN:HD21 | 1.64 | 0.44 |
| 1:N:968:PHE:CD1 | 1:N:1047:PRO:HG2 | 2.53 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:N:1023:ASN:HD21 | 1:N:1184:LEU:HD22 | 1.81 | 0.44 |
| 1:N:1824:HIS:HB2 | 1:N:1827:ASP:CG | 2.43 | 0.44 |
| 1:N:1907:ASN:ND2 | 1:N:1945:PHE:HB3 | 2.33 | 0.44 |
| 1:N:2626:GLU:HB2 | 1:N:2633:LYS:HG3 | 1.98 | 0.44 |
| 1:O:182:GLU:O | 1:O:186:ASN:ND2 | 2.50 | 0.44 |
| 1:O:348:ILE:HD11 | 1:O:367:PHE:CD1 | 2.51 | 0.44 |
| 1:O:756:LYS:HZ2 | 1:O:757:PRO:HD2 | 1.82 | 0.44 |
| 1:O:1436:LEU:HD23 | 1:O:1436:LEU:HA | 1.89 | 0.44 |
| 1:O:1756:ARG:HH12 | 1:P:2102:ARG:CZ | 2.30 | 0.44 |
| 1:O:1801:ASP:OD1 | 1:O:1802:ILE:N | 2.50 | 0.44 |
| 1:O:1816:ASN:N | 1:O:1816:ASN:OD1 | 2.51 | 0.44 |
| 1:O:2136:CYS:HB3 | 1:O:2144:TYR:C | 2.43 | 0.44 |
| 1:O:2604:THR:HG21 | 1:O:2781:PHE:HE1 | 1.82 | 0.44 |
| 1:P:487:ALA:HB2 | 1:P:775:LYS:HB3 | 2.00 | 0.44 |
| 1:P:610:HIS:O | 1:P:613:PRO:HD2 | 2.18 | 0.44 |
| 1:P:695:ARG:NH2 | 1:P:696:PRO:HD2 | 2.32 | 0.44 |
| 1:P:968:PHE:CD1 | 1:P:1047:PRO:HG2 | 2.52 | 0.44 |
| 1:P:1560:PHE:O | 1:P:1609:LEU:HD12 | 2.17 | 0.44 |
| 1:P:2481:LEU:HD23 | 1:P:2482:PRO:HD2 | 2.00 | 0.44 |
| 1:P:2590:THR:HA | 1:P:2594:ALA:HB3 | 2.00 | 0.44 |
| 1:P:2712:VAL:O | 1:P:2715:GLN:HG2 | 2.18 | 0.44 |
| 1:Q:493:MET:HE2 | 1:Q:493:MET:HB3 | 1.86 | 0.44 |
| 1:Q:1159:ARG:C | 1:Q:1160:LYS:HD3 | 2.43 | 0.44 |
| 1:Q:1432:ALA:HA | 1:Q:1594:SER:OG | 2.17 | 0.44 |
| 1:Q:1570:ASP:HB2 | 1:Q:1638:ARG:HB2 | 1.99 | 0.44 |
| 1:Q:2308:VAL:O | 1:Q:2311:GLU:HG3 | 2.17 | 0.44 |
| 1:Q:2376:ASN:O | 1:Q:2380:LEU:HG | 2.17 | 0.44 |
| 1:Q:2876:ILE:HD11 | 1:Q:2885:ALA:O | 2.17 | 0.44 |
| 1:R:1305:CYS:HB2 | 1:R:1312:VAL:O | 2.17 | 0.44 |
| 1:R:1362:ILE:HG22 | 1:R:1380:PHE:HB3 | 1.99 | 0.44 |
| 1:R:1684:THR:HG23 | 1:R:1687:GLU:H | 1.83 | 0.44 |
| 1:R:1848:VAL:HA | 1:R:2026:PHE:CE1 | 2.53 | 0.44 |
| 1:R:2637:SER:HB2 | 1:R:2686:GLY:O | 2.18 | 0.44 |
| 1:R:2655:TYR:HD2 | 1:R:2659:LEU:HD23 | 1.80 | 0.44 |
| 1:R:3160:GLU:CD | 1:R:3160:GLU:H | 2.24 | 0.44 |
| 1:S:580:TYR:OH | 1:S:957:ASN:OD1 | 2.34 | 0.44 |
| 1:S:1195:ASP:HB3 | 1:T:2441:LEU:HD21 | 1.99 | 0.44 |
| 1:S:1422:PHE:HA | 1:S:1425:GLN:HE21 | 1.81 | 0.44 |
| 1:S:2201:ASP:OD1 | 1:S:2203:TRP:N | 2.35 | 0.44 |
| 1:S:2353:LEU:HD13 | 1:S:2355:LYS:HD3 | 1.99 | 0.44 |
| 1:S:2376:ASN:O | 1:S:2380:LEU:HG | 2.18 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:S:3174:PRO:HA | 1:S:3177:ILE:HB | 1.98 | 0.44 |
| 1:T:543:ASP:HB3 | 1:T:546:SER:HB3 | 1.99 | 0.44 |
| 1:T:702:TYR:N | 1:T:703:GLU:OE1 | 2.51 | 0.44 |
| 1:T:1376:GLU:OE2 | 1:T:1377:SER:N | 2.51 | 0.44 |
| 1:T:1884:HIS:O | 1:T:1887:SER:OG | 2.27 | 0.44 |
| 1:T:2041:LYS:HG3 | 1:T:2043:LEU:HD23 | 1.99 | 0.44 |
| 1:A:414:LYS:HA | 1:A:414:LYS:HD2 | 1.67 | 0.44 |
| 1:A:1577:VAL:HG12 | 1:D:337:GLN:HB3 | 2.00 | 0.44 |
| 1:A:1858:HIS:NE2 | 1:A:1884:HIS:HE1 | 2.15 | 0.44 |
| 1:A:2439:ASP:OD2 | 1:A:2440:ARG:NE | 2.48 | 0.44 |
| 1:A:2448:ASP:O | 1:A:2452:GLU:OE1 | 2.36 | 0.44 |
| 1:B:112:PHE:HD2 | 1:B:121:GLN:H | 1.65 | 0.44 |
| 1:B:297:TYR:O | 1:B:301:GLU:OE1 | 2.35 | 0.44 |
| 1:B:788:GLU:OE2 | 1:B:791:ASP:N | 2.41 | 0.44 |
| 1:B:811:LYS:NZ | 1:B:815:GLY:O | 2.38 | 0.44 |
| 1:B:2811:PHE:CE2 | 1:B:2813:ALA:HB3 | 2.53 | 0.44 |
| 1:B:3183:PHE:HB2 | 1:B:3185:TYR:CD1 | 2.52 | 0.44 |
| 1:C:215:HIS:O | 1:C:219:VAL:HG23 | 2.16 | 0.44 |
| 1:C:527:ARG:HG2 | 1:C:528:PRO:HD2 | 1.99 | 0.44 |
| 1:C:885:HIS:ND1 | 1:C:885:HIS:O | 2.50 | 0.44 |
| 1:C:934:LEU:H | 1:C:934:LEU:HD12 | 1.81 | 0.44 |
| 1:C:968:PHE:HA | 1:C:1047:PRO:HG3 | 1.99 | 0.44 |
| 1:C:971:GLY:H | 1:C:978:THR:HG1 | 1.61 | 0.44 |
| 1:C:1666:ASP:HB3 | 1:D:1902:ARG:O | 2.18 | 0.44 |
| 1:C:2027:ASP:OD1 | 1:C:2028:ARG:N | 2.50 | 0.44 |
| 1:C:2848:ASP:OD1 | 1:C:2849:ARG:N | 2.51 | 0.44 |
| 1:D:675:LEU:O | 1:D:676:LYS:HD2 | 2.18 | 0.44 |
| 1:D:3015:ARG:HH12 | 1:D:3194:GLY:H | 1.66 | 0.44 |
| 1:E:294:GLU:H | 1:E:294:GLU:CD | 2.23 | 0.44 |
| 1:E:449:ARG:HD3 | 1:E:541:TYR:CE1 | 2.52 | 0.44 |
| 1:E:579:GLU:HG3 | 1:E:582:ASP:CG | 2.42 | 0.44 |
| 1:E:676:LYS:H | 1:E:676:LYS:HG3 | 1.64 | 0.44 |
| 1:E:704:HIS:HB3 | 1:E:705:GLU:OE1 | 2.17 | 0.44 |
| 1:E:714:GLN:OE1 | 1:E:715:PHE:N | 2.50 | 0.44 |
| 1:E:1152:GLY:HA3 | 1:E:1197:LEU:HD21 | 1.99 | 0.44 |
| 1:E:2056:ARG:HA | 1:E:2056:ARG:HD2 | 1.74 | 0.44 |
| 1:E:2471:TYR:HE1 | 1:E:2488:LYS:HD2 | 1.80 | 0.44 |
| 1:E:2960:HIS:HE1 | 1:E:3119:HIS:HE1 | 1.64 | 0.44 |
| 1:E:3103:MET:HA | 1:E:3109:SER:HA | 1.98 | 0.44 |
| 1:E:3301:THR:H | 1:E:3325:LYS:HG3 | 1.83 | 0.44 |
| 1:F:41:PHE:CD1 | 1:F:47:MET:HE1 | 2.51 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:F:1898:LEU:HD21 | 1:F:1965:ALA:HB1 | 1.99 | 0.44 |
| 1:F:2269:ASN:HD21 | 1:F:2428:LEU:N | 2.15 | 0.44 |
| 1:F:2413:CYS:SG | 1:F:2470:ARG:NE | 2.90 | 0.44 |
| 1:F:2923:ARG:HD3 | 1:F:3008:ILE:O | 2.17 | 0.44 |
| 1:G:718:MET:HE1 | 1:G:723:LEU:HA | 2.00 | 0.44 |
| 1:G:847:VAL:O | 1:G:847:VAL:HG23 | 2.18 | 0.44 |
| 1:G:889:ASN:HB3 | 1:G:900:PHE:O | 2.18 | 0.44 |
| 1:G:954:THR:HG22 | 1:G:965:PRO:HA | 2.00 | 0.44 |
| 1:G:1709:ALA:O | 1:G:1712:SER:OG | 2.30 | 0.44 |
| 1:G:2190:LEU:HD21 | 1:G:2194:PHE:HD2 | 1.82 | 0.44 |
| 1:H:50:LYS:NZ | 1:H:52:ASP:OD2 | 2.45 | 0.44 |
| 1:H:453:SER:HB3 | 1:H:553:PRO:HG3 | 2.00 | 0.44 |
| 1:H:811:LYS:HD2 | 1:H:815:GLY:HA2 | 1.99 | 0.44 |
| 1:H:1056:THR:HA | 1:H:1059:ILE:HD12 | 1.97 | 0.44 |
| 1:H:1165:THR:O | 1:H:1222:SER:N | 2.48 | 0.44 |
| 1:H:1783:ILE:HD13 | 1:H:1794:PRO:HA | 2.00 | 0.44 |
| 1:H:2183:TRP:CD2 | 1:H:2271:ILE:HD11 | 2.53 | 0.44 |
| 1:I:493:MET:HG2 | 1:I:494:ALA:H | 1.81 | 0.44 |
| 1:I:680:PHE:HB2 | 1:I:684:LEU:HD22 | 1.99 | 0.44 |
| 1:I:1607:ASP:OD1 | 1:I:1608:ARG:N | 2.47 | 0.44 |
| 1:I:1852:ILE:HG21 | 1:I:2030:TYR:CE1 | 2.52 | 0.44 |
| 1:I:3381:LEU:HD23 | 1:I:3386:TYR:CD1 | 2.52 | 0.44 |
| 1:J:434:ARG:HB3 | 1:J:710:TYR:HD1 | 1.81 | 0.44 |
| 1:J:705:GLU:HG2 | 1:J:706:LEU:HD22 | 1.99 | 0.44 |
| 1:J:1301:PHE:CG | 1:J:1302:PRO:HA | 2.53 | 0.44 |
| 1:J:1883:LEU:O | 1:J:1886:SER:OG | 2.28 | 0.44 |
| 1:J:2312:LEU:O | 1:J:2316:ARG:NH1 | 2.50 | 0.44 |
| 1:J:2343:ASN:HB3 | 1:J:2349:ARG:NH2 | 2.32 | 0.44 |
| 1:J:2800:ASP:OD1 | 1:J:2899:GLY:N | 2.50 | 0.44 |
| 1:J:3127:GLN:HA | 1:J:3130:GLN:HG3 | 1.98 | 0.44 |
| 1:K:323:ASN:OD1 | 1:K:324:VAL:N | 2.50 | 0.44 |
| 1:K:1723:PRO:HA | 1:K:1728:ARG:NH2 | 2.30 | 0.44 |
| 1:K:1919:PRO:HG3 | 1:K:1940:LYS:NZ | 2.33 | 0.44 |
| 1:K:2470:ARG:NH2 | 1:K:2471:TYR:O | 2.50 | 0.44 |
| 1:L:460:SER:HB2 | 1:L:1277:GLU:OE2 | 2.18 | 0.44 |
| 1:L:845:LEU:HD21 | 1:L:932:ASP:HA | 1.99 | 0.44 |
| 1:L:864:GLU:HA | 1:L:867:GLN:OE1 | 2.16 | 0.44 |
| 1:L:939:TRP:HZ3 | 1:L:1055:ASN:HB3 | 1.83 | 0.44 |
| 1:L:1124:ASP:OD1 | 1:L:1124:ASP:N | 2.49 | 0.44 |
| 1:L:1204:ASP:OD1 | 1:L:1204:ASP:N | 2.50 | 0.44 |
| 1:L:2779:LEU:H | 1:L:2779:LEU:HD23 | 1.81 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:L:3119:HIS:HA | 1:L:3122:ILE:HG22 | 1.99 | 0.44 |
| 1:M:728:ASP:OD2 | 1:M:836:HIS:HB2 | 2.17 | 0.44 |
| 1:N:775:LYS:HA | 1:N:775:LYS:HD3 | 1.76 | 0.44 |
| 1:N:1834:PHE:CE1 | 1:N:1891:ILE:HD13 | 2.52 | 0.44 |
| 1:N:3037:ILE:HG21 | 1:N:3040:ALA:HB3 | 1.98 | 0.44 |
| 1:O:47:MET:C | 1:O:55:ARG:HH12 | 2.25 | 0.44 |
| 1:O:881:ILE:HA | 1:O:884:PHE:CD2 | 2.50 | 0.44 |
| 1:O:939:TRP:CD1 | 1:O:998:ILE:HG21 | 2.53 | 0.44 |
| 1:O:1225:ASP:HB3 | 1:O:1231:ILE:HD11 | 2.00 | 0.44 |
| 1:O:1596:LEU:HD12 | 1:O:1597:GLY:H | 1.83 | 0.44 |
| 1:O:2814:SER:N | 1:O:2838:GLY:O | 2.50 | 0.44 |
| 1:P:1165:THR:N | 1:P:1222:SER:O | 2.39 | 0.44 |
| 1:P:1372:SER:C | 1:P:1374:THR:HG1 | 2.24 | 0.44 |
| 1:P:2848:ASP:OD1 | 1:P:2849:ARG:N | 2.50 | 0.44 |
| 1:Q:315:LEU:HB2 | 1:Q:361:PHE:HD2 | 1.83 | 0.44 |
| 1:Q:559:VAL:HG13 | 1:Q:633:PHE:CE2 | 2.53 | 0.44 |
| 1:Q:1365:ALA:HA | 1:Q:1381:PHE:CZ | 2.53 | 0.44 |
| 1:Q:1829:TRP:NE1 | 1:Q:1833:GLN:HE22 | 2.16 | 0.44 |
| 1:Q:1889:ASP:OD2 | 1:Q:1955:TYR:OH | 2.34 | 0.44 |
| 1:Q:2182:ASP:OD1 | 1:Q:2184:THR:OG1 | 2.32 | 0.44 |
| 1:Q:2194:PHE:HE1 | 1:Q:2213:ALA:HA | 1.81 | 0.44 |
| 1:Q:2529:LYS:HE3 | 1:Q:2620:ASN:OD1 | 2.17 | 0.44 |
| 1:Q:2679:ASN:HD21 | 1:Q:2836:VAL:C | 2.26 | 0.44 |
| 1:Q:2995:PHE:O | 1:Q:2999:LEU:HD23 | 2.17 | 0.44 |
| 1:Q:3089:ASN:ND2 | 1:Q:3247:ILE:HA | 2.32 | 0.44 |
| 1:Q:3095:VAL:HG13 | 1:Q:3103:MET:SD | 2.57 | 0.44 |
| 1:R:299:LEU:O | 1:R:302:GLN:HG3 | 2.17 | 0.44 |
| 1:R:460:SER:HB2 | 1:R:1277:GLU:OE2 | 2.17 | 0.44 |
| 1:R:598:ASP:HB2 | 1:R:601:ASP:HB3 | 1.99 | 0.44 |
| 1:R:1007:GLU:N | 1:R:1008:GLN:OE1 | 2.50 | 0.44 |
| 1:R:1080:ALA:HB1 | 1:R:1083:SER:OG | 2.18 | 0.44 |
| 1:R:1542:GLN:HA | 1:R:1545:GLU:OE2 | 2.18 | 0.44 |
| 1:R:1947:TYR:CZ | 1:R:1948:LYS:HG3 | 2.53 | 0.44 |
| 1:S:193:GLY:HA3 | 1:S:201:SER:H | 1.83 | 0.44 |
| 1:S:915:ARG:HH21 | 1:S:1115:TYR:CB | 2.31 | 0.44 |
| 1:S:1385:ILE:HD12 | 1:S:1385:ILE:H | 1.83 | 0.44 |
| 1:T:32:VAL:O | 1:T:37:ASN:ND2 | 2.50 | 0.44 |
| 1:T:475:ALA:HB3 | 1:T:485:ARG:HB3 | 1.98 | 0.44 |
| 1:T:719:THR:HG22 | 1:T:722:GLN:NE2 | 2.32 | 0.44 |
| 1:T:917:LEU:O | 1:T:920:GLN:NE2 | 2.43 | 0.44 |
| 1:T:1500:ASN:OD1 | 1:T:1500:ASN:N | 2.50 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:T:1802:ILE:HD11 | 1:T:1805:GLU:HB2 | 1.98 | 0.44 |
| 1:T:1848:VAL:HA | 1:T:2026:PHE:HE2 | 1.83 | 0.44 |
| 1:T:2425:ILE:HG21 | 1:T:2442:TYR:HE2 | 1.82 | 0.44 |
| 1:T:2754:ASN:OD1 | 1:T:2755:ASP:N | 2.50 | 0.44 |
| 1:A:148:ARG:HA | 1:A:151:GLN:HE22 | 1.81 | 0.44 |
| 1:A:945:ALA:HA | 1:A:987:PHE:CZ | 2.52 | 0.44 |
| 1:A:1159:ARG:HA | 1:A:1186:ASP:O | 2.17 | 0.44 |
| 1:A:1854:HIS:O | 1:A:1857:ILE:HG22 | 2.17 | 0.44 |
| 1:A:2328:ASN:HB3 | 1:B:1241:VAL:HB | 2.00 | 0.44 |
| 1:A:2421:ARG:HH22 | 1:A:2424:ALA:HB2 | 1.82 | 0.44 |
| 1:A:2567:CYS:HA | 1:A:2577:TRP:CE2 | 2.53 | 0.44 |
| 1:A:2697:GLU:HG2 | 1:A:2841:LEU:HD13 | 1.99 | 0.44 |
| 1:B:130:ILE:O | 1:B:138:HIS:HA | 2.17 | 0.44 |
| 1:B:169:LEU:HD12 | 1:B:177:PHE:HZ | 1.82 | 0.44 |
| 1:B:1041:ARG:HD2 | 1:B:1042:TYR:CZ | 2.53 | 0.44 |
| 1:B:1205:ILE:HD12 | 1:B:1208:LYS:HE3 | 2.00 | 0.44 |
| 1:B:2155:PRO:HB2 | 1:B:2306:TRP:CE3 | 2.52 | 0.44 |
| 1:B:2637:SER:HB3 | 1:B:2686:GLY:O | 2.18 | 0.44 |
| 1:B:3146:ALA:O | 1:B:3150:LEU:HG | 2.18 | 0.44 |
| 1:B:3183:PHE:HD2 | 1:B:3185:TYR:HE1 | 1.66 | 0.44 |
| 1:C:2029:LEU:HD23 | 1:C:2029:LEU:H | 1.82 | 0.44 |
| 1:C:2226:ARG:H | 1:F:113:LYS:NZ | 2.15 | 0.44 |
| 1:C:3329:LYS:HE3 | 1:D:3357:TYR:HB3 | 1.99 | 0.44 |
| 1:D:327:LYS:HG3 | 1:D:343:GLU:O | 2.18 | 0.44 |
| 1:D:412:PRO:HG3 | 1:D:665:HIS:CD2 | 2.52 | 0.44 |
| 1:D:738:VAL:HG23 | 1:D:789:ILE:HG13 | 2.00 | 0.44 |
| 1:D:896:ALA:HB1 | 1:D:899:LYS:HB2 | 1.99 | 0.44 |
| 1:D:1827:ASP:HA | 1:D:1831:TRP:CD1 | 2.52 | 0.44 |
| 1:D:3049:GLN:CD | 1:D:3050:PRO:HD2 | 2.42 | 0.44 |
| 1:D:3230:VAL:C | 1:D:3231:LYS:HD3 | 2.43 | 0.44 |
| 1:E:9:ASP:OD1 | 1:E:9:ASP:N | 2.49 | 0.44 |
| 1:E:51:ASP:N | 1:E:51:ASP:OD1 | 2.48 | 0.44 |
| 1:E:1186:ASP:OD2 | 1:E:1188:TYR:N | 2.48 | 0.44 |
| 1:E:1301:PHE:CG | 1:E:1302:PRO:HA | 2.53 | 0.44 |
| 1:E:1632:ASP:OD1 | 1:F:1917:ARG:NE | 2.50 | 0.44 |
| 1:E:2052:LYS:HD2 | 1:E:2052:LYS:HA | 1.60 | 0.44 |
| 1:E:2446:ILE:HD11 | 1:E:2491:ILE:HD11 | 1.99 | 0.44 |
| 1:F:5:ARG:HD2 | 1:F:283:TYR:CZ | 2.52 | 0.44 |
| 1:F:597:ARG:HD3 | 1:F:658:ARG:HE | 1.83 | 0.44 |
| 1:F:998:ILE:HA | 1:F:1001:MET:HG3 | 2.00 | 0.44 |
| 1:F:1535:PHE:O | 1:F:1538:TRP:HB2 | 2.18 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:F:1839:GLU:HA | 1:F:1902:ARG:HH22 | 1.83 | 0.44 |
| 1:F:1919:PRO:HB2 | 1:F:1924:SER:HB2 | 2.00 | 0.44 |
| 1:F:2954:GLU:CD | 1:F:2954:GLU:H | 2.25 | 0.44 |
| 1:G:646:ARG:HA | 1:G:710:TYR:HE2 | 1.82 | 0.44 |
| 1:G:1058:ARG:NH1 | 1:G:1125:ASP:O | 2.51 | 0.44 |
| 1:G:1362:ILE:HB | 1:G:1394:ARG:HH22 | 1.82 | 0.44 |
| 1:G:2163:LEU:HD22 | 1:G:2363:LEU:HD12 | 2.00 | 0.44 |
| 1:G:2737:ILE:HA | 1:G:2740:LEU:HD12 | 1.99 | 0.44 |
| 1:G:3160:GLU:HG2 | 1:G:3169:ARG:NH2 | 2.32 | 0.44 |
| 1:H:627:THR:OG1 | 1:H:628:LEU:N | 2.48 | 0.44 |
| 1:H:919:VAL:HG11 | 1:H:1119:PHE:CE1 | 2.51 | 0.44 |
| 1:H:1023:ASN:HD21 | 1:H:1184:LEU:HD22 | 1.81 | 0.44 |
| 1:H:1890:ARG:NH2 | 1:H:1959:GLU:OE2 | 2.45 | 0.44 |
| 1:H:2551:HIS:NE2 | 1:H:2567:CYS:SG | 2.90 | 0.44 |
| 1:I:915:ARG:HH21 | 1:I:1115:TYR:CB | 2.30 | 0.44 |
| 1:I:1322:PHE:HD2 | 1:I:1426:PHE:HE2 | 1.66 | 0.44 |
| 1:I:1678:LYS:NZ | 1:I:1683:LEU:HA | 2.33 | 0.44 |
| 1:I:2056:ARG:HD2 | 1:I:2056:ARG:HA | 1.78 | 0.44 |
| 1:I:2114:LEU:HD13 | 1:I:2172:HIS:HE1 | 1.83 | 0.44 |
| 1:I:2232:LEU:HD13 | 1:I:2274:LEU:HD23 | 1.98 | 0.44 |
| 1:I:2360:TYR:HA | 1:I:2363:LEU:HB2 | 2.00 | 0.44 |
| 1:J:409:VAL:HG13 | 1:J:666:CYS:HA | 1.98 | 0.44 |
| 1:J:1851:GLU:O | 1:J:1855:ASN:ND2 | 2.51 | 0.44 |
| 1:J:2111:LEU:HD13 | 1:J:2212:PHE:CE1 | 2.52 | 0.44 |
| 1:J:2977:CYS:HA | 1:J:2987:TRP:CH2 | 2.52 | 0.44 |
| 1:K:438:ASP:N | 1:K:438:ASP:OD1 | 2.48 | 0.44 |
| 1:K:1301:PHE:CG | 1:K:1302:PRO:HA | 2.52 | 0.44 |
| 1:K:1915:LEU:C | 1:K:1916:MET:HE2 | 2.42 | 0.44 |
| 1:K:2848:ASP:OD1 | 1:K:2849:ARG:N | 2.51 | 0.44 |
| 1:K:3133:GLN:OE1 | 1:K:3140:PHE:HB3 | 2.17 | 0.44 |
| 1:L:752:ILE:HB | 1:L:809:SER:HB3 | 1.99 | 0.44 |
| 1:L:1301:PHE:CG | 1:L:1302:PRO:HA | 2.52 | 0.44 |
| 1:L:1880:ILE:HD12 | 1:L:1880:ILE:H | 1.83 | 0.44 |
| 1:L:2227:ASP:HB3 | 1:L:2277:GLY:HA3 | 1.98 | 0.44 |
| 1:L:2414:GLN:HA | 1:L:2467:PHE:HA | 2.00 | 0.44 |
| 1:L:2940:ALA:HA | 1:L:3002:LYS:HB3 | 1.98 | 0.44 |
| 1:L:3079:ASP:OD1 | 1:L:3260:ARG:NH1 | 2.51 | 0.44 |
| 1:M:855:THR:O | 1:M:859:VAL:HG23 | 2.18 | 0.44 |
| 1:M:1433:LEU:HA | 1:M:1436:LEU:HB2 | 2.00 | 0.44 |
| 1:M:1448:LEU:HB3 | 1:M:1596:LEU:HD21 | 1.99 | 0.44 |
| 1:M:1871:HIS:CD2 | 1:M:1873:HIS:HB2 | 2.53 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:M:2147:CYS:O | 1:M:2149:HIS:ND1 | 2.43 | 0.44 |
| 1:M:2197:GLN:HG2 | 1:M:2198:THR:OG1 | 2.17 | 0.44 |
| 1:M:2603:TRP:CD1 | 1:M:2711:ASN:HD22 | 2.35 | 0.44 |
| 1:M:2770:ASP:OD1 | 1:M:2770:ASP:N | 2.49 | 0.44 |
| 1:N:310:LEU:HD13 | 1:N:366:HIS:HB3 | 1.99 | 0.44 |
| 1:N:753:LEU:HD23 | 1:N:766:ALA:HB3 | 1.99 | 0.44 |
| 1:N:2213:ALA:HA | 1:N:2226:ARG:NH2 | 2.32 | 0.44 |
| 1:N:3124:ARG:NH2 | 1:N:3127:GLN:HG2 | 2.33 | 0.44 |
| 1:N:3147:LEU:HA | 1:N:3150:LEU:HD12 | 1.99 | 0.44 |
| 1:O:438:ASP:N | 1:O:438:ASP:OD1 | 2.50 | 0.44 |
| 1:O:1010:ASP:OD2 | 1:O:1012:CYS:HB3 | 2.18 | 0.44 |
| 1:O:1381:PHE:O | 1:O:1394:ARG:NH2 | 2.50 | 0.44 |
| 1:O:2085:GLN:CD | 1:O:2087:LEU:H | 2.24 | 0.44 |
| 1:O:2159:ARG:HD2 | 1:O:2306:TRP:CE3 | 2.52 | 0.44 |
| 1:O:2215:GLY:O | 1:O:2224:THR:N | 2.49 | 0.44 |
| 1:O:2304:LYS:HB2 | 1:O:2367:TYR:HE2 | 1.83 | 0.44 |
| 1:O:2977:CYS:SG | 1:O:3106:LEU:HD11 | 2.57 | 0.44 |
| 1:P:7:ASN:HB3 | 1:P:10:LEU:HG | 2.00 | 0.44 |
| 1:P:477:CYS:HA | 1:P:479:ARG:N | 2.33 | 0.44 |
| 1:P:480:PRO:HA | 1:P:485:ARG:HH22 | 1.82 | 0.44 |
| 1:P:703:GLU:N | 1:P:703:GLU:OE1 | 2.50 | 0.44 |
| 1:P:816:LYS:HZ2 | 1:P:818:TRP:HZ2 | 1.66 | 0.44 |
| 1:P:937:TRP:H | 1:P:1051:LEU:HB2 | 1.82 | 0.44 |
| 1:P:1834:PHE:CE1 | 1:P:1891:ILE:HD13 | 2.52 | 0.44 |
| 1:P:2738:GLN:OE1 | 1:Q:2894:VAL:N | 2.49 | 0.44 |
| 1:P:3395:ARG:HH21 | 1:P:3400:THR:HG1 | 1.66 | 0.44 |
| 1:Q:1153:PHE:HE1 | 1:Q:1166:LEU:HD21 | 1.83 | 0.44 |
| 1:Q:1494:GLN:NE2 | 1:Q:1495:PRO:O | 2.50 | 0.44 |
| 1:Q:1998:ILE:HG13 | 1:Q:2010:ALA:HB3 | 1.99 | 0.44 |
| 1:Q:2414:GLN:O | 1:Q:2416:ASN:N | 2.47 | 0.44 |
| 1:Q:2465:ALA:HB2 | 1:R:1085:ARG:HD2 | 1.98 | 0.44 |
| 1:R:96:TRP:CZ3 | 1:R:218:ASN:HB3 | 2.53 | 0.44 |
| 1:R:331:HIS:CE1 | 1:R:672:HIS:HB3 | 2.53 | 0.44 |
| 1:R:788:GLU:CD | 1:R:791:ASP:H | 2.23 | 0.44 |
| 1:R:1339:ALA:HB1 | 3:rA:1:NAG:H81 | 2.00 | 0.44 |
| 1:R:1433:LEU:HA | 1:R:1436:LEU:HB2 | 1.99 | 0.44 |
| 1:R:1521:ASP:HB3 | 1:R:1525:HIS:CD2 | 2.52 | 0.44 |
| 1:R:1679:SER:OG | 1:R:1680:VAL:N | 2.50 | 0.44 |
| 1:R:2551:HIS:HB2 | 1:R:2700:ALA:HB2 | 1.99 | 0.44 |
| 1:R:2740:LEU:O | 1:R:2763:ALA:HB3 | 2.17 | 0.44 |
| 1:S:129:GLU:HA | 1:S:140:SER:HA | 2.00 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:S:610:HIS:O | 1:S:613:PRO:HD2 | 2.18 | 0.44 |
| 1:S:629:HIS:HA | 1:S:775:LYS:NZ | 2.29 | 0.44 |
| 1:S:914:HIS:CE1 | 1:S:1053:HIS:CE1 | 3.06 | 0.44 |
| 1:S:1265:ARG:NH2 | 1:S:1331:ASP:OD2 | 2.51 | 0.44 |
| 1:S:1812:ASP:HB3 | 1:S:1863:GLY:HA3 | 1.98 | 0.44 |
| 1:S:1991:LYS:O | 1:S:1991:LYS:HD2 | 2.17 | 0.44 |
| 1:T:11:LEU:HD11 | 1:T:92:PRO:HG3 | 2.00 | 0.44 |
| 1:T:473:LEU:H | 1:T:629:HIS:HB3 | 1.82 | 0.44 |
| 1:T:524:ASP:HA | 1:T:643:ASN:ND2 | 2.32 | 0.44 |
| 1:T:591:LEU:HB3 | 1:T:730:ARG:NH2 | 2.32 | 0.44 |
| 1:T:744:ASN:ND2 | 1:T:778:PRO:HA | 2.33 | 0.44 |
| 1:T:1531:ASP:OD1 | 1:T:1532:THR:N | 2.51 | 0.44 |
| 1:T:3026:SER:OG | 1:T:3030:ASN:ND2 | 2.49 | 0.44 |
| 1:A:1624:LYS:HD3 | 1:A:1624:LYS:HA | 1.83 | 0.44 |
| 1:A:2718:ILE:HD13 | 1:A:2779:LEU:HB3 | 1.99 | 0.44 |
| 1:A:3089:ASN:ND2 | 1:A:3247:ILE:HD12 | 2.33 | 0.44 |
| 1:B:245:GLU:HB2 | 1:B:249:LYS:NZ | 2.33 | 0.44 |
| 1:B:337:GLN:CD | 1:I:1588:HIS:H | 2.25 | 0.44 |
| 1:B:2286:LEU:HD23 | 1:B:2286:LEU:H | 1.82 | 0.44 |
| 1:B:3071:THR:HB | 1:B:3072:LEU:HD12 | 1.99 | 0.44 |
| 1:C:606:PHE:CE2 | 1:C:644:VAL:HG13 | 2.52 | 0.44 |
| 1:C:1001:MET:HE2 | 1:C:1001:MET:HB3 | 1.92 | 0.44 |
| 1:C:1644:TYR:N | 1:F:481:ASP:OD2 | 2.50 | 0.44 |
| 1:C:2130:HIS:O | 1:C:2130:HIS:ND1 | 2.45 | 0.44 |
| 1:C:2502:GLU:HG2 | 1:D:1073:PRO:HD3 | 1.99 | 0.44 |
| 1:C:2624:HIS:HB2 | 1:C:2633:LYS:NZ | 2.33 | 0.44 |
| 1:C:2624:HIS:HB2 | 1:C:2633:LYS:HZ1 | 1.83 | 0.44 |
| 1:C:2963:PRO:HD2 | 1:C:2965:LEU:HD23 | 1.99 | 0.44 |
| 1:C:3096:GLY:HA3 | 1:C:3104:SER:HB3 | 1.98 | 0.44 |
| 1:D:627:THR:HG21 | 1:D:630:TYR:HB2 | 1.99 | 0.44 |
| 1:D:795:LYS:HD3 | 1:D:796:LYS:HD3 | 1.99 | 0.44 |
| 1:D:980:ARG:NH2 | 1:D:1046:ASP:OD1 | 2.48 | 0.44 |
| 1:D:2130:HIS:ND1 | 1:D:2130:HIS:O | 2.50 | 0.44 |
| 1:D:2660:LEU:HD21 | 1:D:2803:PHE:HE1 | 1.83 | 0.44 |
| 1:D:2977:CYS:HA | 1:D:2987:TRP:CH2 | 2.53 | 0.44 |
| 1:D:3118:HIS:O | 1:D:3121:SER:OG | 2.28 | 0.44 |
| 1:E:151:GLN:N | 1:E:151:GLN:OE1 | 2.51 | 0.44 |
| 1:E:284:ASP:OD1 | 1:E:285:ASP:N | 2.51 | 0.44 |
| 1:E:1340:ARG:HH12 | 3:p:1:NAG:H61 | 1.82 | 0.44 |
| 1:E:2315:ARG:NH2 | 1:E:2377:LEU:HD12 | 2.33 | 0.44 |
| 1:E:2376:ASN:O | 1:E:2380:LEU:HG | 2.18 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:E:2990:LEU:HB3 | 1:E:3157:PHE:CE1 | 2.52 | 0.44 |
| 1:E:3165:ASN:ND2 | 1:E:3168:THR:OG1 | 2.49 | 0.44 |
| 1:F:254:PHE:HB2 | 1:F:264:THR:HG21 | 2.00 | 0.44 |
| 1:F:1356:ARG:NH2 | 1:F:1402:ASN:H | 2.15 | 0.44 |
| 1:F:1556:LEU:HB2 | 1:F:1625:LEU:HD21 | 2.00 | 0.44 |
| 1:F:1701:ASP:OD1 | 1:F:1701:ASP:N | 2.47 | 0.44 |
| 1:F:1834:PHE:CE1 | 1:F:1891:ILE:HD13 | 2.53 | 0.44 |
| 1:F:1848:VAL:HA | 1:F:2026:PHE:CE2 | 2.53 | 0.44 |
| 1:F:1865:LYS:O | 1:F:1868:SER:OG | 2.30 | 0.44 |
| 1:F:3127:GLN:HA | 1:F:3130:GLN:HG3 | 2.00 | 0.44 |
| 1:F:3179:ASP:OD2 | 1:F:3181:SER:OG | 2.33 | 0.44 |
| 1:G:1722:TYR:CE2 | 1:G:1724:GLU:HB3 | 2.52 | 0.44 |
| 1:G:1811:ARG:HH22 | 1:G:1880:ILE:HB | 1.83 | 0.44 |
| 1:G:2544:TYR:OH | 1:G:2701:TYR:O | 2.35 | 0.44 |
| 1:H:1694:ALA:O | 1:H:1697:SER:OG | 2.31 | 0.44 |
| 1:H:1893:ALA:HA | 1:H:1896:GLN:HG2 | 2.00 | 0.44 |
| 1:H:2641:GLN:HA | 1:H:2644:SER:OG | 2.18 | 0.44 |
| 1:H:3037:ILE:HG21 | 1:H:3040:ALA:HB3 | 1.99 | 0.44 |
| 1:I:973:VAL:HG11 | 1:I:1045:TYR:CG | 2.53 | 0.44 |
| 1:I:1323:PRO:HG3 | 1:I:1426:PHE:CE2 | 2.53 | 0.44 |
| 1:I:1814:LYS:NZ | 1:I:1860:TRP:O | 2.49 | 0.44 |
| 1:I:2655:TYR:O | 1:I:2658:ILE:HG22 | 2.18 | 0.44 |
| 1:I:2848:ASP:OD1 | 1:I:2849:ARG:N | 2.50 | 0.44 |
| 1:I:3287:LEU:HD23 | 1:I:3287:LEU:H | 1.82 | 0.44 |
| 1:J:235:LYS:HE2 | 1:J:235:LYS:HB3 | 1.77 | 0.44 |
| 1:J:475:ALA:HB1 | 1:J:486:TYR:N | 2.32 | 0.44 |
| 1:J:1305:CYS:SG | 1:J:1314:CYS:N | 2.91 | 0.44 |
| 1:J:2010:ALA:HA | 1:J:2037:VAL:HG21 | 1.99 | 0.44 |
| 1:J:2752:ASN:HD21 | 1:J:2757:ILE:HG13 | 1.82 | 0.44 |
| 1:J:2979:HIS:HA | 1:J:2984:PHE:CD2 | 2.50 | 0.44 |
| 1:J:3337:ARG:HD3 | 1:J:3378:ASN:HD21 | 1.83 | 0.44 |
| 1:J:3340:PHE:CE2 | 1:J:3351:VAL:HG11 | 2.53 | 0.44 |
| 1:K:461:VAL:HA | 1:K:1371:ARG:HD3 | 1.99 | 0.44 |
| 1:K:1202:ILE:HG22 | 1:K:1202:ILE:O | 2.17 | 0.44 |
| 1:K:1676:ILE:HG22 | 1:K:1678:LYS:NZ | 2.32 | 0.44 |
| 1:K:3124:ARG:O | 1:K:3128:ILE:HG23 | 2.17 | 0.44 |
| 1:L:635:PRO:O | 1:L:638:ILE:HG22 | 2.17 | 0.44 |
| 1:L:953:GLU:HA | 1:L:969:HIS:HB2 | 2.00 | 0.44 |
| 1:L:1195:ASP:OD1 | 1:L:1195:ASP:N | 2.44 | 0.44 |
| 1:L:2368:ASP:OD1 | 1:L:2368:ASP:N | 2.51 | 0.44 |
| 1:L:2536:GLN:HA | 1:L:2544:TYR:HB3 | 2.00 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:L:2800:ASP:OD1 | 1:L:2899:GLY:N | 2.51 | 0.44 |
| 1:M:1365:ALA:HA | 1:M:1381:PHE:CE2 | 2.53 | 0.44 |
| 1:M:1433:LEU:HD21 | 1:M:1460:HIS:CE1 | 2.52 | 0.44 |
| 1:M:1701:ASP:OD1 | 1:M:1702:SER:N | 2.50 | 0.44 |
| 1:M:3086:MET:HG2 | 1:M:3262:TYR:CZ | 2.53 | 0.44 |
| 1:N:460:SER:OG | 1:N:462:ASN:OD1 | 2.19 | 0.44 |
| 1:N:479:ARG:NH2 | 1:N:482:ALA:HA | 2.32 | 0.44 |
| 1:N:487:ALA:HB2 | 1:N:775:LYS:HG3 | 1.98 | 0.44 |
| 1:N:1148:ARG:HB2 | 1:N:1244:ARG:HB3 | 2.00 | 0.44 |
| 1:N:1286:MET:HE1 | 1:N:1292:PHE:HB2 | 2.00 | 0.44 |
| 1:N:2602:ASP:CG | 1:N:2604:THR:HG1 | 2.24 | 0.44 |
| 1:N:3127:GLN:HA | 1:N:3130:GLN:HG3 | 2.00 | 0.44 |
| 1:O:181:PHE:CZ | 1:O:219:VAL:HG13 | 2.53 | 0.44 |
| 1:O:866:LEU:HD22 | 1:O:968:PHE:CE1 | 2.52 | 0.44 |
| 1:O:1572:GLN:HB2 | 1:O:1636:LYS:HB2 | 1.99 | 0.44 |
| 1:O:2250:LEU:HA | 1:O:2253:GLU:OE1 | 2.18 | 0.44 |
| 1:O:3191:ASN:OD1 | 1:O:3195:HIS:N | 2.51 | 0.44 |
| 1:O:3283:PHE:CD2 | 1:O:3302:PRO:HG3 | 2.53 | 0.44 |
| 1:P:245:GLU:CD | 1:P:245:GLU:H | 2.24 | 0.44 |
| 1:P:737:PHE:CG | 1:P:786:LYS:HB3 | 2.52 | 0.44 |
| 1:P:780:ASN:OD1 | 1:P:781:PHE:N | 2.50 | 0.44 |
| 1:P:1397:GLN:HB2 | 1:P:1400:LEU:HD23 | 2.00 | 0.44 |
| 1:P:1678:LYS:NZ | 1:P:1683:LEU:HA | 2.32 | 0.44 |
| 1:P:1793:ILE:HD13 | 1:P:1793:ILE:HA | 1.89 | 0.44 |
| 1:P:1848:VAL:HG12 | 1:P:2026:PHE:CD2 | 2.51 | 0.44 |
| 1:P:1956:ASP:OD1 | 1:P:1957:THR:N | 2.50 | 0.44 |
| 1:P:2736:ASN:O | 1:P:2740:LEU:HD23 | 2.18 | 0.44 |
| 1:P:3319:PRO:HB2 | 1:P:3343:PRO:HD3 | 1.99 | 0.44 |
| 1:Q:855:THR:H | 1:Q:858:GLN:NE2 | 2.15 | 0.44 |
| 1:Q:1111:GLU:N | 1:Q:1111:GLU:OE1 | 2.50 | 0.44 |
| 1:Q:1223:VAL:HG13 | 1:Q:1231:ILE:HB | 1.99 | 0.44 |
| 1:Q:2780:ASN:OD1 | 1:Q:2784:LEU:N | 2.51 | 0.44 |
| 1:R:1081:ILE:H | 1:R:1081:ILE:HD12 | 1.82 | 0.44 |
| 1:R:1827:ASP:HA | 1:R:1831:TRP:HD1 | 1.83 | 0.44 |
| 1:R:2994:GLN:HG2 | 1:R:3157:PHE:CZ | 2.51 | 0.44 |
| 1:R:3266:VAL:HG21 | 1:R:3283:PHE:CZ | 2.53 | 0.44 |
| 1:R:3393:LYS:HD2 | 1:R:3394:ALA:N | 2.32 | 0.44 |
| 1:S:186:ASN:HB3 | 1:S:351:LEU:HD13 | 2.00 | 0.44 |
| 1:S:997:LYS:O | 1:S:1001:MET:HG3 | 2.18 | 0.44 |
| 1:S:998:ILE:H | 1:S:998:ILE:HD12 | 1.83 | 0.44 |
| 1:S:1025:ILE:HG21 | 1:S:1052:HIS:NE2 | 2.33 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:S:1677:ARG:HB3 | 1:S:1765:TYR:HE2 | 1.82 | 0.44 |
| 1:S:1920:LEU:HD21 | 1:S:1941:PRO:HB3 | 1.98 | 0.44 |
| 1:T:188:ILE:HG21 | 1:T:215:HIS:CE1 | 2.53 | 0.44 |
| 1:T:1324:HIS:HA | 1:T:1519:VAL:HG11 | 1.98 | 0.44 |
| 3:t:2:NAG:H4 | 3:t:3:BMA:H2 | 1.65 | 0.44 |
| 1:A:104:PRO:HA | 1:A:105:ARG:HH11 | 1.82 | 0.44 |
| 1:A:161:LEU:HD21 | 1:A:187:HIS:CD2 | 2.53 | 0.44 |
| 1:A:312:SER:HA | 1:A:365:TYR:O | 2.18 | 0.44 |
| 1:A:376:LEU:HD12 | 1:A:378:LYS:HZ1 | 1.83 | 0.44 |
| 1:A:396:THR:HG21 | 2:U:1:NAG:HN2 | 1.82 | 0.44 |
| 1:A:981:SER:OG | 1:A:1031:GLY:HA3 | 2.18 | 0.44 |
| 1:A:1744:ARG:HH12 | 1:A:1945:PHE:HA | 1.81 | 0.44 |
| 1:A:2095:GLU:CD | 1:A:2097:SER:H | 2.26 | 0.44 |
| 1:A:2773:ASN:CG | 1:A:3141:ASN:HB2 | 2.42 | 0.44 |
| 1:A:3067:GLN:O | 1:A:3071:THR:HG23 | 2.18 | 0.44 |
| 1:A:3131:THR:HA | 1:A:3134:LYS:HG2 | 2.00 | 0.44 |
| 1:B:456:GLN:HE22 | 1:B:553:PRO:HB2 | 1.83 | 0.44 |
| 1:B:514:ARG:HH12 | 1:B:1341:GLY:HA2 | 1.82 | 0.44 |
| 1:B:1307:HIS:O | 1:B:1308:GLU:HG3 | 2.18 | 0.44 |
| 1:B:1827:ASP:HA | 1:B:1831:TRP:HD1 | 1.80 | 0.44 |
| 1:C:222:ILE:HA | 1:C:225:ILE:HG22 | 1.99 | 0.44 |
| 1:C:326:ILE:HD12 | 1:C:326:ILE:HA | 1.80 | 0.44 |
| 1:C:887:GLN:HG3 | 1:C:889:ASN:HD21 | 1.83 | 0.44 |
| 1:C:1638:ARG:HH12 | 1:C:1642:GLY:HA2 | 1.82 | 0.44 |
| 1:C:2510:GLY:HA3 | 1:C:2513:VAL:HB | 2.00 | 0.44 |
| 1:C:3395:ARG:HD3 | 1:C:3400:THR:HB | 1.99 | 0.44 |
| 1:D:48:CYS:HB2 | 1:D:58:CYS:HB2 | 1.48 | 0.44 |
| 1:D:587:PHE:O | 1:D:591:LEU:HG | 2.18 | 0.44 |
| 1:D:917:LEU:O | 1:D:920:GLN:HG3 | 2.18 | 0.44 |
| 1:D:949:ILE:HB | 1:D:968:PHE:CD2 | 2.53 | 0.44 |
| 1:D:981:SER:HB3 | 1:D:1031:GLY:HA3 | 1.99 | 0.44 |
| 1:D:1221:TYR:CE2 | 1:D:1233:SER:HB2 | 2.53 | 0.44 |
| 1:D:1284:ARG:HH21 | 1:D:1287:GLN:HG2 | 1.83 | 0.44 |
| 1:D:1676:ILE:HG13 | 1:D:1761:VAL:HG23 | 2.00 | 0.44 |
| 1:D:3062:ASP:OD2 | 1:D:3064:LEU:HB2 | 2.18 | 0.44 |
| 1:D:3229:ASN:H | 1:D:3286:THR:HG22 | 1.83 | 0.44 |
| 1:E:742:LEU:HB2 | 1:E:781:PHE:CD2 | 2.53 | 0.44 |
| 1:E:1061:ALA:HA | 1:E:1064:GLN:NE2 | 2.33 | 0.44 |
| 1:E:1305:CYS:SG | 1:E:1314:CYS:N | 2.91 | 0.44 |
| 1:E:1385:ILE:H | 1:E:1385:ILE:HD12 | 1.82 | 0.44 |
| 1:E:1932:ASP:OD2 | 1:E:1934:ILE:HG22 | 2.18 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:E:2273:TYR:HA | 1:E:2284:SER:OG | 2.17 | 0.44 |
| 1:E:3155:GLU:HB3 | 1:E:3158:ASN:HD21 | 1.83 | 0.44 |
| 1:E:3317:ILE:HG23 | 1:E:3339:ARG:HB3 | 2.00 | 0.44 |
| 1:F:531:THR:OG1 | 1:F:532:VAL:N | 2.51 | 0.44 |
| 1:F:1022:HIS:HB2 | 1:F:1052:HIS:CE1 | 2.52 | 0.44 |
| 1:F:1098:ASN:HB2 | 1:F:1104:ARG:HD3 | 1.99 | 0.44 |
| 1:F:1159:ARG:O | 1:F:1159:ARG:HD2 | 2.17 | 0.44 |
| 1:F:1315:CYS:C | 1:F:1317:HIS:HD1 | 2.25 | 0.44 |
| 1:F:1940:LYS:HD2 | 1:F:1940:LYS:HA | 1.69 | 0.44 |
| 1:G:971:GLY:N | 1:G:978:THR:OG1 | 2.47 | 0.44 |
| 1:G:1365:ALA:HA | 1:G:1381:PHE:CZ | 2.52 | 0.44 |
| 1:H:103:LEU:HB2 | 1:H:150:PHE:HZ | 1.83 | 0.44 |
| 1:H:325:ARG:HH21 | 1:H:391:TYR:HE2 | 1.65 | 0.44 |
| 1:H:536:ALA:HA | 1:H:552:ASN:HD21 | 1.82 | 0.44 |
| 1:H:755:ILE:HG21 | 1:H:792:ALA:HB1 | 1.99 | 0.44 |
| 1:H:2345:ASN:O | 1:H:2349:ARG:HG2 | 2.18 | 0.44 |
| 1:H:2558:LYS:HD2 | 1:H:2563:THR:HA | 1.99 | 0.44 |
| 1:H:3151:TYR:HA | 1:H:3173:ARG:NH2 | 2.33 | 0.44 |
| 1:I:501:ARG:NH1 | 1:I:648:TRP:HZ3 | 2.16 | 0.44 |
| 1:I:589:GLY:HA2 | 1:I:592:LEU:HG | 1.98 | 0.44 |
| 1:I:850:ASP:OD1 | 1:I:852:SER:OG | 2.29 | 0.44 |
| 1:I:1896:GLN:O | 1:I:1899:GLN:HG3 | 2.18 | 0.44 |
| 1:I:1899:GLN:NE2 | 1:I:1906:PRO:HA | 2.33 | 0.44 |
| 1:I:2091:ARG:HA | 1:I:2093:ARG:HH21 | 1.83 | 0.44 |
| 1:I:2159:ARG:O | 1:I:2162:THR:OG1 | 2.30 | 0.44 |
| 1:I:2572:ALA:HB3 | 1:I:2736:ASN:HD21 | 1.83 | 0.44 |
| 1:I:3301:THR:HG22 | 1:I:3326:LEU:HA | 1.98 | 0.44 |
| 1:J:953:GLU:HA | 1:J:969:HIS:HB2 | 2.00 | 0.44 |
| 1:J:1619:ARG:HD3 | 1:J:1619:ARG:HA | 1.81 | 0.44 |
| 1:K:196:HIS:O | 1:K:199:SER:OG | 2.31 | 0.44 |
| 1:K:1385:ILE:HB | 1:K:1388:THR:HG21 | 1.99 | 0.44 |
| 1:K:1433:LEU:HD21 | 1:K:1460:HIS:CE1 | 2.53 | 0.44 |
| 1:K:2399:LEU:HB3 | 1:K:2436:TRP:HH2 | 1.80 | 0.44 |
| 1:K:2602:ASP:OD1 | 1:K:2604:THR:HG22 | 2.18 | 0.44 |
| 1:K:3204:ILE:HG13 | 1:K:3205:GLU:H | 1.83 | 0.44 |
| 1:L:735:ARG:NH2 | 1:L:790:THR:H | 2.13 | 0.44 |
| 1:L:1968:LEU:HA | 1:L:1971:LEU:HB3 | 1.98 | 0.44 |
| 1:L:2004:GLU:OE1 | 1:L:2004:GLU:N | 2.47 | 0.44 |
| 1:L:2316:ARG:HD3 | 1:L:2316:ARG:H | 1.81 | 0.44 |
| 1:L:3008:ILE:HD13 | 1:L:3116:MET:HB3 | 1.99 | 0.44 |
| 1:M:629:HIS:HA | 1:M:775:LYS:NZ | 2.33 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:M:1433:LEU:HD21 | 1:M:1460:HIS:HE1 | 1.81 | 0.44 |
| 1:M:1855:ASN:ND2 | 1:M:2015:VAL:HA | 2.31 | 0.44 |
| 1:M:2342:LEU:HD23 | 1:M:2342:LEU:HA | 1.84 | 0.44 |
| 1:M:2404:THR:OG1 | 1:M:2405:SER:N | 2.51 | 0.44 |
| 1:M:2448:ASP:O | 1:M:2452:GLU:OE1 | 2.36 | 0.44 |
| 1:M:3228:ALA:O | 1:M:3245:PHE:N | 2.50 | 0.44 |
| 1:N:41:PHE:CD1 | 1:N:47:MET:HE1 | 2.53 | 0.44 |
| 1:N:1321:VAL:HA | 1:N:1324:HIS:CD2 | 2.53 | 0.44 |
| 1:N:2088:PRO:C | 1:N:2090:ASN:H | 2.23 | 0.44 |
| 1:N:2954:GLU:H | 1:N:2954:GLU:CD | 2.26 | 0.44 |
| 1:O:50:LYS:HB3 | 1:O:54:LYS:H | 1.83 | 0.44 |
| 1:O:687:ASN:OD1 | 1:O:688:GLU:N | 2.50 | 0.44 |
| 1:O:1240:THR:HA | 1:P:2328:ASN:HD21 | 1.81 | 0.44 |
| 1:O:1738:THR:HG22 | 1:O:1738:THR:O | 2.18 | 0.44 |
| 1:O:1993:SER:HB2 | 1:O:2017:GLY:H | 1.83 | 0.44 |
| 1:O:2095:GLU:CD | 1:O:2097:SER:H | 2.25 | 0.44 |
| 1:O:2372:LEU:HD23 | 1:O:2372:LEU:HA | 1.87 | 0.44 |
| 1:O:2544:TYR:OH | 1:O:2701:TYR:O | 2.34 | 0.44 |
| 1:O:3037:ILE:HG12 | 1:O:3039:PHE:H | 1.83 | 0.44 |
| 1:O:3231:LYS:HB2 | 1:O:3284:GLN:HG3 | 1.99 | 0.44 |
| 1:P:848:ARG:HE | 1:P:934:LEU:H | 1.66 | 0.44 |
| 1:P:917:LEU:O | 1:P:920:GLN:NE2 | 2.46 | 0.44 |
| 1:P:968:PHE:HD1 | 1:P:1047:PRO:HG2 | 1.82 | 0.44 |
| 1:P:1433:LEU:HD21 | 1:P:1460:HIS:NE2 | 2.32 | 0.44 |
| 1:P:2809:GLN:NE2 | 1:P:2845:TRP:O | 2.51 | 0.44 |
| 1:Q:341:HIS:NE2 | 1:Q:343:GLU:OE2 | 2.48 | 0.44 |
| 1:Q:489:CYS:C | 1:Q:491:HIS:HD1 | 2.25 | 0.44 |
| 1:Q:731:ARG:HA | 1:Q:735:ARG:NH1 | 2.32 | 0.44 |
| 1:Q:989:LYS:HA | 1:Q:989:LYS:HD2 | 1.83 | 0.44 |
| 1:Q:1151:ALA:CB | 1:Q:1202:ILE:HD11 | 2.48 | 0.44 |
| 1:Q:1693:LEU:O | 1:Q:1696:GLN:HG3 | 2.17 | 0.44 |
| 1:Q:1760:LEU:HD23 | 1:Q:1760:LEU:H | 1.83 | 0.44 |
| 1:Q:2848:ASP:OD1 | 1:Q:2849:ARG:N | 2.50 | 0.44 |
| 1:Q:2980:GLY:HA2 | 1:Q:3258:TYR:HE2 | 1.82 | 0.44 |
| 1:Q:3088:HIS:CE1 | 1:Q:3119:HIS:CD2 | 3.06 | 0.44 |
| 1:Q:3131:THR:HA | 1:Q:3134:LYS:HD3 | 1.98 | 0.44 |
| 1:R:220:ASP:O | 1:R:224:VAL:HG13 | 2.18 | 0.44 |
| 1:R:245:GLU:CD | 1:R:245:GLU:H | 2.26 | 0.44 |
| 1:R:567:SER:OG | 1:R:623:TYR:O | 2.32 | 0.44 |
| 1:R:737:PHE:HB2 | 1:R:829:ILE:HB | 1.99 | 0.44 |
| 1:R:1848:VAL:HG23 | 1:R:1849:GLN:OE1 | 2.17 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:R:2433:GLU:N | 1:R:2433:GLU:OE1 | 2.51 | 0.44 |
| 1:R:2794:GLU:HA | 1:R:2794:GLU:OE2 | 2.17 | 0.44 |
| 1:S:50:LYS:HE2 | 1:S:357:MET:SD | 2.57 | 0.44 |
| 1:S:742:LEU:HB2 | 1:S:781:PHE:CD2 | 2.53 | 0.44 |
| 1:S:1171:PRO:HD3 | 1:S:1217:TYR:HA | 2.00 | 0.44 |
| 1:S:1835:LEU:HA | 1:S:1838:LEU:HD12 | 1.99 | 0.44 |
| 1:S:2465:ALA:HB2 | 1:T:1085:ARG:HD2 | 1.99 | 0.44 |
| 1:S:3070:GLU:O | 1:S:3073:GLU:HG2 | 2.17 | 0.44 |
| 1:T:224:VAL:HA | 1:T:227:GLN:OE1 | 2.16 | 0.44 |
| 1:T:420:LYS:HA | 1:T:420:LYS:HD3 | 1.86 | 0.44 |
| 1:T:1037:MET:HB2 | 1:T:1043:THR:HA | 1.99 | 0.44 |
| 1:T:1192:TRP:HZ3 | 1:T:1194:TYR:HB2 | 1.82 | 0.44 |
| 1:T:3266:VAL:HG21 | 1:T:3283:PHE:CE2 | 2.46 | 0.44 |
| 1:A:164:MET:HE2 | 1:A:184:ALA:HA | 1.99 | 0.44 |
| 1:A:304:ARG:HE | 1:A:411:ARG:NH1 | 2.16 | 0.44 |
| 1:A:492:GLY:HA3 | 1:A:779:TRP:CE3 | 2.52 | 0.44 |
| 1:A:1271:LEU:HD11 | 1:A:1275:GLU:HG3 | 1.99 | 0.44 |
| 1:A:1378:ASN:ND2 | 1:A:1380:PHE:HB2 | 2.33 | 0.44 |
| 1:A:1482:ASP:OD1 | 1:A:1483:ASP:N | 2.51 | 0.44 |
| 1:A:2412:VAL:HG23 | 1:A:2422:ALA:HB2 | 1.99 | 0.44 |
| 1:A:3082:VAL:HG13 | 1:A:3083:GLN:N | 2.32 | 0.44 |
| 1:B:737:PHE:CG | 1:B:786:LYS:HB3 | 2.53 | 0.44 |
| 1:B:1024:TYR:OH | 1:B:1180:GLU:OE1 | 2.25 | 0.44 |
| 1:B:1638:ARG:HH11 | 1:B:1644:TYR:HE1 | 1.66 | 0.44 |
| 1:B:2252:LEU:HD23 | 1:B:2309:TRP:HD1 | 1.83 | 0.44 |
| 1:B:3018:LYS:HA | 1:B:3055:ARG:HH12 | 1.82 | 0.44 |
| 1:B:3363:CYS:HB2 | 1:B:3396:CYS:HB3 | 1.84 | 0.44 |
| 1:C:471:HIS:HB3 | 1:C:632:ALA:HB2 | 2.00 | 0.44 |
| 1:C:1507:PHE:HD1 | 1:C:1508:ASP:CG | 2.25 | 0.44 |
| 1:C:1517:ILE:HD12 | 1:C:1517:ILE:H | 1.83 | 0.44 |
| 1:C:3216:GLY:HA2 | 1:C:3262:TYR:O | 2.18 | 0.44 |
| 1:D:5:ARG:HB3 | 1:D:93:TYR:HD2 | 1.82 | 0.44 |
| 1:D:252:GLU:OE1 | 1:D:256:ARG:NH2 | 2.51 | 0.44 |
| 1:D:445:VAL:O | 1:D:448:LEU:HG | 2.18 | 0.44 |
| 1:D:1055:ASN:HA | 1:D:1058:ARG:HG3 | 2.00 | 0.44 |
| 1:D:2298:HIS:O | 1:D:2302:VAL:HG23 | 2.18 | 0.44 |
| 1:D:2660:LEU:HD11 | 1:D:2803:PHE:HZ | 1.82 | 0.44 |
| 1:E:326:ILE:O | 1:E:345:ALA:HB3 | 2.18 | 0.44 |
| 1:E:1356:ARG:HB2 | 1:E:1357:GLN:OE1 | 2.17 | 0.44 |
| 1:E:1421:ASP:OD1 | 1:E:1422:PHE:N | 2.51 | 0.44 |
| 1:E:1433:LEU:HD21 | 1:E:1460:HIS:CE1 | 2.53 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:E:1466:ARG:HA | 1:E:1530:TYR:HE2 | 1.83 | 0.44 |
| 1:E:1515:ARG:O | 1:E:1519:VAL:HG23 | 2.18 | 0.44 |
| 1:E:2246:ASP:OD1 | 1:E:2246:ASP:N | 2.51 | 0.44 |
| 1:E:2663:GLU:HA | 1:E:2793:ILE:HD11 | 2.00 | 0.44 |
| 1:E:2963:PRO:HG3 | 1:E:3039:PHE:CD2 | 2.53 | 0.44 |
| 1:E:3082:VAL:O | 1:E:3086:MET:HG2 | 2.18 | 0.44 |
| 1:E:3209:ASP:HB2 | 1:F:1117:ARG:HH12 | 1.82 | 0.44 |
| 1:F:540:THR:HG22 | 1:F:551:HIS:HA | 1.99 | 0.44 |
| 1:F:2524:GLU:N | 1:F:2524:GLU:OE1 | 2.51 | 0.44 |
| 1:F:2550:ALA:O | 1:F:2565:ALA:HB1 | 2.17 | 0.44 |
| 1:F:3135:LEU:HD23 | 1:F:3135:LEU:HA | 1.87 | 0.44 |
| 1:G:14:GLN:HG2 | 1:G:15:GLU:N | 2.33 | 0.44 |
| 1:G:757:PRO:HB3 | 1:G:798:LEU:HD11 | 1.98 | 0.44 |
| 1:G:1418:SER:OG | 1:G:1419:PHE:N | 2.51 | 0.44 |
| 1:G:2587:ARG:O | 1:G:2591:LEU:HD23 | 2.17 | 0.44 |
| 1:H:811:LYS:NZ | 1:H:817:ASP:OD1 | 2.51 | 0.44 |
| 1:H:1301:PHE:CD1 | 1:H:1302:PRO:HA | 2.53 | 0.44 |
| 1:H:1303:SER:OG | 1:H:1311:LYS:O | 2.26 | 0.44 |
| 1:H:1364:GLU:OE2 | 1:H:1365:ALA:N | 2.46 | 0.44 |
| 1:I:181:PHE:CE2 | 1:I:219:VAL:HG13 | 2.53 | 0.44 |
| 1:I:939:TRP:HZ3 | 1:I:1055:ASN:HB3 | 1.81 | 0.44 |
| 1:I:2712:VAL:HA | 1:I:2715:GLN:HG2 | 1.99 | 0.44 |
| 1:I:3301:THR:HB | 1:I:3325:LYS:HB3 | 2.00 | 0.44 |
| 1:J:365:TYR:CE2 | 1:J:367:PHE:HB2 | 2.52 | 0.44 |
| 1:J:1143:ARG:HB3 | 1:J:1148:ARG:NH2 | 2.33 | 0.44 |
| 1:J:1633:LEU:HD23 | 1:J:1633:LEU:H | 1.83 | 0.44 |
| 1:J:1802:ILE:CD1 | 1:J:1805:GLU:HB2 | 2.48 | 0.44 |
| 1:J:2028:ARG:HB2 | 1:J:2028:ARG:NH1 | 2.32 | 0.44 |
| 1:J:2433:GLU:N | 1:J:2433:GLU:OE1 | 2.51 | 0.44 |
| 1:J:2714:ARG:O | 1:J:2718:ILE:HG12 | 2.18 | 0.44 |
| 1:J:2737:ILE:H | 1:J:2737:ILE:HD12 | 1.83 | 0.44 |
| 1:J:2816:ASP:OD1 | 1:J:2817:VAL:N | 2.51 | 0.44 |
| 1:K:168:ALA:HA | 1:K:180:GLN:HG3 | 2.00 | 0.44 |
| 1:K:580:TYR:OH | 1:K:860:GLN:OE1 | 2.33 | 0.44 |
| 1:K:618:GLY:HA3 | 1:K:626:SER:HB3 | 2.00 | 0.44 |
| 1:K:1307:HIS:O | 1:K:1308:GLU:HG2 | 2.17 | 0.44 |
| 1:K:1626:ASP:OD1 | 1:K:1626:ASP:N | 2.40 | 0.44 |
| 1:K:2227:ASP:HB3 | 1:K:2277:GLY:HA3 | 2.00 | 0.44 |
| 1:K:2232:LEU:HB2 | 1:K:2274:LEU:HD21 | 1.99 | 0.44 |
| 1:K:2912:ASP:OD1 | 1:K:2912:ASP:N | 2.49 | 0.44 |
| 1:K:3211:ASP:OD2 | 1:K:3309:ALA:N | 2.47 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:K:3352:LYS:HA | 1:K:3371:ASN:O | 2.17 | 0.44 |
| 1:L:48:CYS:HB2 | 1:L:58:CYS:HB2 | 1.52 | 0.44 |
| 1:L:702:TYR:N | 1:L:703:GLU:OE1 | 2.51 | 0.44 |
| 1:L:984:ASP:OD1 | 1:L:985:GLU:N | 2.50 | 0.44 |
| 1:L:1305:CYS:HB2 | 1:L:1312:VAL:O | 2.17 | 0.44 |
| 1:L:1750:PHE:CD2 | 1:L:1882:LEU:HD11 | 2.53 | 0.44 |
| 1:L:1878:ASP:OD2 | 1:L:1880:ILE:HB | 2.18 | 0.44 |
| 1:L:2865:ARG:NH1 | 1:L:2866:PRO:HG2 | 2.33 | 0.44 |
| 1:M:527:ARG:HG2 | 1:M:528:PRO:HD2 | 2.00 | 0.44 |
| 1:M:602:PHE:HA | 1:M:605:GLN:NE2 | 2.32 | 0.44 |
| 1:M:2313:GLN:OE1 | 1:M:2318:LEU:HB2 | 2.18 | 0.44 |
| 1:M:2345:ASN:O | 1:M:2349:ARG:HG2 | 2.18 | 0.44 |
| 1:M:2409:ARG:O | 1:M:2471:TYR:HA | 2.17 | 0.44 |
| 1:M:2864:LEU:HD11 | 1:M:2870:TYR:HB3 | 2.00 | 0.44 |
| 1:M:3089:ASN:HD21 | 1:M:3248:LEU:N | 2.11 | 0.44 |
| 1:N:81:LEU:HB3 | 1:N:86:LEU:HD22 | 1.99 | 0.44 |
| 1:N:728:ASP:OD2 | 1:N:836:HIS:ND1 | 2.51 | 0.44 |
| 1:N:1324:HIS:CD2 | 1:N:1324:HIS:H | 2.36 | 0.44 |
| 1:N:1435:SER:HA | 1:N:1446:SER:OG | 2.17 | 0.44 |
| 1:N:2316:ARG:HD3 | 1:N:2316:ARG:H | 1.83 | 0.44 |
| 1:N:2674:TYR:CE1 | 1:N:2712:VAL:HG22 | 2.53 | 0.44 |
| 1:O:1521:ASP:OD2 | 1:O:1524:ASN:HB2 | 2.17 | 0.44 |
| 1:O:2085:GLN:HE21 | 1:O:2366:ARG:NH1 | 2.16 | 0.44 |
| 1:O:2147:CYS:C | 1:O:2149:HIS:HD1 | 2.26 | 0.44 |
| 1:O:2967:PRO:HD3 | 1:O:2974:TYR:CE2 | 2.53 | 0.44 |
| 1:P:68:GLN:HA | 1:P:71:ARG:HG2 | 2.00 | 0.44 |
| 1:P:173:ASP:O | 1:P:177:PHE:HB2 | 2.18 | 0.44 |
| 1:P:1710:LEU:HB3 | 1:P:1750:PHE:CZ | 2.53 | 0.44 |
| 1:P:2127:ALA:HA | 1:P:2161:TYR:HH | 1.83 | 0.44 |
| 1:P:2515:LYS:HA | 1:P:2777:ASP:OD2 | 2.18 | 0.44 |
| 1:P:2542:ARG:HH11 | 1:P:2591:LEU:HD22 | 1.83 | 0.44 |
| 1:P:3395:ARG:C | 1:P:3401:ARG:HH22 | 2.25 | 0.44 |
| 1:Q:75:VAL:O | 1:Q:78:GLU:HG3 | 2.17 | 0.44 |
| 1:Q:169:LEU:HD23 | 1:Q:222:ILE:HD11 | 2.00 | 0.44 |
| 1:Q:580:TYR:OH | 1:Q:860:GLN:NE2 | 2.51 | 0.44 |
| 1:Q:612:LEU:HB2 | 1:Q:613:PRO:HD3 | 2.00 | 0.44 |
| 1:Q:995:LEU:HB3 | 1:Q:999:ALA:HB3 | 2.00 | 0.44 |
| 1:Q:1331:ASP:O | 1:Q:1334:GLU:HG3 | 2.17 | 0.44 |
| 1:Q:1440:ARG:NH2 | 1:T:1368:PHE:HB3 | 2.31 | 0.44 |
| 1:Q:2414:GLN:HE21 | 1:Q:2453:LEU:HD22 | 1.82 | 0.44 |
| 1:Q:2624:HIS:HB2 | 1:Q:2633:LYS:NZ | 2.33 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:Q:2819:PHE:O | 1:Q:2831:ALA:HB3 | 2.18 | 0.44 |
| 1:R:787:VAL:HG23 | 1:R:789:ILE:HD11 | 2.00 | 0.44 |
| 1:R:928:LYS:HG3 | 1:R:929:GLY:N | 2.33 | 0.44 |
| 1:R:976:LYS:HA | 1:R:976:LYS:HD2 | 1.71 | 0.44 |
| 1:R:1978:LYS:NZ | 1:R:1979:SER:O | 2.48 | 0.44 |
| 1:R:2577:TRP:C | 1:R:2577:TRP:CD1 | 2.96 | 0.44 |
| 1:S:287:SER:OG | 1:S:288:LEU:N | 2.49 | 0.44 |
| 1:S:485:ARG:HD3 | 1:S:485:ARG:HA | 1.87 | 0.44 |
| 1:S:2412:VAL:HG23 | 1:S:2422:ALA:HB2 | 1.99 | 0.44 |
| 1:S:3021:PRO:HD2 | 1:S:3024:LEU:HD21 | 2.00 | 0.44 |
| 1:T:443:GLU:HG2 | 1:T:444:GLU:N | 2.33 | 0.44 |
| 1:T:562:LEU:HB3 | 1:T:564:GLU:OE1 | 2.17 | 0.44 |
| 1:T:729:GLU:O | 1:T:732:THR:HG22 | 2.17 | 0.44 |
| 1:T:2286:LEU:HD23 | 1:T:2286:LEU:H | 1.83 | 0.44 |
| 1:T:2516:ASN:OD1 | 1:T:2517:ILE:N | 2.48 | 0.44 |
| 1:T:2944:LEU:HA | 1:T:3002:LYS:HE2 | 1.98 | 0.44 |
| 1:A:612:LEU:HB2 | 1:A:613:PRO:HD3 | 1.99 | 0.44 |
| 1:A:1701:ASP:OD1 | 1:A:1702:SER:N | 2.51 | 0.44 |
| 1:A:1801:ASP:OD1 | 1:A:1802:ILE:N | 2.50 | 0.44 |
| 1:A:3144:ARG:NE | 1:A:3147:LEU:HD21 | 2.33 | 0.44 |
| 1:A:3154:LEU:O | 1:A:3158:ASN:N | 2.50 | 0.44 |
| 1:A:3259:GLU:OE1 | 1:A:3259:GLU:N | 2.41 | 0.44 |
| 1:B:437:VAL:HG12 | 1:B:521:PRO:HG2 | 2.00 | 0.44 |
| 1:B:522:TYR:HE2 | 1:B:524:ASP:HB2 | 1.83 | 0.44 |
| 1:B:533:PRO:HB2 | 1:B:535:ILE:HD12 | 1.99 | 0.44 |
| 1:B:1051:LEU:HD12 | 1:B:1052:HIS:N | 2.33 | 0.44 |
| 1:B:1322:PHE:HB3 | 1:B:1323:PRO:HD3 | 1.98 | 0.44 |
| 1:B:1556:LEU:HB2 | 1:B:1625:LEU:HD11 | 2.00 | 0.44 |
| 1:B:3057:LYS:HD2 | 1:B:3062:ASP:HA | 1.99 | 0.44 |
| 1:C:755:ILE:HG12 | 1:C:765:VAL:HG22 | 2.00 | 0.44 |
| 1:C:2584:THR:HG21 | 1:C:2747:PHE:HE2 | 1.82 | 0.44 |
| 1:C:2994:GLN:OE1 | 1:C:3165:ASN:ND2 | 2.32 | 0.44 |
| 1:D:224:VAL:HA | 1:D:227:GLN:OE1 | 2.18 | 0.44 |
| 1:D:602:PHE:O | 1:D:606:PHE:HB2 | 2.18 | 0.44 |
| 1:D:845:LEU:HD22 | 1:D:926:ARG:HD3 | 2.00 | 0.44 |
| 1:D:1058:ARG:HG2 | 1:D:1123:TYR:CE1 | 2.52 | 0.44 |
| 1:D:2577:TRP:C | 1:D:2577:TRP:CD1 | 2.95 | 0.44 |
| 1:D:2979:HIS:HA | 1:D:2984:PHE:CD2 | 2.50 | 0.44 |
| 1:D:3149:ASN:HD22 | 1:D:3152:ARG:HD3 | 1.82 | 0.44 |
| 1:E:719:THR:H | 1:E:722:GLN:NE2 | 2.16 | 0.44 |
| 1:E:744:ASN:HB3 | 1:E:779:TRP:NE1 | 2.33 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:E:957:ASN:HD21 | 1:E:959:GLU:HB3 | 1.83 | 0.44 |
| 1:E:2354:PRO:O | 1:E:2357:VAL:HG22 | 2.17 | 0.44 |
| 1:E:3081:GLU:HA | 1:E:3084:PHE:HB3 | 1.99 | 0.44 |
| 1:F:24:ARG:HD2 | 1:F:24:ARG:HA | 1.74 | 0.44 |
| 1:F:592:LEU:O | 1:F:595:GLU:HG2 | 2.18 | 0.44 |
| 1:F:887:GLN:HE22 | 1:F:889:ASN:HB2 | 1.82 | 0.44 |
| 1:F:1364:GLU:OE2 | 1:F:1365:ALA:N | 2.47 | 0.44 |
| 1:F:1857:ILE:HD12 | 1:F:1884:HIS:CD2 | 2.52 | 0.44 |
| 1:F:1914:GLU:OE1 | 1:F:1914:GLU:N | 2.41 | 0.44 |
| 1:G:1375:GLU:OE2 | 1:J:1441:GLY:HA3 | 2.18 | 0.44 |
| 1:H:1925:PHE:O | 1:H:1936:LYS:HE2 | 2.18 | 0.44 |
| 1:H:2434:MET:O | 1:H:2436:TRP:HD1 | 2.01 | 0.44 |
| 1:H:3160:GLU:CD | 1:H:3160:GLU:H | 2.25 | 0.44 |
| 1:I:910:PHE:HZ | 1:I:1022:HIS:ND1 | 2.15 | 0.44 |
| 1:I:958:PRO:HA | 1:I:961:ASN:HA | 1.99 | 0.44 |
| 1:I:1161:SER:N | 1:I:1185:GLY:O | 2.51 | 0.44 |
| 1:I:1178:GLU:CG | 1:I:1205:ILE:HG21 | 2.48 | 0.44 |
| 1:I:1931:LEU:HB3 | 1:J:2102:ARG:HB2 | 2.00 | 0.44 |
| 1:I:2412:VAL:HG23 | 1:I:2422:ALA:HB2 | 2.00 | 0.44 |
| 1:I:2603:TRP:CD1 | 1:I:2711:ASN:ND2 | 2.86 | 0.44 |
| 1:I:2746:PRO:O | 1:I:2749:TRP:HB2 | 2.18 | 0.44 |
| 1:I:2819:PHE:O | 1:I:2831:ALA:HB3 | 2.18 | 0.44 |
| 1:J:44:GLU:HB2 | 1:J:204:GLU:CD | 2.43 | 0.44 |
| 1:J:202:THR:HG22 | 1:J:321:SER:HB2 | 1.99 | 0.44 |
| 1:J:486:TYR:HB3 | 1:J:777:MET:HE1 | 2.00 | 0.44 |
| 1:J:1428:ILE:HA | 1:J:1431:ASN:HD21 | 1.83 | 0.44 |
| 1:J:1834:PHE:CE2 | 1:J:1891:ILE:HD13 | 2.53 | 0.44 |
| 1:J:1839:GLU:HB2 | 1:J:1972:ILE:HD12 | 2.00 | 0.44 |
| 1:J:2254:GLN:HE21 | 1:J:2260:PHE:HA | 1.83 | 0.44 |
| 1:J:3057:LYS:HZ3 | 1:J:3062:ASP:HB2 | 1.82 | 0.44 |
| 1:K:591:LEU:HD12 | 1:K:727:ILE:HD13 | 2.00 | 0.44 |
| 1:K:1153:PHE:HB2 | 1:K:1198:PHE:HD2 | 1.83 | 0.44 |
| 1:K:1482:ASP:OD1 | 1:K:1483:ASP:N | 2.50 | 0.44 |
| 1:K:1629:GLY:H | 1:L:1917:ARG:NH2 | 2.16 | 0.44 |
| 1:K:1899:GLN:NE2 | 1:K:1905:ASP:O | 2.50 | 0.44 |
| 1:K:1959:GLU:HG3 | 1:K:1960:LEU:H | 1.83 | 0.44 |
| 1:K:2045:VAL:HG21 | 1:K:2075:TYR:CE2 | 2.53 | 0.44 |
| 1:K:2101:ALA:O | 1:K:2105:MET:HE3 | 2.18 | 0.44 |
| 1:K:2392:ARG:HB3 | 1:K:2394:PHE:CE1 | 2.53 | 0.44 |
| 1:K:2510:GLY:HA3 | 1:K:2513:VAL:HB | 2.00 | 0.44 |
| 1:L:172:ASP:OD1 | 1:L:173:ASP:N | 2.51 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:L:938:ASP:HA | 1:L:1055:ASN:HD22 | 1.83 | 0.44 |
| 1:L:1560:PHE:O | 1:L:1609:LEU:HD12 | 2.17 | 0.44 |
| 1:L:1840:GLN:N | 1:L:1840:GLN:OE1 | 2.51 | 0.44 |
| 1:M:146:ASP:CG | 1:M:148:ARG:HG2 | 2.42 | 0.44 |
| 1:M:489:CYS:O | 1:M:491:HIS:ND1 | 2.51 | 0.44 |
| 1:M:2190:LEU:HD21 | 1:M:2194:PHE:CD2 | 2.53 | 0.44 |
| 1:M:2534:ALA:HA | 1:M:2537:GLN:HE22 | 1.82 | 0.44 |
| 1:M:3074:GLU:OE2 | 1:M:3079:ASP:HB2 | 2.18 | 0.44 |
| 1:M:3276:ASN:OD1 | 1:M:3277:ALA:N | 2.48 | 0.44 |
| 1:N:597:ARG:NH2 | 1:N:655:GLN:HA | 2.28 | 0.44 |
| 1:N:706:LEU:HB3 | 1:N:708:TYR:CD1 | 2.52 | 0.44 |
| 1:N:960:THR:OG1 | 1:N:964:GLU:OE2 | 2.27 | 0.44 |
| 1:N:991:LYS:HD2 | 1:N:992:PHE:N | 2.33 | 0.44 |
| 1:N:1457:PHE:CZ | 1:N:1461:HIS:HE1 | 2.36 | 0.44 |
| 1:O:64:ALA:HB1 | 1:O:174:TYR:CE2 | 2.53 | 0.44 |
| 1:O:307:GLU:OE1 | 1:O:412:PRO:HA | 2.18 | 0.44 |
| 1:O:1405:TYR:HA | 1:O:1408:ASN:HD21 | 1.82 | 0.44 |
| 1:O:1424:ILE:HG12 | 1:O:1606:PHE:CE2 | 2.53 | 0.44 |
| 1:O:1596:LEU:HD12 | 1:O:1597:GLY:N | 2.32 | 0.44 |
| 1:O:1818:LEU:N | 1:O:1860:TRP:HZ2 | 2.15 | 0.44 |
| 1:O:1849:GLN:OE1 | 1:O:1849:GLN:N | 2.47 | 0.44 |
| 1:O:3124:ARG:O | 1:O:3128:ILE:HG23 | 2.18 | 0.44 |
| 1:P:24:ARG:HA | 1:P:24:ARG:HD2 | 1.69 | 0.44 |
| 1:P:371:LYS:HD3 | 1:P:371:LYS:C | 2.42 | 0.44 |
| 1:P:1042:TYR:HA | 1:P:1045:TYR:CE2 | 2.53 | 0.44 |
| 1:P:1893:ALA:O | 1:P:1896:GLN:HB2 | 2.18 | 0.44 |
| 1:Q:129:GLU:HG2 | 1:Q:139:THR:C | 2.43 | 0.44 |
| 1:Q:722:GLN:N | 1:Q:722:GLN:OE1 | 2.51 | 0.44 |
| 1:Q:1317:HIS:HA | 1:Q:1322:PHE:CD1 | 2.52 | 0.44 |
| 1:Q:1720:CYS:HB2 | 1:Q:1731:CYS:HB3 | 1.78 | 0.44 |
| 1:Q:1978:LYS:HA | 1:Q:2078:LYS:HG2 | 2.00 | 0.44 |
| 1:Q:2232:LEU:HD22 | 1:Q:2274:LEU:HD21 | 2.00 | 0.44 |
| 1:Q:2679:ASN:HD21 | 1:Q:2837:LEU:N | 2.16 | 0.44 |
| 1:Q:2991:LEU:HD23 | 1:Q:2991:LEU:HA | 1.83 | 0.44 |
| 1:Q:3089:ASN:HD21 | 1:Q:3247:ILE:HD12 | 1.83 | 0.44 |
| 1:R:788:GLU:OE1 | 1:R:791:ASP:HB2 | 2.18 | 0.44 |
| 1:R:2101:ALA:O | 1:R:2105:MET:HG3 | 2.18 | 0.44 |
| 1:R:2109:ALA:HA | 1:R:2112:ARG:HG2 | 2.00 | 0.44 |
| 1:R:2997:MET:HE3 | 1:R:3000:ARG:HB3 | 1.99 | 0.44 |
| 1:S:46:SER:HB3 | 1:S:57:ALA:HA | 2.00 | 0.44 |
| 1:S:253:PRO:O | 1:S:256:ARG:HG2 | 2.18 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:S:1061:ALA:HA | 1:S:1064:GLN:NE2 | 2.33 | 0.44 |
| 1:S:1466:ARG:HA | 1:S:1530:TYR:HE2 | 1.82 | 0.44 |
| 1:S:3226:ALA:H | 1:S:3247:ILE:HG23 | 1.83 | 0.44 |
| 1:T:627:THR:OG1 | 1:T:628:LEU:N | 2.51 | 0.44 |
| 1:T:872:ASP:HB3 | 1:T:877:GLY:HA2 | 2.00 | 0.44 |
| 1:T:1167:GLU:HA | 1:T:1177:PRO:HA | 2.00 | 0.44 |
| 1:T:2790:GLU:HG2 | 1:T:2791:GLU:OE1 | 2.17 | 0.44 |
| 3:VA:1:NAG:H62 | 3:VA:2:NAG:N2 | 2.30 | 0.44 |
| 1:A:428:SER:OG | 1:A:429:ALA:N | 2.51 | 0.43 |
| 1:A:718:MET:SD | 1:A:722:GLN:NE2 | 2.90 | 0.43 |
| 1:A:744:ASN:HB3 | 1:A:779:TRP:CD1 | 2.52 | 0.43 |
| 1:A:958:PRO:HA | 1:A:961:ASN:HA | 2.00 | 0.43 |
| 1:A:1133:ILE:HD12 | 1:A:1133:ILE:H | 1.83 | 0.43 |
| 1:A:1278:SER:O | 1:A:1281:SER:OG | 2.32 | 0.43 |
| 1:A:2340:VAL:HG12 | 1:A:2349:ARG:HD3 | 1.99 | 0.43 |
| 1:A:2392:ARG:HB3 | 1:A:2394:PHE:CE1 | 2.53 | 0.43 |
| 1:A:2404:THR:OG1 | 1:A:2405:SER:N | 2.51 | 0.43 |
| 1:A:2601:TRP:CZ2 | 1:A:2603:TRP:HB3 | 2.53 | 0.43 |
| 1:A:2811:PHE:HB3 | 1:A:2888:LEU:HD21 | 1.99 | 0.43 |
| 1:B:1283:LEU:HD12 | 1:B:1286:MET:SD | 2.58 | 0.43 |
| 1:B:1384:LYS:HB3 | 1:B:1391:VAL:HG12 | 2.00 | 0.43 |
| 1:B:1843:TYR:HA | 1:B:1895:TRP:HH2 | 1.82 | 0.43 |
| 1:B:3089:ASN:HB3 | 1:B:3248:LEU:HD13 | 1.99 | 0.43 |
| 1:B:3128:ILE:HD11 | 1:B:3190:LEU:HD22 | 2.00 | 0.43 |
| 1:C:674:LEU:HD22 | 1:C:695:ARG:NH2 | 2.33 | 0.43 |
| 1:C:1008:GLN:OE1 | 1:C:1008:GLN:N | 2.45 | 0.43 |
| 1:C:1223:VAL:HG13 | 1:C:1231:ILE:HB | 1.98 | 0.43 |
| 1:C:1246:GLY:O | 1:C:1249:THR:OG1 | 2.28 | 0.43 |
| 1:C:1307:HIS:HB3 | 1:C:1312:VAL:HG11 | 2.00 | 0.43 |
| 1:C:1365:ALA:HA | 1:C:1381:PHE:HZ | 1.83 | 0.43 |
| 1:C:1397:GLN:NE2 | 1:C:1399:GLU:OE2 | 2.29 | 0.43 |
| 1:C:1909:ALA:HB1 | 1:C:1916:MET:HE3 | 2.00 | 0.43 |
| 1:C:2091:ARG:HA | 1:C:2093:ARG:HH21 | 1.83 | 0.43 |
| 1:C:2376:ASN:O | 1:C:2380:LEU:HG | 2.18 | 0.43 |
| 1:C:2405:SER:HB3 | 1:C:2426:PHE:CE1 | 2.53 | 0.43 |
| 1:C:3128:ILE:HG13 | 1:C:3129:TRP:N | 2.33 | 0.43 |
| 1:C:3408:ASP:OD1 | 1:C:3408:ASP:N | 2.49 | 0.43 |
| 1:D:1010:ASP:O | 1:D:1013:THR:OG1 | 2.34 | 0.43 |
| 1:D:1782:PRO:O | 1:D:1795:ASN:N | 2.36 | 0.43 |
| 1:D:2155:PRO:HB2 | 1:D:2306:TRP:CE3 | 2.53 | 0.43 |
| 1:D:2337:PHE:O | 1:D:2349:ARG:NH2 | 2.51 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:D:2488:LYS:HD2 | 1:D:2489:PRO:HD2 | 2.00 | 0.43 |
| 1:D:2787:PRO:HA | 1:D:2790:GLU:OE1 | 2.18 | 0.43 |
| 1:E:181:PHE:HE2 | 1:E:219:VAL:HG13 | 1.83 | 0.43 |
| 1:E:304:ARG:HH21 | 1:E:411:ARG:NH2 | 2.16 | 0.43 |
| 1:E:527:ARG:HG2 | 1:E:528:PRO:HD2 | 2.00 | 0.43 |
| 1:E:1506:GLU:CD | 1:E:1507:PHE:N | 2.76 | 0.43 |
| 1:E:1624:LYS:HD3 | 1:E:1624:LYS:HA | 1.75 | 0.43 |
| 1:E:2811:PHE:HZ | 1:E:2889:LEU:HD12 | 1.82 | 0.43 |
| 1:F:60:VAL:HG23 | 1:F:63:MET:HE2 | 1.99 | 0.43 |
| 1:F:93:TYR:HB2 | 1:F:218:ASN:OD1 | 2.18 | 0.43 |
| 1:F:728:ASP:HB3 | 1:F:836:HIS:CD2 | 2.53 | 0.43 |
| 1:F:737:PHE:CG | 1:F:786:LYS:HB3 | 2.53 | 0.43 |
| 1:F:887:GLN:OE1 | 1:F:901:ALA:HB2 | 2.18 | 0.43 |
| 1:F:912:HIS:NE2 | 1:F:1113:PHE:HE1 | 2.16 | 0.43 |
| 1:F:1026:HIS:HB3 | 1:F:1037:MET:HE1 | 1.99 | 0.43 |
| 1:F:1821:ASP:OD1 | 1:F:1821:ASP:N | 2.46 | 0.43 |
| 1:F:2216:TYR:HD1 | 1:F:2223:TYR:CZ | 2.36 | 0.43 |
| 1:F:2313:GLN:NE2 | 1:F:2318:LEU:O | 2.46 | 0.43 |
| 1:G:1832:LYS:O | 1:G:1835:LEU:HG | 2.17 | 0.43 |
| 1:G:1854:HIS:HE1 | 1:G:1885:HIS:CE1 | 2.36 | 0.43 |
| 1:G:1919:PRO:HG3 | 1:G:1940:LYS:NZ | 2.33 | 0.43 |
| 1:G:2617:LYS:NZ | 1:G:2623:GLU:HG3 | 2.33 | 0.43 |
| 1:G:3049:GLN:CD | 1:G:3051:GLY:H | 2.26 | 0.43 |
| 1:H:334:ASP:OD1 | 1:H:334:ASP:N | 2.49 | 0.43 |
| 1:H:469:GLU:OE1 | 1:H:469:GLU:N | 2.46 | 0.43 |
| 1:H:1136:LEU:HA | 1:H:1139:GLU:OE2 | 2.17 | 0.43 |
| 1:H:2231:GLU:H | 1:H:2231:GLU:CD | 2.24 | 0.43 |
| 1:H:2771:GLN:HG2 | 1:H:2772:PHE:HD1 | 1.82 | 0.43 |
| 1:H:2798:SER:OG | 1:H:2799:GLU:OE1 | 2.30 | 0.43 |
| 1:H:3315:VAL:HG13 | 1:H:3317:ILE:HD11 | 1.99 | 0.43 |
| 1:I:473:LEU:N | 1:I:775:LYS:HE3 | 2.32 | 0.43 |
| 1:I:501:ARG:HH12 | 1:I:702:TYR:HB3 | 1.83 | 0.43 |
| 1:I:598:ASP:OD1 | 1:I:599:PHE:N | 2.50 | 0.43 |
| 1:I:724:ASP:O | 1:I:727:ILE:HG12 | 2.17 | 0.43 |
| 1:I:1260:ALA:HB3 | 1:I:1529:HIS:CD2 | 2.53 | 0.43 |
| 1:I:2250:LEU:HA | 1:I:2253:GLU:OE1 | 2.18 | 0.43 |
| 1:I:2533:ARG:HH22 | 1:I:2620:ASN:N | 2.16 | 0.43 |
| 1:I:2743:PRO:HA | 1:I:2762:ARG:NE | 2.33 | 0.43 |
| 1:J:1275:GLU:OE1 | 1:J:1275:GLU:N | 2.48 | 0.43 |
| 1:J:1824:HIS:HB2 | 1:J:1827:ASP:CG | 2.42 | 0.43 |
| 1:J:2939:ASN:HB3 | 1:J:2943:LYS:HZ1 | 1.82 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:J:3177:ILE:O | 1:J:3177:ILE:HG13 | 2.18 | 0.43 |
| 1:K:1118:SER:OG | 1:K:1119:PHE:N | 2.51 | 0.43 |
| 1:K:1448:LEU:HB3 | 1:K:1596:LEU:HD21 | 2.00 | 0.43 |
| 1:K:1634:GLU:HA | 1:K:1634:GLU:OE2 | 2.18 | 0.43 |
| 1:K:1956:ASP:OD1 | 1:K:1957:THR:N | 2.51 | 0.43 |
| 1:K:3337:ARG:HH12 | 1:K:3379:TYR:N | 2.16 | 0.43 |
| 1:L:135:MET:HG2 | 1:L:137:VAL:HG13 | 1.99 | 0.43 |
| 1:L:614:HIS:CD2 | 1:L:637:PHE:HE1 | 2.36 | 0.43 |
| 1:L:756:LYS:HD3 | 1:L:762:SER:HB2 | 1.99 | 0.43 |
| 1:L:845:LEU:HD22 | 1:L:926:ARG:HD3 | 1.99 | 0.43 |
| 1:L:1695:LEU:HD23 | 1:L:1796:PRO:HG2 | 2.00 | 0.43 |
| 1:L:2105:MET:HA | 1:L:2108:LYS:HG2 | 1.98 | 0.43 |
| 1:L:2162:THR:O | 1:L:2165:VAL:HG22 | 2.17 | 0.43 |
| 1:L:2238:ASP:O | 1:L:2240:LYS:NZ | 2.35 | 0.43 |
| 1:L:2345:ASN:O | 1:L:2349:ARG:HG2 | 2.18 | 0.43 |
| 1:M:41:PHE:CE1 | 1:M:253:PRO:HG2 | 2.53 | 0.43 |
| 1:M:302:GLN:NE2 | 1:M:303:ARG:HG3 | 2.33 | 0.43 |
| 1:M:376:LEU:HB3 | 1:M:378:LYS:HZ3 | 1.82 | 0.43 |
| 1:M:584:THR:HG23 | 1:M:587:PHE:H | 1.82 | 0.43 |
| 1:M:1355:ILE:O | 1:M:1355:ILE:HG13 | 2.18 | 0.43 |
| 1:M:3085:GLU:HG2 | 1:M:3258:TYR:OH | 2.18 | 0.43 |
| 1:M:3196:SER:O | 1:M:3200:ILE:HG12 | 2.17 | 0.43 |
| 1:N:3:LEU:HD13 | 1:N:78:GLU:HG2 | 2.00 | 0.43 |
| 1:N:1221:TYR:OH | 1:N:1233:SER:O | 2.34 | 0.43 |
| 1:N:1884:HIS:O | 1:N:1888:THR:HG23 | 2.17 | 0.43 |
| 1:N:2574:PHE:CE2 | 1:N:2578:HIS:CE1 | 3.06 | 0.43 |
| 1:O:7:ASN:HB3 | 1:O:93:TYR:CZ | 2.53 | 0.43 |
| 1:O:14:GLN:HG2 | 1:O:15:GLU:N | 2.33 | 0.43 |
| 1:O:629:HIS:HA | 1:O:775:LYS:NZ | 2.33 | 0.43 |
| 1:O:647:LEU:HA | 1:O:650:ILE:HG12 | 2.00 | 0.43 |
| 1:O:2448:ASP:O | 1:O:2452:GLU:OE1 | 2.36 | 0.43 |
| 1:O:3227:THR:OG1 | 1:O:3245:PHE:O | 2.29 | 0.43 |
| 1:O:3259:GLU:OE1 | 1:O:3259:GLU:N | 2.41 | 0.43 |
| 1:P:316:HIS:HB3 | 1:P:360:GLU:CD | 2.43 | 0.43 |
| 1:P:452:LEU:HD12 | 1:P:554:PHE:CE1 | 2.53 | 0.43 |
| 1:P:1153:PHE:C | 1:P:1154:MET:HE2 | 2.43 | 0.43 |
| 1:P:1890:ARG:HH12 | 1:P:1959:GLU:HG3 | 1.82 | 0.43 |
| 1:P:2086:GLU:HA | 1:P:2366:ARG:NH1 | 2.32 | 0.43 |
| 1:P:2414:GLN:HA | 1:P:2467:PHE:HA | 2.00 | 0.43 |
| 1:P:2416:ASN:OD1 | 1:P:2417:GLY:N | 2.51 | 0.43 |
| 1:P:2515:LYS:HB3 | 1:P:2519:THR:OG1 | 2.18 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:P:3156:PRO:HB2 | 1:P:3162:LYS:HG3 | 1.99 | 0.43 |
| 1:Q:323:ASN:OD1 | 1:Q:324:VAL:N | 2.51 | 0.43 |
| 1:Q:1145:HIS:NE2 | 1:Q:1524:ASN:OD1 | 2.51 | 0.43 |
| 1:Q:1320:ALA:HA | 1:Q:1423:GLU:OE2 | 2.17 | 0.43 |
| 1:Q:1424:ILE:HD11 | 1:Q:1606:PHE:CE2 | 2.53 | 0.43 |
| 1:Q:1543:LEU:O | 1:Q:1547:LEU:HD23 | 2.18 | 0.43 |
| 1:Q:2448:ASP:O | 1:Q:2452:GLU:OE1 | 2.36 | 0.43 |
| 1:Q:2655:TYR:O | 1:Q:2658:ILE:HG22 | 2.18 | 0.43 |
| 1:R:469:GLU:HA | 1:R:633:PHE:HE1 | 1.82 | 0.43 |
| 1:R:848:ARG:HH11 | 1:R:1123:TYR:HE1 | 1.64 | 0.43 |
| 1:R:2045:VAL:HG13 | 1:R:2046:ASP:OD1 | 2.18 | 0.43 |
| 1:R:2558:LYS:HD2 | 1:R:2563:THR:HA | 2.00 | 0.43 |
| 1:R:2695:THR:OG1 | 1:R:2696:LEU:N | 2.49 | 0.43 |
| 1:R:2787:PRO:HG2 | 1:R:2788:GLN:OE1 | 2.18 | 0.43 |
| 1:S:98:LYS:HG2 | 1:S:99:PRO:HD2 | 2.00 | 0.43 |
| 1:S:579:GLU:HG3 | 1:S:582:ASP:CG | 2.44 | 0.43 |
| 1:S:704:HIS:HB3 | 1:S:705:GLU:OE1 | 2.18 | 0.43 |
| 1:S:750:LEU:HD21 | 1:S:767:LYS:NZ | 2.33 | 0.43 |
| 1:S:891:CYS:HB3 | 1:S:900:PHE:O | 2.18 | 0.43 |
| 1:S:1231:ILE:H | 1:S:1231:ILE:HD12 | 1.83 | 0.43 |
| 1:S:1284:ARG:HH11 | 1:S:1379:PRO:HG3 | 1.83 | 0.43 |
| 1:S:2008:LYS:HG2 | 1:S:2041:LYS:HE2 | 2.00 | 0.43 |
| 1:S:2053:VAL:HG11 | 1:S:2068:ILE:HG21 | 2.00 | 0.43 |
| 1:S:2064:SER:OG | 1:S:2066:SER:OG | 2.34 | 0.43 |
| 1:S:2124:GLN:CD | 1:S:2124:GLN:H | 2.19 | 0.43 |
| 1:S:3399:GLY:HA2 | 1:S:3401:ARG:HH21 | 1.83 | 0.43 |
| 1:T:160:GLN:OE1 | 1:T:164:MET:HE2 | 2.18 | 0.43 |
| 1:T:958:PRO:C | 1:T:961:ASN:H | 2.26 | 0.43 |
| 1:T:1284:ARG:NH1 | 1:T:1379:PRO:HB3 | 2.33 | 0.43 |
| 1:T:1539:THR:H | 1:T:1542:GLN:NE2 | 2.15 | 0.43 |
| 1:T:2829:SER:OG | 1:T:2862:MET:HE1 | 2.18 | 0.43 |
| 1:A:107:VAL:HG12 | 1:A:125:TRP:HB3 | 2.00 | 0.43 |
| 1:A:435:LYS:HZ2 | 1:A:1130:GLY:HA2 | 1.83 | 0.43 |
| 1:A:2112:ARG:HB3 | 1:A:2116:LYS:HZ1 | 1.82 | 0.43 |
| 1:A:2394:PHE:CD2 | 1:A:2443:LYS:HG2 | 2.53 | 0.43 |
| 1:A:2407:GLU:OE2 | 1:A:2424:ALA:HB1 | 2.18 | 0.43 |
| 1:A:2500:ARG:NH1 | 1:A:2502:GLU:OE2 | 2.51 | 0.43 |
| 1:A:2981:MET:HG3 | 1:A:2982:PRO:HD2 | 1.99 | 0.43 |
| 1:A:3205:GLU:C | 1:B:1117:ARG:HH12 | 2.23 | 0.43 |
| 1:A:3395:ARG:HH21 | 1:A:3398:GLN:NE2 | 2.15 | 0.43 |
| 1:B:939:TRP:CZ3 | 1:B:1055:ASN:HB3 | 2.53 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:1276:VAL:O | 1:B:1279:LEU:HG | 2.18 | 0.43 |
| 1:B:2898:PRO:HB3 | 1:C:2917:LYS:NZ | 2.33 | 0.43 |
| 1:C:326:ILE:HG23 | 1:C:345:ALA:HB3 | 2.01 | 0.43 |
| 1:C:434:ARG:HG2 | 1:C:519:GLY:HA3 | 2.00 | 0.43 |
| 1:C:2020:ALA:N | 1:C:2021:GLU:OE1 | 2.51 | 0.43 |
| 1:C:2136:CYS:HB3 | 1:C:2144:TYR:C | 2.43 | 0.43 |
| 1:D:42:HIS:HB2 | 1:D:73:TYR:OH | 2.18 | 0.43 |
| 1:D:741:HIS:C | 1:D:742:LEU:HD12 | 2.43 | 0.43 |
| 1:D:786:LYS:HE2 | 1:D:829:ILE:HG21 | 1.99 | 0.43 |
| 1:D:1284:ARG:NH2 | 1:D:1287:GLN:HG2 | 2.33 | 0.43 |
| 1:D:1560:PHE:O | 1:D:1609:LEU:HD12 | 2.18 | 0.43 |
| 1:D:1946:ASP:HB3 | 1:D:1950:HIS:CD2 | 2.52 | 0.43 |
| 1:D:3081:GLU:HA | 1:D:3084:PHE:HB2 | 2.00 | 0.43 |
| 1:E:193:GLY:HA3 | 1:E:201:SER:H | 1.83 | 0.43 |
| 1:E:222:ILE:O | 1:E:225:ILE:HG22 | 2.17 | 0.43 |
| 1:E:989:LYS:HD2 | 1:E:989:LYS:HA | 1.71 | 0.43 |
| 1:E:998:ILE:H | 1:E:998:ILE:HD12 | 1.83 | 0.43 |
| 1:E:1910:ASN:HB3 | 1:F:1657:PHE:O | 2.18 | 0.43 |
| 1:E:2085:GLN:HE21 | 1:E:2366:ARG:HH22 | 1.65 | 0.43 |
| 1:E:2136:CYS:HB3 | 1:E:2144:TYR:C | 2.43 | 0.43 |
| 1:E:2630:LEU:HD23 | 1:E:2630:LEU:O | 2.19 | 0.43 |
| 1:E:2656:ARG:HD3 | 1:E:2656:ARG:HA | 1.78 | 0.43 |
| 1:F:426:VAL:HG12 | 1:F:428:SER:H | 1.83 | 0.43 |
| 1:F:610:HIS:O | 1:F:613:PRO:HD2 | 2.17 | 0.43 |
| 1:F:1884:HIS:O | 1:F:1887:SER:OG | 2.25 | 0.43 |
| 1:F:2941:LEU:HD12 | 1:F:2941:LEU:HA | 1.89 | 0.43 |
| 1:F:3174:PRO:O | 1:F:3177:ILE:HG22 | 2.18 | 0.43 |
| 1:G:478:PRO:HB2 | 1:G:676:LYS:NZ | 2.33 | 0.43 |
| 1:G:1802:ILE:HG12 | 1:G:1807:THR:O | 2.18 | 0.43 |
| 1:G:2159:ARG:NH2 | 1:G:2360:TYR:HB3 | 2.33 | 0.43 |
| 1:G:2408:VAL:HG12 | 1:G:2473:ILE:HG12 | 2.00 | 0.43 |
| 1:G:3017:SER:OG | 1:G:3019:ALA:O | 2.36 | 0.43 |
| 1:G:3165:ASN:ND2 | 1:G:3168:THR:H | 2.15 | 0.43 |
| 1:G:3329:LYS:HE2 | 1:G:3403:GLN:OE1 | 2.18 | 0.43 |
| 1:H:592:LEU:HD11 | 1:H:737:PHE:CZ | 2.53 | 0.43 |
| 1:H:702:TYR:N | 1:H:703:GLU:OE1 | 2.51 | 0.43 |
| 1:H:703:GLU:N | 1:H:703:GLU:OE1 | 2.50 | 0.43 |
| 1:H:1286:MET:O | 1:H:1291:THR:OG1 | 2.31 | 0.43 |
| 1:H:2101:ALA:O | 1:H:2105:MET:HG3 | 2.18 | 0.43 |
| 1:H:2143:LYS:HB3 | 1:H:2144:TYR:CD2 | 2.53 | 0.43 |
| 1:H:2712:VAL:O | 1:H:2715:GLN:HG2 | 2.18 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:H:2924:TYR:HD2 | 1:H:3006:LEU:HD11 | 1.83 | 0.43 |
| 1:H:3150:LEU:HD23 | 1:H:3174:PRO:HB2 | 2.00 | 0.43 |
| 1:I:580:TYR:HE1 | 1:I:856:ARG:HD2 | 1.82 | 0.43 |
| 1:I:601:ASP:O | 1:I:604:VAL:HG12 | 2.17 | 0.43 |
| 1:I:738:VAL:HG23 | 1:I:789:ILE:HG21 | 2.00 | 0.43 |
| 1:I:1436:LEU:HD23 | 1:I:1436:LEU:HA | 1.82 | 0.43 |
| 1:I:2448:ASP:O | 1:I:2452:GLU:OE1 | 2.36 | 0.43 |
| 1:I:2614:LEU:HG | 1:I:2704:ILE:HD11 | 2.00 | 0.43 |
| 1:J:1126:LEU:H | 1:J:1126:LEU:HD23 | 1.82 | 0.43 |
| 1:J:1167:GLU:HG2 | 1:J:1167:GLU:O | 2.18 | 0.43 |
| 1:J:1167:GLU:HA | 1:J:1177:PRO:HA | 2.00 | 0.43 |
| 1:K:585:ALA:HA | 1:K:588:ASP:OD2 | 2.18 | 0.43 |
| 1:K:914:HIS:NE2 | 1:K:1053:HIS:HE1 | 2.16 | 0.43 |
| 1:K:1159:ARG:O | 1:K:1160:LYS:HD3 | 2.17 | 0.43 |
| 1:K:1178:GLU:HG3 | 1:K:1205:ILE:HG12 | 2.00 | 0.43 |
| 1:K:1420:CYS:HB2 | 1:K:1608:ARG:NH2 | 2.29 | 0.43 |
| 1:K:1698:LEU:HD13 | 1:K:1757:ARG:HD2 | 2.00 | 0.43 |
| 1:K:2149:HIS:CD2 | 1:K:2154:PHE:HE1 | 2.36 | 0.43 |
| 1:K:2154:PHE:HB3 | 1:K:2155:PRO:HD3 | 2.00 | 0.43 |
| 1:K:2633:LYS:HE3 | 1:K:2633:LYS:HB3 | 1.68 | 0.43 |
| 1:L:96:TRP:CZ3 | 1:L:218:ASN:HB3 | 2.53 | 0.43 |
| 1:L:276:TYR:O | 1:L:280:GLY:N | 2.44 | 0.43 |
| 1:L:859:VAL:HG12 | 1:L:863:ARG:CZ | 2.47 | 0.43 |
| 1:L:1274:GLY:O | 1:L:1277:GLU:HG3 | 2.17 | 0.43 |
| 1:L:1817:ARG:HA | 1:L:1820:ASP:OD2 | 2.18 | 0.43 |
| 1:L:1834:PHE:O | 1:L:1838:LEU:HD23 | 2.18 | 0.43 |
| 1:L:2101:ALA:O | 1:L:2105:MET:HG3 | 2.18 | 0.43 |
| 1:L:2816:ASP:OD1 | 1:L:2817:VAL:N | 2.51 | 0.43 |
| 1:L:3150:LEU:HD23 | 1:L:3174:PRO:HB2 | 1.99 | 0.43 |
| 1:M:24:ARG:HH12 | 1:M:125:TRP:CD1 | 2.36 | 0.43 |
| 1:M:2460:VAL:O | 1:N:1085:ARG:NH2 | 2.51 | 0.43 |
| 1:N:198:HIS:HA | 1:N:205:TRP:CD1 | 2.53 | 0.43 |
| 1:N:1556:LEU:HD11 | 1:N:1655:LEU:HD12 | 1.99 | 0.43 |
| 1:N:2712:VAL:HA | 1:N:2715:GLN:CD | 2.43 | 0.43 |
| 1:N:2795:LYS:HE2 | 1:N:2795:LYS:HB2 | 1.61 | 0.43 |
| 1:N:2977:CYS:HA | 1:N:2987:TRP:CH2 | 2.53 | 0.43 |
| 1:N:3266:VAL:HG11 | 1:N:3283:PHE:HZ | 1.83 | 0.43 |
| 1:O:202:THR:OG1 | 1:O:204:GLU:OE1 | 2.36 | 0.43 |
| 1:O:278:GLN:HG2 | 1:O:279:LEU:HD22 | 1.99 | 0.43 |
| 1:O:436:ASP:HB3 | 1:O:522:TYR:CE2 | 2.52 | 0.43 |
| 1:O:493:MET:SD | 1:O:670:MET:HE3 | 2.59 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:O:2750:ASP:HA | 1:O:2758:ARG:HD2 | 1.99 | 0.43 |
| 1:O:3064:LEU:O | 1:O:3067:GLN:HG3 | 2.18 | 0.43 |
| 1:P:5:ARG:HD2 | 1:P:283:TYR:CE1 | 2.54 | 0.43 |
| 1:P:454:ARG:NH2 | 1:P:1338:LEU:O | 2.48 | 0.43 |
| 1:P:554:PHE:O | 1:P:568:ARG:NH2 | 2.51 | 0.43 |
| 1:P:788:GLU:OE2 | 1:P:791:ASP:N | 2.43 | 0.43 |
| 1:P:1325:TRP:HD1 | 1:P:1326:HIS:ND1 | 2.16 | 0.43 |
| 1:P:1463:ASN:O | 1:P:1467:ILE:HG12 | 2.18 | 0.43 |
| 1:P:3256:TRP:H | 1:P:3256:TRP:CD1 | 2.37 | 0.43 |
| 1:Q:173:ASP:O | 1:Q:177:PHE:N | 2.49 | 0.43 |
| 1:Q:181:PHE:CE2 | 1:Q:219:VAL:HG13 | 2.53 | 0.43 |
| 1:Q:866:LEU:HD22 | 1:Q:968:PHE:CE1 | 2.53 | 0.43 |
| 1:Q:1996:VAL:HG22 | 1:Q:2055:LEU:HD13 | 2.00 | 0.43 |
| 1:Q:2095:GLU:OE1 | 1:Q:2098:HIS:N | 2.51 | 0.43 |
| 1:Q:2439:ASP:CG | 1:Q:2440:ARG:HE | 2.26 | 0.43 |
| 1:Q:2673:GLN:NE2 | 1:Q:2852:GLN:H | 2.16 | 0.43 |
| 1:Q:2981:MET:HE3 | 1:Q:3149:ASN:ND2 | 2.30 | 0.43 |
| 1:R:597:ARG:NH2 | 1:R:655:GLN:HA | 2.32 | 0.43 |
| 1:R:978:THR:HB | 1:R:1036:SER:HA | 2.01 | 0.43 |
| 1:R:1425:GLN:O | 1:R:1429:VAL:HG22 | 2.17 | 0.43 |
| 1:R:1963:ILE:HG23 | 1:R:1967:LEU:HD21 | 2.00 | 0.43 |
| 1:S:585:ALA:HA | 1:S:588:ASP:OD2 | 2.18 | 0.43 |
| 1:S:1308:GLU:OE2 | 1:S:1310:ARG:NH2 | 2.51 | 0.43 |
| 1:S:2557:CYS:HB3 | 1:S:2564:VAL:HG23 | 2.00 | 0.43 |
| 1:S:2995:PHE:O | 1:S:2999:LEU:HD23 | 2.18 | 0.43 |
| 1:T:725:HIS:O | 1:T:729:GLU:HG2 | 2.18 | 0.43 |
| 1:T:2488:LYS:NZ | 1:T:2489:PRO:O | 2.51 | 0.43 |
| 1:T:2675:GLU:O | 1:T:2679:ASN:ND2 | 2.50 | 0.43 |
| 1:T:3389:VAL:HG23 | 1:T:3401:ARG:NE | 2.32 | 0.43 |
| 2:CA:1:NAG:O7 | 2:CA:1:NAG:O3 | 2.32 | 0.43 |
| 1:A:169:LEU:HD12 | 1:A:300:LEU:HD21 | 2.00 | 0.43 |
| 1:A:478:PRO:HB2 | 1:A:676:LYS:HZ1 | 1.83 | 0.43 |
| 1:A:592:LEU:HA | 1:A:595:GLU:OE1 | 2.17 | 0.43 |
| 1:A:953:GLU:OE1 | 1:A:969:HIS:ND1 | 2.51 | 0.43 |
| 1:A:1010:ASP:OD2 | 1:A:1013:THR:HG23 | 2.18 | 0.43 |
| 1:A:2409:ARG:HH21 | 1:A:2474:ILE:HD13 | 1.83 | 0.43 |
| 1:A:2529:LYS:HE3 | 1:A:2620:ASN:OD1 | 2.18 | 0.43 |
| 1:A:2943:LYS:HD2 | 1:A:3002:LYS:HG3 | 2.00 | 0.43 |
| 1:B:226:TRP:HA | 1:B:229:LEU:HD12 | 2.00 | 0.43 |
| 1:B:732:THR:HG23 | 1:B:733:LYS:HE3 | 2.00 | 0.43 |
| 1:B:3026:SER:HG | 1:B:3030:ASN:HD22 | 1.63 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:493:MET:HG3 | 1:C:494:ALA:N | 2.33 | 0.43 |
| 1:C:752:ILE:HG13 | 1:C:767:LYS:NZ | 2.34 | 0.43 |
| 1:C:855:THR:H | 1:C:858:GLN:NE2 | 2.16 | 0.43 |
| 1:C:1505:ASN:ND2 | 1:C:1510:THR:OG1 | 2.51 | 0.43 |
| 1:C:3013:TRP:CD1 | 1:C:3013:TRP:H | 2.34 | 0.43 |
| 1:D:105:ARG:HA | 1:D:108:GLN:NE2 | 2.32 | 0.43 |
| 1:D:928:LYS:HG3 | 1:D:929:GLY:N | 2.32 | 0.43 |
| 1:D:1023:ASN:HB3 | 1:D:1182:TYR:HD2 | 1.83 | 0.43 |
| 1:D:1147:GLU:N | 1:D:1147:GLU:OE1 | 2.51 | 0.43 |
| 1:D:1149:VAL:HG11 | 1:D:1206:LEU:HD23 | 1.99 | 0.43 |
| 1:D:1834:PHE:CE1 | 1:D:1891:ILE:HD13 | 2.53 | 0.43 |
| 1:D:2786:ILE:O | 1:D:2790:GLU:OE1 | 2.36 | 0.43 |
| 1:D:3124:ARG:HH11 | 1:D:3124:ARG:HG2 | 1.83 | 0.43 |
| 1:E:748:SER:O | 1:E:813:VAL:N | 2.48 | 0.43 |
| 1:E:751:VAL:CG2 | 1:E:768:LEU:HB3 | 2.48 | 0.43 |
| 1:E:1362:ILE:HD13 | 1:E:1456:LEU:HD11 | 1.99 | 0.43 |
| 1:E:1424:ILE:HG23 | 1:E:1425:GLN:N | 2.33 | 0.43 |
| 1:E:1993:SER:HB2 | 1:E:2017:GLY:H | 1.83 | 0.43 |
| 1:F:362:ASN:HB2 | 1:F:784:LEU:HD21 | 1.99 | 0.43 |
| 1:F:859:VAL:O | 1:F:862:LEU:HG | 2.18 | 0.43 |
| 1:F:972:LEU:HD23 | 1:F:972:LEU:HA | 1.84 | 0.43 |
| 1:F:2126:LEU:HD21 | 1:F:2165:VAL:HG12 | 2.00 | 0.43 |
| 1:F:2394:PHE:HB2 | 1:F:2492:ILE:HB | 2.00 | 0.43 |
| 1:G:197:ASP:OD1 | 1:G:197:ASP:N | 2.51 | 0.43 |
| 1:G:639:LEU:O | 1:G:642:SER:OG | 2.32 | 0.43 |
| 1:G:1152:GLY:HA3 | 1:G:1197:LEU:HD21 | 2.00 | 0.43 |
| 1:G:2064:SER:HB3 | 1:G:2067:LEU:HG | 2.00 | 0.43 |
| 1:G:2158:HIS:O | 1:G:2162:THR:HG23 | 2.18 | 0.43 |
| 1:G:2343:ASN:OD1 | 1:G:2344:GLU:N | 2.51 | 0.43 |
| 1:G:2665:ARG:HH12 | 1:G:2726:ARG:HD2 | 1.83 | 0.43 |
| 1:G:3133:GLN:HG3 | 1:G:3136:ARG:HH21 | 1.83 | 0.43 |
| 1:G:3259:GLU:OE1 | 1:G:3259:GLU:N | 2.44 | 0.43 |
| 1:G:3300:ALA:HA | 1:G:3325:LYS:HE3 | 1.99 | 0.43 |
| 1:H:441:THR:HB | 1:H:444:GLU:OE1 | 2.18 | 0.43 |
| 1:H:456:GLN:OE1 | 1:H:553:PRO:HB2 | 2.17 | 0.43 |
| 1:H:696:PRO:HA | 1:H:699:ILE:HD13 | 1.99 | 0.43 |
| 1:H:1268:LEU:HD23 | 1:H:1268:LEU:H | 1.83 | 0.43 |
| 1:H:1362:ILE:HD13 | 1:H:1456:LEU:HD11 | 1.98 | 0.43 |
| 1:H:1475:GLN:NE2 | 1:H:1478:ARG:HD2 | 2.33 | 0.43 |
| 1:H:1880:ILE:HD12 | 1:H:1880:ILE:H | 1.82 | 0.43 |
| 1:H:2802:VAL:HG23 | 1:H:2855:VAL:HG23 | 2.01 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:H:3333:SER:OG | 1:H:3334:ARG:N | 2.51 | 0.43 |
| 1:I:38:LEU:HD23 | 1:I:77:LEU:HD12 | 2.00 | 0.43 |
| 1:I:1007:GLU:OE1 | 1:I:1007:GLU:N | 2.34 | 0.43 |
| 1:I:1384:LYS:HA | 1:I:1391:VAL:HG12 | 2.00 | 0.43 |
| 1:I:1919:PRO:HG3 | 1:I:1940:LYS:NZ | 2.34 | 0.43 |
| 1:J:371:LYS:HD3 | 1:J:371:LYS:C | 2.43 | 0.43 |
| 1:J:1154:MET:HE1 | 1:J:1197:LEU:HD23 | 1.99 | 0.43 |
| 1:J:1722:TYR:CE2 | 1:J:1724:GLU:HB2 | 2.52 | 0.43 |
| 1:J:1743:HIS:O | 1:J:1747:THR:HG23 | 2.18 | 0.43 |
| 1:J:3289:LYS:HG2 | 1:J:3290:TYR:H | 1.83 | 0.43 |
| 1:J:3334:ARG:NH1 | 1:J:3408:ASP:HA | 2.34 | 0.43 |
| 1:K:171:GLU:OE2 | 1:K:173:ASP:N | 2.51 | 0.43 |
| 1:K:1535:PHE:O | 1:K:1538:TRP:HB2 | 2.19 | 0.43 |
| 1:K:1842:ASN:ND2 | 1:K:1845:ASP:H | 2.16 | 0.43 |
| 1:K:2386:GLN:O | 1:K:2389:SER:OG | 2.30 | 0.43 |
| 1:K:2509:SER:HB3 | 1:K:3138:ARG:HH12 | 1.82 | 0.43 |
| 1:K:2581:PHE:O | 1:K:2584:THR:HG22 | 2.18 | 0.43 |
| 1:K:2976:CYS:HB3 | 1:K:3156:PRO:HD3 | 2.01 | 0.43 |
| 1:K:3308:PRO:HG2 | 1:K:3311:ALA:HB3 | 2.00 | 0.43 |
| 1:L:735:ARG:CZ | 1:L:788:GLU:HG2 | 2.49 | 0.43 |
| 1:L:1254:ILE:HG23 | 1:L:1256:LYS:H | 1.82 | 0.43 |
| 1:L:2823:ASP:OD1 | 1:L:2823:ASP:N | 2.51 | 0.43 |
| 1:M:28:ASP:OD1 | 1:M:29:ASP:N | 2.52 | 0.43 |
| 1:M:1025:ILE:HD12 | 1:M:1028:LEU:HD23 | 2.00 | 0.43 |
| 1:M:1221:TYR:OH | 1:M:1236:PHE:N | 2.43 | 0.43 |
| 1:M:1260:ALA:HB3 | 1:M:1529:HIS:CD2 | 2.53 | 0.43 |
| 1:M:2158:HIS:O | 1:M:2162:THR:HG23 | 2.17 | 0.43 |
| 1:M:2164:GLN:HE22 | 1:M:2348:THR:HG21 | 1.84 | 0.43 |
| 1:M:2819:PHE:O | 1:M:2831:ALA:HB3 | 2.17 | 0.43 |
| 1:M:3068:THR:O | 1:M:3071:THR:OG1 | 2.33 | 0.43 |
| 1:M:3228:ALA:HB3 | 1:M:3245:PHE:HB3 | 2.00 | 0.43 |
| 1:N:729:GLU:O | 1:N:732:THR:HG22 | 2.18 | 0.43 |
| 1:N:744:ASN:HB3 | 1:N:779:TRP:CD1 | 2.54 | 0.43 |
| 1:N:1048:ILE:HA | 1:N:1051:LEU:HG | 1.98 | 0.43 |
| 1:N:1116:GLU:O | 1:N:1120:GLN:HB3 | 2.18 | 0.43 |
| 1:N:2972:ASP:OD1 | 1:N:2972:ASP:N | 2.52 | 0.43 |
| 1:O:133:ASP:HA | 1:O:138:HIS:HE1 | 1.82 | 0.43 |
| 1:O:651:TRP:CH2 | 1:O:655:GLN:HG3 | 2.53 | 0.43 |
| 1:O:704:HIS:HB3 | 1:O:705:GLU:OE1 | 2.19 | 0.43 |
| 1:O:2465:ALA:HB2 | 1:P:1085:ARG:HD2 | 2.00 | 0.43 |
| 1:O:3287:LEU:HD23 | 1:O:3287:LEU:H | 1.82 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:P:59:CYS:C | 1:P:61:HIS:HD1 | 2.25 | 0.43 |
| 1:P:461:VAL:HG22 | 1:P:1277:GLU:CD | 2.43 | 0.43 |
| 1:P:536:ALA:HB2 | 1:P:554:PHE:HD2 | 1.84 | 0.43 |
| 1:P:1085:ARG:HD3 | 1:P:1110:PHE:HE2 | 1.83 | 0.43 |
| 1:P:1596:LEU:HD12 | 1:P:1596:LEU:HA | 1.90 | 0.43 |
| 1:P:1775:LEU:HD12 | 1:P:1776:PRO:HD2 | 1.99 | 0.43 |
| 1:P:2155:PRO:HB2 | 1:P:2306:TRP:CE3 | 2.52 | 0.43 |
| 1:P:3232:LEU:HD12 | 1:P:3283:PHE:CZ | 2.53 | 0.43 |
| 1:Q:164:MET:HE1 | 1:Q:187:HIS:CE1 | 2.53 | 0.43 |
| 1:Q:1741:GLN:O | 1:Q:1744:ARG:HG2 | 2.19 | 0.43 |
| 1:Q:2112:ARG:HH11 | 1:Q:2211:PRO:HG3 | 1.82 | 0.43 |
| 1:Q:2602:ASP:OD2 | 1:Q:2604:THR:HG22 | 2.17 | 0.43 |
| 1:R:5:ARG:HG3 | 1:R:283:TYR:CD2 | 2.53 | 0.43 |
| 1:R:292:ASN:H | 1:R:295:GLN:HB2 | 1.83 | 0.43 |
| 1:R:786:LYS:HE2 | 1:R:829:ILE:HG21 | 2.00 | 0.43 |
| 1:R:1251:LYS:HD3 | 1:R:1251:LYS:HA | 1.68 | 0.43 |
| 1:R:1448:LEU:HD21 | 1:R:1596:LEU:HG | 1.99 | 0.43 |
| 1:R:1607:ASP:OD2 | 1:R:1608:ARG:NH1 | 2.51 | 0.43 |
| 1:R:1842:ASN:HD21 | 1:R:1844:CYS:HB3 | 1.84 | 0.43 |
| 1:R:2326:ALA:HB1 | 1:R:2329:TYR:HB2 | 2.01 | 0.43 |
| 1:R:2668:CYS:HA | 1:R:2671:GLU:OE1 | 2.18 | 0.43 |
| 1:R:2786:ILE:N | 1:R:2787:PRO:HD2 | 2.33 | 0.43 |
| 1:R:2929:LEU:HD12 | 1:R:2933:GLN:HB3 | 1.99 | 0.43 |
| 1:S:580:TYR:OH | 1:S:860:GLN:OE1 | 2.26 | 0.43 |
| 1:S:647:LEU:HA | 1:S:650:ILE:HG12 | 2.00 | 0.43 |
| 1:S:1246:GLY:O | 1:S:1249:THR:OG1 | 2.28 | 0.43 |
| 1:S:1421:ASP:HB3 | 1:S:1608:ARG:NH1 | 2.34 | 0.43 |
| 1:S:1670:LYS:HD2 | 1:S:1670:LYS:HA | 1.82 | 0.43 |
| 1:S:1983:ALA:HB2 | 1:S:2034:ILE:HG21 | 2.00 | 0.43 |
| 1:S:2329:TYR:OH | 1:T:1238:LYS:HD3 | 2.17 | 0.43 |
| 1:S:3165:ASN:ND2 | 1:S:3168:THR:HG23 | 2.34 | 0.43 |
| 1:S:3308:PRO:HG2 | 1:S:3311:ALA:HB3 | 1.99 | 0.43 |
| 1:T:408:GLY:HA3 | 1:T:669:THR:HG21 | 2.00 | 0.43 |
| 1:T:447:GLU:HA | 1:T:450:GLN:NE2 | 2.32 | 0.43 |
| 1:T:1080:ALA:HB1 | 1:T:1083:SER:OG | 2.18 | 0.43 |
| 1:T:2004:GLU:HG2 | 1:T:2006:VAL:HG23 | 2.01 | 0.43 |
| 1:T:2977:CYS:HA | 1:T:2987:TRP:CH2 | 2.53 | 0.43 |
| 1:T:3011:TRP:CZ3 | 1:T:3013:TRP:HA | 2.53 | 0.43 |
| 1:A:485:ARG:HA | 1:A:485:ARG:HD3 | 1.89 | 0.43 |
| 1:A:866:LEU:HD22 | 1:A:968:PHE:HE1 | 1.83 | 0.43 |
| 1:A:1317:HIS:HA | 1:A:1322:PHE:CD1 | 2.53 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:1579:THR:OG1 | 1:A:1584:ARG:NH2 | 2.41 | 0.43 |
| 1:A:1918:GLU:OE2 | 1:A:1921:LYS:NZ | 2.48 | 0.43 |
| 1:A:2052:LYS:HD2 | 1:A:2052:LYS:HA | 1.70 | 0.43 |
| 1:A:2190:LEU:HD21 | 1:A:2194:PHE:HB3 | 1.99 | 0.43 |
| 1:A:2390:LYS:HE2 | 1:A:2390:LYS:HB2 | 1.89 | 0.43 |
| 1:A:2510:GLY:HA3 | 1:A:2513:VAL:HB | 2.00 | 0.43 |
| 1:B:143:ARG:HH22 | 1:B:209:ASP:CG | 2.25 | 0.43 |
| 1:B:453:SER:HB3 | 1:B:553:PRO:HG3 | 2.00 | 0.43 |
| 1:B:845:LEU:HD21 | 1:B:932:ASP:HA | 2.00 | 0.43 |
| 1:B:1884:HIS:O | 1:B:1888:THR:HG23 | 2.18 | 0.43 |
| 1:B:3020:LEU:HD11 | 1:B:3025:THR:HB | 1.99 | 0.43 |
| 1:C:1081:ILE:HD12 | 1:D:2461:PHE:HD1 | 1.84 | 0.43 |
| 1:C:2059:ASN:ND2 | 1:C:2061:SER:OG | 2.51 | 0.43 |
| 1:C:2162:THR:O | 1:C:2165:VAL:HG22 | 2.19 | 0.43 |
| 1:C:2575:PRO:O | 1:C:2579:ARG:HB2 | 2.18 | 0.43 |
| 1:C:2855:VAL:HG12 | 1:C:2855:VAL:O | 2.18 | 0.43 |
| 1:C:3219:LEU:O | 1:C:3258:TYR:HB2 | 2.18 | 0.43 |
| 1:D:41:PHE:CD1 | 1:D:47:MET:HE1 | 2.53 | 0.43 |
| 1:D:313:PHE:HE1 | 1:D:406:PRO:HB3 | 1.82 | 0.43 |
| 1:D:524:ASP:HA | 1:D:643:ASN:ND2 | 2.34 | 0.43 |
| 1:D:845:LEU:HD21 | 1:D:932:ASP:HA | 1.99 | 0.43 |
| 1:D:1162:ALA:HB3 | 1:D:1183:ILE:HD11 | 2.00 | 0.43 |
| 1:D:1714:HIS:NE2 | 1:D:1732:CYS:SG | 2.91 | 0.43 |
| 1:E:169:LEU:HD23 | 1:E:222:ILE:HD11 | 2.01 | 0.43 |
| 1:E:1223:VAL:HG13 | 1:E:1231:ILE:HB | 1.99 | 0.43 |
| 1:E:1426:PHE:CZ | 1:E:1464:VAL:HG13 | 2.53 | 0.43 |
| 1:E:1698:LEU:HD13 | 1:E:1757:ARG:HD2 | 2.00 | 0.43 |
| 1:E:2109:ALA:HA | 1:E:2112:ARG:NH2 | 2.32 | 0.43 |
| 1:E:3305:ILE:HA | 1:E:3315:VAL:O | 2.19 | 0.43 |
| 1:E:3329:LYS:HD2 | 1:F:3357:TYR:HB3 | 1.99 | 0.43 |
| 1:F:297:TYR:O | 1:F:300:LEU:HG | 2.18 | 0.43 |
| 1:F:921:ALA:O | 1:F:925:LEU:HD23 | 2.19 | 0.43 |
| 1:F:1090:PRO:HB2 | 1:F:1093:GLN:HE22 | 1.82 | 0.43 |
| 1:F:1560:PHE:O | 1:F:1609:LEU:HD12 | 2.17 | 0.43 |
| 1:F:1890:ARG:NH1 | 1:F:1959:GLU:O | 2.51 | 0.43 |
| 1:F:2183:TRP:CD2 | 1:F:2271:ILE:HD11 | 2.54 | 0.43 |
| 1:G:508:GLU:OE1 | 1:G:520:ILE:N | 2.34 | 0.43 |
| 1:G:610:HIS:O | 1:G:613:PRO:HD2 | 2.19 | 0.43 |
| 1:G:914:HIS:CE1 | 1:G:1053:HIS:HE1 | 2.36 | 0.43 |
| 1:G:2095:GLU:CD | 1:G:2097:SER:H | 2.24 | 0.43 |
| 1:G:2147:CYS:C | 1:G:2149:HIS:HD1 | 2.26 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:G:2399:LEU:HB3 | 1:G:2436:TRP:CH2 | 2.54 | 0.43 |
| 1:G:2569:HIS:HA | 1:G:2574:PHE:CE1 | 2.53 | 0.43 |
| 1:H:299:LEU:O | 1:H:302:GLN:HG3 | 2.18 | 0.43 |
| 1:H:953:GLU:HA | 1:H:969:HIS:HB2 | 2.01 | 0.43 |
| 1:H:1009:THR:HA | 1:H:1070:ARG:NH2 | 2.34 | 0.43 |
| 1:H:1843:TYR:HD1 | 1:H:1895:TRP:CH2 | 2.37 | 0.43 |
| 1:H:3360:LEU:HD12 | 1:H:3387:PHE:HB3 | 1.99 | 0.43 |
| 1:I:606:PHE:HZ | 1:I:644:VAL:HG13 | 1.82 | 0.43 |
| 1:I:849:SER:HB3 | 1:I:854:LEU:HD21 | 2.00 | 0.43 |
| 1:I:884:PHE:CE1 | 1:I:1090:PRO:HG2 | 2.53 | 0.43 |
| 1:I:2225:VAL:O | 1:I:2279:GLN:NE2 | 2.49 | 0.43 |
| 1:I:2849:ARG:HA | 1:I:2849:ARG:HH11 | 1.82 | 0.43 |
| 1:J:12:THR:N | 1:J:15:GLU:OE2 | 2.47 | 0.43 |
| 1:J:2645:ASP:HB3 | 1:J:2649:GLY:O | 2.18 | 0.43 |
| 1:K:471:HIS:ND1 | 1:K:471:HIS:O | 2.51 | 0.43 |
| 1:K:1397:GLN:HA | 1:K:1398:PRO:HD3 | 1.83 | 0.43 |
| 1:K:3072:LEU:HA | 1:K:3080:PHE:CE1 | 2.53 | 0.43 |
| 1:K:3304:VAL:HG23 | 1:K:3317:ILE:HB | 2.00 | 0.43 |
| 1:L:655:GLN:HG2 | 1:L:662:TYR:HB3 | 1.99 | 0.43 |
| 1:L:981:SER:HB3 | 1:L:1031:GLY:HA3 | 2.00 | 0.43 |
| 1:L:1131:PHE:HB3 | 1:L:1136:LEU:HD21 | 1.98 | 0.43 |
| 1:L:1169:CYS:HA | 1:L:1175:CYS:HA | 2.00 | 0.43 |
| 1:L:1315:CYS:O | 1:L:1317:HIS:ND1 | 2.48 | 0.43 |
| 1:L:1576:CYS:HB2 | 1:L:1632:ASP:OD1 | 2.18 | 0.43 |
| 1:L:2794:GLU:OE2 | 1:L:2794:GLU:HA | 2.19 | 0.43 |
| 1:L:3117:ILE:O | 1:L:3120:SER:OG | 2.28 | 0.43 |
| 1:M:635:PRO:O | 1:M:638:ILE:HG12 | 2.18 | 0.43 |
| 1:M:850:ASP:OD1 | 1:M:852:SER:N | 2.48 | 0.43 |
| 1:M:915:ARG:HH21 | 1:M:1115:TYR:CB | 2.32 | 0.43 |
| 1:M:2544:TYR:HA | 1:M:2547:ILE:HG12 | 2.00 | 0.43 |
| 1:N:357:MET:SD | 1:N:358:PRO:HD2 | 2.58 | 0.43 |
| 1:N:1488:ALA:HB1 | 1:N:1491:ILE:HD13 | 2.00 | 0.43 |
| 1:N:1743:HIS:O | 1:N:1747:THR:HG23 | 2.18 | 0.43 |
| 1:N:2623:GLU:N | 1:N:2623:GLU:OE1 | 2.51 | 0.43 |
| 1:N:2985:PRO:HB2 | 1:N:2989:ARG:NH2 | 2.33 | 0.43 |
| 1:O:204:GLU:OE2 | 1:O:354:ALA:N | 2.44 | 0.43 |
| 1:O:257:ASP:HA | 1:O:265:ARG:NE | 2.28 | 0.43 |
| 1:O:585:ALA:HA | 1:O:588:ASP:OD2 | 2.18 | 0.43 |
| 1:O:1061:ALA:HA | 1:O:1064:GLN:CD | 2.44 | 0.43 |
| 1:O:1974:LYS:HZ1 | 1:O:2361:GLN:HB3 | 1.83 | 0.43 |
| 1:O:2156:HIS:CD2 | 1:O:2306:TRP:HH2 | 2.37 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:O:2164:GLN:HE22 | 1:O:2348:THR:HG21 | 1.83 | 0.43 |
| 1:O:2900:LYS:HE3 | 1:O:2900:LYS:HB3 | 1.79 | 0.43 |
| 1:O:3350:ASN:O | 1:O:3391:SER:N | 2.51 | 0.43 |
| 1:P:580:TYR:HE2 | 1:P:959:GLU:HB3 | 1.83 | 0.43 |
| 1:P:1267:ASN:HB3 | 1:P:1348:TYR:CZ | 2.52 | 0.43 |
| 1:P:1285:ARG:HA | 1:P:1285:ARG:HD2 | 1.80 | 0.43 |
| 1:P:1695:LEU:HG | 1:P:1796:PRO:HB2 | 2.00 | 0.43 |
| 1:P:1960:LEU:N | 1:P:1963:ILE:O | 2.46 | 0.43 |
| 1:P:2343:ASN:HD21 | 1:P:2345:ASN:HB3 | 1.83 | 0.43 |
| 1:P:3266:VAL:HG11 | 1:P:3283:PHE:CZ | 2.53 | 0.43 |
| 1:Q:183:VAL:HG21 | 1:Q:365:TYR:HE1 | 1.82 | 0.43 |
| 1:Q:586:LEU:HD12 | 1:Q:586:LEU:H | 1.83 | 0.43 |
| 1:Q:1649:VAL:HG13 | 1:Q:1650:LEU:HD23 | 2.00 | 0.43 |
| 1:Q:2111:LEU:HD12 | 1:Q:2211:PRO:HG2 | 2.00 | 0.43 |
| 1:Q:2544:TYR:HA | 1:Q:2547:ILE:HG22 | 1.99 | 0.43 |
| 1:Q:3084:PHE:HE1 | 1:Q:3125:ILE:HG23 | 1.83 | 0.43 |
| 1:R:48:CYS:HB2 | 1:R:58:CYS:HB2 | 1.83 | 0.43 |
| 1:R:859:VAL:HG12 | 1:R:863:ARG:CZ | 2.48 | 0.43 |
| 1:R:1324:HIS:CD2 | 1:R:1324:HIS:H | 2.37 | 0.43 |
| 1:R:1405:TYR:CD2 | 1:R:1406:LEU:HD22 | 2.53 | 0.43 |
| 1:R:1547:LEU:O | 1:R:1550:GLN:HG3 | 2.18 | 0.43 |
| 1:R:2247:GLU:OE1 | 1:R:2267:THR:HG22 | 2.18 | 0.43 |
| 1:R:2371:LYS:NZ | 1:R:2377:LEU:H | 2.17 | 0.43 |
| 1:R:2614:LEU:CD1 | 1:R:2636:ARG:HH12 | 2.30 | 0.43 |
| 1:R:2736:ASN:OD1 | 1:S:2893:SER:OG | 2.21 | 0.43 |
| 1:R:3259:GLU:O | 1:R:3331:ILE:HD13 | 2.17 | 0.43 |
| 1:S:189:HIS:HE1 | 1:S:212:PHE:CE1 | 2.36 | 0.43 |
| 1:S:732:THR:HA | 1:S:836:HIS:NE2 | 2.33 | 0.43 |
| 1:S:3100:THR:HA | 1:S:3290:TYR:HE2 | 1.83 | 0.43 |
| 1:T:285:ASP:OD1 | 1:T:286:LEU:N | 2.52 | 0.43 |
| 1:T:331:HIS:HE1 | 1:T:672:HIS:HB3 | 1.82 | 0.43 |
| 1:T:545:ASN:HD21 | 1:T:992:PHE:HE2 | 1.64 | 0.43 |
| 1:T:968:PHE:CD1 | 1:T:1047:PRO:HG2 | 2.54 | 0.43 |
| 1:T:968:PHE:HD1 | 1:T:1047:PRO:HG2 | 1.83 | 0.43 |
| 1:T:1854:HIS:HE1 | 1:T:1885:HIS:NE2 | 2.17 | 0.43 |
| 1:T:3212:ARG:HE | 1:T:3212:ARG:HB2 | 1.70 | 0.43 |
| 1:T:3232:LEU:HD11 | 1:T:3270:LEU:HG | 1.99 | 0.43 |
| 1:T:3337:ARG:HD3 | 1:T:3378:ASN:HD21 | 1.84 | 0.43 |
| 1:A:453:SER:OG | 3:V:1:NAG:O7 | 2.23 | 0.43 |
| 1:A:1733:VAL:C | 1:A:1734:HIS:HD1 | 2.27 | 0.43 |
| 1:A:2311:GLU:HG2 | 1:A:2370:MET:HG2 | 2.00 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:3087:LEU:O | 1:A:3090:THR:OG1 | 2.32 | 0.43 |
| 1:B:56:VAL:HB | 1:B:355:ASN:O | 2.19 | 0.43 |
| 1:B:378:LYS:HZ3 | 1:B:383:ASP:H | 1.67 | 0.43 |
| 1:B:474:PRO:HB2 | 1:B:476:ARG:NH1 | 2.32 | 0.43 |
| 1:B:1372:SER:O | 1:B:1374:THR:OG1 | 2.35 | 0.43 |
| 1:B:1619:ARG:HH21 | 1:B:1625:LEU:HD13 | 1.84 | 0.43 |
| 1:B:1941:PRO:O | 1:B:1944:VAL:HG22 | 2.18 | 0.43 |
| 1:B:1967:LEU:HD23 | 1:B:1967:LEU:H | 1.83 | 0.43 |
| 1:B:2376:ASN:HD21 | 1:B:2378:ASP:HB2 | 1.83 | 0.43 |
| 1:B:2979:HIS:HA | 1:B:2984:PHE:CD2 | 2.50 | 0.43 |
| 1:C:327:LYS:HE2 | 1:C:342:CYS:SG | 2.58 | 0.43 |
| 1:C:650:ILE:HG22 | 1:C:713:LEU:HD12 | 2.00 | 0.43 |
| 1:C:1560:PHE:CE2 | 1:C:1593:PHE:HZ | 2.36 | 0.43 |
| 1:C:2099:LEU:HD13 | 1:C:2103:ALA:HB3 | 2.00 | 0.43 |
| 1:C:3067:GLN:O | 1:C:3071:THR:HG23 | 2.17 | 0.43 |
| 1:C:3351:VAL:HG21 | 1:C:3388:PHE:HB3 | 2.00 | 0.43 |
| 1:C:3353:GLU:HG3 | 1:C:3386:TYR:HD2 | 1.83 | 0.43 |
| 1:D:32:VAL:HA | 1:D:37:ASN:HD21 | 1.83 | 0.43 |
| 1:D:597:ARG:NH2 | 1:D:655:GLN:HA | 2.32 | 0.43 |
| 1:D:914:HIS:O | 1:D:918:THR:HG23 | 2.18 | 0.43 |
| 1:D:1873:HIS:HE2 | 1:D:2020:ALA:CB | 2.25 | 0.43 |
| 1:D:2064:SER:OG | 1:D:2066:SER:OG | 2.27 | 0.43 |
| 1:D:2088:PRO:C | 1:D:2090:ASN:H | 2.26 | 0.43 |
| 1:D:2598:ILE:HD11 | 1:D:2710:SER:HB2 | 2.00 | 0.43 |
| 1:E:704:HIS:ND1 | 1:E:705:GLU:OE2 | 2.52 | 0.43 |
| 1:E:1534:ASN:HA | 1:E:1539:THR:HA | 2.01 | 0.43 |
| 1:E:1745:LEU:HD23 | 1:E:1923:PHE:CD2 | 2.54 | 0.43 |
| 1:E:2381:GLU:HA | 1:E:2384:ILE:HD12 | 2.01 | 0.43 |
| 1:E:3002:LYS:HD3 | 1:E:3002:LYS:HA | 1.70 | 0.43 |
| 1:E:3396:CYS:HA | 1:E:3401:ARG:NH1 | 2.34 | 0.43 |
| 1:F:106:LEU:HD12 | 1:F:125:TRP:HE3 | 1.83 | 0.43 |
| 1:F:580:TYR:CG | 1:F:958:PRO:HG2 | 2.54 | 0.43 |
| 1:F:845:LEU:O | 1:F:926:ARG:NH1 | 2.51 | 0.43 |
| 1:F:872:ASP:HB3 | 1:F:877:GLY:HA2 | 1.99 | 0.43 |
| 1:F:946:LEU:HG | 1:F:951:ALA:HB2 | 2.00 | 0.43 |
| 1:F:1018:TYR:OH | 1:F:1056:THR:HB | 2.18 | 0.43 |
| 1:F:2514:ARG:CZ | 1:F:2774:TYR:HB2 | 2.48 | 0.43 |
| 1:F:2529:LYS:HB3 | 1:F:2529:LYS:HE2 | 1.85 | 0.43 |
| 1:G:133:ASP:OD1 | 1:G:134:SER:N | 2.51 | 0.43 |
| 1:G:183:VAL:HA | 1:G:186:ASN:HD22 | 1.83 | 0.43 |
| 1:G:193:GLY:HA3 | 1:G:201:SER:H | 1.82 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:G:204:GLU:OE2 | 1:G:354:ALA:N | 2.49 | 0.43 |
| 1:G:489:CYS:O | 1:G:491:HIS:ND1 | 2.51 | 0.43 |
| 1:G:2034:ILE:O | 1:G:2038:LEU:HD23 | 2.17 | 0.43 |
| 1:G:2101:ALA:O | 1:G:2105:MET:HE3 | 2.19 | 0.43 |
| 1:G:2376:ASN:O | 1:G:2380:LEU:HG | 2.18 | 0.43 |
| 1:G:2729:ASP:OD2 | 1:G:2916:THR:OG1 | 2.25 | 0.43 |
| 1:G:2741:ARG:HA | 1:G:2762:ARG:HH22 | 1.82 | 0.43 |
| 1:H:80:LYS:NZ | 1:H:261:ILE:HG13 | 2.33 | 0.43 |
| 1:H:799:LYS:N | 1:H:802:ASP:OD2 | 2.47 | 0.43 |
| 1:H:859:VAL:HG12 | 1:H:863:ARG:CZ | 2.48 | 0.43 |
| 1:H:1007:GLU:OE1 | 1:H:1007:GLU:N | 2.50 | 0.43 |
| 1:H:1315:CYS:O | 1:H:1317:HIS:ND1 | 2.50 | 0.43 |
| 1:H:1325:TRP:HD1 | 1:H:1326:HIS:ND1 | 2.16 | 0.43 |
| 1:H:1854:HIS:HE1 | 1:H:1885:HIS:CD2 | 2.37 | 0.43 |
| 1:H:2552:GLY:HA3 | 1:H:2697:GLU:HA | 1.99 | 0.43 |
| 1:H:2977:CYS:HA | 1:H:2987:TRP:CH2 | 2.53 | 0.43 |
| 1:H:3131:THR:HA | 1:H:3134:LYS:HG2 | 1.99 | 0.43 |
| 1:I:307:GLU:OE1 | 1:I:412:PRO:HA | 2.18 | 0.43 |
| 1:I:1362:ILE:HD12 | 1:I:1394:ARG:NH2 | 2.33 | 0.43 |
| 1:I:1495:PRO:HA | 1:I:1516:PRO:HD3 | 2.00 | 0.43 |
| 1:I:2052:LYS:HA | 1:I:2052:LYS:HD2 | 1.62 | 0.43 |
| 1:I:2112:ARG:HB3 | 1:I:2116:LYS:HZ1 | 1.83 | 0.43 |
| 1:J:1023:ASN:HB3 | 1:J:1182:TYR:HD2 | 1.83 | 0.43 |
| 1:J:2665:ARG:CZ | 1:J:2726:ARG:HH21 | 2.32 | 0.43 |
| 1:J:2802:VAL:HG23 | 1:J:2855:VAL:HG23 | 2.00 | 0.43 |
| 1:J:2941:LEU:HD13 | 1:J:2999:LEU:HD21 | 2.01 | 0.43 |
| 1:J:3195:HIS:HB3 | 1:J:3199:GLU:OE2 | 2.19 | 0.43 |
| 1:K:1277:GLU:HA | 1:K:1280:LYS:HG2 | 2.00 | 0.43 |
| 1:K:1425:GLN:O | 1:K:1429:VAL:HG22 | 2.17 | 0.43 |
| 1:K:1559:GLY:C | 1:K:1560:PHE:HD1 | 2.27 | 0.43 |
| 1:K:2112:ARG:NH2 | 1:K:2208:LEU:HD21 | 2.33 | 0.43 |
| 1:K:2252:LEU:HD11 | 1:K:2312:LEU:CD2 | 2.44 | 0.43 |
| 1:K:2805:ASN:ND2 | 1:K:2852:GLN:OE1 | 2.51 | 0.43 |
| 1:K:3329:LYS:HE3 | 1:L:3357:TYR:CD2 | 2.53 | 0.43 |
| 1:K:3340:PHE:CE1 | 1:K:3351:VAL:HG11 | 2.54 | 0.43 |
| 1:L:675:LEU:HD23 | 1:L:675:LEU:HA | 1.81 | 0.43 |
| 1:L:1051:LEU:HD12 | 1:L:1052:HIS:N | 2.33 | 0.43 |
| 1:L:1720:CYS:O | 1:L:1729:TYR:HB2 | 2.18 | 0.43 |
| 1:L:2183:TRP:HZ3 | 1:L:2244:LEU:HB2 | 1.82 | 0.43 |
| 1:L:3232:LEU:HD13 | 1:L:3269:ALA:HB3 | 2.00 | 0.43 |
| 1:M:256:ARG:HE | 1:M:256:ARG:HB3 | 1.72 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:M:826:THR:OG1 | 1:M:827:THR:N | 2.52 | 0.43 |
| 1:M:2271:ILE:HD11 | 1:M:2298:HIS:NE2 | 2.33 | 0.43 |
| 1:M:2301:PHE:O | 1:M:2305:ILE:HG12 | 2.18 | 0.43 |
| 1:M:2313:GLN:CD | 1:M:2318:LEU:HB2 | 2.43 | 0.43 |
| 1:N:81:LEU:HB3 | 1:N:86:LEU:HB2 | 1.99 | 0.43 |
| 1:N:220:ASP:O | 1:N:224:VAL:HG13 | 2.18 | 0.43 |
| 1:N:1802:ILE:HD11 | 1:N:1805:GLU:HB2 | 2.00 | 0.43 |
| 1:N:2669:ASN:OD1 | 1:N:2670:PHE:N | 2.52 | 0.43 |
| 1:N:3144:ARG:NH2 | 1:N:3409:GLU:OE2 | 2.40 | 0.43 |
| 1:N:3334:ARG:NH1 | 1:N:3408:ASP:HA | 2.33 | 0.43 |
| 1:O:343:GLU:OE1 | 1:O:375:HIS:ND1 | 2.52 | 0.43 |
| 1:O:1161:SER:OG | 1:O:1184:LEU:HD12 | 2.18 | 0.43 |
| 1:O:1571:VAL:O | 1:O:1592:SER:HB2 | 2.18 | 0.43 |
| 1:O:1722:TYR:CD1 | 1:O:1724:GLU:HB2 | 2.53 | 0.43 |
| 1:O:2095:GLU:HB3 | 1:O:2098:HIS:HB2 | 2.00 | 0.43 |
| 1:O:2627:ILE:HD11 | 1:O:2632:GLU:HB3 | 2.00 | 0.43 |
| 1:O:2940:ALA:HB1 | 1:O:2999:LEU:CD1 | 2.49 | 0.43 |
| 1:O:2997:MET:HE2 | 1:O:2997:MET:HB2 | 1.86 | 0.43 |
| 1:O:3047:ASP:HB2 | 1:O:3097:GLY:HA3 | 2.01 | 0.43 |
| 1:O:3065:PHE:HA | 1:O:3068:THR:HG22 | 2.00 | 0.43 |
| 1:P:14:GLN:HG2 | 1:P:15:GLU:N | 2.33 | 0.43 |
| 1:P:719:THR:HG22 | 1:P:722:GLN:NE2 | 2.34 | 0.43 |
| 1:P:859:VAL:HG12 | 1:P:863:ARG:CZ | 2.48 | 0.43 |
| 1:P:1301:PHE:CD1 | 1:P:1302:PRO:HA | 2.52 | 0.43 |
| 1:Q:613:PRO:HB2 | 1:Q:640:HIS:HE1 | 1.83 | 0.43 |
| 1:Q:1061:ALA:HA | 1:Q:1064:GLN:NE2 | 2.33 | 0.43 |
| 1:Q:1577:VAL:HG11 | 1:Q:1623:LEU:HD11 | 2.00 | 0.43 |
| 1:Q:1662:ASP:OD1 | 1:Q:1662:ASP:N | 2.49 | 0.43 |
| 1:Q:2273:TYR:HA | 1:Q:2284:SER:OG | 2.19 | 0.43 |
| 1:Q:3086:MET:SD | 1:Q:3245:PHE:HZ | 2.41 | 0.43 |
| 1:R:23:LEU:HD23 | 1:R:123:ASN:ND2 | 2.33 | 0.43 |
| 1:R:217:SER:HA | 1:R:220:ASP:OD1 | 2.19 | 0.43 |
| 1:R:881:ILE:HA | 1:R:884:PHE:HB2 | 2.01 | 0.43 |
| 1:R:1356:ARG:NH1 | 1:R:1356:ARG:HA | 2.34 | 0.43 |
| 1:R:2469:LEU:HD11 | 1:R:2489:PRO:HG2 | 1.99 | 0.43 |
| 1:R:3088:HIS:CE1 | 1:R:3119:HIS:CE1 | 3.07 | 0.43 |
| 1:S:444:GLU:HB3 | 1:S:518:PHE:HZ | 1.84 | 0.43 |
| 1:S:752:ILE:O | 1:S:808:LEU:HA | 2.19 | 0.43 |
| 1:S:1452:ALA:HA | 1:S:1457:PHE:CG | 2.53 | 0.43 |
| 1:S:1741:GLN:N | 1:S:1741:GLN:OE1 | 2.50 | 0.43 |
| 1:S:1897:GLU:HG3 | 1:S:1958:LEU:HD22 | 1.99 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:S:1993:SER:HB2 | 1:S:2017:GLY:H | 1.81 | 0.43 |
| 1:S:2215:GLY:O | 1:S:2224:THR:N | 2.49 | 0.43 |
| 1:S:3231:LYS:HB2 | 1:S:3284:GLN:HG3 | 2.01 | 0.43 |
| 1:T:70:HIS:O | 1:T:74:VAL:HG13 | 2.18 | 0.43 |
| 1:T:859:VAL:HG12 | 1:T:863:ARG:CZ | 2.48 | 0.43 |
| 1:T:1069:TYR:HE2 | 1:T:1137:GLN:HG3 | 1.82 | 0.43 |
| 1:T:1705:THR:HG23 | 1:T:1931:LEU:HD12 | 2.00 | 0.43 |
| 1:T:2313:GLN:HE22 | 1:T:2318:LEU:HB2 | 1.82 | 0.43 |
| 1:T:2959:PHE:O | 1:T:2976:CYS:HB2 | 2.19 | 0.43 |
| 1:T:3058:GLN:N | 1:T:3061:LEU:O | 2.36 | 0.43 |
| 1:T:3340:PHE:CE2 | 1:T:3351:VAL:HG11 | 2.53 | 0.43 |
| 1:T:3395:ARG:HD2 | 1:T:3395:ARG:HA | 1.71 | 0.43 |
| 3:rA:2:NAG:H4 | 3:rA:3:BMA:H2 | 1.76 | 0.43 |
| 1:A:972:LEU:HD23 | 1:A:977:LYS:HB3 | 2.00 | 0.43 |
| 1:A:1323:PRO:HG3 | 1:A:1426:PHE:CE2 | 2.53 | 0.43 |
| 1:A:2027:ASP:OD2 | 1:A:2028:ARG:NH1 | 2.52 | 0.43 |
| 1:A:2126:LEU:O | 1:A:2161:TYR:OH | 2.36 | 0.43 |
| 1:B:107:VAL:HG11 | 1:B:211:LEU:HD21 | 2.00 | 0.43 |
| 1:B:378:LYS:HD2 | 1:B:378:LYS:HA | 1.81 | 0.43 |
| 1:B:552:ASN:ND2 | 1:B:554:PHE:HB2 | 2.33 | 0.43 |
| 1:B:674:LEU:HA | 1:B:695:ARG:NH1 | 2.30 | 0.43 |
| 1:B:1125:ASP:OD1 | 1:B:1125:ASP:N | 2.51 | 0.43 |
| 1:B:1301:PHE:CD1 | 1:B:1302:PRO:HA | 2.54 | 0.43 |
| 1:B:1550:GLN:HA | 1:B:1553:GLN:HE22 | 1.83 | 0.43 |
| 1:B:1579:THR:HG21 | 1:B:1585:ASN:HB3 | 2.00 | 0.43 |
| 1:B:2028:ARG:HB2 | 1:B:2028:ARG:CZ | 2.48 | 0.43 |
| 1:B:2671:GLU:HA | 1:B:2674:TYR:HB3 | 2.01 | 0.43 |
| 1:B:2718:ILE:CD1 | 1:B:2779:LEU:HB2 | 2.49 | 0.43 |
| 1:B:3062:ASP:HB3 | 1:B:3065:PHE:HB3 | 2.00 | 0.43 |
| 1:C:71:ARG:HA | 1:C:74:VAL:HG12 | 2.00 | 0.43 |
| 1:C:689:LYS:HA | 1:C:689:LYS:HD3 | 1.71 | 0.43 |
| 1:C:998:ILE:HD12 | 1:C:998:ILE:H | 1.84 | 0.43 |
| 1:C:2245:PHE:O | 1:C:2249:LEU:HD13 | 2.19 | 0.43 |
| 1:C:2260:PHE:HE1 | 1:C:2309:TRP:HB2 | 1.83 | 0.43 |
| 1:C:2371:LYS:HA | 1:C:2371:LYS:HD2 | 1.90 | 0.43 |
| 1:C:2819:PHE:O | 1:C:2831:ALA:HB3 | 2.18 | 0.43 |
| 1:D:81:LEU:HA | 1:D:84:LYS:HB2 | 2.01 | 0.43 |
| 1:D:501:ARG:HH21 | 1:D:648:TRP:HB3 | 1.83 | 0.43 |
| 1:D:600:CYS:HB3 | 1:D:783:ARG:HH12 | 1.82 | 0.43 |
| 1:D:1062:ILE:HG22 | 1:D:1126:LEU:HB2 | 2.00 | 0.43 |
| 1:D:1143:ARG:HB3 | 1:D:1148:ARG:NH2 | 2.33 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:D:2786:ILE:N | 1:D:2787:PRO:HD2 | 2.34 | 0.43 |
| 1:E:176:HIS:CD2 | 1:E:363:LEU:HD21 | 2.53 | 0.43 |
| 1:E:259:ASN:ND2 | 1:E:264:THR:OG1 | 2.52 | 0.43 |
| 1:E:1168:VAL:N | 1:E:1178:GLU:OE1 | 2.51 | 0.43 |
| 1:E:1350:ASP:HA | 1:E:1463:ASN:ND2 | 2.33 | 0.43 |
| 1:F:673:GLU:C | 1:F:695:ARG:HH12 | 2.25 | 0.43 |
| 1:F:1678:LYS:NZ | 1:F:1683:LEU:HA | 2.34 | 0.43 |
| 1:F:1729:TYR:CE1 | 1:F:2022:MET:HA | 2.53 | 0.43 |
| 1:F:2655:TYR:CD1 | 1:F:2659:LEU:HD23 | 2.54 | 0.43 |
| 1:G:16:VAL:HG21 | 1:G:105:ARG:HH12 | 1.84 | 0.43 |
| 1:G:196:HIS:O | 1:G:199:SER:OG | 2.27 | 0.43 |
| 1:G:453:SER:OG | 3:z:1:NAG:O7 | 2.22 | 0.43 |
| 1:G:2601:TRP:H | 1:G:2707:ILE:CG2 | 2.32 | 0.43 |
| 1:G:3002:LYS:HA | 1:G:3002:LYS:HD3 | 1.58 | 0.43 |
| 1:G:3182:LYS:HE2 | 1:G:3182:LYS:HB3 | 1.87 | 0.43 |
| 1:G:3202:THR:HA | 1:G:3205:GLU:OE2 | 2.18 | 0.43 |
| 1:H:1722:TYR:CE2 | 1:H:1724:GLU:HG2 | 2.53 | 0.43 |
| 1:H:2316:ARG:HD3 | 1:H:2316:ARG:H | 1.83 | 0.43 |
| 1:H:2765:ASP:OD1 | 1:H:2765:ASP:N | 2.49 | 0.43 |
| 1:I:16:VAL:HG21 | 1:I:105:ARG:HH12 | 1.84 | 0.43 |
| 1:I:1486:ASP:OD1 | 1:I:1486:ASP:N | 2.49 | 0.43 |
| 1:I:2029:LEU:HD23 | 1:I:2029:LEU:H | 1.83 | 0.43 |
| 1:J:744:ASN:ND2 | 1:J:778:PRO:HA | 2.33 | 0.43 |
| 1:J:884:PHE:HA | 1:J:888:PRO:HG3 | 2.01 | 0.43 |
| 1:J:1143:ARG:O | 1:J:1148:ARG:NH1 | 2.35 | 0.43 |
| 1:J:1433:LEU:HA | 1:J:1436:LEU:HB2 | 2.00 | 0.43 |
| 1:J:2542:ARG:HD3 | 1:J:2591:LEU:HD23 | 2.01 | 0.43 |
| 1:J:3331:ILE:HA | 1:J:3405:SER:OG | 2.18 | 0.43 |
| 1:K:589:GLY:HA2 | 1:K:592:LEU:HG | 2.01 | 0.43 |
| 1:K:636:ILE:H | 1:K:636:ILE:HD12 | 1.84 | 0.43 |
| 1:K:973:VAL:HG11 | 1:K:1045:TYR:CD2 | 2.54 | 0.43 |
| 1:K:2542:ARG:NH1 | 1:K:2588:ALA:HA | 2.32 | 0.43 |
| 1:K:3263:LYS:HD2 | 1:K:3305:ILE:HD11 | 2.00 | 0.43 |
| 1:L:452:LEU:HD13 | 1:L:554:PHE:CZ | 2.53 | 0.43 |
| 1:L:494:ALA:O | 1:L:497:PRO:HD2 | 2.19 | 0.43 |
| 1:L:618:GLY:HA3 | 1:L:626:SER:N | 2.34 | 0.43 |
| 1:L:636:ILE:O | 1:L:639:LEU:HG | 2.17 | 0.43 |
| 1:L:740:LEU:HB2 | 1:L:785:VAL:HB | 2.00 | 0.43 |
| 1:L:1285:ARG:O | 1:L:1340:ARG:NH1 | 2.52 | 0.43 |
| 1:L:2194:PHE:CD1 | 1:L:2212:PHE:HB3 | 2.53 | 0.43 |
| 1:L:2527:SER:O | 1:L:2530:LYS:HG3 | 2.19 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:L:2712:VAL:HA | 1:L:2715:GLN:NE2 | 2.33 | 0.43 |
| 1:M:849:SER:HB3 | 1:M:854:LEU:HD21 | 2.00 | 0.43 |
| 1:M:1549:ARG:HD2 | 1:M:1549:ARG:HA | 1.80 | 0.43 |
| 1:M:1687:GLU:HA | 1:M:1760:LEU:HD21 | 2.00 | 0.43 |
| 1:M:2471:TYR:HE1 | 1:M:2488:LYS:HD2 | 1.83 | 0.43 |
| 1:M:3065:PHE:O | 1:M:3068:THR:HG22 | 2.18 | 0.43 |
| 1:M:3074:GLU:O | 1:M:3080:PHE:HZ | 2.00 | 0.43 |
| 1:N:469:GLU:OE1 | 1:N:469:GLU:N | 2.48 | 0.43 |
| 1:N:811:LYS:NZ | 1:N:815:GLY:O | 2.39 | 0.43 |
| 1:N:1060:TRP:NE1 | 1:N:1064:GLN:HE22 | 2.17 | 0.43 |
| 1:N:1086:LYS:HZ1 | 1:N:1089:GLN:HE21 | 1.66 | 0.43 |
| 1:N:1880:ILE:H | 1:N:1880:ILE:HD12 | 1.83 | 0.43 |
| 1:N:2124:GLN:CD | 1:N:2124:GLN:H | 2.25 | 0.43 |
| 1:N:2620:ASN:ND2 | 1:N:2623:GLU:OE1 | 2.50 | 0.43 |
| 1:N:2714:ARG:O | 1:N:2718:ILE:HG12 | 2.19 | 0.43 |
| 1:N:3266:VAL:HG11 | 1:N:3283:PHE:CZ | 2.53 | 0.43 |
| 1:O:304:ARG:HH11 | 1:O:304:ARG:HG2 | 1.84 | 0.43 |
| 1:O:997:LYS:HA | 1:O:1000:GLU:CD | 2.44 | 0.43 |
| 1:O:1722:TYR:HD1 | 1:O:1724:GLU:HB2 | 1.83 | 0.43 |
| 1:O:2531:ALA:O | 1:O:2535:VAL:HG23 | 2.19 | 0.43 |
| 1:P:202:THR:HG23 | 1:P:205:TRP:H | 1.83 | 0.43 |
| 1:P:552:ASN:ND2 | 1:P:554:PHE:HB2 | 2.33 | 0.43 |
| 1:P:2919:LYS:HD3 | 1:P:3184:HIS:HB2 | 2.00 | 0.43 |
| 1:Q:997:LYS:O | 1:Q:1001:MET:HG3 | 2.19 | 0.43 |
| 1:Q:1138:ARG:HH22 | 1:Q:1260:ALA:C | 2.26 | 0.43 |
| 1:Q:1421:ASP:HB3 | 1:Q:1608:ARG:NH1 | 2.34 | 0.43 |
| 1:Q:3096:GLY:HA3 | 1:Q:3104:SER:HB3 | 1.99 | 0.43 |
| 1:Q:3289:LYS:HE2 | 1:Q:3291:ASN:HB2 | 2.00 | 0.43 |
| 1:R:149:LEU:HD11 | 1:R:191:LEU:HB3 | 2.00 | 0.43 |
| 1:R:442:ASP:OD1 | 1:R:443:GLU:N | 2.51 | 0.43 |
| 1:R:1204:ASP:N | 1:R:1204:ASP:OD1 | 2.51 | 0.43 |
| 1:R:1795:ASN:HD21 | 1:R:1797:TRP:HB2 | 1.84 | 0.43 |
| 1:R:1849:GLN:O | 1:R:1852:ILE:HG22 | 2.19 | 0.43 |
| 1:R:2271:ILE:HD12 | 1:R:2298:HIS:CE1 | 2.53 | 0.43 |
| 1:R:2336:PRO:HB2 | 1:R:2342:LEU:HD12 | 2.00 | 0.43 |
| 1:R:2397:PHE:CD1 | 1:R:2489:PRO:HB3 | 2.53 | 0.43 |
| 1:R:2788:GLN:O | 1:R:2791:GLU:HG3 | 2.19 | 0.43 |
| 1:S:869:LEU:HG | 1:S:878:PHE:HB2 | 2.00 | 0.43 |
| 1:S:1839:GLU:OE1 | 1:S:1839:GLU:N | 2.43 | 0.43 |
| 1:S:2271:ILE:HG13 | 1:S:2298:HIS:HE1 | 1.83 | 0.43 |
| 1:S:2439:ASP:N | 1:S:2439:ASP:OD1 | 2.49 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:S:3065:PHE:HA | 1:S:3068:THR:HG22 | 1.99 | 0.43 |
| 1:T:1165:THR:N | 1:T:1222:SER:O | 2.36 | 0.43 |
| 1:T:1221:TYR:OH | 1:T:1237:GLY:N | 2.52 | 0.43 |
| 1:T:1338:LEU:HA | 1:T:1342:SER:OG | 2.19 | 0.43 |
| 1:T:1947:TYR:CE1 | 1:T:1948:LYS:HG3 | 2.54 | 0.43 |
| 1:A:30:LYS:HG3 | 1:A:31:THR:H | 1.83 | 0.43 |
| 1:A:646:ARG:HA | 1:A:710:TYR:HE2 | 1.83 | 0.43 |
| 1:A:1162:ALA:HB1 | 1:A:1224:ILE:O | 2.19 | 0.43 |
| 1:A:2229:GLN:HB2 | 1:A:2274:LEU:HD12 | 2.01 | 0.43 |
| 1:B:142:ALA:HB3 | 1:B:196:HIS:CG | 2.54 | 0.43 |
| 1:B:568:ARG:NH1 | 1:B:634:ASP:OD1 | 2.48 | 0.43 |
| 1:B:636:ILE:O | 1:B:639:LEU:HG | 2.19 | 0.43 |
| 1:B:1463:ASN:O | 1:B:1467:ILE:HG12 | 2.18 | 0.43 |
| 1:B:1938:TYR:CE2 | 1:B:1950:HIS:HB3 | 2.54 | 0.43 |
| 1:B:2034:ILE:O | 1:B:2034:ILE:HG13 | 2.19 | 0.43 |
| 1:C:47:MET:C | 1:C:55:ARG:HH12 | 2.27 | 0.43 |
| 1:C:731:ARG:HG2 | 1:C:735:ARG:NH2 | 2.33 | 0.43 |
| 1:C:1061:ALA:HA | 1:C:1064:GLN:CD | 2.43 | 0.43 |
| 1:C:1378:ASN:ND2 | 1:C:1380:PHE:HB2 | 2.33 | 0.43 |
| 1:C:2194:PHE:HE1 | 1:C:2213:ALA:HA | 1.84 | 0.43 |
| 1:C:2238:ASP:OD1 | 1:C:2238:ASP:N | 2.48 | 0.43 |
| 1:C:3046:ARG:NH2 | 1:C:3112:ASP:OD2 | 2.52 | 0.43 |
| 1:D:413:ALA:HB3 | 1:D:416:PHE:HB2 | 2.00 | 0.43 |
| 1:D:1338:LEU:HA | 1:D:1342:SER:OG | 2.18 | 0.43 |
| 1:D:1419:PHE:HE1 | 1:D:1468:TRP:HE1 | 1.66 | 0.43 |
| 1:D:1433:LEU:HD11 | 1:D:1460:HIS:NE2 | 2.32 | 0.43 |
| 1:D:2522:VAL:O | 1:D:2525:THR:N | 2.51 | 0.43 |
| 1:D:3124:ARG:HD2 | 1:D:3187:PHE:CD2 | 2.53 | 0.43 |
| 1:E:173:ASP:O | 1:E:177:PHE:N | 2.46 | 0.43 |
| 1:E:292:ASN:H | 1:E:295:GLN:NE2 | 2.16 | 0.43 |
| 1:E:525:TRP:CE3 | 1:E:586:LEU:HD23 | 2.53 | 0.43 |
| 1:F:246:LEU:HA | 1:F:249:LYS:HE2 | 2.01 | 0.43 |
| 1:F:581:GLY:H | 1:F:856:ARG:HH22 | 1.66 | 0.43 |
| 1:F:587:PHE:O | 1:F:591:LEU:HG | 2.18 | 0.43 |
| 1:F:668:HIS:O | 1:F:671:THR:HG22 | 2.18 | 0.43 |
| 1:F:862:LEU:HD22 | 1:F:935:PRO:HG3 | 2.01 | 0.43 |
| 1:F:2109:ALA:HA | 1:F:2112:ARG:HG2 | 2.01 | 0.43 |
| 1:F:2741:ARG:HH11 | 1:G:2869:VAL:HA | 1.83 | 0.43 |
| 1:F:3052:LEU:O | 1:F:3055:ARG:NH1 | 2.36 | 0.43 |
| 1:G:304:ARG:HA | 1:G:304:ARG:NE | 2.33 | 0.43 |
| 1:G:2705:PHE:HD2 | 1:G:2706:PHE:HD2 | 1.66 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:G:3211:ASP:OD1 | 1:G:3212:ARG:N | 2.52 | 0.43 |
| 1:G:3351:VAL:HG21 | 1:G:3388:PHE:HB3 | 2.00 | 0.43 |
| 1:H:220:ASP:O | 1:H:224:VAL:HG13 | 2.19 | 0.43 |
| 1:H:298:ASN:HA | 1:H:301:GLU:CD | 2.44 | 0.43 |
| 1:H:1773:ASN:OD1 | 1:H:1774:SER:N | 2.51 | 0.43 |
| 1:H:2044:SER:N | 1:H:2047:ASP:OD2 | 2.52 | 0.43 |
| 1:I:169:LEU:HD12 | 1:I:300:LEU:HD21 | 2.00 | 0.43 |
| 1:I:946:LEU:HD13 | 1:I:950:VAL:HG23 | 2.00 | 0.43 |
| 1:I:1152:GLY:HA3 | 1:I:1197:LEU:HD21 | 2.01 | 0.43 |
| 1:I:1295:ILE:HD12 | 1:I:1333:VAL:HG23 | 2.01 | 0.43 |
| 1:I:1732:CYS:HA | 1:I:1742:TRP:CH2 | 2.54 | 0.43 |
| 1:I:2353:LEU:HD22 | 1:I:2355:LYS:HZ2 | 1.82 | 0.43 |
| 1:I:3228:ALA:HB3 | 1:I:3245:PHE:HB3 | 1.99 | 0.43 |
| 1:J:445:VAL:O | 1:J:448:LEU:HG | 2.19 | 0.43 |
| 1:J:612:LEU:HD21 | 1:J:768:LEU:HD13 | 2.00 | 0.43 |
| 1:J:928:LYS:HG3 | 1:J:929:GLY:N | 2.33 | 0.43 |
| 1:J:1143:ARG:HB3 | 1:J:1148:ARG:HH22 | 1.83 | 0.43 |
| 1:J:1677:ARG:HD2 | 1:J:1763:ILE:O | 2.18 | 0.43 |
| 1:J:1979:SER:OG | 1:J:2078:LYS:HD2 | 2.19 | 0.43 |
| 1:J:2340:VAL:HG23 | 1:J:2349:ARG:HD2 | 2.00 | 0.43 |
| 1:K:14:GLN:HG2 | 1:K:15:GLU:N | 2.33 | 0.43 |
| 1:K:275:SER:HB3 | 1:K:278:GLN:HE22 | 1.84 | 0.43 |
| 1:K:307:GLU:OE1 | 1:K:412:PRO:HA | 2.18 | 0.43 |
| 1:K:654:LEU:HD12 | 1:K:723:LEU:HD23 | 2.01 | 0.43 |
| 1:K:850:ASP:OD1 | 1:K:852:SER:N | 2.50 | 0.43 |
| 1:K:1778:PHE:HD2 | 1:K:1779:PHE:HD1 | 1.66 | 0.43 |
| 1:K:2217:ILE:HD12 | 1:K:2217:ILE:HA | 1.84 | 0.43 |
| 1:K:2399:LEU:HB3 | 1:K:2436:TRP:CH2 | 2.53 | 0.43 |
| 1:K:2453:LEU:HD23 | 1:K:2453:LEU:HA | 1.83 | 0.43 |
| 1:K:2791:GLU:O | 1:K:2794:GLU:HG3 | 2.18 | 0.43 |
| 1:L:297:TYR:O | 1:L:301:GLU:OE1 | 2.37 | 0.43 |
| 1:L:456:GLN:NE2 | 1:L:553:PRO:O | 2.48 | 0.43 |
| 1:L:592:LEU:HD21 | 1:L:787:VAL:HA | 2.00 | 0.43 |
| 1:L:1736:MET:N | 1:L:1736:MET:SD | 2.92 | 0.43 |
| 1:L:1970:SER:HB2 | 1:L:2085:GLN:HE22 | 1.83 | 0.43 |
| 1:L:2273:TYR:HB3 | 1:L:2426:PHE:CD1 | 2.53 | 0.43 |
| 1:L:2589:LEU:HG | 1:L:2594:ALA:HB2 | 2.01 | 0.43 |
| 1:L:2987:TRP:CD1 | 1:L:3154:LEU:HD12 | 2.53 | 0.43 |
| 1:M:278:GLN:HG2 | 1:M:279:LEU:HD22 | 2.00 | 0.43 |
| 1:M:425:ASP:OD1 | 1:M:425:ASP:N | 2.43 | 0.43 |
| 1:M:604:VAL:HG12 | 1:M:781:PHE:CD1 | 2.53 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:M:731:ARG:HA | 1:M:735:ARG:NH1 | 2.28 | 0.43 |
| 1:M:1693:LEU:O | 1:M:1696:GLN:HG3 | 2.19 | 0.43 |
| 1:M:1857:ILE:HD12 | 1:M:1857:ILE:HA | 1.86 | 0.43 |
| 1:M:2269:ASN:OD1 | 1:M:2428:LEU:HB2 | 2.19 | 0.43 |
| 1:M:2360:TYR:HA | 1:M:2363:LEU:HB2 | 2.00 | 0.43 |
| 1:M:2972:ASP:OD1 | 1:M:2972:ASP:N | 2.51 | 0.43 |
| 1:N:81:LEU:HA | 1:N:84:LYS:HB2 | 2.00 | 0.43 |
| 1:N:246:LEU:HA | 1:N:249:LYS:HE2 | 2.01 | 0.43 |
| 1:N:719:THR:HG23 | 1:N:722:GLN:H | 1.83 | 0.43 |
| 1:N:2340:VAL:HA | 1:N:2349:ARG:NH1 | 2.33 | 0.43 |
| 1:N:2595:ARG:HG3 | 1:N:2596:VAL:HG13 | 2.00 | 0.43 |
| 1:N:2720:GLN:NE2 | 1:N:2730:TYR:HB2 | 2.17 | 0.43 |
| 1:N:3080:PHE:C | 1:N:3083:GLN:HE22 | 2.26 | 0.43 |
| 1:O:525:TRP:CE3 | 1:O:586:LEU:HD23 | 2.53 | 0.43 |
| 1:O:612:LEU:HD21 | 1:O:768:LEU:HD12 | 1.99 | 0.43 |
| 1:O:672:HIS:O | 1:O:695:ARG:NH2 | 2.41 | 0.43 |
| 1:O:1061:ALA:HA | 1:O:1064:GLN:NE2 | 2.34 | 0.43 |
| 1:O:1693:LEU:O | 1:O:1696:GLN:HG3 | 2.18 | 0.43 |
| 1:O:3045:THR:N | 1:O:3101:TYR:O | 2.40 | 0.43 |
| 1:P:42:HIS:HE1 | 1:P:70:HIS:CD2 | 2.36 | 0.43 |
| 1:P:627:THR:HG21 | 1:P:630:TYR:HD2 | 1.83 | 0.43 |
| 1:P:727:ILE:HG13 | 1:P:728:ASP:N | 2.33 | 0.43 |
| 1:P:753:LEU:HD23 | 1:P:766:ALA:HB3 | 2.01 | 0.43 |
| 1:P:905:HIS:H | 1:P:907:MET:HE1 | 1.84 | 0.43 |
| 1:P:1276:VAL:O | 1:P:1279:LEU:HG | 2.18 | 0.43 |
| 1:P:3124:ARG:HD2 | 1:P:3187:PHE:CD2 | 2.54 | 0.43 |
| 1:Q:736:THR:N | 1:Q:790:THR:OG1 | 2.49 | 0.43 |
| 1:Q:1212:GLU:CD | 1:Q:1214:ASN:H | 2.27 | 0.43 |
| 1:Q:1966:GLU:OE1 | 1:Q:1966:GLU:N | 2.39 | 0.43 |
| 1:Q:2328:ASN:HD21 | 1:R:1240:THR:HA | 1.84 | 0.43 |
| 1:Q:2587:ARG:O | 1:Q:2591:LEU:HD23 | 2.19 | 0.43 |
| 1:R:848:ARG:HE | 1:R:922:GLU:HG3 | 1.84 | 0.43 |
| 1:R:905:HIS:HA | 1:R:910:PHE:CD2 | 2.50 | 0.43 |
| 1:R:1136:LEU:O | 1:R:1140:ILE:HG12 | 2.19 | 0.43 |
| 1:R:2543:GLY:HA3 | 1:R:2546:GLU:CD | 2.44 | 0.43 |
| 1:R:2630:LEU:HG | 1:R:2632:GLU:OE1 | 2.18 | 0.43 |
| 1:R:2723:GLN:HB3 | 1:R:2728:LEU:HD11 | 2.00 | 0.43 |
| 1:S:20:GLU:HB2 | 1:S:24:ARG:CZ | 2.48 | 0.43 |
| 1:S:1133:ILE:HB | 1:S:1134:PRO:HD3 | 1.99 | 0.43 |
| 1:S:1551:ARG:HA | 1:S:1555:ARG:NH1 | 2.33 | 0.43 |
| 1:S:1978:LYS:HD2 | 1:S:2078:LYS:HZ3 | 1.83 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:S:3204:ILE:HG13 | 1:S:3205:GLU:H | 1.83 | 0.43 |
| 1:T:551:HIS:ND1 | 1:T:552:ASN:O | 2.46 | 0.43 |
| 1:T:695:ARG:O | 1:T:697:THR:N | 2.51 | 0.43 |
| 1:T:1051:LEU:HD12 | 1:T:1052:HIS:N | 2.34 | 0.43 |
| 1:T:1542:GLN:HA | 1:T:1545:GLU:OE2 | 2.19 | 0.43 |
| 1:T:1741:GLN:HE21 | 1:T:1945:PHE:HE1 | 1.67 | 0.43 |
| 1:T:3084:PHE:CD2 | 1:T:3122:ILE:HD11 | 2.53 | 0.43 |
| 1:T:3224:VAL:HG21 | 1:T:3295:LEU:HD21 | 1.99 | 0.43 |
| 1:A:869:LEU:HD13 | 1:A:928:LYS:HG3 | 2.01 | 0.43 |
| 1:A:1422:PHE:HA | 1:A:1425:GLN:NE2 | 2.34 | 0.43 |
| 1:A:2075:TYR:O | 1:B:1486:ASP:HB2 | 2.18 | 0.43 |
| 1:A:2376:ASN:N | 1:A:2379:GLU:OE2 | 2.43 | 0.43 |
| 1:A:2674:TYR:CZ | 1:A:2712:VAL:HG22 | 2.54 | 0.43 |
| 1:B:1714:HIS:HB2 | 1:B:1746:TYR:OH | 2.18 | 0.43 |
| 1:B:2574:PHE:O | 1:B:2578:HIS:ND1 | 2.36 | 0.43 |
| 1:B:2576:GLN:HE21 | 1:B:2767:PHE:HE1 | 1.66 | 0.43 |
| 1:C:636:ILE:HA | 1:C:639:LEU:HD12 | 2.00 | 0.43 |
| 1:C:969:HIS:HA | 1:C:980:ARG:HH12 | 1.84 | 0.43 |
| 1:C:1314:CYS:SG | 1:C:1497:LYS:HG2 | 2.59 | 0.43 |
| 1:C:1397:GLN:HB3 | 1:C:1399:GLU:CD | 2.44 | 0.43 |
| 1:C:1730:ALA:N | 1:C:2020:ALA:O | 2.52 | 0.43 |
| 1:C:1865:LYS:HE3 | 1:C:1867:HIS:HB2 | 1.99 | 0.43 |
| 1:C:2448:ASP:O | 1:C:2452:GLU:OE1 | 2.36 | 0.43 |
| 1:C:2573:SER:HB3 | 1:C:2739:GLU:OE2 | 2.19 | 0.43 |
| 1:C:3174:PRO:HA | 1:C:3177:ILE:HD12 | 2.00 | 0.43 |
| 1:D:245:GLU:HB2 | 1:D:249:LYS:NZ | 2.34 | 0.43 |
| 1:D:702:TYR:N | 1:D:703:GLU:OE1 | 2.51 | 0.43 |
| 1:D:1848:VAL:HA | 1:D:2026:PHE:CE1 | 2.54 | 0.43 |
| 1:D:2521:THR:HG23 | 1:D:2524:GLU:OE1 | 2.19 | 0.43 |
| 1:D:2552:GLY:HA3 | 1:D:2697:GLU:HA | 1.99 | 0.43 |
| 1:D:3344:VAL:HG12 | 1:D:3346:SER:H | 1.83 | 0.43 |
| 1:E:718:MET:SD | 1:E:722:GLN:HG2 | 2.59 | 0.43 |
| 1:E:895:ASP:OD1 | 1:E:895:ASP:N | 2.40 | 0.43 |
| 1:E:1195:ASP:OD2 | 1:E:1196:ARG:NE | 2.43 | 0.43 |
| 1:E:2095:GLU:HG3 | 1:E:2098:HIS:CD2 | 2.54 | 0.43 |
| 1:E:2916:THR:C | 1:E:2918:THR:H | 2.26 | 0.43 |
| 1:E:2972:ASP:OD1 | 1:E:2972:ASP:N | 2.51 | 0.43 |
| 1:F:640:HIS:O | 1:F:644:VAL:HG23 | 2.19 | 0.43 |
| 1:F:1124:ASP:OD1 | 1:F:1124:ASP:N | 2.49 | 0.43 |
| 1:F:2642:LEU:HD12 | 1:F:2684:TRP:HE3 | 1.84 | 0.43 |
| 1:F:2898:PRO:HG3 | 1:G:2915:PRO:HB3 | 2.00 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:G:914:HIS:CE1 | 1:G:1053:HIS:CE1 | 3.06 | 0.43 |
| 1:G:1262:SER:OG | 1:G:1263:HIS:N | 2.37 | 0.43 |
| 1:G:2102:ARG:HB3 | 1:H:1931:LEU:HD22 | 2.01 | 0.43 |
| 1:G:2665:ARG:HA | 1:G:2726:ARG:HH22 | 1.83 | 0.43 |
| 1:G:2810:GLY:HA2 | 1:G:2845:TRP:CE2 | 2.54 | 0.43 |
| 1:G:3124:ARG:O | 1:G:3128:ILE:HG23 | 2.19 | 0.43 |
| 1:H:706:LEU:HB3 | 1:H:708:TYR:CD1 | 2.53 | 0.43 |
| 1:H:1277:GLU:HA | 1:H:1280:LYS:HG2 | 2.00 | 0.43 |
| 1:H:1428:ILE:HA | 1:H:1431:ASN:HD21 | 1.83 | 0.43 |
| 1:H:1748:VAL:HA | 1:H:1751:GLU:HG2 | 2.00 | 0.43 |
| 1:H:2602:ASP:OD2 | 1:H:2604:THR:OG1 | 2.30 | 0.43 |
| 1:H:3220:SER:HB2 | 1:H:3256:TRP:O | 2.19 | 0.43 |
| 1:H:3398:GLN:OE1 | 1:H:3400:THR:OG1 | 2.25 | 0.43 |
| 1:I:193:GLY:HA3 | 1:I:201:SER:N | 2.34 | 0.43 |
| 1:I:718:MET:SD | 1:I:722:GLN:HG2 | 2.59 | 0.43 |
| 1:I:2517:ILE:HG13 | 1:I:2518:ASN:N | 2.34 | 0.43 |
| 1:I:2724:ARG:NH1 | 1:I:2730:TYR:OH | 2.42 | 0.43 |
| 1:I:2743:PRO:HA | 1:I:2762:ARG:HE | 1.84 | 0.43 |
| 1:I:2821:LEU:O | 1:I:2828:CYS:HB2 | 2.19 | 0.43 |
| 1:I:3072:LEU:HD23 | 1:I:3129:TRP:CD1 | 2.48 | 0.43 |
| 1:I:3289:LYS:HE2 | 1:I:3293:GLU:HB2 | 2.01 | 0.43 |
| 1:I:3312:ASP:OD1 | 1:I:3312:ASP:N | 2.51 | 0.43 |
| 1:J:912:HIS:NE2 | 1:J:1113:PHE:HE1 | 2.17 | 0.43 |
| 1:J:2516:ASN:OD1 | 1:J:2517:ILE:N | 2.48 | 0.43 |
| 1:J:3011:TRP:CZ3 | 1:J:3013:TRP:HA | 2.53 | 0.43 |
| 1:K:1115:TYR:CE2 | 1:K:1116:GLU:HG2 | 2.53 | 0.43 |
| 1:K:1152:GLY:HA3 | 1:K:1197:LEU:HD21 | 2.01 | 0.43 |
| 1:K:1515:ARG:O | 1:K:1519:VAL:HG23 | 2.18 | 0.43 |
| 1:K:2448:ASP:O | 1:K:2452:GLU:OE1 | 2.37 | 0.43 |
| 1:K:2465:ALA:HB2 | 1:L:1085:ARG:HD2 | 2.00 | 0.43 |
| 1:K:3334:ARG:HH21 | 1:K:3406:ILE:HG23 | 1.83 | 0.43 |
| 1:L:309:ALA:HB2 | 1:L:380:LEU:HD11 | 2.00 | 0.43 |
| 1:L:727:ILE:HG22 | 1:L:730:ARG:HH21 | 1.84 | 0.43 |
| 1:L:1042:TYR:HA | 1:L:1045:TYR:CE2 | 2.54 | 0.43 |
| 1:L:1416:GLN:HE21 | 1:L:1422:PHE:HA | 1.83 | 0.43 |
| 1:L:2093:ARG:HD3 | 1:L:2367:TYR:CE1 | 2.54 | 0.43 |
| 1:L:2494:LYS:HD3 | 1:L:2495:PRO:HD2 | 2.00 | 0.43 |
| 1:L:3032:PHE:HA | 1:L:3113:PRO:HG2 | 2.01 | 0.43 |
| 1:L:3139:SER:OG | 1:L:3142:TYR:HB3 | 2.18 | 0.43 |
| 1:L:3142:TYR:OH | 1:L:3144:ARG:HD3 | 2.18 | 0.43 |
| 1:M:1588:HIS:N | 1:P:337:GLN:OE1 | 2.41 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:M:2402:ILE:HG23 | 1:M:2404:THR:H | 1.83 | 0.43 |
| 1:M:2521:THR:HG23 | 1:M:2524:GLU:H | 1.84 | 0.43 |
| 1:M:2705:PHE:HD2 | 1:M:2706:PHE:HD1 | 1.65 | 0.43 |
| 1:M:2743:PRO:HA | 1:M:2762:ARG:NE | 2.33 | 0.43 |
| 1:N:5:ARG:HD2 | 1:N:283:TYR:CE1 | 2.53 | 0.43 |
| 1:N:471:HIS:ND1 | 1:N:471:HIS:O | 2.52 | 0.43 |
| 1:N:1051:LEU:HD12 | 1:N:1052:HIS:N | 2.33 | 0.43 |
| 1:N:1124:ASP:OD1 | 1:N:1124:ASP:N | 2.52 | 0.43 |
| 1:N:2093:ARG:HD2 | 1:N:2367:TYR:HE1 | 1.84 | 0.43 |
| 1:N:2433:GLU:OE1 | 1:N:2433:GLU:N | 2.52 | 0.43 |
| 1:N:2645:ASP:HB3 | 1:N:2649:GLY:O | 2.19 | 0.43 |
| 1:N:2686:GLY:HA3 | 1:N:2694:SER:H | 1.83 | 0.43 |
| 1:N:2788:GLN:HA | 1:N:2791:GLU:OE2 | 2.18 | 0.43 |
| 1:N:2923:ARG:HD3 | 1:N:3008:ILE:O | 2.19 | 0.43 |
| 1:N:3211:ASP:OD1 | 1:N:3309:ALA:N | 2.52 | 0.43 |
| 1:O:2167:GLN:HG2 | 1:O:2168:ALA:N | 2.34 | 0.43 |
| 1:P:73:TYR:HA | 1:P:76:GLN:OE1 | 2.18 | 0.43 |
| 1:P:848:ARG:HB2 | 1:P:934:LEU:O | 2.18 | 0.43 |
| 1:P:1363:ASN:OD1 | 1:P:1364:GLU:N | 2.50 | 0.43 |
| 1:P:2353:LEU:O | 1:P:2356:GLU:HG3 | 2.18 | 0.43 |
| 1:P:3374:ASP:N | 1:P:3379:TYR:OH | 2.40 | 0.43 |
| 1:Q:100:ILE:HD12 | 1:Q:100:ILE:HA | 1.91 | 0.43 |
| 1:Q:980:ARG:HH21 | 1:Q:1046:ASP:CG | 2.27 | 0.43 |
| 1:Q:1162:ALA:HB1 | 1:Q:1224:ILE:O | 2.19 | 0.43 |
| 1:Q:2124:GLN:OE1 | 1:Q:2124:GLN:N | 2.33 | 0.43 |
| 1:Q:2246:ASP:N | 1:Q:2246:ASP:OD1 | 2.51 | 0.43 |
| 1:Q:2345:ASN:O | 1:Q:2349:ARG:NH1 | 2.51 | 0.43 |
| 1:Q:2743:PRO:HA | 1:Q:2762:ARG:NE | 2.33 | 0.43 |
| 1:Q:2796:ARG:NH2 | 1:Q:2801:ARG:HE | 2.14 | 0.43 |
| 1:Q:3267:THR:O | 1:Q:3271:GLU:OE1 | 2.37 | 0.43 |
| 1:R:306:ARG:O | 1:R:411:ARG:NH2 | 2.47 | 0.43 |
| 1:R:867:GLN:HA | 1:R:870:GLU:HG3 | 2.01 | 0.43 |
| 1:R:887:GLN:HB3 | 1:R:1041:ARG:NH1 | 2.34 | 0.43 |
| 1:R:1305:CYS:SG | 1:R:1314:CYS:N | 2.92 | 0.43 |
| 1:R:1367:TYR:CE2 | 1:R:1369:ASP:HB3 | 2.54 | 0.43 |
| 1:R:1433:LEU:HD21 | 1:R:1460:HIS:HE2 | 1.83 | 0.43 |
| 1:R:1834:PHE:O | 1:R:1838:LEU:HG | 2.18 | 0.43 |
| 1:R:1847:GLU:HA | 1:R:1850:PHE:HB3 | 2.00 | 0.43 |
| 1:R:2369:ASP:OD1 | 1:R:2369:ASP:N | 2.51 | 0.43 |
| 1:R:2718:ILE:CD1 | 1:R:2779:LEU:HB2 | 2.49 | 0.43 |
| 1:R:2802:VAL:HG23 | 1:R:2855:VAL:HG23 | 1.99 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:R:3350:ASN:OD1 | 1:R:3372:SER:HB3 | 2.19 | 0.43 |
| 1:S:764:GLU:OE2 | 1:S:765:VAL:N | 2.52 | 0.43 |
| 1:S:913:TRP:HD1 | 1:S:1088:LEU:HD21 | 1.84 | 0.43 |
| 1:S:1186:ASP:OD2 | 1:S:1188:TYR:N | 2.49 | 0.43 |
| 1:S:1331:ASP:O | 1:S:1334:GLU:HG3 | 2.18 | 0.43 |
| 1:S:1827:ASP:HA | 1:S:1831:TRP:CZ3 | 2.53 | 0.43 |
| 1:T:1294:LYS:O | 1:T:1297:SER:OG | 2.25 | 0.43 |
| 1:T:1321:VAL:HA | 1:T:1324:HIS:CD2 | 2.54 | 0.43 |
| 1:T:2155:PRO:HB2 | 1:T:2306:TRP:CE3 | 2.54 | 0.43 |
| 1:T:2262:VAL:HG23 | 1:T:2438:PHE:CD1 | 2.53 | 0.43 |
| 1:T:2313:GLN:HA | 1:T:2316:ARG:NH1 | 2.34 | 0.43 |
| 1:A:170:GLU:OE2 | 1:A:304:ARG:HD2 | 2.19 | 0.43 |
| 1:A:181:PHE:CE1 | 1:A:219:VAL:HG13 | 2.54 | 0.43 |
| 1:A:189:HIS:HE1 | 1:A:212:PHE:CD1 | 2.37 | 0.43 |
| 1:A:724:ASP:O | 1:A:727:ILE:HG22 | 2.19 | 0.43 |
| 1:A:849:SER:OG | 1:A:850:ASP:N | 2.52 | 0.43 |
| 1:A:989:LYS:HA | 1:A:989:LYS:HD2 | 1.75 | 0.43 |
| 1:A:1145:HIS:NE2 | 1:A:1524:ASN:OD1 | 2.52 | 0.43 |
| 1:A:1225:ASP:HB3 | 1:A:1231:ILE:HD11 | 2.00 | 0.43 |
| 1:A:1295:ILE:HG13 | 1:A:1296:ALA:N | 2.34 | 0.43 |
| 1:A:1405:TYR:HA | 1:A:1408:ASN:HD21 | 1.83 | 0.43 |
| 1:A:2542:ARG:HA | 1:A:2542:ARG:HD2 | 1.85 | 0.43 |
| 1:A:2750:ASP:HA | 1:A:2758:ARG:HD2 | 2.01 | 0.43 |
| 1:A:2805:ASN:HB3 | 1:A:2850:LEU:HD21 | 2.01 | 0.43 |
| 1:A:3074:GLU:HG2 | 1:A:3075:THR:H | 1.84 | 0.43 |
| 1:A:3289:LYS:HE2 | 1:A:3293:GLU:OE1 | 2.19 | 0.43 |
| 1:B:142:ALA:HB3 | 1:B:196:HIS:ND1 | 2.34 | 0.43 |
| 1:B:171:GLU:CD | 1:B:176:HIS:HB3 | 2.43 | 0.43 |
| 1:B:365:TYR:CE2 | 1:B:367:PHE:HB2 | 2.53 | 0.43 |
| 1:B:1283:LEU:HD23 | 1:B:1284:ARG:HH12 | 1.84 | 0.43 |
| 1:B:1299:HIS:NE2 | 1:B:1315:CYS:SG | 2.92 | 0.43 |
| 1:B:1773:ASN:OD1 | 1:B:1774:SER:N | 2.52 | 0.43 |
| 1:B:2152:PRO:HD2 | 1:B:2329:TYR:CE2 | 2.54 | 0.43 |
| 1:B:2508:VAL:HG12 | 1:B:2590:THR:HG23 | 2.00 | 0.43 |
| 1:B:2712:VAL:O | 1:B:2715:GLN:HG2 | 2.19 | 0.43 |
| 1:B:2794:GLU:HA | 1:B:2794:GLU:OE2 | 2.18 | 0.43 |
| 1:B:2985:PRO:HB2 | 1:B:2989:ARG:HH21 | 1.83 | 0.43 |
| 1:B:3088:HIS:CD2 | 1:B:3092:HIS:CD2 | 3.07 | 0.43 |
| 1:C:126:PHE:O | 1:C:143:ARG:NH2 | 2.52 | 0.43 |
| 1:C:173:ASP:O | 1:C:177:PHE:N | 2.50 | 0.43 |
| 1:C:473:LEU:N | 1:C:775:LYS:HE3 | 2.33 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:964:GLU:HB2 | 1:C:965:PRO:HD2 | 2.01 | 0.43 |
| 1:C:1838:LEU:HD23 | 1:C:1895:TRP:HD1 | 1.83 | 0.43 |
| 1:C:1946:ASP:HB3 | 1:C:1950:HIS:CD2 | 2.54 | 0.43 |
| 1:C:3188:ASP:OD1 | 1:C:3189:ASN:N | 2.50 | 0.43 |
| 1:D:8:VAL:HG11 | 1:D:94:TRP:HB2 | 2.00 | 0.43 |
| 1:D:169:LEU:HA | 1:D:177:PHE:CE1 | 2.52 | 0.43 |
| 1:D:864:GLU:HA | 1:D:867:GLN:OE1 | 2.18 | 0.43 |
| 1:D:947:PRO:HB2 | 1:D:950:VAL:HG22 | 2.01 | 0.43 |
| 1:D:1710:LEU:HD13 | 1:D:1750:PHE:CE1 | 2.54 | 0.43 |
| 1:D:1884:HIS:O | 1:D:1888:THR:HG23 | 2.18 | 0.43 |
| 1:D:1910:ASN:O | 1:D:1913:LEU:HG | 2.18 | 0.43 |
| 1:D:2148:LEU:HD21 | 1:D:2153:THR:OG1 | 2.19 | 0.43 |
| 1:D:3332:VAL:O | 1:D:3407:ASP:HB2 | 2.19 | 0.43 |
| 1:E:1025:ILE:O | 1:E:1029:VAL:HG12 | 2.19 | 0.43 |
| 1:E:1163:LEU:HG | 1:E:1182:TYR:CD1 | 2.51 | 0.43 |
| 1:E:1284:ARG:HH21 | 1:E:1379:PRO:HD3 | 1.84 | 0.43 |
| 1:E:2157:TRP:HD1 | 1:E:2334:MET:HG2 | 1.83 | 0.43 |
| 1:E:2912:ASP:N | 1:E:2912:ASP:OD1 | 2.49 | 0.43 |
| 1:E:3017:SER:OG | 1:E:3019:ALA:O | 2.37 | 0.43 |
| 1:E:3091:ILE:O | 1:E:3095:VAL:HG12 | 2.19 | 0.43 |
| 1:F:914:HIS:O | 1:F:917:LEU:HG | 2.18 | 0.43 |
| 1:F:2504:ALA:HA | 1:F:2506:TYR:CE1 | 2.54 | 0.43 |
| 1:F:2581:PHE:O | 1:F:2584:THR:OG1 | 2.33 | 0.43 |
| 1:F:2671:GLU:H | 1:F:2671:GLU:CD | 2.18 | 0.43 |
| 1:F:2986:HIS:HB3 | 1:F:3177:ILE:HG21 | 2.01 | 0.43 |
| 1:F:3389:VAL:HG12 | 1:F:3401:ARG:NE | 2.34 | 0.43 |
| 1:G:41:PHE:HE1 | 1:G:253:PRO:HG2 | 1.82 | 0.43 |
| 1:G:151:GLN:N | 1:G:151:GLN:OE1 | 2.52 | 0.43 |
| 1:G:215:HIS:O | 1:G:219:VAL:HG23 | 2.19 | 0.43 |
| 1:G:312:SER:HA | 1:G:365:TYR:O | 2.18 | 0.43 |
| 1:G:854:LEU:CD1 | 1:G:858:GLN:HE21 | 2.30 | 0.43 |
| 1:G:884:PHE:CE1 | 1:G:1090:PRO:HG2 | 2.54 | 0.43 |
| 1:G:964:GLU:HB2 | 1:G:965:PRO:HD2 | 2.01 | 0.43 |
| 1:G:1307:HIS:O | 1:G:1308:GLU:HG2 | 2.19 | 0.43 |
| 1:G:2614:LEU:HD12 | 1:G:2636:ARG:NH1 | 2.34 | 0.43 |
| 1:G:2926:VAL:HG12 | 1:G:3009:PRO:HB2 | 2.01 | 0.43 |
| 1:G:3043:GLN:HG3 | 1:G:3044:VAL:N | 2.33 | 0.43 |
| 1:G:3049:GLN:HG2 | 1:G:3050:PRO:HD2 | 2.01 | 0.43 |
| 1:G:3254:MET:SD | 1:G:3255:PRO:HD2 | 2.59 | 0.43 |
| 1:H:231:LYS:HB3 | 1:H:237:TYR:CE2 | 2.52 | 0.43 |
| 1:H:300:LEU:O | 1:H:304:ARG:HG2 | 2.18 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:H:542:VAL:HA | 1:H:549:SER:HA | 2.00 | 0.43 |
| 1:H:866:LEU:HD21 | 1:H:967:PRO:HG2 | 2.00 | 0.43 |
| 1:H:954:THR:HB | 1:H:963:PRO:HB2 | 2.01 | 0.43 |
| 1:H:1695:LEU:HD23 | 1:H:1796:PRO:HG2 | 2.01 | 0.43 |
| 1:H:2583:VAL:HG21 | 1:H:2772:PHE:HD2 | 1.83 | 0.43 |
| 1:H:3023:LEU:O | 1:H:3030:ASN:ND2 | 2.50 | 0.43 |
| 1:H:3114:PHE:HD1 | 1:H:3117:ILE:HD11 | 1.84 | 0.43 |
| 1:H:3132:LEU:HG | 1:H:3136:ARG:NH1 | 2.33 | 0.43 |
| 1:I:585:ALA:HA | 1:I:588:ASP:OD2 | 2.19 | 0.43 |
| 1:I:1158:ILE:HD12 | 1:I:1158:ILE:HA | 1.88 | 0.43 |
| 1:I:1775:LEU:HD11 | 1:I:1780:ASN:HD21 | 1.84 | 0.43 |
| 1:I:2090:ASN:O | 1:I:2091:ARG:HD3 | 2.19 | 0.43 |
| 1:I:2986:HIS:HB3 | 1:I:3177:ILE:HD13 | 2.01 | 0.43 |
| 1:J:245:GLU:H | 1:J:245:GLU:CD | 2.27 | 0.43 |
| 1:J:310:LEU:HA | 1:J:367:PHE:O | 2.19 | 0.43 |
| 1:J:1672:GLU:HG3 | 1:J:1673:ARG:HG2 | 2.00 | 0.43 |
| 1:J:1678:LYS:NZ | 1:J:1683:LEU:HA | 2.34 | 0.43 |
| 1:J:2653:PHE:HA | 1:J:2656:ARG:HH22 | 1.83 | 0.43 |
| 1:K:16:VAL:HG21 | 1:K:105:ARG:HH12 | 1.84 | 0.43 |
| 1:K:1137:GLN:O | 1:K:1141:LEU:HD23 | 2.19 | 0.43 |
| 1:K:1384:LYS:HA | 1:K:1391:VAL:HG12 | 2.00 | 0.43 |
| 1:K:1788:VAL:HG12 | 1:K:1789:LEU:HD22 | 2.01 | 0.43 |
| 1:K:2311:GLU:HG2 | 1:K:2370:MET:HG2 | 2.00 | 0.43 |
| 1:K:2587:ARG:O | 1:K:2591:LEU:HD23 | 2.19 | 0.43 |
| 1:K:2870:TYR:H | 1:T:2741:ARG:HH12 | 1.66 | 0.43 |
| 1:K:2977:CYS:HA | 1:K:2987:TRP:CH2 | 2.54 | 0.43 |
| 1:K:3160:GLU:HG2 | 1:K:3169:ARG:NH2 | 2.32 | 0.43 |
| 1:L:735:ARG:NH2 | 1:L:788:GLU:HG2 | 2.34 | 0.43 |
| 1:L:937:TRP:CZ2 | 1:L:947:PRO:HD3 | 2.54 | 0.43 |
| 1:L:946:LEU:HG | 1:L:951:ALA:HB2 | 2.00 | 0.43 |
| 1:L:2994:GLN:HG2 | 1:L:3157:PHE:CZ | 2.54 | 0.43 |
| 1:L:3218:VAL:HA | 1:L:3258:TYR:HD2 | 1.83 | 0.43 |
| 1:M:276:TYR:HA | 1:M:279:LEU:HD23 | 2.00 | 0.43 |
| 1:M:598:ASP:OD1 | 1:M:599:PHE:N | 2.51 | 0.43 |
| 1:M:972:LEU:HD23 | 1:M:977:LYS:HB3 | 2.01 | 0.43 |
| 1:M:1187:GLU:HG2 | 1:M:1188:TYR:CD2 | 2.54 | 0.43 |
| 1:M:2410:PHE:O | 1:M:2422:ALA:HB3 | 2.19 | 0.43 |
| 1:M:3084:PHE:CZ | 1:M:3122:ILE:HG23 | 2.54 | 0.43 |
| 1:M:3389:VAL:HG22 | 1:M:3401:ARG:HG2 | 2.01 | 0.43 |
| 1:N:276:TYR:O | 1:N:280:GLY:N | 2.40 | 0.43 |
| 1:N:702:TYR:N | 1:N:703:GLU:OE1 | 2.52 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:N:732:THR:HG23 | 1:N:733:LYS:HE3 | 2.01 | 0.43 |
| 1:N:848:ARG:HH11 | 1:N:1123:TYR:HE1 | 1.63 | 0.43 |
| 1:N:1084:LEU:HB3 | 1:N:1110:PHE:HE1 | 1.83 | 0.43 |
| 1:N:2160:LEU:HD22 | 1:N:2337:PHE:CE2 | 2.53 | 0.43 |
| 1:N:2163:LEU:HD11 | 1:N:2363:LEU:HB3 | 2.01 | 0.43 |
| 1:N:2369:ASP:HB2 | 1:N:2371:LYS:HG2 | 2.00 | 0.43 |
| 1:O:69:TRP:CD1 | 1:O:251:LEU:HD12 | 2.46 | 0.43 |
| 1:O:471:HIS:O | 1:O:471:HIS:ND1 | 2.51 | 0.43 |
| 1:O:984:ASP:OD1 | 1:O:984:ASP:N | 2.51 | 0.43 |
| 1:O:1169:CYS:HA | 1:O:1175:CYS:HA | 2.00 | 0.43 |
| 1:O:3305:ILE:HA | 1:O:3315:VAL:O | 2.19 | 0.43 |
| 1:P:24:ARG:HD3 | 1:P:123:ASN:HA | 2.00 | 0.43 |
| 1:P:788:GLU:OE1 | 1:P:791:ASP:HB2 | 2.19 | 0.43 |
| 1:P:806:VAL:HG11 | 1:P:825:HIS:O | 2.18 | 0.43 |
| 1:P:849:SER:HA | 1:P:1124:ASP:CG | 2.44 | 0.43 |
| 1:P:1051:LEU:HD12 | 1:P:1052:HIS:N | 2.34 | 0.43 |
| 1:P:1701:ASP:OD1 | 1:P:1701:ASP:N | 2.50 | 0.43 |
| 1:P:1854:HIS:HE1 | 1:P:1885:HIS:NE2 | 2.17 | 0.43 |
| 1:P:1990:ILE:HG22 | 3:jA:2:NAG:H81 | 2.01 | 0.43 |
| 1:P:2109:ALA:HA | 1:P:2112:ARG:HG2 | 2.00 | 0.43 |
| 1:P:3316:LEU:HD11 | 1:P:3338:VAL:HG23 | 2.01 | 0.43 |
| 1:P:3353:GLU:HG2 | 1:P:3388:PHE:CD1 | 2.53 | 0.43 |
| 1:Q:13:ASP:OD1 | 1:Q:14:GLN:N | 2.52 | 0.43 |
| 1:Q:28:ASP:OD1 | 1:Q:29:ASP:N | 2.50 | 0.43 |
| 1:Q:469:GLU:OE1 | 1:Q:474:PRO:HD2 | 2.19 | 0.43 |
| 1:Q:2407:GLU:OE2 | 1:Q:2424:ALA:HB1 | 2.18 | 0.43 |
| 1:Q:2854:ASP:OD1 | 1:Q:2856:THR:HG23 | 2.19 | 0.43 |
| 1:Q:2956:ILE:HD12 | 1:Q:2959:PHE:HE2 | 1.84 | 0.43 |
| 1:Q:3308:PRO:HG2 | 1:Q:3311:ALA:HB3 | 2.01 | 0.43 |
| 1:R:35:TYR:OH | 1:R:208:TYR:HA | 2.19 | 0.43 |
| 1:R:533:PRO:HB2 | 1:R:535:ILE:HD12 | 2.01 | 0.43 |
| 1:R:552:ASN:ND2 | 1:R:554:PHE:HB2 | 2.34 | 0.43 |
| 1:R:735:ARG:NH2 | 1:R:789:ILE:H | 2.17 | 0.43 |
| 1:R:825:HIS:CD2 | 1:R:825:HIS:H | 2.37 | 0.43 |
| 1:R:1501:ASP:OD2 | 1:R:1504:GLN:N | 2.52 | 0.43 |
| 1:R:2527:SER:O | 1:R:2530:LYS:HG3 | 2.18 | 0.43 |
| 1:R:3303:VAL:HG13 | 1:R:3305:ILE:HD11 | 2.01 | 0.43 |
| 1:S:687:ASN:OD1 | 1:S:688:GLU:N | 2.51 | 0.43 |
| 1:S:1204:ASP:OD1 | 1:S:1205:ILE:N | 2.52 | 0.43 |
| 1:S:1220:LYS:NZ | 1:S:1222:SER:HB2 | 2.34 | 0.43 |
| 1:S:1867:HIS:HA | 1:S:1874:TYR:CE2 | 2.54 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:S:1989:GLY:HA2 | 1:S:2024:TRP:NE1 | 2.34 | 0.43 |
| 1:S:2056:ARG:HA | 1:S:2056:ARG:HD2 | 1.83 | 0.43 |
| 1:S:2162:THR:O | 1:S:2165:VAL:HG22 | 2.19 | 0.43 |
| 1:S:2569:HIS:HA | 1:S:2574:PHE:CE2 | 2.54 | 0.43 |
| 1:S:2752:ASN:OD1 | 1:S:2753:PRO:HD2 | 2.18 | 0.43 |
| 1:T:396:THR:HG21 | 4:T:3501:NAG:O7 | 2.18 | 0.43 |
| 1:T:1291:THR:HG22 | 1:T:1294:LYS:HZ3 | 1.84 | 0.43 |
| 1:T:1627:SER:O | 1:T:1627:SER:OG | 2.37 | 0.43 |
| 1:T:1987:LEU:HB3 | 1:T:2024:TRP:HZ3 | 1.83 | 0.43 |
| 1:T:2412:VAL:H | 1:T:2422:ALA:HB2 | 1.84 | 0.43 |
| 1:T:2623:GLU:C | 1:T:2636:ARG:HH22 | 2.27 | 0.43 |
| 1:T:2802:VAL:HG23 | 1:T:2855:VAL:HG23 | 2.00 | 0.43 |
| 1:T:2954:GLU:H | 1:T:2954:GLU:CD | 2.27 | 0.43 |
| 1:A:328:VAL:HG12 | 1:A:345:ALA:HB2 | 2.01 | 0.43 |
| 1:A:574:LEU:HD23 | 1:A:616:LEU:HG | 2.00 | 0.43 |
| 1:A:1571:VAL:HG21 | 1:A:1593:PHE:CE2 | 2.54 | 0.43 |
| 1:A:1843:TYR:O | 1:A:1847:GLU:OE1 | 2.37 | 0.43 |
| 1:A:1899:GLN:OE1 | 1:A:1904:HIS:HB2 | 2.19 | 0.43 |
| 1:A:1919:PRO:HG3 | 1:A:1940:LYS:NZ | 2.34 | 0.43 |
| 1:A:2056:ARG:NH1 | 1:A:2061:SER:O | 2.52 | 0.43 |
| 1:A:2287:HIS:HE1 | 1:A:2432:LEU:HG | 1.83 | 0.43 |
| 1:A:2408:VAL:HA | 1:A:2472:GLU:O | 2.19 | 0.43 |
| 1:B:190:TYR:CD1 | 1:B:201:SER:HB2 | 2.54 | 0.43 |
| 1:B:737:PHE:HB2 | 1:B:829:ILE:HB | 2.01 | 0.43 |
| 1:B:1058:ARG:HG2 | 1:B:1123:TYR:CE1 | 2.53 | 0.43 |
| 1:B:1303:SER:OG | 1:B:1311:LYS:O | 2.32 | 0.43 |
| 1:B:1571:VAL:HB | 1:B:1637:ILE:HG22 | 2.00 | 0.43 |
| 1:B:2264:PHE:HZ | 1:B:2302:VAL:HG13 | 1.84 | 0.43 |
| 1:B:2408:VAL:O | 1:B:2424:ALA:HA | 2.19 | 0.43 |
| 1:B:2923:ARG:HD3 | 1:B:3008:ILE:O | 2.19 | 0.43 |
| 1:B:2967:PRO:O | 1:B:2973:ARG:NH1 | 2.52 | 0.43 |
| 1:B:3203:ILE:HG22 | 1:B:3207:LEU:HD23 | 2.00 | 0.43 |
| 1:C:191:LEU:HG | 1:C:349:PHE:HE2 | 1.83 | 0.43 |
| 1:C:577:LYS:HD3 | 1:C:577:LYS:HA | 1.72 | 0.43 |
| 1:C:1998:ILE:HG13 | 1:C:2010:ALA:HB3 | 2.01 | 0.43 |
| 1:C:2190:LEU:HD21 | 1:C:2194:PHE:HD2 | 1.84 | 0.43 |
| 1:C:3299:LEU:HD23 | 1:C:3299:LEU:HA | 1.84 | 0.43 |
| 1:D:1356:ARG:NH1 | 1:D:1356:ARG:HA | 2.34 | 0.43 |
| 1:D:2805:ASN:HD21 | 1:D:2850:LEU:HB3 | 1.84 | 0.43 |
| 1:D:3171:ASN:OD1 | 1:D:3176:GLN:HB3 | 2.18 | 0.43 |
| 1:D:3225:SER:O | 1:D:3290:TYR:N | 2.52 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:E:193:GLY:HA3 | 1:E:201:SER:N | 2.34 | 0.43 |
| 1:E:254:PHE:HB3 | 1:E:264:THR:HB | 2.00 | 0.43 |
| 1:E:1474:LEU:HD11 | 1:E:1543:LEU:HD11 | 2.00 | 0.43 |
| 1:E:1734:HIS:CD2 | 1:E:2016:LEU:HD11 | 2.53 | 0.43 |
| 1:E:1989:GLY:HA2 | 1:E:2024:TRP:NE1 | 2.34 | 0.43 |
| 1:E:2149:HIS:HA | 1:E:2154:PHE:HD2 | 1.84 | 0.43 |
| 1:E:2570:GLY:H | 1:E:2574:PHE:HE2 | 1.66 | 0.43 |
| 1:E:3205:GLU:O | 1:F:1117:ARG:NH2 | 2.52 | 0.43 |
| 1:F:42:HIS:HB3 | 1:F:207:ALA:HB1 | 2.00 | 0.43 |
| 1:F:1679:SER:OG | 1:F:1680:VAL:N | 2.52 | 0.43 |
| 1:F:2271:ILE:HD12 | 1:F:2298:HIS:CE1 | 2.54 | 0.43 |
| 1:F:2398:LEU:HD12 | 1:F:2399:LEU:H | 1.83 | 0.43 |
| 1:G:94:TRP:HB2 | 1:G:214:LEU:HD12 | 2.01 | 0.43 |
| 1:G:240:ALA:HB2 | 1:G:247:PHE:CD2 | 2.54 | 0.43 |
| 1:G:461:VAL:HA | 1:G:1371:ARG:HD3 | 2.01 | 0.43 |
| 1:G:539:GLU:HA | 1:G:555:PHE:HB2 | 2.00 | 0.43 |
| 1:G:984:ASP:OD1 | 1:G:984:ASP:N | 2.51 | 0.43 |
| 1:G:1460:HIS:O | 1:G:1464:VAL:HG23 | 2.19 | 0.43 |
| 1:G:1760:LEU:HD12 | 1:G:1761:VAL:HB | 2.00 | 0.43 |
| 1:G:2448:ASP:O | 1:G:2452:GLU:OE1 | 2.37 | 0.43 |
| 1:G:2658:ILE:HG23 | 1:G:2659:LEU:HD12 | 2.01 | 0.43 |
| 1:H:1457:PHE:CE1 | 1:H:1461:HIS:HE1 | 2.37 | 0.43 |
| 1:H:2432:LEU:N | 1:H:2433:GLU:OE1 | 2.51 | 0.43 |
| 1:H:3113:PRO:O | 1:H:3117:ILE:HG23 | 2.19 | 0.43 |
| 1:I:14:GLN:HG2 | 1:I:15:GLU:N | 2.33 | 0.43 |
| 1:I:869:LEU:HA | 1:I:869:LEU:HD12 | 1.84 | 0.43 |
| 1:I:1247:SER:HA | 1:I:1250:LYS:HG2 | 2.01 | 0.43 |
| 1:I:1788:VAL:HG12 | 1:I:1789:LEU:HD22 | 2.01 | 0.43 |
| 1:I:1974:LYS:HE3 | 1:I:2361:GLN:HB3 | 2.00 | 0.43 |
| 1:I:2311:GLU:HG2 | 1:I:2370:MET:HG2 | 2.00 | 0.43 |
| 1:I:2876:ILE:HD11 | 1:I:2885:ALA:O | 2.19 | 0.43 |
| 1:J:171:GLU:HB3 | 1:J:177:PHE:HD1 | 1.84 | 0.43 |
| 1:J:1012:CYS:SG | 1:J:1196:ARG:NH1 | 2.88 | 0.43 |
| 1:J:1125:ASP:OD1 | 1:J:1125:ASP:N | 2.50 | 0.43 |
| 1:J:1968:LEU:HA | 1:J:1971:LEU:HB3 | 2.01 | 0.43 |
| 1:J:2504:ALA:HA | 1:J:2506:TYR:CE1 | 2.53 | 0.43 |
| 1:J:2552:GLY:O | 1:J:2555:GLY:N | 2.51 | 0.43 |
| 1:J:2923:ARG:CZ | 1:J:3006:LEU:HB3 | 2.48 | 0.43 |
| 1:K:408:GLY:HA3 | 1:K:669:THR:HG23 | 2.00 | 0.43 |
| 1:K:914:HIS:CE1 | 1:K:1053:HIS:CE1 | 3.07 | 0.43 |
| 1:K:3138:ARG:HD3 | 1:K:3138:ARG:HA | 1.78 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:K:3301:THR:HG22 | 1:K:3326:LEU:HA | 2.00 | 0.43 |
| 1:L:245:GLU:CD | 1:L:245:GLU:H | 2.26 | 0.43 |
| 1:L:720:ILE:HG13 | 1:L:721:ASP:N | 2.34 | 0.43 |
| 1:L:1713:PHE:CZ | 1:L:1929:TYR:HB3 | 2.54 | 0.43 |
| 1:L:2130:HIS:NE2 | 1:L:2147:CYS:SG | 2.92 | 0.43 |
| 1:L:2238:ASP:OD1 | 1:L:2239:GLY:N | 2.52 | 0.43 |
| 1:L:2657:GLN:N | 1:L:2657:GLN:OE1 | 2.52 | 0.43 |
| 1:L:2737:ILE:H | 1:L:2737:ILE:HD12 | 1.84 | 0.43 |
| 1:L:2923:ARG:HD3 | 1:L:3008:ILE:C | 2.44 | 0.43 |
| 1:M:758:LYS:HD3 | 1:M:758:LYS:HA | 1.67 | 0.43 |
| 1:M:1517:ILE:H | 1:M:1517:ILE:HD12 | 1.84 | 0.43 |
| 1:M:1543:LEU:O | 1:M:1547:LEU:HD23 | 2.19 | 0.43 |
| 1:M:1721:PRO:HD3 | 1:M:1729:TYR:CE1 | 2.53 | 0.43 |
| 1:M:1868:SER:O | 1:M:1874:TYR:HB2 | 2.19 | 0.43 |
| 1:M:2867:ASP:N | 1:M:2867:ASP:OD1 | 2.51 | 0.43 |
| 1:N:48:CYS:HB2 | 1:N:58:CYS:HB2 | 1.45 | 0.43 |
| 1:N:327:LYS:HG3 | 1:N:343:GLU:O | 2.19 | 0.43 |
| 1:N:859:VAL:O | 1:N:862:LEU:HG | 2.18 | 0.43 |
| 1:N:1270:ASP:OD1 | 1:N:1271:LEU:N | 2.52 | 0.43 |
| 1:N:1301:PHE:CD1 | 1:N:1302:PRO:HA | 2.54 | 0.43 |
| 1:N:1351:TRP:HZ3 | 1:N:1463:ASN:HB3 | 1.84 | 0.43 |
| 1:N:1908:GLU:OE2 | 1:N:1910:ASN:HB3 | 2.19 | 0.43 |
| 1:N:2656:ARG:O | 1:N:2659:LEU:HG | 2.19 | 0.43 |
| 1:N:2675:GLU:HG3 | 1:N:2847:PHE:CZ | 2.53 | 0.43 |
| 1:N:3200:ILE:HA | 1:N:3203:ILE:HB | 2.00 | 0.43 |
| 1:O:230:GLN:NE2 | 1:O:235:LYS:HB2 | 2.34 | 0.43 |
| 1:O:257:ASP:O | 1:O:265:ARG:NH2 | 2.47 | 0.43 |
| 1:O:455:PHE:HD1 | 1:O:514:ARG:HE | 1.65 | 0.43 |
| 1:O:729:GLU:O | 1:O:732:THR:HG22 | 2.19 | 0.43 |
| 1:O:1161:SER:N | 1:O:1185:GLY:O | 2.52 | 0.43 |
| 1:O:1426:PHE:HZ | 1:O:1464:VAL:HG13 | 1.84 | 0.43 |
| 1:O:2099:LEU:HD13 | 1:O:2103:ALA:HB3 | 2.01 | 0.43 |
| 1:O:2256:ASP:HB3 | 1:O:2259:ASP:HB2 | 2.01 | 0.43 |
| 1:O:2356:GLU:OE1 | 1:O:2356:GLU:N | 2.46 | 0.43 |
| 1:O:3251:ASP:OD1 | 1:O:3251:ASP:N | 2.51 | 0.43 |
| 1:O:3353:GLU:CD | 1:P:3148:ARG:HH12 | 2.27 | 0.43 |
| 1:P:418:ASP:OD2 | 1:P:661:PRO:HA | 2.18 | 0.43 |
| 1:P:1010:ASP:OD1 | 1:P:1011:PHE:N | 2.52 | 0.43 |
| 1:P:1445:LEU:HD23 | 1:P:1445:LEU:HA | 1.82 | 0.43 |
| 1:P:1722:TYR:HD2 | 1:P:1725:ALA:HB2 | 1.84 | 0.43 |
| 1:P:1813:PHE:C | 1:P:1814:LYS:HD3 | 2.44 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:P:2922:VAL:HG22 | 1:P:3186:ASN:OD1 | 2.18 | 0.43 |
| 1:P:2929:LEU:HG | 1:P:2934:VAL:HG23 | 2.00 | 0.43 |
| 1:P:3148:ARG:HG2 | 1:P:3152:ARG:NH1 | 2.34 | 0.43 |
| 1:Q:230:GLN:NE2 | 1:Q:235:LYS:O | 2.52 | 0.43 |
| 1:Q:850:ASP:O | 1:Q:853:SER:OG | 2.35 | 0.43 |
| 1:Q:2304:LYS:HB2 | 1:Q:2367:TYR:CE2 | 2.54 | 0.43 |
| 1:Q:2581:PHE:O | 1:Q:2584:THR:HG22 | 2.19 | 0.43 |
| 1:Q:2878:ALA:HB3 | 1:Q:2882:THR:HB | 2.00 | 0.43 |
| 1:Q:2977:CYS:HA | 1:Q:2987:TRP:CH2 | 2.53 | 0.43 |
| 1:Q:2997:MET:HE2 | 1:Q:2997:MET:HB2 | 1.86 | 0.43 |
| 1:R:24:ARG:HD2 | 1:R:24:ARG:HA | 1.71 | 0.43 |
| 1:R:32:VAL:HA | 1:R:37:ASN:ND2 | 2.33 | 0.43 |
| 1:R:1063:TRP:NE1 | 1:R:1067:GLN:HE22 | 2.17 | 0.43 |
| 1:R:1273:GLU:OE1 | 1:R:1273:GLU:N | 2.48 | 0.43 |
| 1:R:1321:VAL:HA | 1:R:1324:HIS:CD2 | 2.53 | 0.43 |
| 1:R:1605:ILE:HD12 | 1:R:1605:ILE:HA | 1.89 | 0.43 |
| 1:R:2453:LEU:HD23 | 1:R:2453:LEU:HA | 1.92 | 0.43 |
| 1:R:2504:ALA:C | 1:R:2506:TYR:H | 2.27 | 0.43 |
| 1:S:834:THR:OG1 | 1:S:835:THR:N | 2.52 | 0.43 |
| 1:S:855:THR:OG1 | 1:S:856:ARG:N | 2.50 | 0.43 |
| 1:S:1100:ASP:O | 1:S:1104:ARG:NH1 | 2.52 | 0.43 |
| 1:S:1413:ALA:HB1 | 1:S:1425:GLN:OE1 | 2.18 | 0.43 |
| 1:S:1515:ARG:O | 1:S:1519:VAL:HG23 | 2.19 | 0.43 |
| 1:S:2439:ASP:CG | 1:S:2440:ARG:HE | 2.27 | 0.43 |
| 1:S:2448:ASP:O | 1:S:2452:GLU:OE1 | 2.37 | 0.43 |
| 1:S:2664:GLN:NE2 | 1:S:2670:PHE:HA | 2.31 | 0.43 |
| 1:T:887:GLN:OE1 | 1:T:901:ALA:HB2 | 2.19 | 0.43 |
| 1:T:1276:VAL:O | 1:T:1279:LEU:HG | 2.18 | 0.43 |
| 1:T:1912:ALA:O | 1:T:1916:MET:HB2 | 2.18 | 0.43 |
| 1:T:2254:GLN:HE21 | 1:T:2260:PHE:HA | 1.84 | 0.43 |
| 1:T:2313:GLN:NE2 | 1:T:2318:LEU:HB2 | 2.34 | 0.43 |
| 1:T:3148:ARG:HG2 | 1:T:3152:ARG:HH12 | 1.84 | 0.43 |
| 1:T:3325:LYS:HD2 | 1:T:3325:LYS:HA | 1.85 | 0.43 |
| 1:A:1284:ARG:CZ | 1:A:1379:PRO:HG3 | 2.49 | 0.42 |
| 1:A:1645:LEU:HA | 1:D:483:ARG:NH2 | 2.33 | 0.42 |
| 1:A:2162:THR:O | 1:A:2165:VAL:HG22 | 2.19 | 0.42 |
| 1:A:2553:TYR:O | 1:A:2701:TYR:OH | 2.37 | 0.42 |
| 1:A:2641:GLN:HG2 | 1:A:2684:TRP:CH2 | 2.54 | 0.42 |
| 1:B:6:LYS:HD2 | 1:B:11:LEU:HD13 | 2.00 | 0.42 |
| 1:B:8:VAL:HA | 1:B:11:LEU:HD23 | 2.01 | 0.42 |
| 1:B:891:CYS:SG | 1:B:899:LYS:NZ | 2.74 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:2848:ASP:OD1 | 1:B:2849:ARG:N | 2.52 | 0.42 |
| 1:C:855:THR:O | 1:C:859:VAL:HG23 | 2.19 | 0.42 |
| 1:C:1161:SER:HB3 | 1:C:1184:LEU:HA | 2.01 | 0.42 |
| 1:C:1166:LEU:HD22 | 1:C:1200:TYR:HD2 | 1.84 | 0.42 |
| 1:C:1515:ARG:O | 1:C:1519:VAL:HG23 | 2.19 | 0.42 |
| 1:C:2111:LEU:HD12 | 1:C:2211:PRO:HG2 | 2.01 | 0.42 |
| 1:C:2325:CYS:HA | 1:D:1242:VAL:HG13 | 2.01 | 0.42 |
| 1:C:2449:THR:HA | 1:C:2452:GLU:CD | 2.44 | 0.42 |
| 1:C:2531:ALA:O | 1:C:2535:VAL:HG23 | 2.19 | 0.42 |
| 1:C:2533:ARG:HA | 1:C:2536:GLN:OE1 | 2.18 | 0.42 |
| 1:C:2738:GLN:OE1 | 1:C:2738:GLN:N | 2.51 | 0.42 |
| 1:C:2773:ASN:CG | 1:C:3141:ASN:HB2 | 2.44 | 0.42 |
| 1:C:3085:GLU:HG3 | 1:C:3086:MET:HE2 | 2.01 | 0.42 |
| 1:D:68:GLN:O | 1:D:71:ARG:HG2 | 2.18 | 0.42 |
| 1:D:625:LEU:HD12 | 1:D:631:SER:OG | 2.19 | 0.42 |
| 1:D:1136:LEU:O | 1:D:1140:ILE:HG12 | 2.19 | 0.42 |
| 1:D:1165:THR:N | 1:D:1222:SER:O | 2.37 | 0.42 |
| 1:D:1694:ALA:O | 1:D:1697:SER:OG | 2.27 | 0.42 |
| 1:D:1753:ALA:O | 1:D:1757:ARG:HG2 | 2.19 | 0.42 |
| 1:D:2101:ALA:O | 1:D:2105:MET:HG3 | 2.18 | 0.42 |
| 1:E:38:LEU:HD11 | 1:E:76:GLN:OE1 | 2.18 | 0.42 |
| 1:E:460:SER:O | 1:E:1371:ARG:NH1 | 2.48 | 0.42 |
| 1:E:471:HIS:O | 1:E:471:HIS:ND1 | 2.52 | 0.42 |
| 1:E:635:PRO:O | 1:E:638:ILE:HG12 | 2.19 | 0.42 |
| 1:E:754:SER:HA | 1:E:765:VAL:HG23 | 2.01 | 0.42 |
| 1:E:2536:GLN:HE22 | 1:E:2621:PRO:HB2 | 1.84 | 0.42 |
| 1:E:3048:VAL:HG22 | 1:E:3095:VAL:HG23 | 2.01 | 0.42 |
| 1:E:3064:LEU:O | 1:E:3067:GLN:HG3 | 2.19 | 0.42 |
| 1:E:3251:ASP:N | 1:E:3251:ASP:OD1 | 2.52 | 0.42 |
| 1:F:200:LEU:HD23 | 1:F:206:SER:HA | 1.99 | 0.42 |
| 1:F:252:GLU:OE1 | 1:F:256:ARG:NH2 | 2.52 | 0.42 |
| 1:F:984:ASP:OD2 | 1:F:985:GLU:N | 2.51 | 0.42 |
| 1:F:1865:LYS:NZ | 1:F:1866:GLU:OE2 | 2.49 | 0.42 |
| 1:F:2152:PRO:HD2 | 1:F:2329:TYR:HD2 | 1.82 | 0.42 |
| 1:F:3036:GLN:OE1 | 1:F:3042:HIS:N | 2.52 | 0.42 |
| 1:F:3191:ASN:HA | 1:F:3195:HIS:O | 2.18 | 0.42 |
| 1:G:329:CYS:HB3 | 1:G:342:CYS:HB2 | 1.88 | 0.42 |
| 1:G:724:ASP:O | 1:G:727:ILE:HG22 | 2.19 | 0.42 |
| 1:G:989:LYS:HA | 1:G:989:LYS:HD2 | 1.82 | 0.42 |
| 1:G:1272:SER:OG | 1:G:1275:GLU:OE1 | 2.34 | 0.42 |
| 1:G:1452:ALA:HA | 1:G:1457:PHE:CG | 2.54 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:G:2099:LEU:HD13 | 1:G:2103:ALA:HB3 | 2.00 | 0.42 |
| 1:G:2551:HIS:HB2 | 1:G:2581:PHE:CE2 | 2.54 | 0.42 |
| 1:G:2578:HIS:CG | 1:G:2709:HIS:HE1 | 2.37 | 0.42 |
| 1:H:59:CYS:C | 1:H:61:HIS:HD1 | 2.26 | 0.42 |
| 1:H:702:TYR:HB2 | 1:H:708:TYR:CE1 | 2.54 | 0.42 |
| 1:H:914:HIS:O | 1:H:918:THR:HG23 | 2.18 | 0.42 |
| 1:H:1164:VAL:HA | 1:H:1223:VAL:HA | 2.01 | 0.42 |
| 1:H:1452:ALA:HA | 1:H:1457:PHE:CG | 2.54 | 0.42 |
| 1:H:1956:ASP:OD1 | 1:H:1957:THR:N | 2.52 | 0.42 |
| 1:H:2511:ILE:HD12 | 1:H:2773:ASN:HB2 | 2.00 | 0.42 |
| 1:H:2645:ASP:HB3 | 1:H:2649:GLY:O | 2.19 | 0.42 |
| 1:I:9:ASP:OD1 | 1:I:9:ASP:N | 2.51 | 0.42 |
| 1:I:197:ASP:OD1 | 1:I:198:HIS:N | 2.52 | 0.42 |
| 1:I:763:TYR:HE2 | 1:I:792:ALA:HB1 | 1.84 | 0.42 |
| 1:I:1015:GLU:N | 1:I:1015:GLU:OE1 | 2.52 | 0.42 |
| 1:I:1221:TYR:OH | 1:I:1236:PHE:N | 2.41 | 0.42 |
| 1:I:1457:PHE:O | 1:I:1461:HIS:ND1 | 2.35 | 0.42 |
| 1:I:1539:THR:H | 1:I:1542:GLN:NE2 | 2.17 | 0.42 |
| 1:I:1834:PHE:CE1 | 1:I:1853:ALA:HB1 | 2.54 | 0.42 |
| 1:I:2136:CYS:HB3 | 1:I:2144:TYR:C | 2.44 | 0.42 |
| 1:I:2655:TYR:HA | 1:I:2658:ILE:HG22 | 2.00 | 0.42 |
| 1:I:3289:LYS:HE2 | 1:I:3293:GLU:OE1 | 2.19 | 0.42 |
| 1:J:24:ARG:HD2 | 1:J:24:ARG:HA | 1.74 | 0.42 |
| 1:J:30:LYS:HD3 | 1:J:30:LYS:HA | 1.88 | 0.42 |
| 1:J:343:GLU:HG2 | 1:J:376:LEU:HD13 | 2.01 | 0.42 |
| 1:J:657:LYS:NZ | 1:J:724:ASP:OD2 | 2.51 | 0.42 |
| 1:J:1262:SER:OG | 1:J:1263:HIS:N | 2.49 | 0.42 |
| 1:J:1301:PHE:CD1 | 1:J:1302:PRO:HA | 2.54 | 0.42 |
| 1:J:1496:LEU:HD23 | 1:J:1497:LYS:O | 2.18 | 0.42 |
| 1:J:2112:ARG:HH11 | 1:J:2208:LEU:HD22 | 1.84 | 0.42 |
| 1:K:646:ARG:NH2 | 1:K:714:GLN:O | 2.34 | 0.42 |
| 1:K:730:ARG:O | 1:K:735:ARG:NH2 | 2.52 | 0.42 |
| 1:K:888:PRO:HG2 | 1:K:890:TRP:CH2 | 2.54 | 0.42 |
| 1:K:1159:ARG:C | 1:K:1160:LYS:HD3 | 2.44 | 0.42 |
| 1:K:1928:PRO:HD2 | 1:K:1929:TYR:CE1 | 2.54 | 0.42 |
| 1:K:2407:GLU:HB2 | 1:K:2426:PHE:CE2 | 2.53 | 0.42 |
| 1:K:2989:ARG:HH21 | 1:K:3180:ALA:HB2 | 1.83 | 0.42 |
| 1:L:1363:ASN:OD1 | 1:L:1364:GLU:N | 2.52 | 0.42 |
| 1:L:1802:ILE:HG22 | 1:L:1877:TYR:CD1 | 2.54 | 0.42 |
| 1:L:3149:ASN:ND2 | 1:L:3149:ASN:O | 2.52 | 0.42 |
| 1:M:1094:THR:HG22 | 1:M:1095:SER:H | 1.84 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:M:3229:ASN:HB3 | 1:M:3286:THR:OG1 | 2.19 | 0.42 |
| 1:N:185:HIS:CE1 | 1:N:219:VAL:HG21 | 2.53 | 0.42 |
| 1:N:456:GLN:OE1 | 1:N:553:PRO:HB2 | 2.19 | 0.42 |
| 1:N:552:ASN:ND2 | 1:N:554:PHE:HB2 | 2.34 | 0.42 |
| 1:N:635:PRO:O | 1:N:638:ILE:HG22 | 2.18 | 0.42 |
| 1:N:1009:THR:HA | 1:N:1070:ARG:NH2 | 2.33 | 0.42 |
| 1:N:1206:LEU:HD12 | 1:N:1206:LEU:HA | 1.87 | 0.42 |
| 1:N:1301:PHE:CG | 1:N:1302:PRO:HA | 2.53 | 0.42 |
| 1:N:1678:LYS:NZ | 1:N:1683:LEU:HA | 2.33 | 0.42 |
| 1:N:2695:THR:HG21 | 1:N:2698:TYR:CD2 | 2.54 | 0.42 |
| 1:O:72:LEU:HA | 1:O:75:VAL:HG12 | 2.00 | 0.42 |
| 1:O:294:GLU:H | 1:O:294:GLU:CD | 2.25 | 0.42 |
| 1:O:399:ASN:HD21 | 1:O:401:ASN:HD21 | 1.66 | 0.42 |
| 1:O:742:LEU:HB2 | 1:O:781:PHE:HD2 | 1.84 | 0.42 |
| 1:O:1010:ASP:OD2 | 1:O:1013:THR:HG23 | 2.19 | 0.42 |
| 1:O:1249:THR:O | 1:O:1251:LYS:NZ | 2.31 | 0.42 |
| 1:O:2966:CYS:HB3 | 1:O:2974:TYR:O | 2.19 | 0.42 |
| 1:P:148:ARG:HB2 | 1:P:191:LEU:HD11 | 2.00 | 0.42 |
| 1:P:1019:GLU:HA | 1:P:1022:HIS:ND1 | 2.33 | 0.42 |
| 1:P:1055:ASN:O | 1:P:1059:ILE:HG13 | 2.19 | 0.42 |
| 1:P:1131:PHE:HB3 | 1:P:1136:LEU:HD21 | 2.01 | 0.42 |
| 1:P:1895:TRP:HA | 1:P:1898:LEU:HD12 | 1.99 | 0.42 |
| 1:P:2088:PRO:HA | 1:P:2089:PRO:HD2 | 1.91 | 0.42 |
| 1:Q:221:ARG:NH2 | 1:Q:287:SER:O | 2.52 | 0.42 |
| 1:Q:326:ILE:HD12 | 1:Q:326:ILE:HA | 1.89 | 0.42 |
| 1:Q:1001:MET:HE2 | 1:Q:1001:MET:HB3 | 1.92 | 0.42 |
| 1:Q:1138:ARG:NH2 | 1:Q:1261:SER:HB3 | 2.33 | 0.42 |
| 1:Q:1852:ILE:HD13 | 1:Q:2030:TYR:OH | 2.19 | 0.42 |
| 1:Q:1989:GLY:N | 1:Q:2024:TRP:O | 2.51 | 0.42 |
| 1:Q:2112:ARG:HB3 | 1:Q:2116:LYS:HZ1 | 1.84 | 0.42 |
| 1:Q:3100:THR:HA | 1:Q:3290:TYR:CE2 | 2.51 | 0.42 |
| 1:R:71:ARG:NH1 | 1:R:273:LEU:O | 2.31 | 0.42 |
| 1:R:1717:PRO:HA | 1:R:1718:PRO:HD3 | 1.96 | 0.42 |
| 1:R:2516:ASN:OD1 | 1:R:2517:ILE:N | 2.48 | 0.42 |
| 1:S:181:PHE:CE2 | 1:S:219:VAL:HG13 | 2.54 | 0.42 |
| 1:S:1307:HIS:HB3 | 1:S:1312:VAL:HG11 | 2.01 | 0.42 |
| 1:S:2256:ASP:OD2 | 1:S:2258:CYS:HB2 | 2.19 | 0.42 |
| 1:S:2415:GLU:CD | 1:S:2466:PRO:HA | 2.44 | 0.42 |
| 1:T:1560:PHE:HZ | 1:T:1573:LEU:HD11 | 1.83 | 0.42 |
| 1:T:2398:LEU:HD12 | 1:T:2399:LEU:H | 1.84 | 0.42 |
| 1:T:3262:TYR:HE2 | 1:T:3264:TYR:HD2 | 1.67 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:177:PHE:O | 1:A:181:PHE:HB2 | 2.19 | 0.42 |
| 1:A:603:GLU:O | 1:A:607:GLU:OE1 | 2.36 | 0.42 |
| 1:A:1324:HIS:O | 1:A:1328:LEU:HD23 | 2.19 | 0.42 |
| 1:A:1433:LEU:HA | 1:A:1436:LEU:HB2 | 2.01 | 0.42 |
| 1:A:1732:CYS:C | 1:A:1734:HIS:HD1 | 2.26 | 0.42 |
| 1:A:2250:LEU:HA | 1:A:2253:GLU:OE1 | 2.18 | 0.42 |
| 1:A:2392:ARG:HB3 | 1:A:2394:PHE:HE1 | 1.83 | 0.42 |
| 1:A:3013:TRP:CD1 | 1:A:3013:TRP:H | 2.36 | 0.42 |
| 1:A:3103:MET:HA | 1:A:3109:SER:HA | 2.01 | 0.42 |
| 1:B:59:CYS:C | 1:B:61:HIS:HD1 | 2.26 | 0.42 |
| 1:B:703:GLU:N | 1:B:703:GLU:OE1 | 2.52 | 0.42 |
| 1:B:938:ASP:HA | 1:B:1055:ASN:ND2 | 2.33 | 0.42 |
| 1:B:1275:GLU:OE1 | 1:B:1275:GLU:N | 2.44 | 0.42 |
| 1:B:1750:PHE:CG | 1:B:1882:LEU:HD11 | 2.54 | 0.42 |
| 1:C:5:ARG:HD3 | 1:C:5:ARG:HA | 1.87 | 0.42 |
| 1:C:129:GLU:HG2 | 1:C:139:THR:C | 2.44 | 0.42 |
| 1:C:973:VAL:N | 1:C:976:LYS:O | 2.34 | 0.42 |
| 1:C:997:LYS:O | 1:C:1001:MET:HG3 | 2.18 | 0.42 |
| 1:C:1745:LEU:HA | 1:C:1748:VAL:HG12 | 2.01 | 0.42 |
| 1:C:3068:THR:O | 1:C:3071:THR:OG1 | 2.31 | 0.42 |
| 1:D:22:TYR:O | 1:D:25:GLU:HG3 | 2.18 | 0.42 |
| 1:D:866:LEU:HD22 | 1:D:968:PHE:CZ | 2.54 | 0.42 |
| 1:D:1080:ALA:HB1 | 1:D:1083:SER:OG | 2.19 | 0.42 |
| 1:D:1633:LEU:HD11 | 1:D:1653:PRO:HG2 | 2.01 | 0.42 |
| 1:D:1849:GLN:O | 1:D:1852:ILE:HG22 | 2.19 | 0.42 |
| 1:D:2270:ALA:HA | 1:D:2426:PHE:HD2 | 1.84 | 0.42 |
| 1:D:2343:ASN:HD21 | 1:D:2345:ASN:HB3 | 1.83 | 0.42 |
| 1:D:2741:ARG:HH22 | 1:E:2870:TYR:HE1 | 1.66 | 0.42 |
| 1:D:2930:SER:O | 1:D:2934:VAL:HG23 | 2.19 | 0.42 |
| 1:E:481:ASP:OD1 | 1:H:1644:TYR:N | 2.51 | 0.42 |
| 1:E:885:HIS:HD2 | 1:E:913:TRP:CZ3 | 2.37 | 0.42 |
| 1:E:1756:ARG:HH12 | 1:F:2102:ARG:NE | 2.18 | 0.42 |
| 1:E:1913:LEU:HB3 | 1:F:1655:LEU:HD21 | 2.01 | 0.42 |
| 1:E:2353:LEU:HD13 | 1:E:2355:LYS:HD3 | 2.02 | 0.42 |
| 1:E:2371:LYS:HA | 1:E:2371:LYS:HD2 | 1.82 | 0.42 |
| 1:E:2601:TRP:CZ2 | 1:E:2603:TRP:HB3 | 2.54 | 0.42 |
| 1:E:2700:ALA:HA | 1:E:2705:PHE:CD2 | 2.54 | 0.42 |
| 1:F:597:ARG:CZ | 1:F:658:ARG:HG3 | 2.48 | 0.42 |
| 1:F:2964:LYS:HG2 | 1:F:2973:ARG:HB2 | 2.01 | 0.42 |
| 1:F:3225:SER:O | 1:F:3290:TYR:N | 2.44 | 0.42 |
| 1:F:3396:CYS:HA | 1:F:3401:ARG:NH1 | 2.34 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:G:1153:PHE:HB2 | 1:G:1198:PHE:HD2 | 1.85 | 0.42 |
| 1:G:1966:GLU:HG2 | 1:G:1967:LEU:N | 2.35 | 0.42 |
| 1:H:437:VAL:HG12 | 1:H:521:PRO:HG2 | 2.00 | 0.42 |
| 1:H:1359:PRO:HG2 | 1:H:1362:ILE:HG12 | 2.00 | 0.42 |
| 1:H:1744:ARG:HH21 | 1:H:1892:TYR:HD2 | 1.66 | 0.42 |
| 1:H:2392:ARG:HB2 | 1:H:2494:LYS:HB3 | 2.01 | 0.42 |
| 1:H:2695:THR:HG21 | 1:H:2698:TYR:HD2 | 1.84 | 0.42 |
| 1:I:972:LEU:HD23 | 1:I:977:LYS:HB3 | 2.01 | 0.42 |
| 1:I:1025:ILE:HD12 | 1:I:1028:LEU:HD23 | 2.01 | 0.42 |
| 1:I:1420:CYS:HB2 | 1:I:1608:ARG:NH2 | 2.34 | 0.42 |
| 1:I:1577:VAL:H | 1:I:1584:ARG:HH22 | 1.68 | 0.42 |
| 1:I:1829:TRP:NE1 | 1:I:1833:GLN:HE22 | 2.17 | 0.42 |
| 1:I:2956:ILE:HD12 | 1:I:2959:PHE:CE2 | 2.54 | 0.42 |
| 1:I:3019:ALA:HA | 1:I:3053:TYR:CZ | 2.53 | 0.42 |
| 1:I:3342:SER:OG | 1:I:3347:LEU:O | 2.30 | 0.42 |
| 1:J:221:ARG:O | 1:J:225:ILE:HG12 | 2.20 | 0.42 |
| 1:J:847:VAL:HA | 1:J:1122:HIS:O | 2.19 | 0.42 |
| 1:J:1713:PHE:CE1 | 1:J:1929:TYR:HB3 | 2.52 | 0.42 |
| 1:J:2602:ASP:HA | 1:J:2711:ASN:ND2 | 2.33 | 0.42 |
| 1:J:2637:SER:HB3 | 1:J:2686:GLY:O | 2.19 | 0.42 |
| 1:J:2923:ARG:HE | 1:J:2924:TYR:N | 2.14 | 0.42 |
| 1:J:3080:PHE:HA | 1:J:3083:GLN:HE22 | 1.83 | 0.42 |
| 1:J:3301:THR:OG1 | 1:J:3325:LYS:HB2 | 2.19 | 0.42 |
| 1:K:129:GLU:HG2 | 1:K:139:THR:C | 2.44 | 0.42 |
| 1:K:958:PRO:HA | 1:K:961:ASN:HA | 2.00 | 0.42 |
| 1:K:2052:LYS:HA | 1:K:2052:LYS:HD2 | 1.72 | 0.42 |
| 1:K:2112:ARG:HB3 | 1:K:2116:LYS:HZ1 | 1.83 | 0.42 |
| 1:K:2353:LEU:HD23 | 1:K:2353:LEU:HA | 1.88 | 0.42 |
| 1:K:2414:GLN:NE2 | 1:K:2466:PRO:O | 2.52 | 0.42 |
| 1:K:3395:ARG:HH21 | 1:K:3398:GLN:CD | 2.27 | 0.42 |
| 1:L:409:VAL:HG13 | 1:L:666:CYS:HA | 2.01 | 0.42 |
| 1:L:562:LEU:HD12 | 1:L:630:TYR:HE1 | 1.83 | 0.42 |
| 1:L:744:ASN:ND2 | 1:L:778:PRO:HA | 2.34 | 0.42 |
| 1:L:1301:PHE:CD1 | 1:L:1302:PRO:HA | 2.54 | 0.42 |
| 1:L:1677:ARG:HD3 | 1:L:1677:ARG:HA | 1.91 | 0.42 |
| 1:L:2271:ILE:HB | 1:L:2298:HIS:CE1 | 2.54 | 0.42 |
| 1:L:3227:THR:HB | 1:L:3246:TYR:CD2 | 2.54 | 0.42 |
| 1:L:3363:CYS:HB2 | 1:L:3396:CYS:HB3 | 1.90 | 0.42 |
| 1:M:14:GLN:HG2 | 1:M:15:GLU:N | 2.32 | 0.42 |
| 1:M:189:HIS:HE1 | 1:M:212:PHE:HE1 | 1.67 | 0.42 |
| 1:M:601:ASP:O | 1:M:604:VAL:HG22 | 2.19 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:M:1241:VAL:HG13 | 1:N:2327:VAL:HB | 2.01 | 0.42 |
| 1:M:1775:LEU:HD11 | 1:M:1780:ASN:HD21 | 1.84 | 0.42 |
| 1:M:1934:ILE:HD12 | 1:M:1934:ILE:HA | 1.87 | 0.42 |
| 1:M:1977:GLU:O | 1:M:2078:LYS:NZ | 2.36 | 0.42 |
| 1:M:2193:LEU:O | 1:M:2210:ASN:ND2 | 2.53 | 0.42 |
| 1:M:2806:PHE:HB2 | 1:M:2851:PHE:HB3 | 2.01 | 0.42 |
| 1:M:3305:ILE:HA | 1:M:3315:VAL:O | 2.19 | 0.42 |
| 1:N:481:ASP:HA | 1:N:485:ARG:HH12 | 1.84 | 0.42 |
| 1:N:596:GLN:HE22 | 1:N:602:PHE:HD1 | 1.67 | 0.42 |
| 1:N:610:HIS:O | 1:N:613:PRO:HD2 | 2.18 | 0.42 |
| 1:N:860:GLN:NE2 | 1:N:864:GLU:OE2 | 2.52 | 0.42 |
| 1:N:924:ALA:O | 1:N:928:LYS:HG2 | 2.19 | 0.42 |
| 1:N:2305:ILE:HD13 | 1:N:2305:ILE:HA | 1.91 | 0.42 |
| 1:N:2618:ASP:OD1 | 1:N:2618:ASP:N | 2.52 | 0.42 |
| 1:O:483:ARG:HD2 | 1:O:484:VAL:N | 2.34 | 0.42 |
| 1:O:1390:LYS:HD2 | 1:O:1443:TYR:CE2 | 2.54 | 0.42 |
| 1:O:2532:LEU:HA | 1:O:2535:VAL:HB | 2.02 | 0.42 |
| 1:O:2802:VAL:HG12 | 1:O:2856:THR:HG22 | 2.02 | 0.42 |
| 1:O:2940:ALA:O | 1:O:2944:LEU:HD23 | 2.19 | 0.42 |
| 1:O:3131:THR:OG1 | 1:O:3134:LYS:NZ | 2.30 | 0.42 |
| 1:P:634:ASP:OD1 | 1:P:636:ILE:HG12 | 2.19 | 0.42 |
| 1:P:1636:LYS:HE3 | 1:P:1636:LYS:HB2 | 1.83 | 0.42 |
| 1:P:1802:ILE:HG12 | 1:P:1807:THR:O | 2.19 | 0.42 |
| 1:P:1959:GLU:OE1 | 1:P:1962:GLY:N | 2.45 | 0.42 |
| 1:P:3076:ASN:OD1 | 1:P:3079:ASP:N | 2.51 | 0.42 |
| 1:P:3227:THR:OG1 | 1:P:3245:PHE:O | 2.28 | 0.42 |
| 1:Q:409:VAL:HG13 | 1:Q:666:CYS:HA | 2.01 | 0.42 |
| 1:Q:849:SER:OG | 1:Q:853:SER:OG | 2.36 | 0.42 |
| 1:Q:2773:ASN:CG | 1:Q:3141:ASN:HB2 | 2.43 | 0.42 |
| 1:R:157:GLU:N | 1:R:157:GLU:OE1 | 2.52 | 0.42 |
| 1:R:434:ARG:HH11 | 1:R:710:TYR:HE1 | 1.67 | 0.42 |
| 1:R:1321:VAL:HG11 | 1:R:1491:ILE:HG21 | 2.01 | 0.42 |
| 1:R:1772:GLN:HB2 | 1:R:1818:LEU:HD11 | 2.01 | 0.42 |
| 1:R:2210:ASN:ND2 | 1:R:2212:PHE:HB2 | 2.33 | 0.42 |
| 1:R:2553:TYR:HA | 1:R:2554:PRO:HA | 1.80 | 0.42 |
| 1:R:3357:TYR:CD1 | 1:R:3360:LEU:HD22 | 2.54 | 0.42 |
| 1:S:1709:ALA:O | 1:S:1712:SER:OG | 2.25 | 0.42 |
| 1:S:2271:ILE:HG13 | 1:S:2298:HIS:CE1 | 2.54 | 0.42 |
| 1:S:2525:THR:O | 1:S:2529:LYS:HG2 | 2.18 | 0.42 |
| 1:S:3188:ASP:OD1 | 1:S:3189:ASN:N | 2.49 | 0.42 |
| 1:S:3226:ALA:HA | 1:S:3289:LYS:HA | 2.00 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:T:452:LEU:HD12 | 1:T:452:LEU:HA | 1.79 | 0.42 |
| 1:T:460:SER:HB2 | 1:T:1277:GLU:OE2 | 2.19 | 0.42 |
| 1:T:533:PRO:HB2 | 1:T:535:ILE:HD12 | 2.00 | 0.42 |
| 1:T:1684:THR:HG23 | 1:T:1687:GLU:H | 1.84 | 0.42 |
| 1:T:1883:LEU:O | 1:T:1886:SER:OG | 2.31 | 0.42 |
| 1:T:2345:ASN:O | 1:T:2349:ARG:HG2 | 2.19 | 0.42 |
| 1:T:2504:ALA:HA | 1:T:2506:TYR:CE1 | 2.54 | 0.42 |
| 3:1A:2:NAG:H4 | 3:1A:3:BMA:H2 | 1.72 | 0.42 |
| 1:A:60:VAL:HG11 | 1:A:65:THR:OG1 | 2.18 | 0.42 |
| 1:A:222:ILE:O | 1:A:225:ILE:HG22 | 2.19 | 0.42 |
| 1:A:525:TRP:CD1 | 1:A:640:HIS:CD2 | 3.08 | 0.42 |
| 1:A:849:SER:HB3 | 1:A:854:LEU:HD21 | 2.01 | 0.42 |
| 1:A:1693:LEU:O | 1:A:1696:GLN:HG3 | 2.19 | 0.42 |
| 1:B:1722:TYR:CE2 | 1:B:1724:GLU:HB3 | 2.54 | 0.42 |
| 1:B:1745:LEU:HD12 | 1:B:1745:LEU:HA | 1.88 | 0.42 |
| 1:B:1848:VAL:HA | 1:B:2026:PHE:CE2 | 2.54 | 0.42 |
| 1:B:3218:VAL:HG23 | 1:B:3261:VAL:HG13 | 2.01 | 0.42 |
| 1:B:3260:ARG:NH2 | 1:B:3407:ASP:OD2 | 2.51 | 0.42 |
| 1:C:744:ASN:HB3 | 1:C:779:TRP:NE1 | 2.34 | 0.42 |
| 1:C:884:PHE:HE1 | 1:C:1090:PRO:HG2 | 1.84 | 0.42 |
| 1:C:1220:LYS:NZ | 1:C:1222:SER:HB2 | 2.35 | 0.42 |
| 1:C:1351:TRP:HE1 | 1:C:1460:HIS:CD2 | 2.34 | 0.42 |
| 1:C:1411:LEU:HA | 1:C:1414:LEU:CD2 | 2.49 | 0.42 |
| 1:C:1880:ILE:HG13 | 1:C:1883:LEU:HD12 | 2.01 | 0.42 |
| 1:C:1978:LYS:NZ | 1:C:1979:SER:O | 2.39 | 0.42 |
| 1:C:2175:THR:OG1 | 1:D:1757:ARG:NH1 | 2.52 | 0.42 |
| 1:C:2250:LEU:HA | 1:C:2253:GLU:OE1 | 2.19 | 0.42 |
| 1:C:2369:ASP:OD1 | 1:C:2369:ASP:N | 2.51 | 0.42 |
| 1:C:2796:ARG:HH12 | 1:C:2801:ARG:CZ | 2.32 | 0.42 |
| 1:C:2837:LEU:HD12 | 1:C:2837:LEU:HA | 1.88 | 0.42 |
| 1:D:19:LEU:HD13 | 1:D:86:LEU:HD11 | 2.01 | 0.42 |
| 1:D:24:ARG:HD2 | 1:D:24:ARG:HA | 1.75 | 0.42 |
| 1:D:180:GLN:OE1 | 1:D:366:HIS:N | 2.26 | 0.42 |
| 1:D:245:GLU:CD | 1:D:245:GLU:H | 2.26 | 0.42 |
| 1:D:297:TYR:O | 1:D:300:LEU:HG | 2.19 | 0.42 |
| 1:D:455:PHE:HA | 1:D:514:ARG:NH2 | 2.34 | 0.42 |
| 1:D:998:ILE:HD12 | 1:D:998:ILE:H | 1.84 | 0.42 |
| 1:D:1328:LEU:HD22 | 1:D:1499:PHE:CE2 | 2.54 | 0.42 |
| 1:D:1568:SER:OG | 1:D:1597:GLY:O | 2.29 | 0.42 |
| 1:D:2558:LYS:HD2 | 1:D:2563:THR:HA | 2.00 | 0.42 |
| 1:E:453:SER:OG | 3:p:1:NAG:O7 | 2.21 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:E:580:TYR:CG | 1:E:958:PRO:HG2 | 2.54 | 0.42 |
| 1:E:1421:ASP:O | 1:E:1424:ILE:HG22 | 2.19 | 0.42 |
| 1:E:1599:GLU:OE2 | 1:E:1600:THR:OG1 | 2.37 | 0.42 |
| 1:E:3332:VAL:HB | 1:E:3406:ILE:HG12 | 2.01 | 0.42 |
| 1:F:153:VAL:HG21 | 1:F:159:THR:HA | 2.02 | 0.42 |
| 1:F:198:HIS:HA | 1:F:205:TRP:CD1 | 2.54 | 0.42 |
| 1:F:634:ASP:OD1 | 1:F:636:ILE:HG12 | 2.19 | 0.42 |
| 1:F:1019:GLU:HA | 1:F:1022:HIS:ND1 | 2.33 | 0.42 |
| 1:F:1315:CYS:SG | 1:F:1325:TRP:NE1 | 2.92 | 0.42 |
| 1:F:1385:ILE:HG23 | 1:F:1453:PHE:CE2 | 2.55 | 0.42 |
| 1:G:170:GLU:HB2 | 1:G:300:LEU:HG | 2.01 | 0.42 |
| 1:G:171:GLU:OE2 | 1:G:173:ASP:N | 2.52 | 0.42 |
| 1:G:381:ASN:HB3 | 1:G:410:TYR:CZ | 2.55 | 0.42 |
| 1:G:449:ARG:HD3 | 1:G:541:TYR:CE1 | 2.54 | 0.42 |
| 1:G:590:MET:HE2 | 1:G:590:MET:HA | 2.02 | 0.42 |
| 1:G:1746:TYR:HE2 | 1:G:1881:PHE:CE1 | 2.37 | 0.42 |
| 1:G:1956:ASP:OD1 | 1:G:1957:THR:N | 2.51 | 0.42 |
| 1:G:2075:TYR:O | 1:H:1486:ASP:HB2 | 2.20 | 0.42 |
| 1:G:2655:TYR:O | 1:G:2658:ILE:HG22 | 2.19 | 0.42 |
| 1:G:2740:LEU:HB3 | 1:G:2764:VAL:HG22 | 2.00 | 0.42 |
| 1:H:859:VAL:O | 1:H:862:LEU:HG | 2.18 | 0.42 |
| 1:H:896:ALA:HB1 | 1:H:899:LYS:HB2 | 2.00 | 0.42 |
| 1:H:1085:ARG:HA | 1:H:1110:PHE:CZ | 2.53 | 0.42 |
| 1:H:1168:VAL:HG23 | 1:H:1219:VAL:HG22 | 2.01 | 0.42 |
| 1:H:1865:LYS:HA | 1:H:1865:LYS:HD2 | 1.89 | 0.42 |
| 1:H:2088:PRO:O | 1:H:2090:ASN:N | 2.44 | 0.42 |
| 1:H:2271:ILE:HB | 1:H:2298:HIS:CE1 | 2.53 | 0.42 |
| 1:H:2667:TYR:CD1 | 1:H:2667:TYR:C | 2.97 | 0.42 |
| 1:H:3036:GLN:OE1 | 1:H:3042:HIS:N | 2.52 | 0.42 |
| 1:H:3208:ARG:NH1 | 1:H:3310:ASN:HA | 2.34 | 0.42 |
| 1:H:3241:ASP:OD1 | 1:H:3242:VAL:N | 2.53 | 0.42 |
| 1:I:111:ILE:HD13 | 1:I:122:LYS:HA | 2.02 | 0.42 |
| 1:I:228:GLU:OE1 | 1:I:229:LEU:HD22 | 2.18 | 0.42 |
| 1:I:580:TYR:OH | 1:I:957:ASN:OD1 | 2.36 | 0.42 |
| 1:I:720:ILE:HA | 1:I:723:LEU:HB3 | 2.01 | 0.42 |
| 1:I:1670:LYS:HD2 | 1:I:1670:LYS:HA | 1.66 | 0.42 |
| 1:I:2271:ILE:HG13 | 1:I:2298:HIS:CE1 | 2.52 | 0.42 |
| 1:I:2533:ARG:HA | 1:I:2536:GLN:OE1 | 2.18 | 0.42 |
| 1:I:2603:TRP:CZ3 | 1:I:2681:ILE:HD11 | 2.54 | 0.42 |
| 1:I:2831:ALA:HA | 1:I:2858:VAL:HG11 | 2.01 | 0.42 |
| 1:I:3084:PHE:CE1 | 1:I:3125:ILE:HG23 | 2.54 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:J:192:VAL:HG13 | 1:J:200:LEU:HB2 | 2.01 | 0.42 |
| 1:J:456:GLN:OE1 | 1:J:553:PRO:HB2 | 2.19 | 0.42 |
| 1:J:524:ASP:OD2 | 1:J:527:ARG:HG2 | 2.19 | 0.42 |
| 1:J:719:THR:HG23 | 1:J:722:GLN:H | 1.85 | 0.42 |
| 1:J:784:LEU:O | 1:J:786:LYS:NZ | 2.33 | 0.42 |
| 1:J:1268:LEU:HD23 | 1:J:1268:LEU:H | 1.85 | 0.42 |
| 1:J:1940:LYS:HD2 | 1:J:1940:LYS:HA | 1.72 | 0.42 |
| 1:J:2304:LYS:HA | 1:J:2367:TYR:CE2 | 2.54 | 0.42 |
| 1:J:2657:GLN:OE1 | 1:J:2657:GLN:N | 2.42 | 0.42 |
| 1:K:28:ASP:OD1 | 1:K:29:ASP:N | 2.52 | 0.42 |
| 1:K:869:LEU:HD12 | 1:K:869:LEU:HA | 1.90 | 0.42 |
| 1:K:1178:GLU:CG | 1:K:1205:ILE:HG21 | 2.49 | 0.42 |
| 1:K:1231:ILE:H | 1:K:1231:ILE:HD12 | 1.85 | 0.42 |
| 1:K:1568:SER:OG | 1:K:1595:VAL:O | 2.34 | 0.42 |
| 1:K:1816:ASN:OD1 | 1:K:1816:ASN:N | 2.52 | 0.42 |
| 1:K:2387:HIS:O | 1:K:2392:ARG:NH1 | 2.49 | 0.42 |
| 1:K:2814:SER:N | 1:K:2838:GLY:O | 2.53 | 0.42 |
| 1:K:2991:LEU:HD23 | 1:K:2991:LEU:HA | 1.85 | 0.42 |
| 1:L:257:ASP:HA | 1:L:265:ARG:HD3 | 2.01 | 0.42 |
| 1:L:337:GLN:N | 1:L:337:GLN:OE1 | 2.52 | 0.42 |
| 1:L:680:PHE:O | 1:L:685:ASN:ND2 | 2.52 | 0.42 |
| 1:L:1946:ASP:HB3 | 1:L:1950:HIS:CD2 | 2.54 | 0.42 |
| 1:M:110:PRO:HA | 1:M:126:PHE:CG | 2.55 | 0.42 |
| 1:M:129:GLU:HG2 | 1:M:139:THR:C | 2.44 | 0.42 |
| 1:M:253:PRO:O | 1:M:256:ARG:HG2 | 2.19 | 0.42 |
| 1:M:379:LYS:HD3 | 1:M:379:LYS:HA | 1.66 | 0.42 |
| 1:M:964:GLU:HB2 | 1:M:965:PRO:HD2 | 2.01 | 0.42 |
| 1:M:973:VAL:HG11 | 1:M:1045:TYR:CG | 2.54 | 0.42 |
| 1:M:2190:LEU:HG | 1:M:2191:PRO:HD2 | 2.00 | 0.42 |
| 1:M:2811:PHE:CE2 | 1:M:2836:VAL:HG11 | 2.54 | 0.42 |
| 1:M:3100:THR:HA | 1:M:3290:TYR:CE2 | 2.54 | 0.42 |
| 1:M:3208:ARG:HA | 1:M:3212:ARG:HH12 | 1.84 | 0.42 |
| 1:M:3217:PHE:CE1 | 1:M:3302:PRO:HB3 | 2.52 | 0.42 |
| 1:N:646:ARG:HA | 1:N:710:TYR:HE2 | 1.85 | 0.42 |
| 1:N:1428:ILE:HA | 1:N:1431:ASN:HD21 | 1.84 | 0.42 |
| 1:N:2095:GLU:CD | 1:N:2097:SER:H | 2.27 | 0.42 |
| 1:N:2626:GLU:OE1 | 1:N:2627:ILE:N | 2.52 | 0.42 |
| 1:N:3043:GLN:N | 1:N:3043:GLN:OE1 | 2.53 | 0.42 |
| 1:N:3135:LEU:HD23 | 1:N:3135:LEU:HA | 1.91 | 0.42 |
| 1:N:3179:ASP:OD2 | 1:N:3181:SER:OG | 2.31 | 0.42 |
| 1:O:561:PHE:CE2 | 1:O:562:LEU:HG | 2.55 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:O:988:GLU:OE2 | 1:O:996:THR:OG1 | 2.26 | 0.42 |
| 1:O:1728:ARG:HH12 | 2:SA:1:NAG:H83 | 1.83 | 0.42 |
| 1:O:2681:ILE:O | 1:O:2685:ILE:HG22 | 2.19 | 0.42 |
| 1:O:3072:LEU:HD23 | 1:O:3129:TRP:CD1 | 2.48 | 0.42 |
| 1:P:299:LEU:O | 1:P:302:GLN:HG3 | 2.20 | 0.42 |
| 1:P:307:GLU:HG3 | 1:P:413:ALA:HA | 2.01 | 0.42 |
| 1:P:1036:SER:O | 1:P:1042:TYR:HB2 | 2.19 | 0.42 |
| 1:P:1304:LEU:HD23 | 1:P:1304:LEU:HA | 1.88 | 0.42 |
| 1:P:1534:ASN:ND2 | 1:P:1538:TRP:O | 2.52 | 0.42 |
| 1:P:1978:LYS:NZ | 1:P:1979:SER:O | 2.44 | 0.42 |
| 1:P:3088:HIS:CE1 | 1:P:3119:HIS:HE1 | 2.37 | 0.42 |
| 1:Q:488:CYS:HB2 | 1:Q:677:PRO:HD3 | 2.01 | 0.42 |
| 1:Q:1366:SER:CB | 1:Q:1377:SER:HA | 2.49 | 0.42 |
| 1:Q:1919:PRO:HB2 | 1:Q:1924:SER:HB2 | 2.00 | 0.42 |
| 1:Q:2382:GLU:O | 1:Q:2385:ARG:HG2 | 2.19 | 0.42 |
| 1:Q:2648:ARG:HD2 | 1:Q:2656:ARG:HH21 | 1.84 | 0.42 |
| 1:Q:3082:VAL:O | 1:Q:3086:MET:HG2 | 2.19 | 0.42 |
| 1:R:588:ASP:HA | 1:R:591:LEU:HD12 | 2.01 | 0.42 |
| 1:R:1363:ASN:OD1 | 1:R:1364:GLU:N | 2.51 | 0.42 |
| 1:R:2001:CYS:HB2 | 1:R:2050:THR:OG1 | 2.19 | 0.42 |
| 1:R:3227:THR:HB | 1:R:3246:TYR:CD2 | 2.55 | 0.42 |
| 1:R:3289:LYS:HG2 | 1:R:3290:TYR:H | 1.84 | 0.42 |
| 1:S:146:ASP:CG | 1:S:148:ARG:HG2 | 2.44 | 0.42 |
| 1:S:1020:ILE:HD11 | 1:S:1181:PHE:HD2 | 1.84 | 0.42 |
| 1:S:1577:VAL:N | 1:S:1584:ARG:HH22 | 2.18 | 0.42 |
| 1:S:2112:ARG:NE | 1:S:2208:LEU:HD21 | 2.33 | 0.42 |
| 1:S:2147:CYS:C | 1:S:2149:HIS:HD1 | 2.25 | 0.42 |
| 1:S:2675:GLU:N | 1:S:2675:GLU:OE1 | 2.51 | 0.42 |
| 1:S:2750:ASP:HA | 1:S:2758:ARG:HD2 | 2.01 | 0.42 |
| 1:S:2864:LEU:HD11 | 1:S:2870:TYR:HB3 | 2.01 | 0.42 |
| 1:S:2990:LEU:HD12 | 1:S:3168:THR:HG22 | 2.00 | 0.42 |
| 1:S:3091:ILE:O | 1:S:3095:VAL:HG12 | 2.19 | 0.42 |
| 1:S:3191:ASN:OD1 | 1:S:3195:HIS:N | 2.52 | 0.42 |
| 1:T:171:GLU:HB3 | 1:T:177:PHE:HD1 | 1.83 | 0.42 |
| 1:T:244:VAL:HG23 | 1:T:248:ARG:HE | 1.84 | 0.42 |
| 1:T:801:ASP:OD1 | 1:T:801:ASP:N | 2.51 | 0.42 |
| 1:T:867:GLN:HA | 1:T:870:GLU:HG3 | 2.00 | 0.42 |
| 1:T:991:LYS:H | 1:T:994:ARG:NH2 | 2.17 | 0.42 |
| 1:T:1075:ASN:HB2 | 1:T:1113:PHE:HB3 | 2.01 | 0.42 |
| 1:T:1230:LYS:HD2 | 1:T:1230:LYS:HA | 1.77 | 0.42 |
| 1:T:1301:PHE:CD1 | 1:T:1302:PRO:HA | 2.54 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:T:1433:LEU:HA | 1:T:1436:LEU:HB2 | 2.01 | 0.42 |
| 1:T:1878:ASP:OD2 | 1:T:1880:ILE:HB | 2.19 | 0.42 |
| 1:T:2112:ARG:HB3 | 1:T:2211:PRO:HG3 | 2.01 | 0.42 |
| 1:T:2112:ARG:HH11 | 1:T:2208:LEU:HD22 | 1.84 | 0.42 |
| 1:A:1061:ALA:HA | 1:A:1064:GLN:NE2 | 2.34 | 0.42 |
| 1:A:1440:ARG:HE | 1:D:1368:PHE:HB3 | 1.84 | 0.42 |
| 1:A:1588:HIS:HB2 | 1:D:337:GLN:CD | 2.43 | 0.42 |
| 1:A:1596:LEU:HD12 | 1:A:1597:GLY:N | 2.34 | 0.42 |
| 1:A:2147:CYS:C | 1:A:2149:HIS:HD1 | 2.27 | 0.42 |
| 1:A:2198:THR:HA | 1:A:2209:GLU:HA | 2.00 | 0.42 |
| 1:A:2354:PRO:O | 1:A:2357:VAL:HG22 | 2.18 | 0.42 |
| 1:A:3310:ASN:OD1 | 1:B:1117:ARG:NE | 2.50 | 0.42 |
| 1:B:105:ARG:HA | 1:B:108:GLN:NE2 | 2.33 | 0.42 |
| 1:B:596:GLN:HE22 | 1:B:602:PHE:HD1 | 1.67 | 0.42 |
| 1:B:739:GLY:HA3 | 1:B:784:LEU:HB3 | 2.01 | 0.42 |
| 1:B:788:GLU:OE1 | 1:B:791:ASP:HB2 | 2.19 | 0.42 |
| 1:B:1998:ILE:HG13 | 1:B:2010:ALA:HB3 | 2.02 | 0.42 |
| 1:B:3259:GLU:O | 1:B:3331:ILE:HD13 | 2.19 | 0.42 |
| 1:C:181:PHE:CE2 | 1:C:219:VAL:HG13 | 2.54 | 0.42 |
| 1:C:937:TRP:CD1 | 1:C:938:ASP:H | 2.36 | 0.42 |
| 1:C:1495:PRO:HD2 | 1:C:1500:ASN:HD21 | 1.84 | 0.42 |
| 1:C:1495:PRO:HG3 | 1:C:1515:ARG:HD2 | 2.01 | 0.42 |
| 1:C:1687:GLU:OE1 | 1:C:1687:GLU:N | 2.47 | 0.42 |
| 1:C:2271:ILE:HG13 | 1:C:2298:HIS:CE1 | 2.55 | 0.42 |
| 1:C:2517:ILE:HG13 | 1:C:2518:ASN:N | 2.34 | 0.42 |
| 1:D:254:PHE:CD1 | 1:D:264:THR:HB | 2.54 | 0.42 |
| 1:D:925:LEU:HD22 | 1:D:928:LYS:NZ | 2.31 | 0.42 |
| 1:D:1229:LYS:HE3 | 1:D:1229:LYS:HB3 | 1.82 | 0.42 |
| 1:D:3218:VAL:HA | 1:D:3258:TYR:HD2 | 1.85 | 0.42 |
| 1:E:129:GLU:HA | 1:E:140:SER:HA | 2.00 | 0.42 |
| 1:E:1436:LEU:HD23 | 1:E:1436:LEU:HA | 1.91 | 0.42 |
| 1:E:1548:LYS:HE2 | 1:E:1548:LYS:HB2 | 1.92 | 0.42 |
| 1:E:1571:VAL:HG22 | 1:E:1593:PHE:O | 2.20 | 0.42 |
| 1:E:2313:GLN:CD | 1:E:2318:LEU:HB2 | 2.45 | 0.42 |
| 1:E:3337:ARG:HH11 | 1:E:3378:ASN:HB2 | 1.85 | 0.42 |
| 1:F:73:TYR:HA | 1:F:76:GLN:OE1 | 2.19 | 0.42 |
| 1:F:596:GLN:CD | 1:F:598:ASP:H | 2.27 | 0.42 |
| 1:F:711:ASP:OD1 | 1:F:711:ASP:N | 2.52 | 0.42 |
| 1:F:1276:VAL:O | 1:F:1279:LEU:HG | 2.19 | 0.42 |
| 1:F:2671:GLU:OE1 | 1:F:2671:GLU:N | 2.38 | 0.42 |
| 1:F:3103:MET:HE3 | 1:F:3114:PHE:HD2 | 1.83 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:F:3142:TYR:CZ | 1:F:3144:ARG:HD3 | 2.55 | 0.42 |
| 1:F:3213:VAL:HA | 1:F:3306:SER:HA | 2.00 | 0.42 |
| 1:F:3225:SER:HB2 | 1:F:3290:TYR:CD1 | 2.54 | 0.42 |
| 1:G:33:ASN:HB3 | 1:G:80:LYS:HD2 | 1.99 | 0.42 |
| 1:G:479:ARG:HG3 | 1:G:676:LYS:NZ | 2.34 | 0.42 |
| 1:G:953:GLU:OE1 | 1:G:969:HIS:ND1 | 2.52 | 0.42 |
| 1:G:1263:HIS:HB2 | 1:G:1528:TYR:HB2 | 2.00 | 0.42 |
| 1:G:1535:PHE:O | 1:G:1538:TRP:HB2 | 2.19 | 0.42 |
| 1:G:2334:MET:N | 1:G:2334:MET:SD | 2.93 | 0.42 |
| 1:G:2703:PRO:O | 1:G:2707:ILE:HG12 | 2.18 | 0.42 |
| 1:G:2806:PHE:O | 1:G:2850:LEU:HD12 | 2.19 | 0.42 |
| 1:G:3013:TRP:CZ3 | 1:G:3064:LEU:HB3 | 2.44 | 0.42 |
| 1:G:3305:ILE:HA | 1:G:3315:VAL:O | 2.19 | 0.42 |
| 1:H:2210:ASN:HD21 | 1:H:2212:PHE:HB2 | 1.85 | 0.42 |
| 1:H:2821:LEU:HD13 | 1:H:2872:PHE:CE1 | 2.54 | 0.42 |
| 1:H:3077:TYR:HE1 | 1:H:3126:TRP:HE1 | 1.67 | 0.42 |
| 1:H:3153:PRO:HA | 1:H:3173:ARG:HD2 | 2.00 | 0.42 |
| 1:I:161:LEU:HD21 | 1:I:187:HIS:CD2 | 2.54 | 0.42 |
| 1:I:256:ARG:HE | 1:I:256:ARG:HB3 | 1.69 | 0.42 |
| 1:I:469:GLU:OE1 | 1:I:474:PRO:HD2 | 2.20 | 0.42 |
| 1:I:850:ASP:OD1 | 1:I:852:SER:N | 2.49 | 0.42 |
| 1:I:1049:PHE:HD2 | 1:I:1050:PHE:HD1 | 1.67 | 0.42 |
| 1:I:1301:PHE:CD1 | 1:I:1302:PRO:HA | 2.53 | 0.42 |
| 1:I:1584:ARG:HE | 1:I:1585:ASN:N | 2.17 | 0.42 |
| 1:I:1662:ASP:OD1 | 1:I:1662:ASP:N | 2.51 | 0.42 |
| 1:I:3128:ILE:HA | 1:I:3131:THR:HG22 | 2.01 | 0.42 |
| 1:J:187:HIS:CE1 | 1:J:191:LEU:HD11 | 2.54 | 0.42 |
| 1:J:1315:CYS:C | 1:J:1317:HIS:HD1 | 2.27 | 0.42 |
| 1:J:1556:LEU:HB2 | 1:J:1625:LEU:HD11 | 1.99 | 0.42 |
| 1:J:1928:PRO:HD2 | 1:J:1929:TYR:CD2 | 2.53 | 0.42 |
| 1:J:2922:VAL:HG22 | 1:J:3186:ASN:OD1 | 2.19 | 0.42 |
| 1:K:903:CYS:C | 1:K:905:HIS:HD1 | 2.25 | 0.42 |
| 1:K:2063:LEU:HB3 | 1:K:2067:LEU:HD12 | 2.01 | 0.42 |
| 1:K:2162:THR:O | 1:K:2165:VAL:HG22 | 2.18 | 0.42 |
| 1:L:225:ILE:O | 1:L:229:LEU:HG | 2.18 | 0.42 |
| 1:L:646:ARG:O | 1:L:650:ILE:HG12 | 2.19 | 0.42 |
| 1:L:729:GLU:O | 1:L:732:THR:HG22 | 2.20 | 0.42 |
| 1:L:2433:GLU:N | 1:L:2433:GLU:OE1 | 2.52 | 0.42 |
| 1:L:2997:MET:CE | 1:L:3165:ASN:HD21 | 2.33 | 0.42 |
| 1:L:3058:GLN:N | 1:L:3061:LEU:O | 2.40 | 0.42 |
| 1:L:3122:ILE:HA | 1:L:3125:ILE:HG12 | 2.00 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:M:111:ILE:HG13 | 1:P:2214:ARG:HH21 | 1.84 | 0.42 |
| 1:M:161:LEU:HD21 | 1:M:187:HIS:CD2 | 2.54 | 0.42 |
| 1:M:259:ASN:O | 1:M:265:ARG:NH2 | 2.52 | 0.42 |
| 1:M:307:GLU:OE2 | 1:M:413:ALA:N | 2.43 | 0.42 |
| 1:M:689:LYS:HD3 | 1:M:689:LYS:HA | 1.73 | 0.42 |
| 1:M:1286:MET:HA | 1:M:1289:ASP:OD2 | 2.20 | 0.42 |
| 1:M:1509:LEU:O | 1:M:1513:TYR:N | 2.48 | 0.42 |
| 1:M:1666:ASP:HB3 | 1:N:1902:ARG:O | 2.20 | 0.42 |
| 1:M:1691:LEU:HD23 | 1:M:1691:LEU:HA | 1.86 | 0.42 |
| 1:M:1778:PHE:HD2 | 1:M:1779:PHE:HD2 | 1.67 | 0.42 |
| 1:M:2095:GLU:OE1 | 1:M:2097:SER:OG | 2.31 | 0.42 |
| 1:M:2990:LEU:O | 1:M:2993:VAL:HG12 | 2.20 | 0.42 |
| 1:M:3133:GLN:NE2 | 1:M:3138:ARG:HB3 | 2.34 | 0.42 |
| 1:N:1557:PHE:HD2 | 1:N:1611:LYS:HD3 | 1.85 | 0.42 |
| 1:N:1869:MET:HE1 | 1:N:1881:PHE:CD2 | 2.54 | 0.42 |
| 1:N:2371:LYS:HD3 | 1:N:2376:ASN:HA | 2.01 | 0.42 |
| 1:N:2533:ARG:O | 1:N:2537:GLN:OE1 | 2.38 | 0.42 |
| 1:N:2568:HIS:C | 1:N:2569:HIS:HD1 | 2.27 | 0.42 |
| 1:N:2839:GLY:O | 1:N:2842:GLU:HG2 | 2.19 | 0.42 |
| 1:N:2989:ARG:NH2 | 1:N:3126:TRP:CD1 | 2.87 | 0.42 |
| 1:O:738:VAL:HG23 | 1:O:789:ILE:HG21 | 2.00 | 0.42 |
| 1:O:1509:LEU:HA | 1:O:1513:TYR:HB2 | 2.01 | 0.42 |
| 1:O:1932:ASP:OD2 | 1:O:1934:ILE:HG22 | 2.20 | 0.42 |
| 1:O:2162:THR:O | 1:O:2165:VAL:HG22 | 2.19 | 0.42 |
| 1:O:2249:LEU:HD23 | 1:O:2383:GLU:OE2 | 2.20 | 0.42 |
| 1:O:2394:PHE:HD2 | 1:O:2443:LYS:HG2 | 1.84 | 0.42 |
| 1:O:2616:ASP:OD1 | 1:O:2616:ASP:N | 2.52 | 0.42 |
| 1:O:2625:GLY:C | 1:O:2633:LYS:HZ2 | 2.27 | 0.42 |
| 1:O:3103:MET:HA | 1:O:3109:SER:HA | 2.00 | 0.42 |
| 1:P:96:TRP:CZ3 | 1:P:218:ASN:HB3 | 2.54 | 0.42 |
| 1:P:953:GLU:HA | 1:P:969:HIS:HB2 | 2.00 | 0.42 |
| 1:P:1350:ASP:HA | 1:P:1463:ASN:ND2 | 2.34 | 0.42 |
| 1:P:1425:GLN:O | 1:P:1429:VAL:HG22 | 2.19 | 0.42 |
| 1:P:1842:ASN:OD1 | 1:P:1843:TYR:N | 2.52 | 0.42 |
| 1:P:2286:LEU:HD23 | 1:P:2286:LEU:H | 1.83 | 0.42 |
| 1:P:2313:GLN:NE2 | 1:P:2320:TYR:HB3 | 2.35 | 0.42 |
| 1:P:2550:ALA:O | 1:P:2565:ALA:HB1 | 2.19 | 0.42 |
| 1:P:2714:ARG:O | 1:P:2718:ILE:HG12 | 2.19 | 0.42 |
| 1:P:3117:ILE:O | 1:P:3120:SER:OG | 2.30 | 0.42 |
| 1:Q:1385:ILE:H | 1:Q:1385:ILE:HD12 | 1.85 | 0.42 |
| 1:Q:1969:LEU:HA | 1:Q:1972:ILE:HG12 | 2.01 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:Q:2117:ASP:OD1 | 1:Q:2119:THR:OG1 | 2.22 | 0.42 |
| 1:Q:2425:ILE:HD13 | 1:Q:2425:ILE:HA | 1.91 | 0.42 |
| 1:Q:2797:ARG:HA | 1:Q:2801:ARG:HH22 | 1.85 | 0.42 |
| 1:R:253:PRO:O | 1:R:256:ARG:HG2 | 2.19 | 0.42 |
| 1:R:444:GLU:HA | 1:R:447:GLU:CD | 2.44 | 0.42 |
| 1:R:1052:HIS:O | 1:R:1056:THR:HG23 | 2.19 | 0.42 |
| 1:R:1834:PHE:CE1 | 1:R:1891:ILE:HD13 | 2.54 | 0.42 |
| 1:R:3015:ARG:HG3 | 1:R:3016:PRO:HD2 | 2.01 | 0.42 |
| 1:S:559:VAL:HG13 | 1:S:633:PHE:CE2 | 2.55 | 0.42 |
| 1:S:606:PHE:HZ | 1:S:644:VAL:HG13 | 1.84 | 0.42 |
| 1:S:719:THR:OG1 | 1:S:722:GLN:NE2 | 2.52 | 0.42 |
| 1:S:1219:VAL:HG23 | 1:S:1239:VAL:HG13 | 2.00 | 0.42 |
| 1:S:2035:THR:O | 1:S:2038:LEU:HG | 2.19 | 0.42 |
| 1:S:3002:LYS:HD3 | 1:S:3002:LYS:HA | 1.60 | 0.42 |
| 1:S:3013:TRP:HH2 | 1:S:3087:LEU:HD21 | 1.84 | 0.42 |
| 1:T:160:GLN:HE22 | 1:T:161:LEU:HG | 1.84 | 0.42 |
| 1:T:197:ASP:CG | 1:T:198:HIS:HD2 | 2.26 | 0.42 |
| 1:T:788:GLU:OE1 | 1:T:791:ASP:HB2 | 2.20 | 0.42 |
| 1:T:1004:LEU:O | 1:T:1008:GLN:NE2 | 2.37 | 0.42 |
| 1:T:2004:GLU:OE1 | 1:T:2004:GLU:N | 2.45 | 0.42 |
| 1:T:2603:TRP:CD1 | 1:T:2654:PHE:HD2 | 2.38 | 0.42 |
| 1:A:24:ARG:HH12 | 1:A:125:TRP:CD1 | 2.38 | 0.42 |
| 1:A:284:ASP:OD1 | 1:A:285:ASP:N | 2.53 | 0.42 |
| 1:A:559:VAL:HG13 | 1:A:633:PHE:CE2 | 2.54 | 0.42 |
| 1:A:687:ASN:OD1 | 1:A:688:GLU:N | 2.53 | 0.42 |
| 1:A:1446:SER:OG | 1:A:1447:SER:N | 2.53 | 0.42 |
| 1:A:1490:ASN:ND2 | 1:B:2049:PHE:O | 2.48 | 0.42 |
| 1:A:2213:ALA:HA | 1:A:2226:ARG:HH22 | 1.85 | 0.42 |
| 1:A:2705:PHE:CE1 | 1:A:2709:HIS:CD2 | 3.07 | 0.42 |
| 1:A:2819:PHE:O | 1:A:2831:ALA:HB3 | 2.19 | 0.42 |
| 1:A:3270:LEU:HD11 | 1:A:3277:ALA:HA | 2.02 | 0.42 |
| 1:B:7:ASN:HB3 | 1:B:10:LEU:HG | 2.01 | 0.42 |
| 1:B:859:VAL:HG12 | 1:B:863:ARG:CZ | 2.50 | 0.42 |
| 1:B:1193:GLN:OE1 | 1:B:1194:TYR:N | 2.52 | 0.42 |
| 1:B:1305:CYS:HB2 | 1:B:1312:VAL:O | 2.20 | 0.42 |
| 1:B:1321:VAL:HA | 1:B:1324:HIS:CD2 | 2.54 | 0.42 |
| 1:B:1776:PRO:HG2 | 1:B:1779:PHE:CZ | 2.54 | 0.42 |
| 1:B:2786:ILE:N | 1:B:2787:PRO:HD2 | 2.35 | 0.42 |
| 1:B:2816:ASP:OD1 | 1:B:2817:VAL:N | 2.52 | 0.42 |
| 1:C:1407:LEU:O | 1:C:1411:LEU:HD13 | 2.19 | 0.42 |
| 1:C:1835:LEU:HG | 1:C:1968:LEU:HD11 | 2.01 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:1845:ASP:OD1 | 1:C:2028:ARG:HD2 | 2.20 | 0.42 |
| 1:C:1855:ASN:ND2 | 1:C:2015:VAL:HA | 2.33 | 0.42 |
| 1:C:2190:LEU:HD21 | 1:C:2194:PHE:HB3 | 2.01 | 0.42 |
| 1:C:2359:ASN:O | 1:C:2363:LEU:HD23 | 2.20 | 0.42 |
| 1:C:2514:ARG:HH12 | 1:C:2774:TYR:HE2 | 1.67 | 0.42 |
| 1:C:2544:TYR:HA | 1:C:2547:ILE:HG22 | 2.01 | 0.42 |
| 1:C:2581:PHE:HA | 1:C:2747:PHE:HZ | 1.84 | 0.42 |
| 1:D:5:ARG:HD2 | 1:D:283:TYR:CE1 | 2.53 | 0.42 |
| 1:D:435:LYS:CG | 1:D:436:ASP:H | 2.31 | 0.42 |
| 1:D:612:LEU:HD21 | 1:D:768:LEU:HD13 | 2.02 | 0.42 |
| 1:D:695:ARG:O | 1:D:697:THR:N | 2.52 | 0.42 |
| 1:D:1075:ASN:HB2 | 1:D:1113:PHE:HB3 | 2.01 | 0.42 |
| 1:D:1679:SER:OG | 1:D:1680:VAL:N | 2.53 | 0.42 |
| 1:D:3381:LEU:HD23 | 1:D:3386:TYR:CZ | 2.55 | 0.42 |
| 1:E:980:ARG:NE | 1:E:1046:ASP:OD2 | 2.34 | 0.42 |
| 1:E:2448:ASP:O | 1:E:2452:GLU:OE1 | 2.37 | 0.42 |
| 1:E:2864:LEU:HD21 | 1:E:2870:TYR:CD1 | 2.55 | 0.42 |
| 1:F:1472:GLN:NE2 | 1:F:1482:ASP:OD2 | 2.52 | 0.42 |
| 1:F:2567:CYS:C | 1:F:2569:HIS:HD1 | 2.27 | 0.42 |
| 1:G:222:ILE:HA | 1:G:225:ILE:HG22 | 2.01 | 0.42 |
| 1:G:983:ARG:HD3 | 1:G:1031:GLY:HA2 | 2.01 | 0.42 |
| 1:G:1078:ASN:HB3 | 1:H:2493:PHE:HB3 | 2.00 | 0.42 |
| 1:G:1461:HIS:HA | 1:G:1464:VAL:HB | 2.01 | 0.42 |
| 1:G:1964:ASN:ND2 | 1:G:1966:GLU:OE2 | 2.53 | 0.42 |
| 1:G:2155:PRO:HB2 | 1:G:2306:TRP:CH2 | 2.55 | 0.42 |
| 1:G:2354:PRO:O | 1:G:2357:VAL:HG22 | 2.19 | 0.42 |
| 1:G:2517:ILE:HA | 1:G:2520:LEU:HB2 | 2.00 | 0.42 |
| 1:H:297:TYR:O | 1:H:301:GLU:OE1 | 2.37 | 0.42 |
| 1:H:1075:ASN:HB2 | 1:H:1113:PHE:HB3 | 2.01 | 0.42 |
| 1:H:1153:PHE:HZ | 1:H:1166:LEU:HD22 | 1.83 | 0.42 |
| 1:H:1294:LYS:O | 1:H:1297:SER:OG | 2.23 | 0.42 |
| 1:H:1966:GLU:N | 1:H:1966:GLU:OE1 | 2.52 | 0.42 |
| 1:H:2433:GLU:OE1 | 1:H:2433:GLU:N | 2.52 | 0.42 |
| 1:H:3008:ILE:HD13 | 1:H:3116:MET:HB3 | 2.02 | 0.42 |
| 1:H:3008:ILE:HG21 | 1:H:3116:MET:HB3 | 2.00 | 0.42 |
| 1:I:1397:GLN:HB2 | 1:I:1436:LEU:O | 2.20 | 0.42 |
| 1:I:2021:GLU:N | 1:I:2021:GLU:OE1 | 2.52 | 0.42 |
| 1:I:2572:ALA:HB1 | 1:I:2671:GLU:OE2 | 2.19 | 0.42 |
| 1:I:3204:ILE:O | 1:I:3207:LEU:HG | 2.20 | 0.42 |
| 1:I:3217:PHE:CE1 | 1:I:3302:PRO:HB3 | 2.55 | 0.42 |
| 1:I:3337:ARG:NH2 | 1:I:3380:SER:HB2 | 2.34 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:J:412:PRO:HG3 | 1:J:665:HIS:CD2 | 2.53 | 0.42 |
| 1:J:479:ARG:HE | 1:J:481:ASP:HB3 | 1.83 | 0.42 |
| 1:J:735:ARG:NH1 | 1:J:788:GLU:HG2 | 2.35 | 0.42 |
| 1:J:1193:GLN:OE1 | 1:J:1194:TYR:N | 2.50 | 0.42 |
| 1:J:1378:ASN:HD21 | 1:J:1380:PHE:HB2 | 1.83 | 0.42 |
| 1:J:1447:SER:O | 1:J:1451:SER:N | 2.41 | 0.42 |
| 1:J:1507:PHE:CZ | 1:J:1509:LEU:HB3 | 2.54 | 0.42 |
| 1:J:2041:LYS:HG3 | 1:J:2043:LEU:HD23 | 2.00 | 0.42 |
| 1:J:2368:ASP:OD1 | 1:J:2368:ASP:N | 2.51 | 0.42 |
| 1:J:3133:GLN:HB3 | 1:J:3138:ARG:HB2 | 2.02 | 0.42 |
| 1:J:3266:VAL:HG21 | 1:J:3283:PHE:CE1 | 2.55 | 0.42 |
| 1:K:276:TYR:HA | 1:K:279:LEU:HD23 | 2.02 | 0.42 |
| 1:K:687:ASN:OD1 | 1:K:688:GLU:N | 2.52 | 0.42 |
| 1:K:2810:GLY:HA2 | 1:K:2845:TRP:CE2 | 2.54 | 0.42 |
| 1:L:5:ARG:HG3 | 1:L:221:ARG:HH22 | 1.85 | 0.42 |
| 1:L:461:VAL:HG22 | 1:L:1277:GLU:OE2 | 2.19 | 0.42 |
| 1:L:640:HIS:O | 1:L:644:VAL:HG23 | 2.20 | 0.42 |
| 1:L:2576:GLN:OE1 | 1:L:2576:GLN:N | 2.42 | 0.42 |
| 1:M:418:ASP:OD2 | 1:M:662:TYR:N | 2.53 | 0.42 |
| 1:M:1284:ARG:HE | 1:M:1379:PRO:HG3 | 1.83 | 0.42 |
| 1:M:3083:GLN:NE2 | 1:M:3263:LYS:HB3 | 2.34 | 0.42 |
| 1:N:13:ASP:O | 1:N:17:LEU:HD23 | 2.19 | 0.42 |
| 1:N:68:GLN:O | 1:N:71:ARG:HG2 | 2.20 | 0.42 |
| 1:N:445:VAL:O | 1:N:448:LEU:HG | 2.20 | 0.42 |
| 1:N:1075:ASN:HB2 | 1:N:1113:PHE:HB3 | 2.02 | 0.42 |
| 1:N:1710:LEU:HD13 | 1:N:1750:PHE:CE1 | 2.54 | 0.42 |
| 1:N:1857:ILE:HD12 | 1:N:1884:HIS:CD2 | 2.54 | 0.42 |
| 1:N:1947:TYR:CZ | 1:N:1948:LYS:HG3 | 2.54 | 0.42 |
| 1:N:2376:ASN:O | 1:N:2379:GLU:HG3 | 2.19 | 0.42 |
| 1:N:2923:ARG:HE | 1:N:2924:TYR:N | 2.17 | 0.42 |
| 1:O:1162:ALA:HB1 | 1:O:1224:ILE:O | 2.19 | 0.42 |
| 1:O:2126:LEU:O | 1:O:2161:TYR:OH | 2.35 | 0.42 |
| 1:O:3021:PRO:HD2 | 1:O:3024:LEU:HD21 | 2.02 | 0.42 |
| 1:P:69:TRP:O | 1:P:72:LEU:HG | 2.20 | 0.42 |
| 1:P:190:TYR:HD2 | 1:P:349:PHE:CD2 | 2.34 | 0.42 |
| 1:P:408:GLY:O | 1:P:669:THR:OG1 | 2.27 | 0.42 |
| 1:P:727:ILE:HG22 | 1:P:730:ARG:NH2 | 2.34 | 0.42 |
| 1:P:1538:TRP:CD1 | 1:P:1542:GLN:HG3 | 2.54 | 0.42 |
| 1:P:1646:GLU:OE1 | 1:P:1648:SER:OG | 2.21 | 0.42 |
| 1:P:2105:MET:HA | 1:P:2108:LYS:HG2 | 2.00 | 0.42 |
| 1:P:2155:PRO:HB2 | 1:P:2306:TRP:CZ3 | 2.54 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:P:3124:ARG:NH2 | 1:P:3127:GLN:HG2 | 2.35 | 0.42 |
| 1:P:3127:GLN:O | 1:P:3130:GLN:HG3 | 2.19 | 0.42 |
| 1:Q:836:HIS:HE1 | 1:Q:838:GLU:HB3 | 1.83 | 0.42 |
| 1:Q:1061:ALA:HA | 1:Q:1064:GLN:CD | 2.44 | 0.42 |
| 1:Q:1283:LEU:HD21 | 1:Q:1287:GLN:HE22 | 1.83 | 0.42 |
| 1:Q:1413:ALA:HB2 | 1:Q:1425:GLN:HG2 | 2.01 | 0.42 |
| 1:Q:1495:PRO:HD2 | 1:Q:1500:ASN:HD21 | 1.83 | 0.42 |
| 1:Q:2000:VAL:O | 1:Q:2041:LYS:NZ | 2.46 | 0.42 |
| 1:Q:2473:ILE:HG21 | 1:Q:2481:LEU:HB2 | 2.00 | 0.42 |
| 1:Q:2990:LEU:HD12 | 1:Q:3168:THR:HG22 | 2.00 | 0.42 |
| 1:Q:3047:ASP:HB2 | 1:Q:3097:GLY:HA3 | 2.01 | 0.42 |
| 1:Q:3063:SER:O | 1:Q:3067:GLN:HG3 | 2.20 | 0.42 |
| 1:Q:3066:TYR:O | 1:Q:3069:LEU:HG | 2.20 | 0.42 |
| 1:R:376:LEU:HD12 | 1:R:376:LEU:HA | 1.83 | 0.42 |
| 1:R:650:ILE:HD13 | 1:R:713:LEU:HB3 | 2.02 | 0.42 |
| 1:R:1495:PRO:HA | 1:R:1515:ARG:NH2 | 2.33 | 0.42 |
| 1:R:2055:LEU:HB2 | 1:R:2063:LEU:HB2 | 2.02 | 0.42 |
| 1:R:2158:HIS:HD2 | 1:R:2299:HIS:CD2 | 2.37 | 0.42 |
| 1:R:2488:LYS:HZ3 | 1:R:2489:PRO:HG2 | 1.84 | 0.42 |
| 1:R:2620:ASN:HB3 | 1:R:2623:GLU:OE1 | 2.20 | 0.42 |
| 1:R:2709:HIS:O | 1:R:2712:VAL:HG12 | 2.19 | 0.42 |
| 1:R:2922:VAL:HG22 | 1:R:3186:ASN:OD1 | 2.19 | 0.42 |
| 1:R:3036:GLN:OE1 | 1:R:3042:HIS:N | 2.53 | 0.42 |
| 1:S:744:ASN:ND2 | 1:S:778:PRO:HA | 2.35 | 0.42 |
| 1:S:893:SER:OG | 1:S:895:ASP:OD2 | 2.37 | 0.42 |
| 1:S:911:PRO:HG3 | 1:S:1011:PHE:HZ | 1.84 | 0.42 |
| 1:S:1168:VAL:N | 1:S:1178:GLU:OE1 | 2.53 | 0.42 |
| 1:S:1559:GLY:C | 1:S:1560:PHE:HD2 | 2.27 | 0.42 |
| 1:S:1830:LEU:HG | 1:S:1834:PHE:HE2 | 1.83 | 0.42 |
| 1:S:2051:VAL:HB | 1:S:2071:PRO:HG2 | 2.01 | 0.42 |
| 1:S:2342:LEU:HD23 | 1:S:2342:LEU:HA | 1.82 | 0.42 |
| 1:T:221:ARG:O | 1:T:225:ILE:HG12 | 2.20 | 0.42 |
| 1:T:1678:LYS:NZ | 1:T:1683:LEU:HA | 2.34 | 0.42 |
| 1:T:3148:ARG:HG2 | 1:T:3152:ARG:NH1 | 2.34 | 0.42 |
| 3:X:1:NAG:H62 | 3:X:2:NAG:H82 | 2.01 | 0.42 |
| 1:A:326:ILE:HA | 1:A:326:ILE:HD12 | 1.79 | 0.42 |
| 1:A:954:THR:HA | 1:A:965:PRO:HA | 2.01 | 0.42 |
| 1:A:1210:LYS:HE3 | 1:A:1210:LYS:HB3 | 1.91 | 0.42 |
| 1:A:1588:HIS:HB2 | 1:D:337:GLN:NE2 | 2.35 | 0.42 |
| 1:A:1932:ASP:OD2 | 1:A:1934:ILE:HG22 | 2.19 | 0.42 |
| 1:B:111:ILE:HG13 | 1:I:2214:ARG:HH11 | 1.85 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:235:LYS:HE2 | 1:B:235:LYS:HB3 | 1.87 | 0.42 |
| 1:B:1353:GLN:NE2 | 1:B:1536:ASN:OD1 | 2.53 | 0.42 |
| 1:B:1687:GLU:O | 1:B:1691:LEU:HD23 | 2.20 | 0.42 |
| 1:B:2165:VAL:HG11 | 1:B:2296:PHE:CE2 | 2.54 | 0.42 |
| 1:B:2865:ARG:NH1 | 1:B:2866:PRO:HG2 | 2.34 | 0.42 |
| 1:C:506:GLN:HB2 | 1:C:690:THR:HG21 | 2.02 | 0.42 |
| 1:C:561:PHE:CE2 | 1:C:562:LEU:HG | 2.54 | 0.42 |
| 1:C:2008:LYS:HB2 | 1:C:2008:LYS:HE3 | 1.79 | 0.42 |
| 1:C:2382:GLU:O | 1:C:2386:GLN:HG2 | 2.19 | 0.42 |
| 1:C:2404:THR:OG1 | 1:C:2405:SER:N | 2.52 | 0.42 |
| 1:C:2805:ASN:ND2 | 1:C:2852:GLN:OE1 | 2.53 | 0.42 |
| 1:C:2960:HIS:HE1 | 1:C:3119:HIS:CE1 | 2.36 | 0.42 |
| 1:C:3089:ASN:O | 1:C:3092:HIS:HB2 | 2.19 | 0.42 |
| 1:D:504:VAL:O | 1:D:507:VAL:HG22 | 2.19 | 0.42 |
| 1:D:618:GLY:HA3 | 1:D:626:SER:N | 2.34 | 0.42 |
| 1:D:636:ILE:O | 1:D:640:HIS:ND1 | 2.31 | 0.42 |
| 1:D:788:GLU:OE1 | 1:D:791:ASP:HB2 | 2.20 | 0.42 |
| 1:D:914:HIS:O | 1:D:917:LEU:HG | 2.20 | 0.42 |
| 1:D:1152:GLY:HA2 | 1:D:1198:PHE:O | 2.19 | 0.42 |
| 1:D:1824:HIS:HB2 | 1:D:1827:ASP:CG | 2.45 | 0.42 |
| 1:E:870:GLU:HA | 1:E:878:PHE:HB3 | 2.02 | 0.42 |
| 1:E:1061:ALA:HA | 1:E:1064:GLN:CD | 2.45 | 0.42 |
| 1:E:1161:SER:N | 1:E:1185:GLY:O | 2.52 | 0.42 |
| 1:E:1405:TYR:CD2 | 1:E:1406:LEU:HD22 | 2.55 | 0.42 |
| 1:E:1421:ASP:HA | 1:E:1608:ARG:HD2 | 2.01 | 0.42 |
| 1:E:2954:GLU:OE2 | 1:E:3035:TYR:OH | 2.29 | 0.42 |
| 1:F:69:TRP:O | 1:F:72:LEU:HG | 2.18 | 0.42 |
| 1:F:1428:ILE:HA | 1:F:1431:ASN:HD21 | 1.83 | 0.42 |
| 1:F:1767:ASP:OD2 | 1:F:1890:ARG:NH2 | 2.53 | 0.42 |
| 1:F:1849:GLN:O | 1:F:1852:ILE:HG22 | 2.18 | 0.42 |
| 1:F:3011:TRP:CZ3 | 1:F:3013:TRP:HA | 2.55 | 0.42 |
| 1:G:755:ILE:HD11 | 1:G:763:TYR:HD2 | 1.84 | 0.42 |
| 1:G:758:LYS:HD3 | 1:G:758:LYS:HA | 1.72 | 0.42 |
| 1:G:812:ASP:OD2 | 1:G:818:TRP:NE1 | 2.37 | 0.42 |
| 1:G:2580:LEU:HA | 1:G:2583:VAL:HG12 | 2.02 | 0.42 |
| 1:G:2729:ASP:OD2 | 1:G:2915:PRO:HG2 | 2.19 | 0.42 |
| 1:G:3353:GLU:HG3 | 1:G:3386:TYR:HD2 | 1.85 | 0.42 |
| 1:H:81:LEU:HD12 | 1:H:86:LEU:HD13 | 2.02 | 0.42 |
| 1:H:446:TYR:OH | 1:H:543:ASP:OD1 | 2.35 | 0.42 |
| 1:H:1219:VAL:HB | 1:H:1239:VAL:HG21 | 2.01 | 0.42 |
| 1:H:1452:ALA:HA | 1:H:1457:PHE:CD2 | 2.55 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:H:1556:LEU:C | 1:H:1557:PHE:HD1 | 2.28 | 0.42 |
| 1:H:1801:ASP:OD1 | 1:H:1802:ILE:N | 2.52 | 0.42 |
| 1:H:2159:ARG:O | 1:H:2162:THR:OG1 | 2.31 | 0.42 |
| 1:I:131:ASN:HA | 1:I:138:HIS:HA | 2.01 | 0.42 |
| 1:I:629:HIS:HA | 1:I:775:LYS:NZ | 2.34 | 0.42 |
| 1:I:1966:GLU:H | 1:I:1966:GLU:CD | 2.27 | 0.42 |
| 1:I:1989:GLY:HA2 | 1:I:2024:TRP:NE1 | 2.34 | 0.42 |
| 1:I:1991:LYS:HE3 | 3:BA:2:NAG:H83 | 2.01 | 0.42 |
| 1:I:2648:ARG:HD2 | 1:I:2651:GLU:HB2 | 2.01 | 0.42 |
| 1:I:2941:LEU:HD12 | 1:I:2944:LEU:HD11 | 2.02 | 0.42 |
| 1:I:3078:CYS:O | 1:I:3082:VAL:HG13 | 2.19 | 0.42 |
| 1:J:248:ARG:NH2 | 1:J:801:ASP:HA | 2.34 | 0.42 |
| 1:J:535:ILE:H | 1:J:535:ILE:HD12 | 1.85 | 0.42 |
| 1:J:759:ASP:OD1 | 1:J:760:GLY:N | 2.53 | 0.42 |
| 1:J:2093:ARG:HD2 | 1:J:2367:TYR:HE1 | 1.84 | 0.42 |
| 1:J:3081:GLU:N | 1:J:3081:GLU:OE1 | 2.53 | 0.42 |
| 1:K:425:ASP:OD1 | 1:K:425:ASP:N | 2.48 | 0.42 |
| 1:K:910:PHE:HZ | 1:K:1022:HIS:ND1 | 2.17 | 0.42 |
| 1:K:971:GLY:H | 1:K:978:THR:HG1 | 1.61 | 0.42 |
| 1:K:1178:GLU:HG3 | 1:K:1205:ILE:HG21 | 2.01 | 0.42 |
| 1:K:1385:ILE:HD12 | 1:K:1385:ILE:H | 1.85 | 0.42 |
| 1:K:1596:LEU:HD12 | 1:K:1597:GLY:H | 1.85 | 0.42 |
| 1:K:2705:PHE:HD2 | 1:K:2706:PHE:CD1 | 2.37 | 0.42 |
| 1:L:523:TRP:HB3 | 1:L:639:LEU:HD13 | 2.02 | 0.42 |
| 1:L:869:LEU:HB3 | 1:L:928:LYS:HE3 | 2.00 | 0.42 |
| 1:L:1153:PHE:O | 1:L:1154:MET:HE2 | 2.20 | 0.42 |
| 1:L:1775:LEU:HD11 | 1:L:1779:PHE:HE1 | 1.84 | 0.42 |
| 1:L:2754:ASN:OD1 | 1:L:2755:ASP:N | 2.53 | 0.42 |
| 1:L:2953:TYR:HA | 1:L:2956:ILE:HG12 | 2.00 | 0.42 |
| 1:M:50:LYS:HE3 | 1:M:56:VAL:HB | 2.00 | 0.42 |
| 1:M:508:GLU:OE1 | 1:M:520:ILE:HB | 2.19 | 0.42 |
| 1:M:756:LYS:HB3 | 1:M:805:ASP:HB2 | 2.01 | 0.42 |
| 1:M:792:ALA:O | 1:M:795:LYS:HG2 | 2.19 | 0.42 |
| 1:M:996:THR:HG23 | 1:M:999:ALA:H | 1.84 | 0.42 |
| 1:M:1689:ARG:HA | 1:M:1692:VAL:HG22 | 2.01 | 0.42 |
| 1:M:2108:LYS:HA | 1:M:2111:LEU:HG | 2.00 | 0.42 |
| 1:M:2175:THR:HG23 | 1:N:1757:ARG:HD2 | 2.01 | 0.42 |
| 1:M:2514:ARG:HD3 | 1:M:2598:ILE:HG23 | 2.02 | 0.42 |
| 1:M:2676:VAL:HG21 | 1:M:2851:PHE:CZ | 2.55 | 0.42 |
| 1:N:1405:TYR:CD2 | 1:N:1406:LEU:HD22 | 2.55 | 0.42 |
| 1:N:1564:ASN:HD22 | 1:N:1603:PRO:HA | 1.84 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:N:2416:ASN:OD1 | 1:N:2417:GLY:N | 2.53 | 0.42 |
| 1:N:2712:VAL:HG23 | 1:N:2715:GLN:NE2 | 2.34 | 0.42 |
| 1:N:2757:ILE:O | 1:N:2761:ALA:HB2 | 2.20 | 0.42 |
| 1:N:3032:PHE:HA | 1:N:3113:PRO:HG2 | 2.01 | 0.42 |
| 1:N:3071:THR:HG23 | 1:N:3083:GLN:CG | 2.49 | 0.42 |
| 1:N:3129:TRP:O | 1:N:3133:GLN:HG2 | 2.20 | 0.42 |
| 1:N:3232:LEU:HD13 | 1:N:3269:ALA:HB3 | 2.01 | 0.42 |
| 1:O:302:GLN:NE2 | 1:O:303:ARG:HG3 | 2.35 | 0.42 |
| 1:O:1587:ASN:OD1 | 1:O:1588:HIS:ND1 | 2.52 | 0.42 |
| 1:O:2329:TYR:OH | 1:P:1238:LYS:HD3 | 2.20 | 0.42 |
| 1:P:105:ARG:HA | 1:P:108:GLN:NE2 | 2.34 | 0.42 |
| 1:P:477:CYS:HB2 | 1:P:478:PRO:HA | 2.02 | 0.42 |
| 1:P:493:MET:HE2 | 1:P:670:MET:SD | 2.59 | 0.42 |
| 1:P:872:ASP:HB3 | 1:P:877:GLY:HA2 | 2.01 | 0.42 |
| 1:P:1020:ILE:HG13 | 1:P:1021:ALA:N | 2.34 | 0.42 |
| 1:P:1153:PHE:O | 1:P:1198:PHE:HB3 | 2.19 | 0.42 |
| 1:Q:884:PHE:HE1 | 1:Q:1090:PRO:HG2 | 1.84 | 0.42 |
| 1:Q:949:ILE:HG23 | 1:Q:950:VAL:HG13 | 1.99 | 0.42 |
| 1:Q:1385:ILE:HB | 1:Q:1388:THR:HG21 | 2.01 | 0.42 |
| 1:Q:1684:THR:O | 1:Q:1688:ARG:HB3 | 2.20 | 0.42 |
| 1:Q:2714:ARG:NH2 | 1:Q:2778:ASP:O | 2.53 | 0.42 |
| 1:Q:2822:CYS:HA | 1:Q:2828:CYS:HB3 | 2.02 | 0.42 |
| 1:R:1143:ARG:HB3 | 1:R:1148:ARG:NH2 | 2.35 | 0.42 |
| 1:R:1159:ARG:NH2 | 1:R:1160:LYS:HE3 | 2.35 | 0.42 |
| 1:R:1333:VAL:HG22 | 1:R:1458:PHE:HE1 | 1.84 | 0.42 |
| 1:R:2086:GLU:C | 1:R:2087:LEU:HD12 | 2.45 | 0.42 |
| 1:R:3062:ASP:OD2 | 1:R:3064:LEU:HB2 | 2.19 | 0.42 |
| 1:R:3363:CYS:HB2 | 1:R:3396:CYS:HB3 | 1.89 | 0.42 |
| 1:S:304:ARG:HA | 1:S:304:ARG:NE | 2.35 | 0.42 |
| 1:S:441:THR:OG1 | 1:S:443:GLU:OE1 | 2.38 | 0.42 |
| 1:S:954:THR:HA | 1:S:965:PRO:HA | 2.01 | 0.42 |
| 1:S:1272:SER:OG | 1:S:1275:GLU:OE1 | 2.37 | 0.42 |
| 1:S:2273:TYR:HD1 | 1:S:2284:SER:HG | 1.66 | 0.42 |
| 1:S:3058:GLN:NE2 | 1:S:3268:ASP:OD2 | 2.52 | 0.42 |
| 1:S:3149:ASN:HD22 | 1:S:3152:ARG:NH2 | 2.16 | 0.42 |
| 1:S:3407:ASP:OD1 | 1:S:3407:ASP:N | 2.44 | 0.42 |
| 1:T:437:VAL:HG12 | 1:T:535:ILE:HD13 | 2.01 | 0.42 |
| 1:T:477:CYS:HA | 1:T:479:ARG:N | 2.35 | 0.42 |
| 1:T:944:THR:HG22 | 1:T:987:PHE:HB3 | 2.00 | 0.42 |
| 1:T:983:ARG:H | 1:T:986:LEU:HD12 | 1.83 | 0.42 |
| 1:T:1077:ALA:H | 1:T:1113:PHE:HE2 | 1.67 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:T:2923:ARG:NH1 | 1:T:3007:GLY:O | 2.49 | 0.42 |
| 1:T:3079:ASP:OD2 | 1:T:3333:SER:OG | 2.34 | 0.42 |
| 1:A:104:PRO:HA | 1:A:105:ARG:NH1 | 2.35 | 0.42 |
| 1:A:178:GLU:O | 1:A:182:GLU:HG2 | 2.19 | 0.42 |
| 1:A:728:ASP:OD2 | 1:A:836:HIS:HB2 | 2.20 | 0.42 |
| 1:A:734:ASP:HB3 | 1:A:833:GLY:N | 2.34 | 0.42 |
| 1:A:782:ASP:OD1 | 1:A:783:ARG:N | 2.53 | 0.42 |
| 1:A:997:LYS:HE2 | 1:A:997:LYS:H | 1.85 | 0.42 |
| 1:A:1204:ASP:OD1 | 1:A:1205:ILE:N | 2.52 | 0.42 |
| 1:A:1829:TRP:NE1 | 1:A:1833:GLN:HE22 | 2.17 | 0.42 |
| 1:A:2443:LYS:HZ1 | 1:A:2494:LYS:HD3 | 1.85 | 0.42 |
| 1:A:2525:THR:O | 1:A:2529:LYS:HG2 | 2.20 | 0.42 |
| 1:A:2605:GLU:OE1 | 1:A:2605:GLU:N | 2.48 | 0.42 |
| 1:A:2976:CYS:HB3 | 1:A:3156:PRO:HD3 | 2.01 | 0.42 |
| 1:A:2986:HIS:O | 1:A:2990:LEU:HD23 | 2.20 | 0.42 |
| 1:B:1878:ASP:OD2 | 1:B:1880:ILE:HB | 2.20 | 0.42 |
| 1:B:2087:LEU:H | 1:B:2366:ARG:HH12 | 1.66 | 0.42 |
| 1:B:2553:TYR:HA | 1:B:2554:PRO:HA | 1.75 | 0.42 |
| 1:C:330:ASP:OD1 | 1:C:331:HIS:N | 2.53 | 0.42 |
| 1:C:398:LEU:HD12 | 1:C:399:ASN:H | 1.84 | 0.42 |
| 1:C:530:THR:HG23 | 1:C:574:LEU:HB2 | 2.02 | 0.42 |
| 1:C:767:LYS:HD3 | 1:C:768:LEU:N | 2.34 | 0.42 |
| 1:C:1061:ALA:HA | 1:C:1064:GLN:NE2 | 2.34 | 0.42 |
| 1:C:1145:HIS:NE2 | 1:C:1524:ASN:OD1 | 2.53 | 0.42 |
| 1:C:1662:ASP:N | 1:C:1662:ASP:OD1 | 2.52 | 0.42 |
| 1:C:1778:PHE:HD2 | 1:C:1779:PHE:HD2 | 1.67 | 0.42 |
| 1:C:1912:ALA:O | 1:C:1916:MET:HG2 | 2.19 | 0.42 |
| 1:C:2654:PHE:HA | 1:C:2657:GLN:OE1 | 2.20 | 0.42 |
| 1:C:2743:PRO:HA | 1:C:2762:ARG:HE | 1.83 | 0.42 |
| 1:D:500:HIS:CD2 | 1:D:641:HIS:CE1 | 3.08 | 0.42 |
| 1:D:905:HIS:HA | 1:D:910:PHE:CD2 | 2.52 | 0.42 |
| 1:D:1134:PRO:O | 1:D:1138:ARG:HG3 | 2.19 | 0.42 |
| 1:D:1305:CYS:HB2 | 1:D:1312:VAL:O | 2.19 | 0.42 |
| 1:D:1646:GLU:CD | 1:D:1648:SER:H | 2.28 | 0.42 |
| 1:D:1928:PRO:HD2 | 1:D:1929:TYR:CD2 | 2.54 | 0.42 |
| 1:D:2041:LYS:HE2 | 1:D:2043:LEU:HD23 | 2.00 | 0.42 |
| 1:E:332:ASP:OD1 | 1:E:332:ASP:N | 2.53 | 0.42 |
| 1:E:1278:SER:O | 1:E:1281:SER:OG | 2.26 | 0.42 |
| 1:E:1722:TYR:CD1 | 1:E:1724:GLU:HB2 | 2.55 | 0.42 |
| 1:F:198:HIS:HD1 | 1:F:205:TRP:CD1 | 2.38 | 0.42 |
| 1:F:496:PHE:HB3 | 1:F:497:PRO:HD3 | 2.02 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:F:966:ASN:HD21 | 1:F:968:PHE:HD2 | 1.67 | 0.42 |
| 1:F:1036:SER:O | 1:F:1042:TYR:HB2 | 2.19 | 0.42 |
| 1:F:1159:ARG:HG2 | 1:F:1186:ASP:C | 2.45 | 0.42 |
| 1:F:1543:LEU:O | 1:F:1546:VAL:HG12 | 2.20 | 0.42 |
| 1:F:2108:LYS:HE3 | 1:F:2108:LYS:HB3 | 1.69 | 0.42 |
| 1:G:687:ASN:OD1 | 1:G:688:GLU:N | 2.53 | 0.42 |
| 1:G:1122:HIS:ND1 | 1:G:1123:TYR:O | 2.51 | 0.42 |
| 1:G:1852:ILE:HG21 | 1:G:2030:TYR:CZ | 2.55 | 0.42 |
| 1:G:1928:PRO:HD2 | 1:G:1929:TYR:CE1 | 2.54 | 0.42 |
| 1:G:1968:LEU:O | 1:G:1972:ILE:HG23 | 2.20 | 0.42 |
| 1:G:2101:ALA:O | 1:G:2104:THR:OG1 | 2.23 | 0.42 |
| 1:G:2163:LEU:HA | 1:G:2166:GLU:OE1 | 2.20 | 0.42 |
| 1:G:2287:HIS:HE1 | 1:G:2432:LEU:HG | 1.84 | 0.42 |
| 1:G:2330:MET:HE3 | 1:G:2330:MET:O | 2.18 | 0.42 |
| 1:H:48:CYS:HB2 | 1:H:58:CYS:HB2 | 1.55 | 0.42 |
| 1:H:663:LYS:HD2 | 1:H:664:ALA:O | 2.20 | 0.42 |
| 1:H:732:THR:HG23 | 1:H:733:LYS:HE3 | 2.01 | 0.42 |
| 1:H:2487:SER:OG | 1:H:2488:LYS:N | 2.52 | 0.42 |
| 1:H:2953:TYR:HA | 1:H:2956:ILE:HG12 | 2.01 | 0.42 |
| 1:H:3227:THR:HB | 1:H:3246:TYR:CD2 | 2.55 | 0.42 |
| 1:I:129:GLU:HG2 | 1:I:139:THR:C | 2.44 | 0.42 |
| 1:I:527:ARG:HG2 | 1:I:528:PRO:HD2 | 2.02 | 0.42 |
| 1:I:903:CYS:O | 1:I:905:HIS:ND1 | 2.40 | 0.42 |
| 1:I:1169:CYS:HA | 1:I:1175:CYS:HA | 2.02 | 0.42 |
| 1:I:1365:ALA:HA | 1:I:1381:PHE:CE2 | 2.55 | 0.42 |
| 1:I:3351:VAL:HG21 | 1:I:3388:PHE:HB3 | 2.01 | 0.42 |
| 1:J:8:VAL:HG11 | 1:J:94:TRP:HB2 | 2.02 | 0.42 |
| 1:J:130:ILE:O | 1:J:138:HIS:HA | 2.19 | 0.42 |
| 1:J:1060:TRP:NE1 | 1:J:1064:GLN:HE22 | 2.17 | 0.42 |
| 1:J:1649:VAL:HG23 | 1:J:1650:LEU:HD22 | 2.02 | 0.42 |
| 1:J:1809:VAL:HG22 | 1:J:1811:ARG:HH12 | 1.83 | 0.42 |
| 1:J:2754:ASN:ND2 | 1:J:2757:ILE:HG12 | 2.34 | 0.42 |
| 1:K:704:HIS:ND1 | 1:K:705:GLU:OE2 | 2.53 | 0.42 |
| 1:K:881:ILE:HA | 1:K:884:PHE:HD2 | 1.83 | 0.42 |
| 1:K:891:CYS:HB3 | 1:K:900:PHE:O | 2.20 | 0.42 |
| 1:K:2286:LEU:HD12 | 1:K:2429:GLY:HA2 | 2.02 | 0.42 |
| 1:K:2297:THR:O | 1:K:2300:THR:OG1 | 2.27 | 0.42 |
| 1:K:2390:LYS:HB2 | 1:K:2392:ARG:HH12 | 1.84 | 0.42 |
| 1:L:135:MET:SD | 1:L:135:MET:N | 2.93 | 0.42 |
| 1:L:751:VAL:HG22 | 1:L:810:ILE:HD13 | 2.01 | 0.42 |
| 1:L:2343:ASN:OD1 | 1:L:2344:GLU:N | 2.52 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:L:3357:TYR:HE1 | 1:L:3360:LEU:HD22 | 1.84 | 0.42 |
| 1:M:1687:GLU:HB2 | 1:M:1760:LEU:HD11 | 2.02 | 0.42 |
| 1:M:1776:PRO:HD2 | 1:M:1779:PHE:CZ | 2.55 | 0.42 |
| 1:M:2313:GLN:HG2 | 1:M:2320:TYR:HB3 | 2.00 | 0.42 |
| 1:M:2407:GLU:HB2 | 1:M:2426:PHE:CE2 | 2.54 | 0.42 |
| 1:M:2762:ARG:HG3 | 1:M:2764:VAL:HG22 | 2.00 | 0.42 |
| 1:N:122:LYS:HE3 | 1:N:122:LYS:HB3 | 1.77 | 0.42 |
| 1:N:695:ARG:NH2 | 1:N:696:PRO:HD2 | 2.34 | 0.42 |
| 1:N:1285:ARG:HA | 1:N:1285:ARG:HD2 | 1.86 | 0.42 |
| 1:N:1711:ALA:HA | 1:N:1876:SER:HB2 | 2.02 | 0.42 |
| 1:N:1883:LEU:O | 1:N:1886:SER:OG | 2.32 | 0.42 |
| 1:N:1966:GLU:N | 1:N:1966:GLU:OE1 | 2.53 | 0.42 |
| 1:N:2141:ALA:HB3 | 1:N:2143:LYS:HZ2 | 1.85 | 0.42 |
| 1:N:2305:ILE:HA | 1:N:2308:VAL:HG12 | 2.02 | 0.42 |
| 1:N:2822:CYS:HB2 | 1:N:2871:HIS:NE2 | 2.34 | 0.42 |
| 1:O:89:ILE:HG22 | 1:O:90:GLY:O | 2.19 | 0.42 |
| 1:O:228:GLU:OE1 | 1:O:229:LEU:HD22 | 2.20 | 0.42 |
| 1:O:997:LYS:O | 1:O:1001:MET:HG3 | 2.20 | 0.42 |
| 1:O:1016:VAL:O | 1:O:1019:GLU:HG3 | 2.18 | 0.42 |
| 1:O:1470:ILE:HD13 | 1:O:1533:LEU:HD12 | 2.01 | 0.42 |
| 1:O:2371:LYS:HA | 1:O:2371:LYS:HD2 | 1.86 | 0.42 |
| 1:O:2415:GLU:CD | 1:O:2466:PRO:HA | 2.45 | 0.42 |
| 1:O:3089:ASN:ND2 | 1:O:3247:ILE:HA | 2.35 | 0.42 |
| 1:O:3128:ILE:HG13 | 1:O:3129:TRP:N | 2.33 | 0.42 |
| 1:P:17:LEU:HD13 | 1:P:20:GLU:OE2 | 2.20 | 0.42 |
| 1:P:409:VAL:HG22 | 1:P:666:CYS:HA | 2.00 | 0.42 |
| 1:P:486:TYR:HB3 | 1:P:777:MET:HE1 | 2.01 | 0.42 |
| 1:P:1229:LYS:HE3 | 1:P:1229:LYS:HB3 | 1.89 | 0.42 |
| 1:P:1275:GLU:OE1 | 1:P:1275:GLU:N | 2.50 | 0.42 |
| 1:P:2112:ARG:HE | 1:P:2116:LYS:NZ | 2.14 | 0.42 |
| 1:P:2343:ASN:OD1 | 1:P:2344:GLU:N | 2.53 | 0.42 |
| 1:P:2527:SER:O | 1:P:2530:LYS:HG3 | 2.20 | 0.42 |
| 1:P:2559:ASP:OD1 | 1:P:2559:ASP:N | 2.53 | 0.42 |
| 1:P:2676:VAL:HA | 1:P:2679:ASN:HD21 | 1.85 | 0.42 |
| 1:P:3086:MET:HE1 | 1:P:3258:TYR:CE2 | 2.54 | 0.42 |
| 1:P:3342:SER:OG | 1:P:3344:VAL:O | 2.35 | 0.42 |
| 1:Q:330:ASP:OD1 | 1:Q:331:HIS:N | 2.53 | 0.42 |
| 1:Q:647:LEU:O | 1:Q:650:ILE:HG12 | 2.20 | 0.42 |
| 1:Q:689:LYS:HD3 | 1:Q:689:LYS:HA | 1.70 | 0.42 |
| 1:Q:1114:ASP:OD1 | 1:Q:1114:ASP:N | 2.46 | 0.42 |
| 1:Q:1317:HIS:HA | 1:Q:1322:PHE:HD1 | 1.84 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:Q:1485:SER:OG | 1:Q:1486:ASP:N | 2.52 | 0.42 |
| 1:Q:2567:CYS:C | 1:Q:2569:HIS:HD1 | 2.26 | 0.42 |
| 1:Q:2986:HIS:HB3 | 1:Q:3177:ILE:CD1 | 2.50 | 0.42 |
| 1:Q:3154:LEU:O | 1:Q:3158:ASN:N | 2.53 | 0.42 |
| 1:R:591:LEU:HB3 | 1:R:730:ARG:NH2 | 2.35 | 0.42 |
| 1:R:695:ARG:HH21 | 1:R:696:PRO:HD2 | 1.85 | 0.42 |
| 1:R:944:THR:HA | 1:R:987:PHE:CD1 | 2.55 | 0.42 |
| 1:R:968:PHE:CE1 | 1:R:1047:PRO:HG2 | 2.53 | 0.42 |
| 1:R:1101:HIS:CD2 | 1:R:1104:ARG:HH22 | 2.37 | 0.42 |
| 1:R:1315:CYS:C | 1:R:1317:HIS:HD1 | 2.27 | 0.42 |
| 1:R:2113:ASP:HA | 1:R:2116:LYS:HZ2 | 1.84 | 0.42 |
| 1:R:2569:HIS:HD2 | 1:R:2837:LEU:HD21 | 1.85 | 0.42 |
| 1:R:3002:LYS:HA | 1:R:3002:LYS:HD3 | 1.78 | 0.42 |
| 1:R:3146:ALA:O | 1:R:3150:LEU:HG | 2.19 | 0.42 |
| 1:R:3227:THR:OG1 | 1:R:3245:PHE:O | 2.31 | 0.42 |
| 1:S:93:TYR:HA | 1:S:217:SER:OG | 2.20 | 0.42 |
| 1:S:161:LEU:HD21 | 1:S:187:HIS:CD2 | 2.55 | 0.42 |
| 1:S:611:ASN:HD22 | 1:S:771:LEU:H | 1.68 | 0.42 |
| 1:S:811:LYS:HZ2 | 1:S:815:GLY:C | 2.27 | 0.42 |
| 1:S:1327:ARG:NH1 | 1:S:1465:ASP:OD1 | 2.53 | 0.42 |
| 1:S:2114:LEU:HD13 | 1:S:2172:HIS:CE1 | 2.54 | 0.42 |
| 1:S:2229:GLN:HB2 | 1:S:2274:LEU:HD12 | 2.01 | 0.42 |
| 1:S:2812:LYS:HD3 | 1:S:2812:LYS:HA | 1.89 | 0.42 |
| 1:T:158:ASN:HB3 | 1:T:162:PHE:CD2 | 2.55 | 0.42 |
| 1:T:442:ASP:OD1 | 1:T:443:GLU:N | 2.53 | 0.42 |
| 1:T:663:LYS:HB3 | 1:T:665:HIS:CE1 | 2.55 | 0.42 |
| 1:T:946:LEU:HG | 1:T:951:ALA:HB2 | 2.01 | 0.42 |
| 1:T:1125:ASP:N | 1:T:1125:ASP:OD1 | 2.52 | 0.42 |
| 1:T:1564:ASN:HD22 | 1:T:1603:PRO:HA | 1.85 | 0.42 |
| 1:T:1773:ASN:OD1 | 1:T:1773:ASN:N | 2.52 | 0.42 |
| 1:T:2481:LEU:HD13 | 1:T:2482:PRO:HD2 | 2.02 | 0.42 |
| 1:T:2695:THR:HG21 | 1:T:2698:TYR:HD2 | 1.84 | 0.42 |
| 1:A:14:GLN:HG2 | 1:A:15:GLU:N | 2.34 | 0.42 |
| 1:A:129:GLU:HG2 | 1:A:139:THR:C | 2.44 | 0.42 |
| 1:A:855:THR:HG22 | 1:A:858:GLN:HE22 | 1.84 | 0.42 |
| 1:A:1307:HIS:CE1 | 1:A:1602:MET:HE1 | 2.55 | 0.42 |
| 1:A:2022:MET:HE3 | 1:A:2022:MET:HB3 | 1.89 | 0.42 |
| 1:A:2029:LEU:HD23 | 1:A:2029:LEU:H | 1.84 | 0.42 |
| 1:A:2598:ILE:HD11 | 1:A:2707:ILE:HD13 | 2.01 | 0.42 |
| 1:A:2616:ASP:C | 1:A:2617:LYS:HE2 | 2.45 | 0.42 |
| 1:A:2991:LEU:HD23 | 1:A:2991:LEU:HA | 1.90 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:3064:LEU:O | 1:A:3067:GLN:HG3 | 2.20 | 0.42 |
| 1:A:3083:GLN:O | 1:A:3087:LEU:HD13 | 2.20 | 0.42 |
| 1:A:3299:LEU:HD23 | 1:A:3299:LEU:HA | 1.93 | 0.42 |
| 1:A:3330:VAL:HB | 1:A:3404:ILE:HD12 | 2.01 | 0.42 |
| 1:B:80:LYS:O | 1:B:83:LYS:HG2 | 2.20 | 0.42 |
| 1:B:225:ILE:HA | 1:B:228:GLU:OE2 | 2.19 | 0.42 |
| 1:B:1143:ARG:HB3 | 1:B:1148:ARG:NH2 | 2.35 | 0.42 |
| 1:B:1500:ASN:OD1 | 1:B:1500:ASN:N | 2.52 | 0.42 |
| 1:B:1852:ILE:HD11 | 1:B:2013:PHE:HD2 | 1.84 | 0.42 |
| 1:B:2345:ASN:ND2 | 1:B:2348:THR:OG1 | 2.53 | 0.42 |
| 1:B:2948:ASP:OD1 | 1:B:2948:ASP:N | 2.51 | 0.42 |
| 1:B:3077:TYR:HE1 | 1:B:3126:TRP:HE1 | 1.67 | 0.42 |
| 1:C:647:LEU:HA | 1:C:650:ILE:HG12 | 2.00 | 0.42 |
| 1:C:792:ALA:HA | 1:C:795:LYS:HG2 | 2.01 | 0.42 |
| 1:C:1867:HIS:HA | 1:C:1874:TYR:CD2 | 2.55 | 0.42 |
| 1:C:2153:THR:HA | 1:C:2156:HIS:ND1 | 2.34 | 0.42 |
| 1:C:2582:VAL:O | 1:C:2586:GLU:OE1 | 2.38 | 0.42 |
| 1:C:2602:ASP:HA | 1:C:2711:ASN:ND2 | 2.34 | 0.42 |
| 1:C:2603:TRP:CD1 | 1:C:2711:ASN:HD22 | 2.38 | 0.42 |
| 1:C:3212:ARG:HG3 | 1:C:3214:TYR:CZ | 2.54 | 0.42 |
| 1:D:4:VAL:HG23 | 1:D:284:ASP:HB3 | 2.01 | 0.42 |
| 1:D:435:LYS:O | 1:D:521:PRO:HA | 2.19 | 0.42 |
| 1:D:614:HIS:HA | 1:D:625:LEU:HG | 2.02 | 0.42 |
| 1:D:847:VAL:HA | 1:D:1122:HIS:O | 2.20 | 0.42 |
| 1:D:1166:LEU:HB3 | 1:D:1179:GLY:O | 2.19 | 0.42 |
| 1:D:1376:GLU:OE2 | 1:D:1377:SER:N | 2.52 | 0.42 |
| 1:D:1547:LEU:O | 1:D:1550:GLN:HG3 | 2.20 | 0.42 |
| 1:D:1894:LEU:HD11 | 1:D:1959:GLU:O | 2.20 | 0.42 |
| 1:D:2487:SER:OG | 1:D:2488:LYS:N | 2.52 | 0.42 |
| 1:D:2521:THR:O | 1:D:2525:THR:HG23 | 2.20 | 0.42 |
| 1:E:133:ASP:HA | 1:E:138:HIS:HE1 | 1.84 | 0.42 |
| 1:E:2605:GLU:OE1 | 1:E:2605:GLU:N | 2.52 | 0.42 |
| 1:E:2819:PHE:O | 1:E:2831:ALA:HB3 | 2.19 | 0.42 |
| 1:E:3089:ASN:ND2 | 1:E:3247:ILE:HD12 | 2.35 | 0.42 |
| 1:F:443:GLU:HG2 | 1:F:444:GLU:N | 2.34 | 0.42 |
| 1:F:1022:HIS:HD2 | 1:F:1026:HIS:NE2 | 2.18 | 0.42 |
| 1:F:1624:LYS:HD2 | 1:F:1624:LYS:HA | 1.90 | 0.42 |
| 1:F:2617:LYS:HD3 | 1:F:2617:LYS:HA | 1.78 | 0.42 |
| 1:F:2989:ARG:HG2 | 1:F:3123:ASP:OD1 | 2.20 | 0.42 |
| 1:F:3331:ILE:HA | 1:F:3405:SER:OG | 2.19 | 0.42 |
| 1:G:182:GLU:O | 1:G:186:ASN:ND2 | 2.53 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:G:381:ASN:HB3 | 1:G:410:TYR:CE1 | 2.54 | 0.42 |
| 1:G:854:LEU:HD12 | 1:G:858:GLN:HG3 | 2.02 | 0.42 |
| 1:G:1067:GLN:NE2 | 1:G:1073:PRO:O | 2.50 | 0.42 |
| 1:G:1084:LEU:HG | 1:G:1110:PHE:HE1 | 1.84 | 0.42 |
| 1:G:1534:ASN:HA | 1:G:1539:THR:HA | 2.01 | 0.42 |
| 1:G:1635:ILE:O | 1:G:1647:SER:OG | 2.37 | 0.42 |
| 1:G:2958:SER:HA | 1:G:2962:ALA:O | 2.20 | 0.42 |
| 1:H:74:VAL:HA | 1:H:77:LEU:HD23 | 2.00 | 0.42 |
| 1:H:973:VAL:O | 1:H:974:GLU:HG3 | 2.20 | 0.42 |
| 1:H:1135:GLN:O | 1:H:1136:LEU:C | 2.63 | 0.42 |
| 1:H:1736:MET:N | 1:H:1736:MET:SD | 2.93 | 0.42 |
| 1:H:1890:ARG:NH1 | 1:H:1957:THR:O | 2.53 | 0.42 |
| 1:H:2526:GLU:HA | 1:H:2529:LYS:HG2 | 2.02 | 0.42 |
| 1:H:3068:THR:O | 1:H:3071:THR:HB | 2.20 | 0.42 |
| 1:I:1508:ASP:OD2 | 1:I:1509:LEU:HG | 2.19 | 0.42 |
| 1:I:1723:PRO:C | 1:I:1728:ARG:HH12 | 2.26 | 0.42 |
| 1:I:1745:LEU:HA | 1:I:1748:VAL:HG12 | 2.02 | 0.42 |
| 1:I:2022:MET:SD | 1:I:2022:MET:N | 2.93 | 0.42 |
| 1:I:2225:VAL:C | 1:I:2226:ARG:HD3 | 2.45 | 0.42 |
| 1:I:2470:ARG:NH1 | 1:I:2471:TYR:H | 2.18 | 0.42 |
| 1:I:2663:GLU:OE2 | 1:I:2801:ARG:NH2 | 2.53 | 0.42 |
| 1:I:2941:LEU:HD23 | 1:I:3031:PRO:HG2 | 2.01 | 0.42 |
| 1:I:3227:THR:OG1 | 1:I:3245:PHE:O | 2.23 | 0.42 |
| 1:J:198:HIS:HD1 | 1:J:205:TRP:NE1 | 2.18 | 0.42 |
| 1:J:309:ALA:HB2 | 1:J:380:LEU:HD11 | 2.01 | 0.42 |
| 1:J:562:LEU:HB3 | 1:J:564:GLU:OE1 | 2.20 | 0.42 |
| 1:J:756:LYS:HB3 | 1:J:805:ASP:HB2 | 2.02 | 0.42 |
| 1:J:1142:HIS:HD2 | 1:J:1143:ARG:HH12 | 1.67 | 0.42 |
| 1:J:2407:GLU:O | 1:J:2473:ILE:HA | 2.20 | 0.42 |
| 1:J:3102:SER:O | 1:J:3105:THR:OG1 | 2.31 | 0.42 |
| 1:K:215:HIS:O | 1:K:219:VAL:HG23 | 2.19 | 0.42 |
| 1:K:844:GLU:HB2 | 1:K:846:HIS:CE1 | 2.53 | 0.42 |
| 1:K:2095:GLU:OE1 | 1:K:2098:HIS:N | 2.52 | 0.42 |
| 1:K:3071:THR:HG22 | 1:K:3083:GLN:HG2 | 2.01 | 0.42 |
| 1:L:337:GLN:CD | 1:S:1588:HIS:H | 2.25 | 0.42 |
| 1:L:848:ARG:HB2 | 1:L:934:LEU:O | 2.20 | 0.42 |
| 1:L:1133:ILE:H | 1:L:1133:ILE:HD12 | 1.85 | 0.42 |
| 1:L:1143:ARG:HB3 | 1:L:1148:ARG:NH2 | 2.35 | 0.42 |
| 1:L:1437:VAL:HG23 | 1:L:1445:LEU:HD12 | 2.02 | 0.42 |
| 1:L:1802:ILE:CD1 | 1:L:1805:GLU:HB2 | 2.50 | 0.42 |
| 1:L:2001:CYS:HB2 | 1:L:2050:THR:OG1 | 2.20 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:L:2210:ASN:ND2 | 1:L:2212:PHE:HB2 | 2.33 | 0.42 |
| 1:L:2578:HIS:CD2 | 1:L:2709:HIS:CD2 | 3.08 | 0.42 |
| 1:L:3036:GLN:OE1 | 1:L:3042:HIS:N | 2.53 | 0.42 |
| 1:L:3092:HIS:HA | 1:L:3103:MET:HE1 | 2.02 | 0.42 |
| 1:L:3256:TRP:HZ3 | 1:L:3258:TYR:CE1 | 2.38 | 0.42 |
| 1:M:131:ASN:HA | 1:M:138:HIS:HA | 2.02 | 0.42 |
| 1:M:811:LYS:HB2 | 1:M:811:LYS:HE2 | 1.87 | 0.42 |
| 1:M:915:ARG:HH21 | 1:M:1115:TYR:HB3 | 1.85 | 0.42 |
| 1:M:1518:ASP:CG | 1:M:1525:HIS:HD1 | 2.27 | 0.42 |
| 1:M:2405:SER:HB2 | 1:M:2476:VAL:HB | 2.00 | 0.42 |
| 1:M:2686:GLY:HA2 | 1:M:2693:MET:HG3 | 2.01 | 0.42 |
| 1:M:2923:ARG:HD3 | 1:M:3187:PHE:CE1 | 2.54 | 0.42 |
| 1:M:2939:ASN:O | 1:M:2943:LYS:HE2 | 2.19 | 0.42 |
| 1:N:221:ARG:HH12 | 1:N:285:ASP:HB3 | 1.85 | 0.42 |
| 1:N:627:THR:OG1 | 1:N:628:LEU:N | 2.53 | 0.42 |
| 1:N:859:VAL:O | 1:N:863:ARG:NE | 2.48 | 0.42 |
| 1:N:1992:THR:C | 1:N:2017:GLY:O | 2.63 | 0.42 |
| 1:N:2169:LEU:HB3 | 1:N:2174:SER:HB3 | 2.02 | 0.42 |
| 1:N:2752:ASN:HD21 | 1:N:2757:ILE:HG13 | 1.83 | 0.42 |
| 1:N:3214:TYR:HD1 | 1:N:3265:ASP:HA | 1.84 | 0.42 |
| 1:N:3282:GLY:C | 1:N:3283:PHE:HD1 | 2.26 | 0.42 |
| 1:N:3382:GLU:O | 1:N:3386:TYR:OH | 2.34 | 0.42 |
| 1:O:269:THR:OG1 | 1:O:270:ALA:N | 2.53 | 0.42 |
| 1:O:561:PHE:CD2 | 1:O:562:LEU:HG | 2.54 | 0.42 |
| 1:O:601:ASP:O | 1:O:604:VAL:HG22 | 2.20 | 0.42 |
| 1:O:799:LYS:HD2 | 1:O:799:LYS:HA | 1.77 | 0.42 |
| 1:O:1489:LEU:HD11 | 1:P:2075:TYR:HB2 | 2.01 | 0.42 |
| 1:O:2656:ARG:H | 1:O:2656:ARG:CD | 2.29 | 0.42 |
| 1:P:111:ILE:HG22 | 1:P:121:GLN:O | 2.20 | 0.42 |
| 1:P:196:HIS:HE1 | 1:P:198:HIS:HB2 | 1.82 | 0.42 |
| 1:P:224:VAL:HA | 1:P:227:GLN:OE1 | 2.19 | 0.42 |
| 1:P:1328:LEU:HG | 1:P:1499:PHE:HE2 | 1.85 | 0.42 |
| 1:P:1839:GLU:N | 1:P:1839:GLU:OE1 | 2.53 | 0.42 |
| 1:P:2297:THR:O | 1:P:2300:THR:OG1 | 2.34 | 0.42 |
| 1:P:3230:VAL:HG22 | 1:P:3283:PHE:HD2 | 1.85 | 0.42 |
| 1:Q:729:GLU:O | 1:Q:732:THR:HG22 | 2.20 | 0.42 |
| 1:Q:968:PHE:HA | 1:Q:1047:PRO:HG3 | 2.00 | 0.42 |
| 1:Q:1159:ARG:NE | 1:Q:1186:ASP:O | 2.50 | 0.42 |
| 1:Q:1482:ASP:OD1 | 1:Q:1483:ASP:N | 2.51 | 0.42 |
| 1:Q:1492:MET:O | 1:Q:1516:PRO:HD2 | 2.20 | 0.42 |
| 1:Q:1515:ARG:O | 1:Q:1519:VAL:HG23 | 2.20 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:Q:1739:PHE:HB3 | 1:Q:1740:PRO:HD3 | 2.02 | 0.42 |
| 1:Q:1903:GLY:HA3 | 1:R:1667:GLN:HB2 | 2.02 | 0.42 |
| 1:Q:2225:VAL:HG23 | 1:T:113:LYS:HE2 | 2.00 | 0.42 |
| 1:Q:2271:ILE:HG13 | 1:Q:2298:HIS:CE1 | 2.54 | 0.42 |
| 1:Q:2421:ARG:HH22 | 1:Q:2424:ALA:HB2 | 1.85 | 0.42 |
| 1:Q:2576:GLN:NE2 | 1:Q:2767:PHE:HD1 | 2.18 | 0.42 |
| 1:Q:2770:ASP:N | 1:Q:2770:ASP:OD1 | 2.53 | 0.42 |
| 1:Q:2821:LEU:O | 1:Q:2828:CYS:HB2 | 2.20 | 0.42 |
| 1:Q:2900:LYS:HE3 | 1:Q:2900:LYS:HB3 | 1.78 | 0.42 |
| 1:R:801:ASP:OD1 | 1:R:801:ASP:N | 2.52 | 0.42 |
| 1:R:1500:ASN:N | 1:R:1500:ASN:OD1 | 2.50 | 0.42 |
| 1:R:1788:VAL:HG12 | 1:R:1789:LEU:HD22 | 2.02 | 0.42 |
| 1:R:1893:ALA:O | 1:R:1896:GLN:HB2 | 2.20 | 0.42 |
| 1:R:1941:PRO:O | 1:R:1944:VAL:HG22 | 2.18 | 0.42 |
| 1:R:1992:THR:HA | 1:R:2017:GLY:O | 2.20 | 0.42 |
| 1:R:2041:LYS:HE2 | 1:R:2043:LEU:HD23 | 2.02 | 0.42 |
| 1:R:2305:ILE:HA | 1:R:2308:VAL:HG12 | 2.02 | 0.42 |
| 1:S:168:ALA:HA | 1:S:180:GLN:HG2 | 2.02 | 0.42 |
| 1:S:307:GLU:OE1 | 1:S:412:PRO:HA | 2.20 | 0.42 |
| 1:S:473:LEU:N | 1:S:775:LYS:HE3 | 2.35 | 0.42 |
| 1:S:1247:SER:O | 1:S:1250:LYS:HG2 | 2.20 | 0.42 |
| 1:S:2012:ASP:OD1 | 1:S:2012:ASP:N | 2.52 | 0.42 |
| 1:S:2330:MET:HE2 | 1:S:2355:LYS:HG3 | 2.01 | 0.42 |
| 1:S:2390:LYS:HB2 | 1:S:2390:LYS:HE2 | 1.92 | 0.42 |
| 1:S:2416:ASN:OD1 | 1:S:2417:GLY:N | 2.46 | 0.42 |
| 1:S:2653:PHE:HA | 1:S:2656:ARG:HH12 | 1.84 | 0.42 |
| 1:S:3078:CYS:O | 1:S:3082:VAL:HG13 | 2.20 | 0.42 |
| 1:S:3091:ILE:HA | 1:S:3094:LEU:HD23 | 2.01 | 0.42 |
| 1:T:160:GLN:NE2 | 1:T:161:LEU:HG | 2.34 | 0.42 |
| 1:T:215:HIS:O | 1:T:219:VAL:HG23 | 2.20 | 0.42 |
| 1:T:327:LYS:HE2 | 1:T:327:LYS:HB3 | 1.82 | 0.42 |
| 1:T:735:ARG:NH2 | 1:T:789:ILE:H | 2.18 | 0.42 |
| 1:T:1139:GLU:OE2 | 1:T:1143:ARG:NH1 | 2.51 | 0.42 |
| 1:T:2945:GLN:HG3 | 1:T:3035:TYR:HE1 | 1.85 | 0.42 |
| 1:T:3081:GLU:OE1 | 1:T:3081:GLU:N | 2.52 | 0.42 |
| 1:T:3174:PRO:O | 1:T:3177:ILE:HG22 | 2.20 | 0.42 |
| 1:A:168:ALA:HA | 1:A:180:GLN:HG3 | 2.02 | 0.42 |
| 1:A:483:ARG:HD2 | 1:A:484:VAL:N | 2.34 | 0.42 |
| 1:A:811:LYS:HZ3 | 1:A:816:LYS:C | 2.27 | 0.42 |
| 1:A:914:HIS:HE1 | 1:A:1022:HIS:HE1 | 1.68 | 0.42 |
| 1:A:920:GLN:HE22 | 1:A:1100:ASP:CB | 2.33 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:1263:HIS:N | 1:A:1263:HIS:CD2 | 2.88 | 0.42 |
| 1:A:1286:MET:HA | 1:A:1289:ASP:OD2 | 2.20 | 0.42 |
| 1:A:1413:ALA:O | 1:A:1425:GLN:NE2 | 2.53 | 0.42 |
| 1:A:1899:GLN:NE2 | 1:A:1905:ASP:O | 2.51 | 0.42 |
| 1:A:2034:ILE:HB | 1:A:2038:LEU:HD23 | 2.02 | 0.42 |
| 1:A:2939:ASN:O | 1:A:2943:LYS:HG2 | 2.20 | 0.42 |
| 1:B:435:LYS:NZ | 1:B:439:THR:OG1 | 2.51 | 0.42 |
| 1:B:501:ARG:HE | 1:B:645:ASP:CG | 2.21 | 0.42 |
| 1:B:1650:LEU:HD12 | 1:B:1650:LEU:HA | 1.87 | 0.42 |
| 1:B:1889:ASP:OD1 | 1:B:1955:TYR:OH | 2.30 | 0.42 |
| 1:C:635:PRO:O | 1:C:638:ILE:HG12 | 2.19 | 0.42 |
| 1:C:757:PRO:HB3 | 1:C:798:LEU:HD11 | 2.02 | 0.42 |
| 1:C:1286:MET:HA | 1:C:1289:ASP:OD2 | 2.19 | 0.42 |
| 1:C:1770:ASN:OD1 | 1:C:1772:GLN:NE2 | 2.53 | 0.42 |
| 1:C:2775:GLN:N | 1:C:2775:GLN:OE1 | 2.51 | 0.42 |
| 1:C:2819:PHE:CZ | 1:C:2832:GLY:HA3 | 2.55 | 0.42 |
| 1:D:96:TRP:CZ3 | 1:D:218:ASN:HB3 | 2.55 | 0.42 |
| 1:D:444:GLU:HA | 1:D:447:GLU:CD | 2.45 | 0.42 |
| 1:D:458:ASP:HB2 | 1:D:1341:GLY:HA3 | 2.02 | 0.42 |
| 1:D:614:HIS:CG | 1:D:771:LEU:HD11 | 2.55 | 0.42 |
| 1:D:688:GLU:HG2 | 1:D:689:LYS:N | 2.35 | 0.42 |
| 1:D:1557:PHE:CD2 | 1:D:1611:LYS:HD3 | 2.55 | 0.42 |
| 1:D:1766:TRP:CD1 | 1:D:1766:TRP:C | 2.98 | 0.42 |
| 1:D:2416:ASN:ND2 | 1:D:2418:LYS:O | 2.46 | 0.42 |
| 1:D:3120:SER:O | 1:D:3124:ARG:HG2 | 2.19 | 0.42 |
| 1:E:305:ALA:HA | 1:E:414:LYS:HG3 | 2.01 | 0.42 |
| 1:E:1284:ARG:HH12 | 1:E:1376:GLU:CD | 2.25 | 0.42 |
| 1:E:1440:ARG:NH2 | 1:H:1368:PHE:HB3 | 2.35 | 0.42 |
| 1:E:1557:PHE:CG | 1:E:1611:LYS:HD2 | 2.54 | 0.42 |
| 1:E:1567:THR:HG21 | 2:q:1:NAG:H62 | 2.00 | 0.42 |
| 1:E:1741:GLN:O | 1:E:1744:ARG:HG2 | 2.20 | 0.42 |
| 1:E:2156:HIS:HB3 | 1:E:2357:VAL:HG21 | 2.02 | 0.42 |
| 1:E:2529:LYS:HE2 | 1:E:2621:PRO:HD2 | 2.01 | 0.42 |
| 1:E:2581:PHE:O | 1:E:2584:THR:HG22 | 2.19 | 0.42 |
| 1:E:3013:TRP:CD1 | 1:E:3013:TRP:H | 2.36 | 0.42 |
| 1:E:3072:LEU:HD23 | 1:E:3129:TRP:CD1 | 2.49 | 0.42 |
| 1:E:3231:LYS:CB | 1:E:3284:GLN:HE21 | 2.31 | 0.42 |
| 1:E:3353:GLU:HG3 | 1:E:3386:TYR:CD2 | 2.55 | 0.42 |
| 1:F:146:ASP:CG | 1:F:148:ARG:HG2 | 2.44 | 0.42 |
| 1:F:399:ASN:HD21 | 1:F:401:ASN:HD21 | 1.68 | 0.42 |
| 1:F:744:ASN:ND2 | 1:F:778:PRO:HA | 2.35 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:F:788:GLU:OE1 | 1:F:791:ASP:HB2 | 2.19 | 0.42 |
| 1:F:1576:CYS:N | 1:F:1632:ASP:O | 2.44 | 0.42 |
| 1:F:2823:ASP:OD1 | 1:F:2823:ASP:N | 2.53 | 0.42 |
| 1:F:3096:GLY:HA3 | 1:F:3104:SER:HB3 | 2.02 | 0.42 |
| 1:G:376:LEU:HD12 | 1:G:378:LYS:HZ1 | 1.85 | 0.42 |
| 1:G:502:LEU:HD23 | 1:G:502:LEU:HA | 1.85 | 0.42 |
| 1:G:667:ALA:O | 1:G:671:THR:HG23 | 2.20 | 0.42 |
| 1:G:676:LYS:H | 1:G:676:LYS:HG3 | 1.73 | 0.42 |
| 1:G:741:HIS:HD2 | 1:G:743:GLN:HE22 | 1.68 | 0.42 |
| 1:G:1637:ILE:HG21 | 1:G:1645:LEU:HD12 | 2.01 | 0.42 |
| 1:G:2604:THR:HG23 | 1:G:2782:HIS:NE2 | 2.35 | 0.42 |
| 1:G:2743:PRO:HA | 1:G:2762:ARG:HH11 | 1.85 | 0.42 |
| 1:G:3041:GLN:O | 1:G:3042:HIS:ND1 | 2.53 | 0.42 |
| 1:G:3385:ASP:C | 1:H:3148:ARG:HH22 | 2.28 | 0.42 |
| 1:H:1221:TYR:OH | 1:H:1233:SER:O | 2.30 | 0.42 |
| 1:H:1535:PHE:O | 1:H:1538:TRP:HB2 | 2.19 | 0.42 |
| 1:H:1630:ASP:OD1 | 1:H:1630:ASP:N | 2.49 | 0.42 |
| 1:H:1720:CYS:O | 1:H:1729:TYR:HB2 | 2.20 | 0.42 |
| 1:H:1802:ILE:HA | 1:H:1877:TYR:CE1 | 2.55 | 0.42 |
| 1:H:2313:GLN:HG2 | 1:H:2320:TYR:HB3 | 2.01 | 0.42 |
| 1:I:126:PHE:O | 1:I:143:ARG:NH1 | 2.53 | 0.42 |
| 1:I:580:TYR:CG | 1:I:958:PRO:HG2 | 2.55 | 0.42 |
| 1:I:887:GLN:HG3 | 1:I:889:ASN:HD21 | 1.84 | 0.42 |
| 1:I:1315:CYS:C | 1:I:1317:HIS:HD1 | 2.28 | 0.42 |
| 1:I:2056:ARG:HH22 | 1:I:2060:GLY:HA2 | 1.85 | 0.42 |
| 1:I:2439:ASP:OD1 | 1:I:2440:ARG:N | 2.52 | 0.42 |
| 1:I:2542:ARG:HH21 | 1:I:2591:LEU:HB2 | 1.85 | 0.42 |
| 1:I:3289:LYS:HB3 | 1:I:3295:LEU:HD11 | 2.01 | 0.42 |
| 1:J:220:ASP:OD2 | 1:J:283:TYR:OH | 2.36 | 0.42 |
| 1:J:468:ALA:HB1 | 1:J:632:ALA:O | 2.19 | 0.42 |
| 1:J:500:HIS:CD2 | 1:J:641:HIS:CE1 | 3.07 | 0.42 |
| 1:J:568:ARG:HH12 | 1:J:636:ILE:HG12 | 1.85 | 0.42 |
| 1:J:925:LEU:HD22 | 1:J:928:LYS:NZ | 2.34 | 0.42 |
| 1:J:946:LEU:HG | 1:J:951:ALA:HB2 | 2.01 | 0.42 |
| 1:J:1385:ILE:HG23 | 1:J:1453:PHE:CE2 | 2.54 | 0.42 |
| 1:J:2394:PHE:HD1 | 1:J:2445:ASP:HA | 1.85 | 0.42 |
| 1:J:3200:ILE:HA | 1:J:3203:ILE:HB | 2.01 | 0.42 |
| 1:J:3382:GLU:O | 1:J:3386:TYR:OH | 2.25 | 0.42 |
| 1:K:240:ALA:HB2 | 1:K:247:PHE:CE2 | 2.55 | 0.42 |
| 1:K:916:LEU:HA | 1:K:916:LEU:HD23 | 1.84 | 0.42 |
| 1:K:2977:CYS:SG | 1:K:3106:LEU:HD11 | 2.60 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:K:2980:GLY:HA2 | 1:K:3258:TYR:CE1 | 2.54 | 0.42 |
| 1:K:3088:HIS:O | 1:K:3092:HIS:ND1 | 2.53 | 0.42 |
| 1:L:671:THR:HG23 | 1:L:696:PRO:HG2 | 2.02 | 0.42 |
| 1:L:738:VAL:HG13 | 1:L:827:THR:O | 2.19 | 0.42 |
| 1:L:968:PHE:CD1 | 1:L:1047:PRO:HG2 | 2.55 | 0.42 |
| 1:L:1126:LEU:HD11 | 1:L:1133:ILE:HD11 | 2.01 | 0.42 |
| 1:L:1294:LYS:O | 1:L:1297:SER:OG | 2.27 | 0.42 |
| 1:L:1428:ILE:HA | 1:L:1431:ASN:HD21 | 1.84 | 0.42 |
| 1:L:1452:ALA:HA | 1:L:1457:PHE:CG | 2.55 | 0.42 |
| 1:L:1500:ASN:OD1 | 1:L:1500:ASN:N | 2.53 | 0.42 |
| 1:L:1646:GLU:OE2 | 1:L:1649:VAL:HG13 | 2.20 | 0.42 |
| 1:L:1857:ILE:HD12 | 1:L:1884:HIS:NE2 | 2.35 | 0.42 |
| 1:L:2541:PRO:HD2 | 1:L:2542:ARG:N | 2.31 | 0.42 |
| 1:L:2647:GLU:OE2 | 1:L:2656:ARG:NH2 | 2.41 | 0.42 |
| 1:L:2926:VAL:HG12 | 1:L:3011:TRP:HB3 | 2.02 | 0.42 |
| 1:L:3106:LEU:HA | 1:L:3109:SER:HB3 | 2.01 | 0.42 |
| 1:M:222:ILE:O | 1:M:225:ILE:HG22 | 2.20 | 0.42 |
| 1:M:704:HIS:HB3 | 1:M:705:GLU:OE1 | 2.20 | 0.42 |
| 1:M:724:ASP:OD1 | 1:M:725:HIS:N | 2.53 | 0.42 |
| 1:M:1002:VAL:HG12 | 1:M:1006:PHE:CE2 | 2.55 | 0.42 |
| 1:M:1010:ASP:OD2 | 1:M:1013:THR:HG23 | 2.20 | 0.42 |
| 1:M:1314:CYS:SG | 1:M:1497:LYS:HG2 | 2.59 | 0.42 |
| 1:M:1741:GLN:O | 1:M:1745:LEU:HD23 | 2.19 | 0.42 |
| 1:M:2034:ILE:HB | 1:M:2038:LEU:HD23 | 2.01 | 0.42 |
| 1:M:2181:TRP:H | 1:M:2297:THR:HG22 | 1.84 | 0.42 |
| 1:M:2364:ASN:OD1 | 1:M:2366:ARG:NH1 | 2.24 | 0.42 |
| 1:M:2947:ASP:OD2 | 1:M:3002:LYS:NZ | 2.48 | 0.42 |
| 1:N:247:PHE:HB3 | 1:N:271:LYS:HD2 | 2.00 | 0.42 |
| 1:N:331:HIS:CE1 | 1:N:672:HIS:HB3 | 2.55 | 0.42 |
| 1:N:695:ARG:O | 1:N:697:THR:N | 2.53 | 0.42 |
| 1:N:1060:TRP:CD1 | 1:N:1064:GLN:HE22 | 2.37 | 0.42 |
| 1:N:2109:ALA:HA | 1:N:2112:ARG:HG2 | 2.01 | 0.42 |
| 1:N:2271:ILE:O | 1:N:2275:VAL:HG12 | 2.20 | 0.42 |
| 1:N:2278:HIS:N | 1:N:2279:GLN:OE1 | 2.53 | 0.42 |
| 1:N:2469:LEU:HD11 | 1:N:2489:PRO:HG2 | 2.02 | 0.42 |
| 1:N:3011:TRP:CZ3 | 1:N:3013:TRP:HA | 2.55 | 0.42 |
| 1:N:3183:PHE:HB2 | 1:N:3185:TYR:CD1 | 2.55 | 0.42 |
| 1:N:3212:ARG:HD2 | 1:N:3214:TYR:OH | 2.20 | 0.42 |
| 1:O:222:ILE:O | 1:O:225:ILE:HG22 | 2.20 | 0.42 |
| 1:O:501:ARG:O | 1:O:504:VAL:HG12 | 2.20 | 0.42 |
| 1:O:1286:MET:HA | 1:O:1289:ASP:OD2 | 2.20 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:O:2201:ASP:OD1 | 1:O:2203:TRP:N | 2.37 | 0.42 |
| 1:O:3013:TRP:CD1 | 1:O:3013:TRP:H | 2.37 | 0.42 |
| 1:P:847:VAL:HA | 1:P:1122:HIS:O | 2.20 | 0.42 |
| 1:P:1017:GLN:HA | 1:P:1020:ILE:HG12 | 2.02 | 0.42 |
| 1:P:1283:LEU:HD12 | 1:P:1286:MET:SD | 2.59 | 0.42 |
| 1:P:1305:CYS:HB2 | 1:P:1312:VAL:O | 2.19 | 0.42 |
| 1:P:1705:THR:HG23 | 1:P:1931:LEU:HD12 | 2.01 | 0.42 |
| 1:P:1736:MET:N | 1:P:1736:MET:SD | 2.93 | 0.42 |
| 1:P:1766:TRP:C | 1:P:1766:TRP:CD1 | 2.98 | 0.42 |
| 1:P:2260:PHE:O | 1:P:2264:PHE:HB3 | 2.18 | 0.42 |
| 1:P:2695:THR:HG21 | 1:P:2698:TYR:CD2 | 2.53 | 0.42 |
| 1:P:2823:ASP:OD1 | 1:P:2823:ASP:N | 2.50 | 0.42 |
| 1:P:3225:SER:O | 1:P:3290:TYR:N | 2.50 | 0.42 |
| 1:Q:314:THR:C | 1:Q:315:LEU:HD12 | 2.45 | 0.42 |
| 1:Q:453:SER:OG | 3:nA:1:NAG:O7 | 2.21 | 0.42 |
| 1:Q:608:VAL:HG11 | 1:Q:785:VAL:HG21 | 2.01 | 0.42 |
| 1:Q:1325:TRP:HE1 | 1:Q:1498:PRO:CG | 2.31 | 0.42 |
| 1:Q:1721:PRO:HD3 | 1:Q:1729:TYR:CZ | 2.54 | 0.42 |
| 1:Q:3174:PRO:O | 1:Q:3177:ILE:HG22 | 2.20 | 0.42 |
| 1:Q:3227:THR:HG22 | 1:Q:3288:THR:O | 2.20 | 0.42 |
| 1:Q:3289:LYS:HG2 | 1:Q:3295:LEU:HD21 | 2.01 | 0.42 |
| 1:R:112:PHE:HB3 | 1:R:121:GLN:O | 2.20 | 0.42 |
| 1:R:780:ASN:OD1 | 1:R:781:PHE:N | 2.51 | 0.42 |
| 1:R:1437:VAL:HG23 | 1:R:1445:LEU:HD12 | 2.01 | 0.42 |
| 1:R:2313:GLN:HE21 | 1:R:2320:TYR:HB3 | 1.85 | 0.42 |
| 1:R:2953:TYR:HA | 1:R:2956:ILE:HG12 | 2.02 | 0.42 |
| 1:R:3108:TYR:HD1 | 1:R:3111:PHE:HE2 | 1.68 | 0.42 |
| 1:S:248:ARG:CZ | 1:S:803:GLU:HA | 2.50 | 0.42 |
| 1:S:254:PHE:HB3 | 1:S:264:THR:HB | 2.02 | 0.42 |
| 1:S:392:SER:OG | 1:S:393:VAL:N | 2.53 | 0.42 |
| 1:S:580:TYR:CG | 1:S:958:PRO:HG2 | 2.55 | 0.42 |
| 1:S:1061:ALA:HA | 1:S:1064:GLN:CD | 2.45 | 0.42 |
| 1:S:1433:LEU:HD21 | 1:S:1460:HIS:CD2 | 2.54 | 0.42 |
| 1:S:2212:PHE:O | 1:S:2226:ARG:NH2 | 2.53 | 0.42 |
| 1:S:3204:ILE:O | 1:S:3207:LEU:HG | 2.19 | 0.42 |
| 1:S:3351:VAL:O | 1:S:3372:SER:HA | 2.19 | 0.42 |
| 1:T:5:ARG:HG3 | 1:T:283:TYR:CD2 | 2.55 | 0.42 |
| 1:T:135:MET:HG2 | 1:T:137:VAL:HG13 | 2.01 | 0.42 |
| 1:T:847:VAL:HA | 1:T:1122:HIS:O | 2.20 | 0.42 |
| 1:T:907:MET:SD | 1:T:907:MET:N | 2.89 | 0.42 |
| 1:T:1894:LEU:O | 1:T:1898:LEU:HG | 2.20 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:T:1967:LEU:HD23 | 1:T:1967:LEU:H | 1.84 | 0.42 |
| 1:T:2312:LEU:O | 1:T:2316:ARG:NH1 | 2.53 | 0.42 |
| 1:T:2469:LEU:HD11 | 1:T:2489:PRO:HB2 | 2.01 | 0.42 |
| 1:T:2553:TYR:HA | 1:T:2554:PRO:HA | 1.77 | 0.42 |
| 1:T:3270:LEU:HD22 | 1:T:3275:LEU:HB2 | 2.02 | 0.42 |
| 1:A:230:GLN:NE2 | 1:A:235:LYS:HB2 | 2.35 | 0.42 |
| 1:A:514:ARG:NH1 | 1:A:1343:ALA:HA | 2.35 | 0.42 |
| 1:A:595:GLU:OE1 | 1:A:595:GLU:N | 2.46 | 0.42 |
| 1:A:651:TRP:CH2 | 1:A:655:GLN:HG3 | 2.54 | 0.42 |
| 1:A:1118:SER:OG | 1:A:1119:PHE:N | 2.53 | 0.42 |
| 1:A:1541:PRO:HD2 | 1:A:1542:GLN:OE1 | 2.20 | 0.42 |
| 1:A:1865:LYS:HE3 | 1:A:1867:HIS:HB2 | 2.01 | 0.42 |
| 1:A:2000:VAL:O | 1:A:2041:LYS:NZ | 2.48 | 0.42 |
| 1:A:2136:CYS:HB3 | 1:A:2144:TYR:C | 2.45 | 0.42 |
| 1:A:2790:GLU:HA | 1:A:2793:ILE:HG22 | 2.01 | 0.42 |
| 1:A:3114:PHE:HD1 | 1:A:3117:ILE:HD11 | 1.84 | 0.42 |
| 1:A:3251:ASP:OD1 | 1:A:3251:ASP:N | 2.53 | 0.42 |
| 1:B:225:ILE:HD13 | 1:B:228:GLU:OE2 | 2.20 | 0.42 |
| 1:B:654:LEU:HD13 | 1:B:723:LEU:HD11 | 2.01 | 0.42 |
| 1:B:863:ARG:O | 1:B:866:LEU:HB3 | 2.20 | 0.42 |
| 1:B:1966:GLU:OE1 | 1:B:1966:GLU:N | 2.52 | 0.42 |
| 1:B:2416:ASN:OD1 | 1:B:2417:GLY:N | 2.52 | 0.42 |
| 1:B:2511:ILE:HD12 | 1:B:2772:PHE:O | 2.20 | 0.42 |
| 1:B:2703:PRO:O | 1:B:2707:ILE:HG12 | 2.20 | 0.42 |
| 1:C:489:CYS:O | 1:C:491:HIS:ND1 | 2.53 | 0.42 |
| 1:C:1407:LEU:O | 1:C:1410:VAL:HG12 | 2.19 | 0.42 |
| 1:C:1720:CYS:HA | 1:C:1721:PRO:C | 2.44 | 0.42 |
| 1:C:2022:MET:SD | 1:C:2022:MET:N | 2.92 | 0.42 |
| 1:C:2405:SER:HB3 | 1:C:2426:PHE:HE1 | 1.85 | 0.42 |
| 1:C:2977:CYS:HA | 1:C:2987:TRP:CH2 | 2.55 | 0.42 |
| 1:C:3268:ASP:OD1 | 1:C:3268:ASP:N | 2.52 | 0.42 |
| 1:D:23:LEU:HD23 | 1:D:123:ASN:ND2 | 2.32 | 0.42 |
| 1:D:229:LEU:HB3 | 1:D:233:ARG:NH2 | 2.35 | 0.42 |
| 1:D:461:VAL:H | 1:D:1277:GLU:CD | 2.28 | 0.42 |
| 1:D:634:ASP:OD1 | 1:D:636:ILE:HG12 | 2.20 | 0.42 |
| 1:D:1036:SER:O | 1:D:1042:TYR:HB2 | 2.20 | 0.42 |
| 1:D:1951:PHE:O | 1:D:1952:ASN:ND2 | 2.53 | 0.42 |
| 1:D:3392:ASN:OD1 | 1:D:3395:ARG:N | 2.52 | 0.42 |
| 1:E:601:ASP:OD1 | 1:E:602:PHE:N | 2.53 | 0.42 |
| 1:E:887:GLN:HG3 | 1:E:889:ASN:HD21 | 1.85 | 0.42 |
| 1:E:962:LEU:HD12 | 1:E:962:LEU:HA | 1.95 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:E:1357:GLN:HG2 | 1:E:1358:LEU:O | 2.20 | 0.42 |
| 1:E:1756:ARG:HH12 | 1:F:2102:ARG:CZ | 2.33 | 0.42 |
| 1:E:2326:ALA:HB1 | 1:E:2329:TYR:HB2 | 2.02 | 0.42 |
| 1:E:2401:GLY:HA2 | 1:E:2436:TRP:CE2 | 2.55 | 0.42 |
| 1:E:2768:ASP:OD1 | 1:E:2769:TYR:N | 2.51 | 0.42 |
| 1:E:3091:ILE:HG22 | 1:E:3094:LEU:HD12 | 2.01 | 0.42 |
| 1:F:293:ILE:O | 1:F:296:LEU:HG | 2.20 | 0.42 |
| 1:F:2112:ARG:HD2 | 1:F:2208:LEU:HD11 | 2.02 | 0.42 |
| 1:F:2313:GLN:HA | 1:F:2316:ARG:NH1 | 2.34 | 0.42 |
| 1:F:2494:LYS:HD3 | 1:F:2494:LYS:HA | 1.81 | 0.42 |
| 1:F:2552:GLY:O | 1:F:2555:GLY:N | 2.53 | 0.42 |
| 1:F:2771:GLN:HG2 | 1:F:2772:PHE:CD1 | 2.53 | 0.42 |
| 1:G:851:VAL:HG12 | 1:G:935:PRO:HB2 | 2.02 | 0.42 |
| 1:G:2258:CYS:HA | 1:G:2261:GLU:HG2 | 2.02 | 0.42 |
| 1:H:81:LEU:HA | 1:H:84:LYS:HB2 | 2.02 | 0.42 |
| 1:H:257:ASP:HA | 1:H:265:ARG:HD3 | 2.01 | 0.42 |
| 1:H:735:ARG:NH2 | 1:H:788:GLU:HG2 | 2.35 | 0.42 |
| 1:H:740:LEU:O | 1:H:784:LEU:HA | 2.20 | 0.42 |
| 1:H:1153:PHE:O | 1:H:1154:MET:HE2 | 2.20 | 0.42 |
| 1:H:1307:HIS:CD2 | 1:H:1602:MET:HE1 | 2.55 | 0.42 |
| 1:H:1359:PRO:O | 1:H:1363:ASN:ND2 | 2.53 | 0.42 |
| 1:H:1362:ILE:HG22 | 1:H:1380:PHE:HB3 | 2.01 | 0.42 |
| 1:H:1497:LYS:HE2 | 1:H:1497:LYS:HB3 | 1.88 | 0.42 |
| 1:H:2481:LEU:HD21 | 3:6:1:NAG:H62 | 2.02 | 0.42 |
| 1:H:2553:TYR:HA | 1:H:2554:PRO:HA | 1.76 | 0.42 |
| 1:H:3393:LYS:HE3 | 1:H:3393:LYS:HB3 | 1.96 | 0.42 |
| 1:I:41:PHE:CE1 | 1:I:253:PRO:HG2 | 2.55 | 0.42 |
| 1:I:181:PHE:HE2 | 1:I:219:VAL:HG13 | 1.85 | 0.42 |
| 1:I:997:LYS:O | 1:I:1001:MET:HG3 | 2.20 | 0.42 |
| 1:I:1093:GLN:HB2 | 1:I:1097:ILE:HG21 | 2.02 | 0.42 |
| 1:I:1490:ASN:ND2 | 1:J:2049:PHE:O | 2.53 | 0.42 |
| 1:I:1559:GLY:HA2 | 1:I:1610:TYR:O | 2.19 | 0.42 |
| 1:I:2769:TYR:HA | 1:I:2772:PHE:HD2 | 1.85 | 0.42 |
| 1:I:3028:ASP:OD1 | 1:I:3028:ASP:N | 2.53 | 0.42 |
| 1:I:3089:ASN:HD21 | 1:I:3247:ILE:HA | 1.85 | 0.42 |
| 1:I:3390:SER:HB3 | 1:I:3395:ARG:HG3 | 2.02 | 0.42 |
| 1:J:198:HIS:HA | 1:J:205:TRP:CD1 | 2.55 | 0.42 |
| 1:J:2266:VAL:HG21 | 1:J:2442:TYR:CZ | 2.55 | 0.42 |
| 1:J:2286:LEU:HD23 | 1:J:2286:LEU:H | 1.84 | 0.42 |
| 1:J:2454:HIS:CE1 | 1:J:2456:ARG:HH12 | 2.38 | 0.42 |
| 1:J:2712:VAL:HA | 1:J:2715:GLN:NE2 | 2.35 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:J:3043:GLN:N | 1:J:3043:GLN:OE1 | 2.53 | 0.42 |
| 1:J:3090:THR:HG22 | 1:J:3246:TYR:H | 1.85 | 0.42 |
| 1:K:986:LEU:HD12 | 1:K:1028:LEU:HG | 2.01 | 0.42 |
| 1:K:2158:HIS:O | 1:K:2162:THR:HG23 | 2.19 | 0.42 |
| 1:K:2271:ILE:HG13 | 1:K:2298:HIS:CE1 | 2.55 | 0.42 |
| 1:K:2714:ARG:NH2 | 1:K:2778:ASP:O | 2.51 | 0.42 |
| 1:L:187:HIS:O | 1:L:191:LEU:HG | 2.20 | 0.42 |
| 1:L:526:THR:OG1 | 1:L:527:ARG:NH1 | 2.53 | 0.42 |
| 1:L:529:GLY:HA2 | 1:L:575:SER:HA | 2.01 | 0.42 |
| 1:L:970:HIS:CD2 | 1:L:972:LEU:HG | 2.55 | 0.42 |
| 1:L:2790:GLU:OE1 | 1:L:2790:GLU:N | 2.50 | 0.42 |
| 1:L:2807:MET:HB3 | 1:L:2890:GLU:OE2 | 2.19 | 0.42 |
| 1:L:2822:CYS:HB2 | 1:L:2871:HIS:CE1 | 2.55 | 0.42 |
| 1:L:3266:VAL:HG11 | 1:L:3283:PHE:CE1 | 2.55 | 0.42 |
| 1:M:731:ARG:HH21 | 1:M:834:THR:HG21 | 1.85 | 0.42 |
| 1:M:1137:GLN:O | 1:M:1140:ILE:HG22 | 2.20 | 0.42 |
| 1:M:1272:SER:OG | 1:M:1275:GLU:OE1 | 2.38 | 0.42 |
| 1:M:2137:PRO:HD2 | 1:M:2141:ALA:O | 2.20 | 0.42 |
| 1:M:2335:GLN:NE2 | 1:M:2336:PRO:HB3 | 2.35 | 0.42 |
| 1:M:2359:ASN:OD1 | 1:M:2361:GLN:HG2 | 2.20 | 0.42 |
| 1:M:2392:ARG:HB3 | 1:M:2394:PHE:CE1 | 2.54 | 0.42 |
| 1:M:3203:ILE:HD12 | 1:M:3206:ASN:HB2 | 2.02 | 0.42 |
| 1:M:3351:VAL:HG21 | 1:M:3388:PHE:HB3 | 2.02 | 0.42 |
| 1:M:3381:LEU:HD23 | 1:M:3386:TYR:CD1 | 2.55 | 0.42 |
| 1:N:171:GLU:HB3 | 1:N:177:PHE:HD1 | 1.84 | 0.42 |
| 1:N:789:ILE:HG22 | 1:N:793:LEU:HD23 | 2.01 | 0.42 |
| 1:N:1062:ILE:HG22 | 1:N:1126:LEU:HD12 | 2.02 | 0.42 |
| 1:N:1254:ILE:HG23 | 1:N:1256:LYS:H | 1.85 | 0.42 |
| 1:N:1649:VAL:HG23 | 1:N:1650:LEU:HD22 | 2.02 | 0.42 |
| 1:N:2108:LYS:HB3 | 1:N:2108:LYS:HE3 | 1.80 | 0.42 |
| 1:N:2577:TRP:C | 1:N:2577:TRP:CD1 | 2.97 | 0.42 |
| 1:N:3334:ARG:HE | 1:N:3335:GLY:N | 2.16 | 0.42 |
| 1:O:310:LEU:HD23 | 1:O:366:HIS:HB3 | 2.02 | 0.42 |
| 1:O:428:SER:OG | 1:O:429:ALA:N | 2.52 | 0.42 |
| 1:O:502:LEU:HA | 1:O:505:VAL:HG12 | 2.01 | 0.42 |
| 1:O:573:GLU:HB3 | 1:O:616:LEU:HD11 | 2.02 | 0.42 |
| 1:O:1378:ASN:ND2 | 1:O:1380:PHE:HB2 | 2.35 | 0.42 |
| 1:O:1649:VAL:HG13 | 1:O:1650:LEU:HD23 | 2.01 | 0.42 |
| 1:O:2509:SER:H | 1:O:3138:ARG:HH12 | 1.68 | 0.42 |
| 1:O:3013:TRP:HZ3 | 1:O:3064:LEU:HB3 | 1.85 | 0.42 |
| 1:O:3089:ASN:ND2 | 1:O:3247:ILE:HD12 | 2.35 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:O:3308:PRO:HG2 | 1:O:3311:ALA:HB3 | 2.02 | 0.42 |
| 1:P:471:HIS:HB3 | 1:P:632:ALA:HB1 | 2.02 | 0.42 |
| 1:P:1433:LEU:HD23 | 1:P:1433:LEU:H | 1.85 | 0.42 |
| 1:P:1630:ASP:OD1 | 1:P:1630:ASP:N | 2.53 | 0.42 |
| 1:P:2028:ARG:CZ | 1:P:2028:ARG:HB2 | 2.49 | 0.42 |
| 1:P:2985:PRO:O | 1:P:2989:ARG:HG3 | 2.20 | 0.42 |
| 1:P:3303:VAL:HG13 | 1:P:3305:ILE:HD11 | 2.02 | 0.42 |
| 1:Q:489:CYS:O | 1:Q:491:HIS:ND1 | 2.48 | 0.42 |
| 1:Q:913:TRP:HD1 | 1:Q:1088:LEU:HD11 | 1.84 | 0.42 |
| 1:Q:1156:HIS:HB3 | 1:Q:1193:GLN:NE2 | 2.33 | 0.42 |
| 1:Q:1855:ASN:ND2 | 1:Q:2015:VAL:HA | 2.34 | 0.42 |
| 1:Q:2509:SER:C | 1:Q:3138:ARG:HH22 | 2.25 | 0.42 |
| 1:Q:2601:TRP:HB3 | 1:Q:2707:ILE:HG21 | 2.02 | 0.42 |
| 1:Q:2653:PHE:HA | 1:Q:2656:ARG:HH12 | 1.85 | 0.42 |
| 1:Q:3202:THR:HA | 1:Q:3205:GLU:OE2 | 2.19 | 0.42 |
| 1:R:57:ALA:H | 1:R:355:ASN:HB3 | 1.84 | 0.42 |
| 1:R:480:PRO:HA | 1:R:485:ARG:HH22 | 1.85 | 0.42 |
| 1:R:695:ARG:NH2 | 1:R:696:PRO:HD2 | 2.34 | 0.42 |
| 1:R:702:TYR:HB2 | 1:R:708:TYR:CE1 | 2.55 | 0.42 |
| 1:R:1023:ASN:HD21 | 1:R:1184:LEU:HB2 | 1.85 | 0.42 |
| 1:R:1143:ARG:HB3 | 1:R:1148:ARG:HH22 | 1.85 | 0.42 |
| 1:R:1166:LEU:HB3 | 1:R:1179:GLY:O | 2.20 | 0.42 |
| 1:R:2169:LEU:HB3 | 1:R:2174:SER:HB3 | 2.02 | 0.42 |
| 1:R:2250:LEU:O | 1:R:2253:GLU:HG3 | 2.20 | 0.42 |
| 1:R:2557:CYS:HB2 | 1:R:2566:CYS:HB3 | 1.85 | 0.42 |
| 1:S:16:VAL:HG21 | 1:S:105:ARG:NH2 | 2.35 | 0.42 |
| 1:S:1496:LEU:O | 1:S:1500:ASN:ND2 | 2.53 | 0.42 |
| 1:S:1852:ILE:HG21 | 1:S:2030:TYR:CE1 | 2.55 | 0.42 |
| 1:S:2080:ARG:HB3 | 1:S:2314:LYS:HE3 | 2.01 | 0.42 |
| 1:T:668:HIS:O | 1:T:671:THR:OG1 | 2.32 | 0.42 |
| 1:T:1284:ARG:HH12 | 1:T:1379:PRO:CB | 2.33 | 0.42 |
| 1:T:1538:TRP:CD1 | 1:T:1542:GLN:HG3 | 2.54 | 0.42 |
| 1:T:2469:LEU:HD22 | 1:T:2491:ILE:HD11 | 2.02 | 0.42 |
| 1:T:2527:SER:O | 1:T:2530:LYS:HG3 | 2.20 | 0.42 |
| 1:T:2529:LYS:HB3 | 1:T:2529:LYS:HE2 | 1.84 | 0.42 |
| 1:T:2567:CYS:O | 1:T:2569:HIS:ND1 | 2.50 | 0.42 |
| 1:T:2574:PHE:HB3 | 1:T:2575:PRO:HD3 | 2.02 | 0.42 |
| 1:T:2574:PHE:HE1 | 1:T:2578:HIS:CE1 | 2.38 | 0.42 |
| 1:T:2637:SER:HB3 | 1:T:2686:GLY:O | 2.20 | 0.42 |
| 1:T:2771:GLN:OE1 | 1:T:2771:GLN:N | 2.49 | 0.42 |
| 1:T:3118:HIS:O | 1:T:3121:SER:OG | 2.24 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:104:PRO:HG2 | 1:A:107:VAL:HG22 | 2.02 | 0.41 |
| 1:A:1061:ALA:HA | 1:A:1064:GLN:CD | 2.45 | 0.41 |
| 1:A:1421:ASP:OD1 | 1:A:1422:PHE:N | 2.52 | 0.41 |
| 1:A:2967:PRO:HD3 | 1:A:2974:TYR:CE2 | 2.55 | 0.41 |
| 1:A:3176:GLN:H | 1:A:3176:GLN:HG3 | 1.72 | 0.41 |
| 1:A:3209:ASP:HB2 | 1:B:1117:ARG:NH1 | 2.35 | 0.41 |
| 1:A:3216:GLY:HA2 | 1:A:3262:TYR:O | 2.20 | 0.41 |
| 1:A:3268:ASP:OD1 | 1:A:3268:ASP:N | 2.52 | 0.41 |
| 1:B:35:TYR:OH | 1:B:208:TYR:HA | 2.19 | 0.41 |
| 1:B:81:LEU:HB3 | 1:B:86:LEU:HB2 | 2.02 | 0.41 |
| 1:B:103:LEU:HG | 1:B:104:PRO:HD2 | 2.02 | 0.41 |
| 1:B:437:VAL:HG21 | 1:B:533:PRO:HG3 | 2.02 | 0.41 |
| 1:B:471:HIS:CD2 | 1:B:500:HIS:HE1 | 2.37 | 0.41 |
| 1:B:1363:ASN:OD1 | 1:B:1364:GLU:N | 2.52 | 0.41 |
| 1:B:1684:THR:HG23 | 1:B:1687:GLU:H | 1.85 | 0.41 |
| 1:B:1834:PHE:CE1 | 1:B:1891:ILE:HD13 | 2.54 | 0.41 |
| 1:B:2363:LEU:HB2 | 1:B:2365:PHE:HE1 | 1.85 | 0.41 |
| 1:B:2919:LYS:HB3 | 1:B:2920:ASP:H | 1.50 | 0.41 |
| 1:B:3142:TYR:OH | 1:B:3144:ARG:HB3 | 2.20 | 0.41 |
| 1:B:3230:VAL:HG22 | 1:B:3283:PHE:HD2 | 1.85 | 0.41 |
| 1:C:171:GLU:OE2 | 1:C:173:ASP:N | 2.52 | 0.41 |
| 1:C:409:VAL:HG13 | 1:C:666:CYS:HA | 2.01 | 0.41 |
| 1:C:539:GLU:N | 1:C:539:GLU:OE1 | 2.52 | 0.41 |
| 1:C:660:LEU:HD23 | 1:C:660:LEU:HA | 1.84 | 0.41 |
| 1:C:913:TRP:CE3 | 1:C:914:HIS:HD2 | 2.37 | 0.41 |
| 1:C:1695:LEU:HD12 | 1:C:1695:LEU:HA | 1.87 | 0.41 |
| 1:C:1722:TYR:HD1 | 1:C:1724:GLU:HB2 | 1.84 | 0.41 |
| 1:C:2977:CYS:HA | 1:C:2987:TRP:CZ3 | 2.55 | 0.41 |
| 1:D:31:THR:O | 1:D:36:GLN:NE2 | 2.29 | 0.41 |
| 1:D:192:VAL:HG13 | 1:D:200:LEU:HB2 | 2.02 | 0.41 |
| 1:D:695:ARG:HH21 | 1:D:696:PRO:HD2 | 1.85 | 0.41 |
| 1:D:1457:PHE:CE2 | 1:D:1461:HIS:HE1 | 2.37 | 0.41 |
| 1:D:1500:ASN:OD1 | 1:D:1500:ASN:N | 2.53 | 0.41 |
| 1:D:2522:VAL:HG23 | 1:D:2523:ALA:N | 2.35 | 0.41 |
| 1:D:2543:GLY:HA3 | 1:D:2546:GLU:CD | 2.45 | 0.41 |
| 1:D:2580:LEU:O | 1:D:2584:THR:HG23 | 2.20 | 0.41 |
| 1:D:2798:SER:O | 1:D:2900:LYS:N | 2.41 | 0.41 |
| 1:D:3025:THR:HA | 1:D:3046:ARG:HH22 | 1.84 | 0.41 |
| 1:D:3058:GLN:NE2 | 1:D:3268:ASP:OD2 | 2.52 | 0.41 |
| 1:D:3082:VAL:O | 1:D:3086:MET:HG2 | 2.20 | 0.41 |
| 1:E:5:ARG:HH21 | 1:E:90:GLY:HA3 | 1.84 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:E:1330:VAL:HA | 1:E:1333:VAL:HG22 | 2.02 | 0.41 |
| 1:E:1359:PRO:HB2 | 1:E:1362:ILE:HG12 | 2.02 | 0.41 |
| 1:E:3049:GLN:HG2 | 1:E:3050:PRO:HD2 | 2.01 | 0.41 |
| 1:F:450:GLN:O | 1:F:453:SER:OG | 2.26 | 0.41 |
| 1:F:523:TRP:HB3 | 1:F:639:LEU:HD13 | 2.01 | 0.41 |
| 1:F:1301:PHE:CD1 | 1:F:1302:PRO:HA | 2.54 | 0.41 |
| 1:F:1547:LEU:O | 1:F:1550:GLN:HG3 | 2.20 | 0.41 |
| 1:F:1736:MET:SD | 1:F:1736:MET:N | 2.93 | 0.41 |
| 1:F:1802:ILE:HG22 | 1:F:1877:TYR:CG | 2.55 | 0.41 |
| 1:F:2333:ALA:HB1 | 1:F:2338:ASN:HD22 | 1.84 | 0.41 |
| 1:F:2413:CYS:HA | 1:F:2419:CYS:HB3 | 2.02 | 0.41 |
| 1:F:2516:ASN:OD1 | 1:F:2517:ILE:N | 2.48 | 0.41 |
| 1:F:2686:GLY:HA3 | 1:F:2694:SER:H | 1.85 | 0.41 |
| 1:F:2821:LEU:HD13 | 1:F:2872:PHE:CE1 | 2.55 | 0.41 |
| 1:F:2923:ARG:NH2 | 1:F:3006:LEU:HD13 | 2.35 | 0.41 |
| 1:G:183:VAL:HG23 | 1:G:184:ALA:N | 2.35 | 0.41 |
| 1:G:473:LEU:N | 1:G:775:LYS:HE3 | 2.35 | 0.41 |
| 1:G:1385:ILE:HB | 1:G:1388:THR:HG21 | 2.02 | 0.41 |
| 1:G:2390:LYS:HE2 | 1:G:2390:LYS:HB2 | 1.86 | 0.41 |
| 1:H:196:HIS:CE1 | 1:H:198:HIS:HB2 | 2.55 | 0.41 |
| 1:H:224:VAL:HA | 1:H:227:GLN:OE1 | 2.20 | 0.41 |
| 1:H:946:LEU:HG | 1:H:951:ALA:HB2 | 2.02 | 0.41 |
| 1:H:1998:ILE:HG12 | 1:H:2011:GLY:O | 2.20 | 0.41 |
| 1:H:2152:PRO:HD2 | 1:H:2329:TYR:CD2 | 2.55 | 0.41 |
| 1:H:2450:LEU:HD23 | 1:H:2450:LEU:HA | 1.87 | 0.41 |
| 1:H:2453:LEU:HD23 | 1:H:2453:LEU:HA | 1.93 | 0.41 |
| 1:I:1066:LEU:HD21 | 1:I:1070:ARG:NH2 | 2.35 | 0.41 |
| 1:I:1079:CYS:O | 1:J:2492:ILE:HD13 | 2.20 | 0.41 |
| 1:I:1349:TRP:CE2 | 1:I:1359:PRO:HG3 | 2.55 | 0.41 |
| 1:I:2475:ALA:C | 1:I:2478:GLY:H | 2.28 | 0.41 |
| 1:I:2533:ARG:HH12 | 1:I:2621:PRO:HD3 | 1.84 | 0.41 |
| 1:I:3260:ARG:HE | 1:I:3261:VAL:H | 1.68 | 0.41 |
| 1:I:3359:SER:HA | 1:I:3362:LEU:HB3 | 2.02 | 0.41 |
| 1:J:143:ARG:NH2 | 1:J:209:ASP:OD2 | 2.53 | 0.41 |
| 1:J:253:PRO:O | 1:J:256:ARG:HG2 | 2.20 | 0.41 |
| 1:J:614:HIS:CD2 | 1:J:637:PHE:HE1 | 2.37 | 0.41 |
| 1:J:695:ARG:O | 1:J:697:THR:N | 2.53 | 0.41 |
| 1:J:1710:LEU:HB3 | 1:J:1750:PHE:HZ | 1.83 | 0.41 |
| 1:J:1802:ILE:HG12 | 1:J:1807:THR:O | 2.20 | 0.41 |
| 1:J:1854:HIS:HE1 | 1:J:1885:HIS:CE1 | 2.38 | 0.41 |
| 1:J:2217:ILE:HG13 | 1:J:2291:TYR:HD2 | 1.85 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:J:2709:HIS:O | 1:J:2712:VAL:HG22 | 2.20 | 0.41 |
| 1:J:3334:ARG:HE | 1:J:3335:GLY:N | 2.16 | 0.41 |
| 1:J:3351:VAL:HG12 | 1:J:3373:TYR:O | 2.20 | 0.41 |
| 1:K:293:ILE:H | 1:K:293:ILE:HD12 | 1.85 | 0.41 |
| 1:K:376:LEU:HB3 | 1:K:378:LYS:HZ3 | 1.85 | 0.41 |
| 1:K:561:PHE:CD2 | 1:K:562:LEU:HG | 2.54 | 0.41 |
| 1:K:574:LEU:HD23 | 1:K:616:LEU:HG | 2.02 | 0.41 |
| 1:K:954:THR:HA | 1:K:965:PRO:HA | 2.01 | 0.41 |
| 1:K:2271:ILE:HG13 | 1:K:2298:HIS:HE1 | 1.85 | 0.41 |
| 1:K:3268:ASP:N | 1:K:3268:ASP:OD1 | 2.53 | 0.41 |
| 1:L:610:HIS:O | 1:L:613:PRO:HD2 | 2.20 | 0.41 |
| 1:L:750:LEU:HD12 | 1:L:769:ALA:HB2 | 2.00 | 0.41 |
| 1:L:2165:VAL:HG11 | 1:L:2296:PHE:CE2 | 2.54 | 0.41 |
| 1:L:2170:LEU:HD12 | 1:L:2174:SER:OG | 2.20 | 0.41 |
| 1:L:2718:ILE:HD13 | 1:L:2779:LEU:HD12 | 2.02 | 0.41 |
| 1:L:3011:TRP:CZ3 | 1:L:3013:TRP:HA | 2.55 | 0.41 |
| 1:L:3088:HIS:NE2 | 1:L:3119:HIS:HE1 | 2.18 | 0.41 |
| 1:M:1061:ALA:HA | 1:M:1064:GLN:CD | 2.45 | 0.41 |
| 1:M:1720:CYS:HB2 | 1:M:1731:CYS:HB3 | 1.78 | 0.41 |
| 1:M:2088:PRO:HA | 1:M:2089:PRO:HD3 | 1.88 | 0.41 |
| 1:M:2340:VAL:HG12 | 1:M:2349:ARG:HD2 | 2.02 | 0.41 |
| 1:N:627:THR:HG21 | 1:N:630:TYR:HD2 | 1.84 | 0.41 |
| 1:N:704:HIS:HB3 | 1:N:705:GLU:OE1 | 2.20 | 0.41 |
| 1:N:1023:ASN:HB3 | 1:N:1182:TYR:HD2 | 1.83 | 0.41 |
| 1:N:1355:ILE:HD12 | 1:N:1355:ILE:HA | 1.92 | 0.41 |
| 1:N:1385:ILE:HG23 | 1:N:1453:PHE:CE2 | 2.55 | 0.41 |
| 1:N:1426:PHE:CZ | 1:N:1464:VAL:HG13 | 2.55 | 0.41 |
| 1:N:1672:GLU:HG3 | 1:N:1673:ARG:HG2 | 2.02 | 0.41 |
| 1:N:1687:GLU:OE1 | 1:N:1761:VAL:HG12 | 2.20 | 0.41 |
| 1:N:2087:LEU:H | 1:N:2366:ARG:NH1 | 2.17 | 0.41 |
| 1:N:2414:GLN:HA | 1:N:2467:PHE:HA | 2.02 | 0.41 |
| 1:N:3062:ASP:OD2 | 1:N:3064:LEU:HB2 | 2.20 | 0.41 |
| 1:O:441:THR:OG1 | 1:O:443:GLU:OE1 | 2.36 | 0.41 |
| 1:O:744:ASN:HB3 | 1:O:779:TRP:NE1 | 2.35 | 0.41 |
| 1:O:1145:HIS:NE2 | 1:O:1524:ASN:OD1 | 2.53 | 0.41 |
| 1:O:2158:HIS:CE1 | 1:O:2299:HIS:HE1 | 2.38 | 0.41 |
| 1:O:3165:ASN:ND2 | 1:O:3168:THR:H | 2.18 | 0.41 |
| 1:O:3289:LYS:NZ | 1:O:3293:GLU:HB2 | 2.35 | 0.41 |
| 1:P:246:LEU:HA | 1:P:249:LYS:HE2 | 2.03 | 0.41 |
| 1:P:363:LEU:HD23 | 1:P:363:LEU:HA | 1.85 | 0.41 |
| 1:P:914:HIS:HA | 1:P:917:LEU:HG | 2.02 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:P:2126:LEU:HD21 | 1:P:2165:VAL:HG12 | 2.02 | 0.41 |
| 1:P:2316:ARG:HD3 | 1:P:2316:ARG:H | 1.84 | 0.41 |
| 1:P:2392:ARG:HD2 | 1:P:2394:PHE:CE1 | 2.55 | 0.41 |
| 1:P:2994:GLN:HG2 | 1:P:3157:PHE:CZ | 2.55 | 0.41 |
| 1:Q:114:ASP:OD2 | 1:Q:117:GLY:N | 2.47 | 0.41 |
| 1:Q:328:VAL:HG12 | 1:Q:345:ALA:HB2 | 2.02 | 0.41 |
| 1:Q:434:ARG:HD2 | 1:Q:710:TYR:CE1 | 2.50 | 0.41 |
| 1:Q:596:GLN:HG2 | 1:Q:605:GLN:HE22 | 1.84 | 0.41 |
| 1:Q:988:GLU:OE2 | 1:Q:996:THR:OG1 | 2.26 | 0.41 |
| 1:Q:1905:ASP:HB3 | 1:Q:1908:GLU:HB2 | 2.02 | 0.41 |
| 1:R:50:LYS:H | 1:R:50:LYS:HG2 | 1.69 | 0.41 |
| 1:R:257:ASP:HA | 1:R:265:ARG:HD3 | 2.02 | 0.41 |
| 1:R:1472:GLN:O | 1:R:1475:GLN:HB2 | 2.19 | 0.41 |
| 1:S:240:ALA:HB2 | 1:S:247:PHE:CE2 | 2.54 | 0.41 |
| 1:S:294:GLU:OE1 | 1:S:294:GLU:N | 2.38 | 0.41 |
| 1:S:968:PHE:HA | 1:S:1047:PRO:HG3 | 2.00 | 0.41 |
| 1:S:1828:ASN:HB3 | 1:S:1831:TRP:HB3 | 2.02 | 0.41 |
| 1:S:2095:GLU:CD | 1:S:2097:SER:H | 2.26 | 0.41 |
| 1:S:2238:ASP:OD1 | 1:S:2239:GLY:N | 2.53 | 0.41 |
| 1:S:2314:LYS:HA | 1:S:2314:LYS:HD2 | 1.95 | 0.41 |
| 1:S:2601:TRP:CE3 | 1:S:2603:TRP:HD1 | 2.38 | 0.41 |
| 1:S:2676:VAL:HG11 | 1:S:2851:PHE:CZ | 2.55 | 0.41 |
| 1:S:2752:ASN:H | 1:S:2758:ARG:HD3 | 1.84 | 0.41 |
| 1:S:2777:ASP:O | 1:S:3137:HIS:NE2 | 2.53 | 0.41 |
| 1:S:3063:SER:O | 1:S:3067:GLN:HG3 | 2.20 | 0.41 |
| 1:S:3338:VAL:HG12 | 1:S:3379:TYR:O | 2.20 | 0.41 |
| 1:T:113:LYS:O | 1:T:115:PRO:HD3 | 2.20 | 0.41 |
| 1:T:974:GLU:OE2 | 1:T:1035:TYR:OH | 2.36 | 0.41 |
| 1:T:1303:SER:OG | 1:T:1311:LYS:O | 2.30 | 0.41 |
| 1:T:1315:CYS:C | 1:T:1317:HIS:HD1 | 2.27 | 0.41 |
| 1:T:1437:VAL:HG23 | 1:T:1445:LEU:HD12 | 2.02 | 0.41 |
| 1:T:1641:ASN:HD22 | 3:2A:1:NAG:H83 | 1.85 | 0.41 |
| 1:T:2645:ASP:HB3 | 1:T:2649:GLY:O | 2.20 | 0.41 |
| 1:A:100:ILE:HD12 | 1:A:100:ILE:HA | 1.95 | 0.41 |
| 1:A:278:GLN:OE1 | 1:A:278:GLN:N | 2.43 | 0.41 |
| 1:A:885:HIS:ND1 | 1:A:885:HIS:O | 2.52 | 0.41 |
| 1:A:913:TRP:HE3 | 1:A:914:HIS:CD2 | 2.36 | 0.41 |
| 1:A:1025:ILE:HG21 | 1:A:1052:HIS:NE2 | 2.35 | 0.41 |
| 1:A:1148:ARG:HG3 | 1:A:1244:ARG:HB3 | 2.02 | 0.41 |
| 1:A:1362:ILE:CD1 | 1:A:1380:PHE:HB3 | 2.48 | 0.41 |
| 1:A:1384:LYS:HA | 1:A:1391:VAL:HG12 | 2.02 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:2158:HIS:O | 1:A:2162:THR:HG23 | 2.20 | 0.41 |
| 1:A:2199:PHE:O | 1:A:2208:LEU:N | 2.46 | 0.41 |
| 1:A:2578:HIS:CG | 1:A:2709:HIS:CE1 | 3.08 | 0.41 |
| 1:A:2848:ASP:HB2 | 1:J:2850:LEU:HD21 | 2.02 | 0.41 |
| 1:B:299:LEU:O | 1:B:302:GLN:HG3 | 2.20 | 0.41 |
| 1:B:674:LEU:HD12 | 1:B:695:ARG:HH22 | 1.85 | 0.41 |
| 1:B:959:GLU:OE2 | 1:B:960:THR:HG23 | 2.21 | 0.41 |
| 1:B:1718:PRO:HG2 | 1:B:1728:ARG:HB3 | 2.02 | 0.41 |
| 1:B:1857:ILE:HD12 | 1:B:1884:HIS:CD2 | 2.55 | 0.41 |
| 1:B:2456:ARG:H | 1:B:2456:ARG:HG2 | 1.68 | 0.41 |
| 1:B:3232:LEU:HD12 | 1:B:3283:PHE:CZ | 2.54 | 0.41 |
| 1:C:1436:LEU:HD23 | 1:C:1436:LEU:HA | 1.90 | 0.41 |
| 1:C:1570:ASP:HB2 | 1:C:1638:ARG:HB2 | 2.02 | 0.41 |
| 1:C:2102:ARG:HG3 | 1:C:2103:ALA:N | 2.35 | 0.41 |
| 1:C:2301:PHE:O | 1:C:2305:ILE:HG12 | 2.20 | 0.41 |
| 1:C:2981:MET:HE2 | 1:C:3149:ASN:HB2 | 2.01 | 0.41 |
| 1:C:3043:GLN:HG3 | 1:C:3044:VAL:H | 1.84 | 0.41 |
| 1:D:496:PHE:HB3 | 1:D:497:PRO:HD3 | 2.00 | 0.41 |
| 1:D:1857:ILE:HB | 1:D:1884:HIS:CE1 | 2.55 | 0.41 |
| 1:D:1984:GLY:C | 1:D:1985:PHE:HD2 | 2.27 | 0.41 |
| 1:D:2045:VAL:HG13 | 1:D:2046:ASP:OD1 | 2.21 | 0.41 |
| 1:D:2105:MET:HA | 1:D:2108:LYS:HG2 | 2.01 | 0.41 |
| 1:E:80:LYS:O | 1:E:83:LYS:HG2 | 2.21 | 0.41 |
| 1:E:913:TRP:HD1 | 1:E:1088:LEU:HD23 | 1.85 | 0.41 |
| 1:E:1358:LEU:O | 1:E:1363:ASN:ND2 | 2.53 | 0.41 |
| 1:E:2095:GLU:HG3 | 1:E:2098:HIS:HD2 | 1.84 | 0.41 |
| 1:E:2250:LEU:O | 1:E:2254:GLN:NE2 | 2.51 | 0.41 |
| 1:E:2383:GLU:OE2 | 1:E:2384:ILE:HG13 | 2.20 | 0.41 |
| 1:E:2585:LEU:HD22 | 1:E:2706:PHE:CE2 | 2.55 | 0.41 |
| 1:E:2922:VAL:HG23 | 1:E:3006:LEU:HG | 2.02 | 0.41 |
| 1:E:3351:VAL:O | 1:E:3372:SER:HA | 2.20 | 0.41 |
| 1:F:441:THR:HB | 1:F:444:GLU:OE1 | 2.20 | 0.41 |
| 1:F:806:VAL:HG11 | 1:F:825:HIS:O | 2.19 | 0.41 |
| 1:F:1783:ILE:HD13 | 1:F:1794:PRO:HA | 2.01 | 0.41 |
| 1:F:2124:GLN:OE1 | 1:F:2124:GLN:N | 2.45 | 0.41 |
| 1:F:3363:CYS:HB2 | 1:F:3396:CYS:HB3 | 1.88 | 0.41 |
| 1:G:408:GLY:HA3 | 1:G:669:THR:HG23 | 2.01 | 0.41 |
| 1:G:1169:CYS:HA | 1:G:1175:CYS:HA | 2.03 | 0.41 |
| 1:G:1238:LYS:HA | 1:G:1238:LYS:HD2 | 1.90 | 0.41 |
| 1:G:1440:ARG:NH2 | 1:J:1368:PHE:HB3 | 2.34 | 0.41 |
| 1:G:2287:HIS:CD2 | 1:G:2430:GLY:HA3 | 2.55 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:G:2353:LEU:HD13 | 1:G:2355:LYS:HD3 | 2.02 | 0.41 |
| 1:G:2376:ASN:H | 1:G:2379:GLU:CD | 2.27 | 0.41 |
| 1:G:2542:ARG:NH1 | 1:G:2588:ALA:HA | 2.35 | 0.41 |
| 1:H:171:GLU:CD | 1:H:176:HIS:HB3 | 2.45 | 0.41 |
| 1:H:533:PRO:HB2 | 1:H:535:ILE:HD12 | 2.01 | 0.41 |
| 1:H:656:ILE:HD12 | 1:H:656:ILE:H | 1.86 | 0.41 |
| 1:H:1210:LYS:HA | 1:H:1210:LYS:HE3 | 2.02 | 0.41 |
| 1:H:1221:TYR:CE2 | 1:H:1233:SER:HB2 | 2.55 | 0.41 |
| 1:H:1559:GLY:HA2 | 1:H:1610:TYR:O | 2.20 | 0.41 |
| 1:H:1854:HIS:O | 1:H:1884:HIS:HE1 | 2.03 | 0.41 |
| 1:H:2130:HIS:NE2 | 1:H:2147:CYS:SG | 2.93 | 0.41 |
| 1:H:2460:VAL:HG22 | 1:H:2467:PHE:HE2 | 1.85 | 0.41 |
| 1:H:3353:GLU:HB3 | 1:H:3371:ASN:HB3 | 2.01 | 0.41 |
| 1:I:253:PRO:O | 1:I:256:ARG:HG2 | 2.20 | 0.41 |
| 1:I:428:SER:OG | 1:I:429:ALA:N | 2.53 | 0.41 |
| 1:I:1067:GLN:HG2 | 1:I:1074:TYR:HB3 | 2.01 | 0.41 |
| 1:I:1187:GLU:HG2 | 1:I:1188:TYR:CD2 | 2.55 | 0.41 |
| 1:I:1378:ASN:ND2 | 1:I:1380:PHE:HB2 | 2.35 | 0.41 |
| 1:I:2752:ASN:H | 1:I:2758:ARG:HD3 | 1.84 | 0.41 |
| 1:I:2805:ASN:HB3 | 1:I:2850:LEU:HD21 | 2.02 | 0.41 |
| 1:I:3036:GLN:OE1 | 1:I:3043:GLN:NE2 | 2.53 | 0.41 |
| 1:J:418:ASP:OD2 | 1:J:661:PRO:HA | 2.20 | 0.41 |
| 1:J:1736:MET:SD | 1:J:1736:MET:N | 2.93 | 0.41 |
| 1:J:2944:LEU:HD22 | 1:J:2999:LEU:HA | 2.02 | 0.41 |
| 1:K:38:LEU:HD23 | 1:K:77:LEU:HD12 | 2.01 | 0.41 |
| 1:K:1212:GLU:CD | 1:K:1214:ASN:H | 2.28 | 0.41 |
| 1:K:2012:ASP:OD1 | 1:K:2012:ASP:N | 2.53 | 0.41 |
| 1:K:2112:ARG:HH11 | 1:K:2211:PRO:HG3 | 1.85 | 0.41 |
| 1:L:445:VAL:O | 1:L:448:LEU:HG | 2.20 | 0.41 |
| 1:L:735:ARG:NH2 | 1:L:789:ILE:H | 2.18 | 0.41 |
| 1:L:847:VAL:HA | 1:L:1122:HIS:O | 2.21 | 0.41 |
| 1:L:1164:VAL:HA | 1:L:1223:VAL:HA | 2.01 | 0.41 |
| 1:L:1384:LYS:HB3 | 1:L:1391:VAL:HG12 | 2.02 | 0.41 |
| 1:L:1576:CYS:HA | 1:L:1586:CYS:HB3 | 2.02 | 0.41 |
| 1:L:2040:LYS:HE3 | 1:L:2040:LYS:HB3 | 1.87 | 0.41 |
| 1:L:2754:ASN:HD22 | 1:L:2757:ILE:HG12 | 1.84 | 0.41 |
| 1:L:3159:TYR:O | 1:L:3169:ARG:NH1 | 2.52 | 0.41 |
| 1:L:3198:SER:O | 1:L:3201:ASN:HB2 | 2.20 | 0.41 |
| 1:L:3245:PHE:HB3 | 1:L:3264:TYR:HE2 | 1.85 | 0.41 |
| 1:M:706:LEU:O | 1:M:707:GLU:HG2 | 2.20 | 0.41 |
| 1:M:996:THR:OG1 | 1:M:997:LYS:N | 2.53 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:M:997:LYS:O | 1:M:1001:MET:HG3 | 2.20 | 0.41 |
| 1:M:1263:HIS:HB2 | 1:M:1528:TYR:HB2 | 2.02 | 0.41 |
| 1:M:1990:ILE:HG22 | 1:M:1992:THR:HG22 | 2.02 | 0.41 |
| 1:M:2052:LYS:HD2 | 1:M:2052:LYS:HA | 1.61 | 0.41 |
| 1:M:2960:HIS:CE1 | 1:M:3119:HIS:HE1 | 2.35 | 0.41 |
| 1:M:3173:ARG:O | 1:M:3177:ILE:HG13 | 2.19 | 0.41 |
| 1:M:3197:VAL:O | 1:M:3201:ASN:ND2 | 2.53 | 0.41 |
| 1:N:17:LEU:HA | 1:N:20:GLU:HG2 | 2.02 | 0.41 |
| 1:N:24:ARG:HD2 | 1:N:24:ARG:HA | 1.75 | 0.41 |
| 1:N:70:HIS:O | 1:N:74:VAL:HG13 | 2.20 | 0.41 |
| 1:N:562:LEU:HB3 | 1:N:564:GLU:OE1 | 2.20 | 0.41 |
| 1:N:1005:ALA:HA | 1:N:1008:GLN:NE2 | 2.29 | 0.41 |
| 1:N:1011:PHE:HA | 1:N:1063:TRP:CH2 | 2.55 | 0.41 |
| 1:N:1871:HIS:CD2 | 1:N:1873:HIS:HB2 | 2.55 | 0.41 |
| 1:N:2448:ASP:OD1 | 1:N:2448:ASP:N | 2.53 | 0.41 |
| 1:O:1040:LEU:HB2 | 1:O:1184:LEU:HD11 | 2.01 | 0.41 |
| 1:O:1114:ASP:N | 1:O:1114:ASP:OD1 | 2.46 | 0.41 |
| 1:O:1926:GLY:HA2 | 1:O:1936:LYS:NZ | 2.35 | 0.41 |
| 1:O:2154:PHE:HB3 | 1:O:2155:PRO:HD3 | 2.02 | 0.41 |
| 1:O:2630:LEU:O | 1:O:2630:LEU:HD23 | 2.20 | 0.41 |
| 1:O:2820:ASP:HA | 1:O:2831:ALA:HB3 | 2.01 | 0.41 |
| 1:P:81:LEU:HB3 | 1:P:86:LEU:HD22 | 2.02 | 0.41 |
| 1:P:599:PHE:O | 1:P:602:PHE:HB3 | 2.20 | 0.41 |
| 1:P:599:PHE:O | 1:P:603:GLU:OE1 | 2.38 | 0.41 |
| 1:P:702:TYR:N | 1:P:703:GLU:OE1 | 2.53 | 0.41 |
| 1:P:1465:ASP:HB3 | 1:P:1530:TYR:OH | 2.21 | 0.41 |
| 1:P:1857:ILE:HD12 | 1:P:1884:HIS:CD2 | 2.55 | 0.41 |
| 1:P:2896:PHE:C | 1:Q:2734:ASN:HD21 | 2.28 | 0.41 |
| 1:P:3283:PHE:HB2 | 1:P:3302:PRO:HG2 | 2.02 | 0.41 |
| 1:Q:143:ARG:HH21 | 1:Q:209:ASP:CG | 2.27 | 0.41 |
| 1:Q:158:ASN:HB2 | 1:Q:162:PHE:CD2 | 2.55 | 0.41 |
| 1:Q:758:LYS:NZ | 1:Q:803:GLU:OE2 | 2.43 | 0.41 |
| 1:Q:1992:THR:C | 1:Q:2017:GLY:O | 2.63 | 0.41 |
| 1:Q:2052:LYS:HD2 | 1:Q:2052:LYS:HA | 1.61 | 0.41 |
| 1:Q:2164:GLN:OE1 | 1:Q:2167:GLN:NE2 | 2.53 | 0.41 |
| 1:Q:2217:ILE:HD13 | 1:Q:2291:TYR:CE1 | 2.55 | 0.41 |
| 1:Q:2537:GLN:OE1 | 1:Q:2537:GLN:N | 2.43 | 0.41 |
| 1:Q:2944:LEU:HD22 | 1:Q:3002:LYS:HE3 | 2.02 | 0.41 |
| 1:R:5:ARG:HH21 | 1:R:91:VAL:H | 1.68 | 0.41 |
| 1:R:379:LYS:HD3 | 1:R:381:ASN:H | 1.85 | 0.41 |
| 1:R:435:LYS:HG2 | 1:R:436:ASP:N | 2.34 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:R:456:GLN:OE1 | 1:R:553:PRO:HB2 | 2.20 | 0.41 |
| 1:S:446:TYR:OH | 1:S:543:ASP:OD2 | 2.37 | 0.41 |
| 1:S:637:PHE:CZ | 1:S:641:HIS:HE1 | 2.39 | 0.41 |
| 1:S:1844:CYS:HB3 | 1:S:2027:ASP:OD2 | 2.20 | 0.41 |
| 1:S:2533:ARG:HA | 1:S:2536:GLN:OE1 | 2.20 | 0.41 |
| 1:S:2696:LEU:O | 1:S:2699:SER:OG | 2.31 | 0.41 |
| 1:S:3047:ASP:HB2 | 1:S:3097:GLY:HA3 | 2.01 | 0.41 |
| 1:S:3068:THR:O | 1:S:3071:THR:OG1 | 2.32 | 0.41 |
| 1:S:3276:ASN:OD1 | 1:S:3277:ALA:N | 2.53 | 0.41 |
| 1:S:3307:ARG:NH1 | 1:S:3312:ASP:O | 2.54 | 0.41 |
| 1:T:525:TRP:CD1 | 1:T:586:LEU:HD13 | 2.55 | 0.41 |
| 1:T:587:PHE:O | 1:T:591:LEU:HG | 2.20 | 0.41 |
| 1:T:1267:ASN:HB3 | 1:T:1348:TYR:CE1 | 2.55 | 0.41 |
| 1:T:1424:ILE:HD12 | 1:T:1424:ILE:HA | 1.89 | 0.41 |
| 1:T:1496:LEU:HD23 | 1:T:1497:LYS:O | 2.21 | 0.41 |
| 1:T:2152:PRO:HA | 1:T:2261:GLU:CD | 2.45 | 0.41 |
| 1:T:2156:HIS:HE1 | 1:T:2257:TYR:OH | 2.03 | 0.41 |
| 1:T:2213:ALA:HA | 1:T:2226:ARG:NH2 | 2.35 | 0.41 |
| 1:T:2581:PHE:O | 1:T:2584:THR:OG1 | 2.33 | 0.41 |
| 1:T:2618:ASP:OD1 | 1:T:2618:ASP:N | 2.50 | 0.41 |
| 1:T:3055:ARG:HB3 | 1:T:3062:ASP:OD1 | 2.20 | 0.41 |
| 1:T:3185:TYR:CD2 | 1:T:3187:PHE:HE1 | 2.37 | 0.41 |
| 1:A:821:ASN:OD1 | 1:A:821:ASN:N | 2.52 | 0.41 |
| 1:A:847:VAL:HG23 | 1:A:847:VAL:O | 2.20 | 0.41 |
| 1:A:866:LEU:HD22 | 1:A:968:PHE:CE1 | 2.54 | 0.41 |
| 1:A:2100:ASP:O | 1:A:2104:THR:HG23 | 2.20 | 0.41 |
| 1:A:2661:ALA:HB2 | 1:A:2673:GLN:HG3 | 2.02 | 0.41 |
| 1:A:2743:PRO:HA | 1:A:2762:ARG:HE | 1.84 | 0.41 |
| 1:A:3273:LEU:HD23 | 1:A:3273:LEU:HA | 1.93 | 0.41 |
| 1:B:215:HIS:O | 1:B:219:VAL:HG23 | 2.19 | 0.41 |
| 1:B:720:ILE:HG13 | 1:B:721:ASP:N | 2.35 | 0.41 |
| 1:B:1135:GLN:HA | 1:B:1138:ARG:CZ | 2.49 | 0.41 |
| 1:B:2516:ASN:OD1 | 1:B:2517:ILE:N | 2.45 | 0.41 |
| 1:B:2578:HIS:CD2 | 1:B:2709:HIS:CD2 | 3.08 | 0.41 |
| 1:B:3260:ARG:HH12 | 1:B:3333:SER:HA | 1.85 | 0.41 |
| 1:B:3331:ILE:HA | 1:B:3405:SER:OG | 2.20 | 0.41 |
| 1:C:38:LEU:O | 1:C:41:PHE:HB2 | 2.20 | 0.41 |
| 1:C:881:ILE:HA | 1:C:884:PHE:CD2 | 2.49 | 0.41 |
| 1:C:1684:THR:O | 1:C:1688:ARG:HB3 | 2.20 | 0.41 |
| 1:C:1690:SER:O | 1:C:1693:LEU:HG | 2.20 | 0.41 |
| 1:C:2256:ASP:OD2 | 1:C:2440:ARG:NH2 | 2.53 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:2470:ARG:NH1 | 1:C:2471:TYR:H | 2.18 | 0.41 |
| 1:C:2997:MET:HE2 | 1:C:2997:MET:HB2 | 1.86 | 0.41 |
| 1:C:3022:SER:HA | 1:C:3025:THR:OG1 | 2.20 | 0.41 |
| 1:D:190:TYR:CD1 | 1:D:201:SER:HB2 | 2.54 | 0.41 |
| 1:D:293:ILE:O | 1:D:296:LEU:HG | 2.20 | 0.41 |
| 1:D:1322:PHE:CE1 | 1:D:1326:HIS:CE1 | 3.08 | 0.41 |
| 1:D:1630:ASP:OD1 | 1:D:1630:ASP:N | 2.51 | 0.41 |
| 1:D:1714:HIS:HB2 | 1:D:1746:TYR:OH | 2.20 | 0.41 |
| 1:D:1746:TYR:CD2 | 1:D:1750:PHE:HE2 | 2.37 | 0.41 |
| 1:D:1777:ALA:HA | 1:D:1780:ASN:HB3 | 2.02 | 0.41 |
| 1:D:2158:HIS:CD2 | 1:D:2299:HIS:CD2 | 3.08 | 0.41 |
| 1:D:2623:GLU:N | 1:D:2623:GLU:OE1 | 2.53 | 0.41 |
| 1:D:3388:PHE:HB2 | 1:D:3402:VAL:HG13 | 2.02 | 0.41 |
| 1:E:5:ARG:HE | 1:E:90:GLY:C | 2.28 | 0.41 |
| 1:E:559:VAL:HG13 | 1:E:633:PHE:CE2 | 2.55 | 0.41 |
| 1:E:561:PHE:CE2 | 1:E:562:LEU:HG | 2.56 | 0.41 |
| 1:E:637:PHE:CE1 | 1:E:641:HIS:HE1 | 2.38 | 0.41 |
| 1:E:724:ASP:O | 1:E:727:ILE:HG22 | 2.19 | 0.41 |
| 1:E:1689:ARG:HA | 1:E:1692:VAL:HG12 | 2.02 | 0.41 |
| 1:E:2112:ARG:HH11 | 1:E:2211:PRO:HG3 | 1.86 | 0.41 |
| 1:E:3165:ASN:ND2 | 1:E:3168:THR:H | 2.17 | 0.41 |
| 1:E:3200:ILE:O | 1:E:3204:ILE:HG12 | 2.19 | 0.41 |
| 1:F:221:ARG:O | 1:F:225:ILE:HG12 | 2.19 | 0.41 |
| 1:F:695:ARG:NE | 1:F:696:PRO:HD2 | 2.36 | 0.41 |
| 1:F:1019:GLU:O | 1:F:1022:HIS:ND1 | 2.53 | 0.41 |
| 1:F:1324:HIS:CD2 | 1:F:1324:HIS:H | 2.38 | 0.41 |
| 1:F:1919:PRO:O | 1:F:1921:LYS:NZ | 2.37 | 0.41 |
| 1:F:2038:LEU:HD12 | 1:F:2039:GLU:N | 2.35 | 0.41 |
| 1:F:2312:LEU:O | 1:F:2316:ARG:NH1 | 2.53 | 0.41 |
| 1:F:3232:LEU:HD13 | 1:F:3269:ALA:HB3 | 2.03 | 0.41 |
| 1:G:42:HIS:NE2 | 1:G:59:CYS:SG | 2.93 | 0.41 |
| 1:G:744:ASN:HB3 | 1:G:779:TRP:CD1 | 2.55 | 0.41 |
| 1:G:835:THR:OG1 | 1:G:836:HIS:N | 2.52 | 0.41 |
| 1:G:881:ILE:HD12 | 1:G:884:PHE:CE2 | 2.55 | 0.41 |
| 1:G:973:VAL:HG11 | 1:G:1045:TYR:CG | 2.56 | 0.41 |
| 1:G:1079:CYS:O | 1:H:2492:ILE:HD13 | 2.20 | 0.41 |
| 1:G:1693:LEU:O | 1:G:1696:GLN:HG3 | 2.20 | 0.41 |
| 1:G:1730:ALA:H | 1:G:2020:ALA:HB1 | 1.84 | 0.41 |
| 1:G:2802:VAL:H | 1:G:2856:THR:HG22 | 1.86 | 0.41 |
| 1:H:1496:LEU:HD23 | 1:H:1497:LYS:O | 2.21 | 0.41 |
| 1:H:1847:GLU:HA | 1:H:1850:PHE:HB3 | 2.01 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:I:678:PHE:O | 1:I:685:ASN:ND2 | 2.52 | 0.41 |
| 1:I:719:THR:H | 1:I:722:GLN:NE2 | 2.17 | 0.41 |
| 1:I:1033:GLU:O | 1:I:1036:SER:OG | 2.25 | 0.41 |
| 1:I:1723:PRO:HA | 1:I:1728:ARG:HH12 | 1.85 | 0.41 |
| 1:I:1816:ASN:OD1 | 1:I:1816:ASN:N | 2.51 | 0.41 |
| 1:J:221:ARG:O | 1:J:224:VAL:HG22 | 2.20 | 0.41 |
| 1:J:225:ILE:HA | 1:J:228:GLU:OE2 | 2.20 | 0.41 |
| 1:J:720:ILE:HG13 | 1:J:721:ASP:N | 2.35 | 0.41 |
| 1:J:735:ARG:HE | 1:J:736:THR:N | 2.17 | 0.41 |
| 1:J:750:LEU:HD12 | 1:J:768:LEU:O | 2.20 | 0.41 |
| 1:J:1502:LYS:HD3 | 1:J:1511:ASN:HD22 | 1.85 | 0.41 |
| 1:J:1564:ASN:HD22 | 1:J:1603:PRO:HA | 1.86 | 0.41 |
| 1:J:1842:ASN:OD1 | 1:J:1843:TYR:N | 2.54 | 0.41 |
| 1:J:2511:ILE:H | 1:J:2773:ASN:HB3 | 1.85 | 0.41 |
| 1:K:1303:SER:CB | 1:K:1311:LYS:HB3 | 2.51 | 0.41 |
| 1:K:1507:PHE:CD2 | 1:K:1508:ASP:HB2 | 2.55 | 0.41 |
| 1:K:1964:ASN:ND2 | 1:K:1966:GLU:OE2 | 2.53 | 0.41 |
| 1:K:2356:GLU:OE1 | 1:K:2356:GLU:N | 2.46 | 0.41 |
| 1:K:2390:LYS:HB2 | 1:K:2390:LYS:HE2 | 1.92 | 0.41 |
| 1:K:2696:LEU:HD11 | 1:K:2842:GLU:HG2 | 2.03 | 0.41 |
| 1:K:2941:LEU:HD23 | 1:K:3031:PRO:HG2 | 2.01 | 0.41 |
| 1:K:3357:TYR:HB3 | 1:L:3329:LYS:HD3 | 2.02 | 0.41 |
| 1:L:244:VAL:HG23 | 1:L:248:ARG:HE | 1.85 | 0.41 |
| 1:L:499:TRP:HE3 | 1:L:500:HIS:CD2 | 2.38 | 0.41 |
| 1:L:2359:ASN:OD1 | 1:L:2359:ASN:N | 2.53 | 0.41 |
| 1:L:2376:ASN:O | 1:L:2379:GLU:HG3 | 2.20 | 0.41 |
| 1:L:2448:ASP:O | 1:L:2452:GLU:OE1 | 2.38 | 0.41 |
| 1:L:3131:THR:HA | 1:L:3134:LYS:HG2 | 2.03 | 0.41 |
| 1:M:2311:GLU:OE1 | 1:M:2377:LEU:HD21 | 2.21 | 0.41 |
| 1:M:2585:LEU:HD23 | 1:M:2585:LEU:HA | 1.78 | 0.41 |
| 1:M:3308:PRO:HG2 | 1:M:3311:ALA:HB3 | 2.03 | 0.41 |
| 1:N:180:GLN:OE1 | 1:N:366:HIS:N | 2.39 | 0.41 |
| 1:N:728:ASP:HB3 | 1:N:836:HIS:CD2 | 2.55 | 0.41 |
| 1:N:735:ARG:HH22 | 1:N:790:THR:H | 1.66 | 0.41 |
| 1:N:2704:ILE:HD13 | 1:N:2707:ILE:HD12 | 2.03 | 0.41 |
| 1:N:2980:GLY:HA3 | 1:N:3256:TRP:CZ3 | 2.55 | 0.41 |
| 1:O:284:ASP:OD1 | 1:O:285:ASP:N | 2.53 | 0.41 |
| 1:O:1635:ILE:HD11 | 1:O:1653:PRO:HG3 | 2.02 | 0.41 |
| 1:O:1654:SER:OG | 1:O:1655:LEU:N | 2.54 | 0.41 |
| 1:O:2752:ASN:OD1 | 1:O:2753:PRO:HD2 | 2.21 | 0.41 |
| 1:O:2991:LEU:HD22 | 1:O:3157:PHE:CZ | 2.54 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:P:913:TRP:NE1 | 1:P:1089:GLN:O | 2.53 | 0.41 |
| 1:P:1328:LEU:HD11 | 1:P:1510:THR:HB | 2.01 | 0.41 |
| 1:P:1828:ASN:ND2 | 1:P:1831:TRP:HB2 | 2.36 | 0.41 |
| 1:P:2661:ALA:HA | 1:P:2664:GLN:HE22 | 1.86 | 0.41 |
| 1:Q:502:LEU:HD23 | 1:Q:502:LEU:HA | 1.88 | 0.41 |
| 1:Q:914:HIS:HE1 | 1:Q:1022:HIS:CE1 | 2.38 | 0.41 |
| 1:Q:1394:ARG:CZ | 1:Q:1456:LEU:HD11 | 2.50 | 0.41 |
| 1:Q:1461:HIS:O | 1:Q:1464:VAL:HB | 2.20 | 0.41 |
| 1:Q:1739:PHE:HZ | 1:Q:1854:HIS:CD2 | 2.38 | 0.41 |
| 1:Q:1832:LYS:O | 1:Q:1835:LEU:HG | 2.20 | 0.41 |
| 1:Q:2009:ASP:OD1 | 1:Q:2010:ALA:N | 2.53 | 0.41 |
| 1:R:1165:THR:O | 1:R:1222:SER:N | 2.54 | 0.41 |
| 1:R:1351:TRP:HZ3 | 1:R:1463:ASN:HB3 | 1.84 | 0.41 |
| 1:R:1894:LEU:O | 1:R:1898:LEU:HG | 2.20 | 0.41 |
| 1:R:2413:CYS:SG | 1:R:2470:ARG:NH2 | 2.89 | 0.41 |
| 1:R:2660:LEU:HD21 | 1:R:2803:PHE:HE1 | 1.85 | 0.41 |
| 1:R:3174:PRO:O | 1:R:3177:ILE:HG22 | 2.19 | 0.41 |
| 1:R:3269:ALA:O | 1:R:3272:LYS:HG3 | 2.21 | 0.41 |
| 1:S:31:THR:OG1 | 1:S:32:VAL:N | 2.54 | 0.41 |
| 1:S:473:LEU:HD23 | 1:S:775:LYS:HZ2 | 1.85 | 0.41 |
| 1:S:654:LEU:HD21 | 1:S:658:ARG:NH2 | 2.35 | 0.41 |
| 1:S:1315:CYS:C | 1:S:1317:HIS:HD1 | 2.27 | 0.41 |
| 1:S:1507:PHE:CG | 1:S:1508:ASP:N | 2.88 | 0.41 |
| 1:S:1824:HIS:H | 1:S:1827:ASP:CG | 2.27 | 0.41 |
| 1:S:2022:MET:SD | 1:S:2022:MET:N | 2.93 | 0.41 |
| 1:S:2064:SER:HG | 1:S:2066:SER:HG | 1.66 | 0.41 |
| 1:S:2354:PRO:O | 1:S:2357:VAL:HG22 | 2.19 | 0.41 |
| 1:S:2603:TRP:CD1 | 1:S:2711:ASN:HD22 | 2.38 | 0.41 |
| 1:S:2987:TRP:NE1 | 1:S:3157:PHE:HE1 | 2.19 | 0.41 |
| 1:T:245:GLU:CD | 1:T:245:GLU:H | 2.27 | 0.41 |
| 1:T:750:LEU:HD12 | 1:T:768:LEU:O | 2.20 | 0.41 |
| 1:T:912:HIS:NE2 | 1:T:1113:PHE:HE1 | 2.18 | 0.41 |
| 1:T:1133:ILE:HB | 1:T:1134:PRO:HD3 | 2.01 | 0.41 |
| 1:T:1222:SER:HB3 | 1:T:1230:LYS:HZ1 | 1.85 | 0.41 |
| 1:T:1405:TYR:CD2 | 1:T:1406:LEU:HD22 | 2.55 | 0.41 |
| 1:T:2530:LYS:HA | 1:T:2533:ARG:NH1 | 2.36 | 0.41 |
| 1:A:50:LYS:NZ | 1:A:357:MET:HG3 | 2.35 | 0.41 |
| 1:A:585:ALA:HA | 1:A:588:ASP:OD2 | 2.20 | 0.41 |
| 1:A:1153:PHE:HB2 | 1:A:1198:PHE:HD2 | 1.86 | 0.41 |
| 1:A:1555:ARG:HH21 | 1:A:1557:PHE:HE2 | 1.69 | 0.41 |
| 1:A:1818:LEU:N | 1:A:1860:TRP:HZ2 | 2.18 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:2101:ALA:O | 1:A:2104:THR:OG1 | 2.27 | 0.41 |
| 1:A:2190:LEU:HD21 | 1:A:2194:PHE:HD2 | 1.84 | 0.41 |
| 1:A:3300:ALA:HA | 1:A:3325:LYS:HE3 | 2.03 | 0.41 |
| 1:B:741:HIS:CE1 | 1:B:780:ASN:HD21 | 2.39 | 0.41 |
| 1:B:1149:VAL:HG11 | 1:B:1206:LEU:HD23 | 2.02 | 0.41 |
| 1:B:1273:GLU:OE1 | 1:B:1273:GLU:N | 2.53 | 0.41 |
| 1:B:1766:TRP:CD1 | 1:B:1766:TRP:C | 2.97 | 0.41 |
| 1:B:1852:ILE:HA | 1:B:1855:ASN:HD21 | 1.85 | 0.41 |
| 1:B:1956:ASP:OD1 | 1:B:1957:THR:N | 2.53 | 0.41 |
| 1:C:1670:LYS:HA | 1:C:1670:LYS:HD3 | 1.85 | 0.41 |
| 1:C:2279:GLN:CD | 1:C:2282:SER:HB3 | 2.45 | 0.41 |
| 1:C:2343:ASN:HD22 | 1:C:2349:ARG:HH22 | 1.69 | 0.41 |
| 1:C:2746:PRO:O | 1:C:2749:TRP:HB2 | 2.20 | 0.41 |
| 1:D:1018:TYR:HE1 | 1:D:1056:THR:HB | 1.84 | 0.41 |
| 1:D:1049:PHE:CD2 | 1:D:1053:HIS:HE1 | 2.38 | 0.41 |
| 1:D:1135:GLN:O | 1:D:1139:GLU:OE1 | 2.37 | 0.41 |
| 1:D:1802:ILE:CD1 | 1:D:1805:GLU:HB2 | 2.50 | 0.41 |
| 1:D:2022:MET:HE3 | 1:D:2022:MET:HB3 | 1.89 | 0.41 |
| 1:D:2972:ASP:OD1 | 1:D:2972:ASP:N | 2.48 | 0.41 |
| 1:D:3155:GLU:CD | 1:D:3158:ASN:HD21 | 2.28 | 0.41 |
| 1:E:86:LEU:HD12 | 1:E:86:LEU:HA | 1.87 | 0.41 |
| 1:E:911:PRO:HB3 | 1:E:1018:TYR:HE1 | 1.85 | 0.41 |
| 1:E:1017:GLN:HA | 1:E:1020:ILE:HG22 | 2.03 | 0.41 |
| 1:E:1190:ILE:HD12 | 1:E:1191:PRO:HD2 | 2.03 | 0.41 |
| 1:E:1559:GLY:HA2 | 1:E:1609:LEU:HD21 | 2.03 | 0.41 |
| 1:E:1750:PHE:HD2 | 1:E:1882:LEU:HD21 | 1.85 | 0.41 |
| 1:E:1829:TRP:NE1 | 1:E:1833:GLN:HE22 | 2.19 | 0.41 |
| 1:E:2061:SER:HB3 | 3:r:1:NAG:H82 | 2.02 | 0.41 |
| 1:E:2129:PHE:HE1 | 1:E:2342:LEU:HD13 | 1.84 | 0.41 |
| 1:E:2298:HIS:O | 1:E:2302:VAL:HG23 | 2.21 | 0.41 |
| 1:E:2775:GLN:N | 1:E:2775:GLN:OE1 | 2.54 | 0.41 |
| 1:E:2853:TYR:HD1 | 1:E:2855:VAL:HG22 | 1.84 | 0.41 |
| 1:E:2900:LYS:HE3 | 1:E:2900:LYS:HB3 | 1.83 | 0.41 |
| 1:E:3203:ILE:HD12 | 1:E:3206:ASN:HB2 | 2.02 | 0.41 |
| 1:F:48:CYS:HB2 | 1:F:58:CYS:HB2 | 1.75 | 0.41 |
| 1:F:812:ASP:OD1 | 1:F:812:ASP:N | 2.52 | 0.41 |
| 1:F:991:LYS:H | 1:F:994:ARG:NH2 | 2.18 | 0.41 |
| 1:F:1430:HIS:HE1 | 1:F:1461:HIS:NE2 | 2.18 | 0.41 |
| 1:F:2155:PRO:HB2 | 1:F:2306:TRP:CE3 | 2.55 | 0.41 |
| 1:F:2371:LYS:HB3 | 1:F:2371:LYS:HE3 | 1.83 | 0.41 |
| 1:F:2932:GLU:O | 1:F:2935:SER:OG | 2.34 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:F:3149:ASN:HA | 1:F:3152:ARG:HD3 | 2.01 | 0.41 |
| 1:F:3218:VAL:HA | 1:F:3258:TYR:CD2 | 2.55 | 0.41 |
| 1:F:3220:SER:HB2 | 1:F:3256:TRP:O | 2.20 | 0.41 |
| 1:G:28:ASP:OD1 | 1:G:29:ASP:N | 2.54 | 0.41 |
| 1:G:874:SER:O | 1:G:877:GLY:N | 2.45 | 0.41 |
| 1:G:995:LEU:HB3 | 1:G:999:ALA:HB3 | 2.02 | 0.41 |
| 1:G:1145:HIS:NE2 | 1:G:1524:ASN:OD1 | 2.53 | 0.41 |
| 1:G:1277:GLU:HA | 1:G:1280:LYS:HG2 | 2.03 | 0.41 |
| 1:G:1899:GLN:HE22 | 1:G:1905:ASP:C | 2.27 | 0.41 |
| 1:G:2306:TRP:NE1 | 1:G:2310:GLN:HE22 | 2.18 | 0.41 |
| 1:G:2314:LYS:HA | 1:G:2314:LYS:HD2 | 1.90 | 0.41 |
| 1:G:2990:LEU:HD12 | 1:G:3168:THR:HG22 | 2.02 | 0.41 |
| 1:G:3144:ARG:NH1 | 1:G:3147:LEU:HD11 | 2.35 | 0.41 |
| 1:H:42:HIS:NE2 | 1:H:59:CYS:SG | 2.94 | 0.41 |
| 1:H:94:TRP:HZ2 | 1:H:100:ILE:HD12 | 1.85 | 0.41 |
| 1:H:228:GLU:HA | 1:H:231:LYS:HG3 | 2.02 | 0.41 |
| 1:H:599:PHE:O | 1:H:603:GLU:OE1 | 2.38 | 0.41 |
| 1:H:1108:VAL:HA | 1:H:1109:PRO:HD3 | 1.89 | 0.41 |
| 1:H:1153:PHE:CE1 | 1:H:1239:VAL:HG12 | 2.55 | 0.41 |
| 1:H:1305:CYS:HB2 | 1:H:1312:VAL:O | 2.20 | 0.41 |
| 1:H:1415:GLU:OE2 | 1:H:1551:ARG:HG2 | 2.20 | 0.41 |
| 1:H:1802:ILE:CD1 | 1:H:1805:GLU:HB2 | 2.50 | 0.41 |
| 1:H:1852:ILE:HD12 | 1:H:1852:ILE:HA | 1.97 | 0.41 |
| 1:H:2095:GLU:CD | 1:H:2097:SER:H | 2.28 | 0.41 |
| 1:H:2209:GLU:H | 1:H:2209:GLU:CD | 2.27 | 0.41 |
| 1:H:2412:VAL:H | 1:H:2422:ALA:HB2 | 1.85 | 0.41 |
| 1:I:1022:HIS:HD2 | 1:I:1052:HIS:HE1 | 1.67 | 0.41 |
| 1:I:1247:SER:O | 1:I:1250:LYS:HG2 | 2.20 | 0.41 |
| 1:I:1286:MET:HA | 1:I:1289:ASP:OD2 | 2.20 | 0.41 |
| 1:I:1721:PRO:HD3 | 1:I:1729:TYR:CZ | 2.55 | 0.41 |
| 1:I:2216:TYR:HA | 1:I:2223:TYR:HA | 2.02 | 0.41 |
| 1:I:2216:TYR:CD1 | 1:I:2223:TYR:HB3 | 2.55 | 0.41 |
| 1:I:2410:PHE:O | 1:I:2422:ALA:HB3 | 2.20 | 0.41 |
| 1:I:2976:CYS:HB3 | 1:I:3156:PRO:HD3 | 2.01 | 0.41 |
| 1:I:3095:VAL:HG21 | 1:I:3114:PHE:CE2 | 2.56 | 0.41 |
| 1:J:480:PRO:HD3 | 1:J:680:PHE:CZ | 2.56 | 0.41 |
| 1:J:581:GLY:H | 1:J:856:ARG:NH2 | 2.18 | 0.41 |
| 1:J:634:ASP:OD1 | 1:J:635:PRO:HD2 | 2.20 | 0.41 |
| 1:J:675:LEU:HD12 | 1:J:694:ALA:O | 2.20 | 0.41 |
| 1:J:938:ASP:OD2 | 1:J:940:THR:OG1 | 2.38 | 0.41 |
| 1:J:1040:LEU:HD21 | 1:J:1184:LEU:HD11 | 2.02 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:J:1093:GLN:N | 1:J:1093:GLN:OE1 | 2.53 | 0.41 |
| 1:J:1884:HIS:O | 1:J:1888:THR:HG23 | 2.20 | 0.41 |
| 1:J:2087:LEU:H | 1:J:2366:ARG:NH1 | 2.18 | 0.41 |
| 1:J:3057:LYS:NZ | 1:J:3062:ASP:HB2 | 2.35 | 0.41 |
| 1:J:3127:GLN:O | 1:J:3130:GLN:HG3 | 2.21 | 0.41 |
| 1:J:3213:VAL:O | 1:J:3267:THR:OG1 | 2.33 | 0.41 |
| 1:K:88:ASP:OD1 | 1:K:89:ILE:N | 2.51 | 0.41 |
| 1:K:1397:GLN:HB3 | 1:K:1400:LEU:HD13 | 2.01 | 0.41 |
| 1:K:1556:LEU:HD11 | 1:K:1655:LEU:HD21 | 2.02 | 0.41 |
| 1:K:1676:ILE:HG22 | 1:K:1678:LYS:HZ2 | 1.85 | 0.41 |
| 1:K:2353:LEU:HB3 | 1:K:2355:LYS:HD3 | 2.02 | 0.41 |
| 1:K:2377:LEU:O | 1:K:2381:GLU:HG2 | 2.20 | 0.41 |
| 1:K:2648:ARG:HH11 | 1:K:2656:ARG:NH2 | 2.17 | 0.41 |
| 1:K:2729:ASP:OD2 | 1:K:2915:PRO:HB2 | 2.20 | 0.41 |
| 1:K:3017:SER:OG | 1:K:3019:ALA:O | 2.37 | 0.41 |
| 1:L:235:LYS:HE2 | 1:L:235:LYS:HB3 | 1.91 | 0.41 |
| 1:L:612:LEU:HD21 | 1:L:768:LEU:HD13 | 2.02 | 0.41 |
| 1:L:2240:LYS:HB2 | 1:L:2240:LYS:HE2 | 1.89 | 0.41 |
| 1:L:2397:PHE:CD1 | 1:L:2489:PRO:HB3 | 2.55 | 0.41 |
| 1:L:2413:CYS:SG | 1:L:2470:ARG:NE | 2.92 | 0.41 |
| 1:M:1161:SER:HB3 | 1:M:1184:LEU:HA | 2.01 | 0.41 |
| 1:M:1356:ARG:HE | 1:M:1356:ARG:HB3 | 1.69 | 0.41 |
| 1:M:1551:ARG:HG2 | 1:M:1661:GLU:HG3 | 2.02 | 0.41 |
| 1:M:1722:TYR:CD1 | 1:M:1724:GLU:HB2 | 2.55 | 0.41 |
| 1:M:1896:GLN:O | 1:M:1899:GLN:HG3 | 2.20 | 0.41 |
| 1:M:2162:THR:O | 1:M:2165:VAL:HG22 | 2.20 | 0.41 |
| 1:M:2863:HIS:HE1 | 1:N:1536:ASN:HD21 | 1.69 | 0.41 |
| 1:N:444:GLU:HA | 1:N:447:GLU:CD | 2.44 | 0.41 |
| 1:N:454:ARG:C | 1:N:514:ARG:HH12 | 2.27 | 0.41 |
| 1:N:535:ILE:H | 1:N:535:ILE:HD12 | 1.85 | 0.41 |
| 1:N:634:ASP:OD1 | 1:N:636:ILE:HG12 | 2.20 | 0.41 |
| 1:N:1280:LYS:HD2 | 1:N:1367:TYR:CZ | 2.55 | 0.41 |
| 1:N:1322:PHE:CE1 | 1:N:1326:HIS:CE1 | 3.09 | 0.41 |
| 1:N:1556:LEU:HD11 | 1:N:1655:LEU:HB2 | 2.03 | 0.41 |
| 1:N:1713:PHE:CE1 | 1:N:1929:TYR:HB3 | 2.55 | 0.41 |
| 1:N:2149:HIS:CD2 | 1:N:2154:PHE:HE2 | 2.39 | 0.41 |
| 1:N:2941:LEU:HD13 | 1:N:2999:LEU:HD21 | 2.01 | 0.41 |
| 1:N:2985:PRO:O | 1:N:2989:ARG:HG3 | 2.19 | 0.41 |
| 1:O:418:ASP:OD2 | 1:O:663:LYS:N | 2.46 | 0.41 |
| 1:O:704:HIS:ND1 | 1:O:705:GLU:OE2 | 2.53 | 0.41 |
| 1:O:754:SER:HA | 1:O:765:VAL:HG23 | 2.03 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:O:1268:LEU:HB3 | 1:O:1347:PRO:HB2 | 2.02 | 0.41 |
| 1:O:1428:ILE:HG21 | 1:O:1610:TYR:CZ | 2.56 | 0.41 |
| 1:O:1507:PHE:CG | 1:O:1508:ASP:N | 2.89 | 0.41 |
| 1:O:1705:THR:OG1 | 1:O:1931:LEU:HD13 | 2.21 | 0.41 |
| 1:O:1869:MET:HA | 1:O:1875:ALA:HA | 2.02 | 0.41 |
| 1:O:1899:GLN:OE1 | 1:O:1904:HIS:HB2 | 2.21 | 0.41 |
| 1:O:2088:PRO:HA | 1:O:2089:PRO:HD2 | 1.87 | 0.41 |
| 1:O:2392:ARG:HB3 | 1:O:2394:PHE:CE1 | 2.55 | 0.41 |
| 1:O:2655:TYR:HA | 1:O:2658:ILE:HG22 | 2.01 | 0.41 |
| 1:P:504:VAL:O | 1:P:507:VAL:HG22 | 2.20 | 0.41 |
| 1:P:525:TRP:CD1 | 1:P:586:LEU:HD13 | 2.55 | 0.41 |
| 1:P:1283:LEU:HA | 1:P:1286:MET:HG3 | 2.03 | 0.41 |
| 1:P:1824:HIS:HB2 | 1:P:1827:ASP:CG | 2.46 | 0.41 |
| 1:P:2099:LEU:HD23 | 1:P:2099:LEU:HA | 1.84 | 0.41 |
| 1:P:2132:VAL:HG13 | 1:P:2287:HIS:HD1 | 1.85 | 0.41 |
| 1:Q:869:LEU:HA | 1:Q:869:LEU:HD12 | 1.81 | 0.41 |
| 1:Q:1495:PRO:HG3 | 1:Q:1515:ARG:HD2 | 2.03 | 0.41 |
| 1:Q:1860:TRP:HA | 1:Q:1860:TRP:CE3 | 2.55 | 0.41 |
| 1:Q:2929:LEU:HD22 | 1:Q:2933:GLN:HE21 | 1.85 | 0.41 |
| 1:Q:3317:ILE:HA | 1:Q:3339:ARG:O | 2.21 | 0.41 |
| 1:R:70:HIS:CD2 | 1:R:216:HIS:CE1 | 3.07 | 0.41 |
| 1:R:74:VAL:HA | 1:R:77:LEU:HD23 | 2.02 | 0.41 |
| 1:R:135:MET:HG2 | 1:R:137:VAL:HG13 | 2.03 | 0.41 |
| 1:R:914:HIS:O | 1:R:917:LEU:HG | 2.20 | 0.41 |
| 1:R:1332:GLN:OE1 | 1:R:1505:ASN:ND2 | 2.43 | 0.41 |
| 1:R:1883:LEU:O | 1:R:1886:SER:OG | 2.34 | 0.41 |
| 1:R:2821:LEU:HD13 | 1:R:2872:PHE:CE1 | 2.55 | 0.41 |
| 1:R:3381:LEU:HD23 | 1:R:3386:TYR:CZ | 2.55 | 0.41 |
| 1:S:76:GLN:HG3 | 1:S:264:THR:HG21 | 2.02 | 0.41 |
| 1:S:263:LEU:HD12 | 1:S:263:LEU:HA | 1.86 | 0.41 |
| 1:S:612:LEU:HD21 | 1:S:768:LEU:HA | 2.02 | 0.41 |
| 1:S:706:LEU:O | 1:S:707:GLU:HG2 | 2.20 | 0.41 |
| 1:S:1283:LEU:HD13 | 1:S:1380:PHE:HE1 | 1.86 | 0.41 |
| 1:S:1548:LYS:HE2 | 1:S:1548:LYS:HB2 | 1.89 | 0.41 |
| 1:S:2232:LEU:HB2 | 1:S:2274:LEU:HD11 | 2.03 | 0.41 |
| 1:S:3045:THR:N | 1:S:3101:TYR:O | 2.46 | 0.41 |
| 1:S:3075:THR:HA | 1:S:3136:ARG:NH2 | 2.35 | 0.41 |
| 1:T:13:ASP:O | 1:T:17:LEU:HD23 | 2.20 | 0.41 |
| 1:T:81:LEU:HB3 | 1:T:86:LEU:HB2 | 2.02 | 0.41 |
| 1:T:270:ALA:HA | 1:T:273:LEU:HD12 | 2.02 | 0.41 |
| 1:T:378:LYS:NZ | 1:T:383:ASP:H | 2.19 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:T:531:THR:OG1 | 1:T:532:VAL:N | 2.54 | 0.41 |
| 1:T:986:LEU:HD11 | 1:T:1028:LEU:HB3 | 2.01 | 0.41 |
| 1:T:1709:ALA:O | 1:T:1712:SER:OG | 2.28 | 0.41 |
| 1:T:2552:GLY:HA3 | 1:T:2697:GLU:HA | 2.02 | 0.41 |
| 1:T:2585:LEU:HG | 1:T:2589:LEU:HD23 | 2.03 | 0.41 |
| 1:T:3149:ASN:O | 1:T:3174:PRO:HG2 | 2.20 | 0.41 |
| 1:T:3332:VAL:HG22 | 1:T:3406:ILE:HA | 2.01 | 0.41 |
| 1:T:3383:PRO:HA | 1:T:3406:ILE:HB | 2.02 | 0.41 |
| 1:A:101:THR:HA | 1:A:150:PHE:HB3 | 2.02 | 0.41 |
| 1:A:131:ASN:HA | 1:A:138:HIS:HA | 2.01 | 0.41 |
| 1:A:2156:HIS:CD2 | 1:A:2306:TRP:HH2 | 2.37 | 0.41 |
| 1:A:2376:ASN:O | 1:A:2380:LEU:HG | 2.21 | 0.41 |
| 1:A:3074:GLU:O | 1:A:3080:PHE:HZ | 2.03 | 0.41 |
| 1:B:2240:LYS:HB2 | 1:B:2240:LYS:HE2 | 1.82 | 0.41 |
| 1:B:2535:VAL:HA | 1:B:2538:GLN:HG3 | 2.03 | 0.41 |
| 1:B:2630:LEU:HG | 1:B:2632:GLU:OE1 | 2.21 | 0.41 |
| 1:B:2676:VAL:HA | 1:B:2679:ASN:HD21 | 1.85 | 0.41 |
| 1:B:2803:PHE:CD1 | 1:B:2852:GLN:HB3 | 2.55 | 0.41 |
| 1:C:602:PHE:HA | 1:C:605:GLN:NE2 | 2.36 | 0.41 |
| 1:C:654:LEU:HD12 | 1:C:723:LEU:HD22 | 2.02 | 0.41 |
| 1:C:1351:TRP:NE1 | 1:C:1460:HIS:HD2 | 2.17 | 0.41 |
| 1:C:3289:LYS:HE2 | 1:C:3291:ASN:HB2 | 2.03 | 0.41 |
| 1:D:303:ARG:HD3 | 1:D:303:ARG:HA | 1.82 | 0.41 |
| 1:D:994:ARG:HE | 1:D:995:LEU:N | 2.18 | 0.41 |
| 1:D:1116:GLU:O | 1:D:1120:GLN:HB3 | 2.20 | 0.41 |
| 1:D:1321:VAL:HA | 1:D:1324:HIS:CD2 | 2.56 | 0.41 |
| 1:D:1852:ILE:HA | 1:D:1855:ASN:HD21 | 1.85 | 0.41 |
| 1:D:1947:TYR:CE1 | 1:D:1948:LYS:HG3 | 2.55 | 0.41 |
| 1:D:3160:GLU:HA | 1:D:3169:ARG:HE | 1.86 | 0.41 |
| 1:D:3270:LEU:HD11 | 1:D:3281:PHE:CZ | 2.54 | 0.41 |
| 1:D:3363:CYS:HB2 | 1:D:3396:CYS:HB3 | 1.91 | 0.41 |
| 1:E:593:ALA:HA | 1:E:605:GLN:HG3 | 2.01 | 0.41 |
| 1:E:878:PHE:O | 1:E:881:ILE:HG22 | 2.20 | 0.41 |
| 1:E:1297:SER:HB2 | 1:E:1302:PRO:HD2 | 2.03 | 0.41 |
| 1:E:1521:ASP:OD2 | 1:E:1524:ASN:HB2 | 2.21 | 0.41 |
| 1:E:1693:LEU:O | 1:E:1696:GLN:HG3 | 2.19 | 0.41 |
| 1:E:2063:LEU:HD11 | 3:r:1:NAG:H5 | 2.02 | 0.41 |
| 1:E:2112:ARG:HB3 | 1:E:2116:LYS:HZ1 | 1.86 | 0.41 |
| 1:E:2288:TYR:HA | 1:E:2291:TYR:HE2 | 1.85 | 0.41 |
| 1:E:2470:ARG:NH1 | 1:E:2471:TYR:H | 2.18 | 0.41 |
| 1:E:2491:ILE:HG22 | 1:F:1082:ALA:H | 1.86 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:F:178:GLU:O | 1:F:182:GLU:HG2 | 2.19 | 0.41 |
| 1:F:202:THR:HG23 | 1:F:205:TRP:H | 1.84 | 0.41 |
| 1:F:811:LYS:NZ | 1:F:817:ASP:OD1 | 2.53 | 0.41 |
| 1:F:832:GLU:N | 1:F:832:GLU:OE1 | 2.54 | 0.41 |
| 1:F:2676:VAL:HA | 1:F:2679:ASN:HD21 | 1.85 | 0.41 |
| 1:F:3132:LEU:HG | 1:F:3136:ARG:HH12 | 1.84 | 0.41 |
| 1:F:3340:PHE:CE2 | 1:F:3351:VAL:HG11 | 2.55 | 0.41 |
| 1:G:23:LEU:HD12 | 1:G:23:LEU:HA | 1.87 | 0.41 |
| 1:G:469:GLU:OE1 | 1:G:474:PRO:HD2 | 2.20 | 0.41 |
| 1:G:792:ALA:O | 1:G:795:LYS:HG2 | 2.20 | 0.41 |
| 1:G:1220:LYS:HZ1 | 1:G:1222:SER:HB2 | 1.86 | 0.41 |
| 1:G:2348:THR:HG1 | 1:G:2349:ARG:NH1 | 2.17 | 0.41 |
| 1:G:2405:SER:HB3 | 1:G:2426:PHE:CE1 | 2.45 | 0.41 |
| 1:G:2673:GLN:OE1 | 1:G:2673:GLN:HA | 2.21 | 0.41 |
| 1:G:2849:ARG:HH11 | 1:G:2849:ARG:HA | 1.85 | 0.41 |
| 1:H:1273:GLU:CD | 1:H:1273:GLU:H | 2.28 | 0.41 |
| 1:H:1424:ILE:HD13 | 1:H:1424:ILE:HA | 1.93 | 0.41 |
| 1:H:1731:CYS:SG | 1:H:1921:LYS:HB3 | 2.60 | 0.41 |
| 1:H:1817:ARG:HA | 1:H:1820:ASP:OD2 | 2.21 | 0.41 |
| 1:H:2149:HIS:HA | 1:H:2154:PHE:CD2 | 2.51 | 0.41 |
| 1:H:2521:THR:HG22 | 1:H:2524:GLU:OE2 | 2.20 | 0.41 |
| 1:H:2676:VAL:HA | 1:H:2679:ASN:HD21 | 1.85 | 0.41 |
| 1:H:3213:VAL:HG22 | 1:H:3267:THR:HG23 | 2.03 | 0.41 |
| 1:I:69:TRP:CD1 | 1:I:251:LEU:HD12 | 2.38 | 0.41 |
| 1:I:635:PRO:O | 1:I:638:ILE:HG12 | 2.20 | 0.41 |
| 1:I:1405:TYR:CD2 | 1:I:1406:LEU:HD22 | 2.55 | 0.41 |
| 1:I:2159:ARG:HD2 | 1:I:2306:TRP:CE3 | 2.56 | 0.41 |
| 1:I:2398:LEU:HB2 | 1:I:2441:LEU:HD22 | 2.03 | 0.41 |
| 1:I:2553:TYR:CG | 1:I:2554:PRO:HA | 2.55 | 0.41 |
| 1:I:2728:LEU:HD21 | 1:I:2912:ASP:OD2 | 2.20 | 0.41 |
| 1:I:3022:SER:HA | 1:I:3025:THR:OG1 | 2.20 | 0.41 |
| 1:J:475:ALA:HB3 | 1:J:485:ARG:HB3 | 2.02 | 0.41 |
| 1:J:887:GLN:OE1 | 1:J:901:ALA:HB2 | 2.20 | 0.41 |
| 1:J:1051:LEU:HD12 | 1:J:1052:HIS:N | 2.35 | 0.41 |
| 1:J:2664:GLN:HB3 | 1:J:2669:ASN:ND2 | 2.36 | 0.41 |
| 1:J:2790:GLU:HG2 | 1:J:2791:GLU:N | 2.36 | 0.41 |
| 1:K:181:PHE:CE1 | 1:K:219:VAL:HG13 | 2.55 | 0.41 |
| 1:K:586:LEU:H | 1:K:586:LEU:HD12 | 1.85 | 0.41 |
| 1:K:682:PRO:HB2 | 1:K:1273:GLU:OE2 | 2.20 | 0.41 |
| 1:K:733:LYS:HB2 | 1:K:733:LYS:HE2 | 1.82 | 0.41 |
| 1:K:1331:ASP:O | 1:K:1334:GLU:HG3 | 2.19 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:K:2570:GLY:HA2 | 1:K:2847:PHE:CE1 | 2.47 | 0.41 |
| 1:K:3307:ARG:NH2 | 1:K:3314:ASP:OD2 | 2.54 | 0.41 |
| 1:L:742:LEU:HD23 | 1:L:781:PHE:CE2 | 2.56 | 0.41 |
| 1:L:1164:VAL:HG12 | 1:L:1181:PHE:H | 1.86 | 0.41 |
| 1:L:1624:LYS:HD3 | 1:L:1626:ASP:H | 1.86 | 0.41 |
| 1:L:1666:ASP:O | 1:L:1668:THR:HG23 | 2.21 | 0.41 |
| 1:L:2213:ALA:HA | 1:L:2226:ARG:NH2 | 2.35 | 0.41 |
| 1:L:2412:VAL:HG12 | 1:L:2422:ALA:HB2 | 2.01 | 0.41 |
| 1:L:2432:LEU:N | 1:L:2433:GLU:OE1 | 2.54 | 0.41 |
| 1:L:2533:ARG:O | 1:L:2537:GLN:OE1 | 2.38 | 0.41 |
| 1:L:3395:ARG:HA | 1:L:3395:ARG:HD2 | 1.89 | 0.41 |
| 1:M:435:LYS:HA | 1:M:711:ASP:OD2 | 2.21 | 0.41 |
| 1:M:501:ARG:NH1 | 1:M:702:TYR:HB3 | 2.34 | 0.41 |
| 1:M:1416:GLN:OE1 | 1:M:1425:GLN:NE2 | 2.48 | 0.41 |
| 1:M:1662:ASP:N | 1:M:1662:ASP:OD1 | 2.53 | 0.41 |
| 1:N:5:ARG:HD2 | 1:N:283:TYR:CZ | 2.56 | 0.41 |
| 1:N:735:ARG:HH21 | 1:N:789:ILE:H | 1.67 | 0.41 |
| 1:N:953:GLU:HA | 1:N:969:HIS:HB2 | 2.02 | 0.41 |
| 1:N:1152:GLY:C | 1:N:1153:PHE:HD1 | 2.28 | 0.41 |
| 1:N:1888:THR:HA | 1:N:1891:ILE:HD12 | 2.02 | 0.41 |
| 1:N:2199:PHE:CZ | 1:N:2208:LEU:HD23 | 2.55 | 0.41 |
| 1:N:2262:VAL:HG23 | 1:N:2438:PHE:CD1 | 2.55 | 0.41 |
| 1:N:2301:PHE:O | 1:N:2304:LYS:HB3 | 2.20 | 0.41 |
| 1:N:2660:LEU:O | 1:N:2664:GLN:NE2 | 2.51 | 0.41 |
| 1:N:2712:VAL:HA | 1:N:2715:GLN:OE1 | 2.21 | 0.41 |
| 1:O:88:ASP:OD1 | 1:O:89:ILE:N | 2.52 | 0.41 |
| 1:O:185:HIS:NE2 | 1:O:216:HIS:HE1 | 2.18 | 0.41 |
| 1:O:331:HIS:CD2 | 1:O:332:ASP:H | 2.37 | 0.41 |
| 1:O:1334:GLU:HG3 | 1:O:1346:VAL:HG12 | 2.01 | 0.41 |
| 1:O:1852:ILE:HD13 | 1:O:2030:TYR:CZ | 2.56 | 0.41 |
| 1:O:1896:GLN:O | 1:O:1899:GLN:HG3 | 2.19 | 0.41 |
| 1:O:2587:ARG:NE | 1:O:2754:ASN:HB2 | 2.35 | 0.41 |
| 1:O:3352:LYS:HA | 1:O:3371:ASN:O | 2.20 | 0.41 |
| 1:O:3408:ASP:N | 1:O:3408:ASP:OD1 | 2.52 | 0.41 |
| 1:P:133:ASP:OD1 | 1:P:133:ASP:N | 2.52 | 0.41 |
| 1:P:614:HIS:CG | 1:P:771:LEU:HD11 | 2.56 | 0.41 |
| 1:P:848:ARG:O | 1:P:1124:ASP:N | 2.52 | 0.41 |
| 1:P:907:MET:SD | 1:P:907:MET:N | 2.90 | 0.41 |
| 1:P:1164:VAL:HG12 | 1:P:1181:PHE:H | 1.85 | 0.41 |
| 1:P:1743:HIS:O | 1:P:1747:THR:HG23 | 2.20 | 0.41 |
| 1:P:2413:CYS:SG | 1:P:2470:ARG:NH2 | 2.92 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:P:2494:LYS:HD3 | 1:P:2494:LYS:HA | 1.89 | 0.41 |
| 1:P:3127:GLN:HA | 1:P:3130:GLN:HG3 | 2.03 | 0.41 |
| 1:Q:513:SER:HG | 1:Q:514:ARG:HH11 | 1.63 | 0.41 |
| 1:Q:577:LYS:HD3 | 1:Q:577:LYS:HA | 1.83 | 0.41 |
| 1:Q:579:GLU:HG3 | 1:Q:582:ASP:CG | 2.46 | 0.41 |
| 1:Q:675:LEU:HD11 | 1:Q:696:PRO:HG3 | 2.02 | 0.41 |
| 1:Q:938:ASP:HA | 1:Q:1055:ASN:ND2 | 2.34 | 0.41 |
| 1:Q:1865:LYS:HE3 | 1:Q:1867:HIS:HB2 | 2.01 | 0.41 |
| 1:Q:2165:VAL:O | 1:Q:2169:LEU:HD23 | 2.20 | 0.41 |
| 1:Q:2495:PRO:HB2 | 1:Q:2500:ARG:HD2 | 2.01 | 0.41 |
| 1:Q:2889:LEU:HD23 | 1:Q:2890:GLU:O | 2.21 | 0.41 |
| 1:Q:2940:ALA:O | 1:Q:2944:LEU:HD23 | 2.21 | 0.41 |
| 1:Q:2941:LEU:HD23 | 1:Q:3031:PRO:HG2 | 2.02 | 0.41 |
| 1:Q:2986:HIS:HB3 | 1:Q:3177:ILE:HD13 | 2.02 | 0.41 |
| 1:Q:3069:LEU:HA | 1:Q:3072:LEU:HD12 | 2.02 | 0.41 |
| 1:R:343:GLU:HG3 | 1:R:375:HIS:CE1 | 2.55 | 0.41 |
| 1:R:418:ASP:OD2 | 1:R:661:PRO:HA | 2.21 | 0.41 |
| 1:R:614:HIS:CD2 | 1:R:637:PHE:HE1 | 2.37 | 0.41 |
| 1:R:742:LEU:HD23 | 1:R:781:PHE:CE2 | 2.56 | 0.41 |
| 1:R:1010:ASP:OD1 | 1:R:1013:THR:OG1 | 2.20 | 0.41 |
| 1:R:1101:HIS:CD2 | 1:R:1101:HIS:N | 2.89 | 0.41 |
| 1:R:1465:ASP:HB3 | 1:R:1530:TYR:OH | 2.21 | 0.41 |
| 1:R:1722:TYR:CE2 | 1:R:1724:GLU:HG2 | 2.55 | 0.41 |
| 1:R:2018:GLY:O | 1:R:2021:GLU:HG2 | 2.20 | 0.41 |
| 1:R:2108:LYS:HE3 | 1:R:2108:LYS:HB3 | 1.83 | 0.41 |
| 1:R:2313:GLN:HA | 1:R:2316:ARG:NH1 | 2.35 | 0.41 |
| 1:R:2550:ALA:O | 1:R:2565:ALA:HB1 | 2.20 | 0.41 |
| 1:R:3124:ARG:HG2 | 1:R:3124:ARG:HH11 | 1.86 | 0.41 |
| 1:S:719:THR:H | 1:S:722:GLN:NE2 | 2.18 | 0.41 |
| 1:S:1348:TYR:OH | 1:S:1531:ASP:OD2 | 2.37 | 0.41 |
| 1:S:1366:SER:OG | 1:S:1377:SER:HA | 2.21 | 0.41 |
| 1:S:2611:PRO:O | 1:S:2615:THR:HG23 | 2.20 | 0.41 |
| 1:T:30:LYS:NZ | 1:T:131:ASN:HD21 | 2.17 | 0.41 |
| 1:T:1159:ARG:HG2 | 1:T:1186:ASP:C | 2.46 | 0.41 |
| 1:T:1270:ASP:OD1 | 1:T:1271:LEU:N | 2.53 | 0.41 |
| 1:T:1828:ASN:ND2 | 1:T:1831:TRP:HB2 | 2.36 | 0.41 |
| 1:T:2712:VAL:HA | 1:T:2715:GLN:NE2 | 2.36 | 0.41 |
| 1:T:3108:TYR:HB3 | 1:T:3111:PHE:CD2 | 2.56 | 0.41 |
| 1:T:3126:TRP:CZ3 | 1:T:3130:GLN:HG2 | 2.56 | 0.41 |
| 1:T:3156:PRO:HB2 | 1:T:3162:LYS:HG3 | 2.01 | 0.41 |
| 3:fA:1:NAG:H62 | 3:fA:2:NAG:N2 | 2.28 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:920:GLN:HE22 | 1:A:1100:ASP:HB3 | 1.86 | 0.41 |
| 1:A:1974:LYS:HE3 | 1:A:2361:GLN:HB3 | 2.02 | 0.41 |
| 1:A:2439:ASP:CG | 1:A:2440:ARG:HE | 2.29 | 0.41 |
| 1:B:538:LYS:HA | 1:B:538:LYS:HD2 | 1.85 | 0.41 |
| 1:B:614:HIS:CD2 | 1:B:637:PHE:HE1 | 2.39 | 0.41 |
| 1:B:1556:LEU:HD23 | 1:B:1557:PHE:N | 2.36 | 0.41 |
| 1:B:1845:ASP:O | 1:B:1848:VAL:HG22 | 2.20 | 0.41 |
| 1:B:1978:LYS:HA | 1:B:2078:LYS:NZ | 2.36 | 0.41 |
| 1:B:1982:PHE:CD1 | 1:B:2031:ARG:HB3 | 2.55 | 0.41 |
| 1:B:1990:ILE:O | 1:B:1991:LYS:HG2 | 2.20 | 0.41 |
| 1:B:2247:GLU:OE2 | 1:B:2267:THR:HG22 | 2.20 | 0.41 |
| 1:B:2359:ASN:OD1 | 1:B:2359:ASN:N | 2.53 | 0.41 |
| 1:B:2738:GLN:O | 1:B:2742:GLN:NE2 | 2.48 | 0.41 |
| 1:C:302:GLN:NE2 | 1:C:303:ARG:HG3 | 2.36 | 0.41 |
| 1:C:718:MET:SD | 1:C:722:GLN:HG2 | 2.61 | 0.41 |
| 1:C:1013:THR:O | 1:C:1016:VAL:HG12 | 2.20 | 0.41 |
| 1:C:1722:TYR:CD1 | 1:C:1724:GLU:HB2 | 2.56 | 0.41 |
| 1:C:1869:MET:HA | 1:C:1875:ALA:HA | 2.03 | 0.41 |
| 1:C:2110:ALA:HB1 | 1:C:2172:HIS:HB3 | 2.03 | 0.41 |
| 1:C:2603:TRP:H | 1:C:2711:ASN:ND2 | 2.18 | 0.41 |
| 1:D:441:THR:HB | 1:D:444:GLU:OE1 | 2.21 | 0.41 |
| 1:D:592:LEU:HD11 | 1:D:737:PHE:CE1 | 2.55 | 0.41 |
| 1:D:625:LEU:HD11 | 1:D:637:PHE:HD1 | 1.85 | 0.41 |
| 1:D:1910:ASN:OD1 | 1:D:1911:CYS:N | 2.54 | 0.41 |
| 1:D:2379:GLU:OE2 | 1:D:2380:LEU:HD12 | 2.21 | 0.41 |
| 1:D:2784:LEU:HD12 | 1:D:2788:GLN:HB3 | 2.01 | 0.41 |
| 1:D:3334:ARG:NH1 | 1:D:3408:ASP:HA | 2.35 | 0.41 |
| 1:E:1365:ALA:HA | 1:E:1381:PHE:CE2 | 2.56 | 0.41 |
| 1:E:2373:GLY:O | 1:E:2375:LEU:HG | 2.21 | 0.41 |
| 1:E:2415:GLU:CD | 1:E:2466:PRO:HA | 2.46 | 0.41 |
| 1:E:2449:THR:HA | 1:E:2452:GLU:CD | 2.46 | 0.41 |
| 1:E:2752:ASN:OD1 | 1:E:2753:PRO:HD2 | 2.20 | 0.41 |
| 1:E:2938:ARG:NH1 | 1:E:3030:ASN:HA | 2.35 | 0.41 |
| 1:F:307:GLU:OE1 | 1:F:413:ALA:HA | 2.20 | 0.41 |
| 1:F:752:ILE:HD12 | 1:F:767:LYS:HG2 | 2.02 | 0.41 |
| 1:F:788:GLU:O | 1:F:789:ILE:HD13 | 2.21 | 0.41 |
| 1:F:825:HIS:CD2 | 1:F:825:HIS:H | 2.38 | 0.41 |
| 1:F:1085:ARG:HD3 | 1:F:1110:PHE:CE2 | 2.55 | 0.41 |
| 1:F:1267:ASN:HB3 | 1:F:1348:TYR:CE1 | 2.56 | 0.41 |
| 1:F:1405:TYR:CD2 | 1:F:1406:LEU:HD22 | 2.56 | 0.41 |
| 1:F:1956:ASP:CG | 1:F:1957:THR:HG23 | 2.46 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:F:2028:ARG:CZ | 1:F:2028:ARG:HB2 | 2.50 | 0.41 |
| 1:F:2530:LYS:HA | 1:F:2533:ARG:NH1 | 2.35 | 0.41 |
| 1:F:2780:ASN:OD1 | 1:F:2780:ASN:N | 2.51 | 0.41 |
| 1:F:2817:VAL:O | 1:F:2833:THR:OG1 | 2.26 | 0.41 |
| 1:F:2953:TYR:CE1 | 1:F:2995:PHE:HE1 | 2.38 | 0.41 |
| 1:F:3127:GLN:O | 1:F:3130:GLN:HG3 | 2.19 | 0.41 |
| 1:F:3266:VAL:HG11 | 1:F:3283:PHE:HZ | 1.86 | 0.41 |
| 1:G:1010:ASP:OD1 | 1:G:1013:THR:OG1 | 2.33 | 0.41 |
| 1:G:1061:ALA:HA | 1:G:1064:GLN:NE2 | 2.36 | 0.41 |
| 1:G:1588:HIS:HD1 | 1:J:337:GLN:CD | 2.28 | 0.41 |
| 1:G:1756:ARG:NH1 | 1:H:2175:THR:HB | 2.33 | 0.41 |
| 1:G:2056:ARG:HH22 | 1:G:2060:GLY:HA2 | 1.85 | 0.41 |
| 1:G:2297:THR:O | 1:G:2300:THR:OG1 | 2.32 | 0.41 |
| 1:G:2330:MET:HE1 | 1:G:2354:PRO:HG2 | 2.02 | 0.41 |
| 1:G:2392:ARG:HE | 1:G:2447:THR:HG21 | 1.85 | 0.41 |
| 1:G:2517:ILE:HD11 | 1:G:2601:TRP:CD1 | 2.54 | 0.41 |
| 1:G:2533:ARG:HE | 1:G:2621:PRO:HB3 | 1.86 | 0.41 |
| 1:H:11:LEU:HD11 | 1:H:92:PRO:HG3 | 2.02 | 0.41 |
| 1:H:306:ARG:C | 1:H:411:ARG:HH21 | 2.28 | 0.41 |
| 1:H:328:VAL:HG22 | 1:H:386:VAL:HG22 | 2.03 | 0.41 |
| 1:H:695:ARG:O | 1:H:697:THR:N | 2.53 | 0.41 |
| 1:H:695:ARG:HE | 1:H:696:PRO:HD2 | 1.86 | 0.41 |
| 1:H:744:ASN:HB3 | 1:H:779:TRP:CD1 | 2.56 | 0.41 |
| 1:H:801:ASP:OD1 | 1:H:801:ASP:N | 2.47 | 0.41 |
| 1:H:1095:SER:HA | 1:H:1104:ARG:HD3 | 2.02 | 0.41 |
| 1:H:1135:GLN:O | 1:H:1139:GLU:OE1 | 2.39 | 0.41 |
| 1:H:1775:LEU:HD11 | 1:H:1779:PHE:CE1 | 2.55 | 0.41 |
| 1:H:1878:ASP:OD2 | 1:H:1880:ILE:HB | 2.20 | 0.41 |
| 1:H:2191:PRO:HG2 | 1:H:2194:PHE:CE2 | 2.56 | 0.41 |
| 1:I:9:ASP:C | 1:I:10:LEU:HD12 | 2.45 | 0.41 |
| 1:I:182:GLU:O | 1:I:186:ASN:ND2 | 2.53 | 0.41 |
| 1:I:409:VAL:HG22 | 1:I:666:CYS:HA | 2.03 | 0.41 |
| 1:I:1260:ALA:HB3 | 1:I:1529:HIS:HD2 | 1.85 | 0.41 |
| 1:I:2150:GLY:H | 1:I:2265:GLU:CD | 2.27 | 0.41 |
| 1:I:2464:ASP:O | 1:J:1085:ARG:NH1 | 2.53 | 0.41 |
| 1:I:2714:ARG:HB2 | 1:I:2776:TYR:CE1 | 2.56 | 0.41 |
| 1:I:3272:LYS:HE3 | 1:I:3272:LYS:HB3 | 1.92 | 0.41 |
| 1:J:11:LEU:HD21 | 1:J:92:PRO:HB3 | 2.01 | 0.41 |
| 1:J:96:TRP:CZ3 | 1:J:218:ASN:HB3 | 2.55 | 0.41 |
| 1:J:552:ASN:HD21 | 1:J:554:PHE:HB2 | 1.84 | 0.41 |
| 1:J:655:GLN:HG2 | 1:J:662:TYR:HB3 | 2.02 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:J:735:ARG:HH12 | 1:J:788:GLU:HG2 | 1.85 | 0.41 |
| 1:J:1283:LEU:HA | 1:J:1286:MET:HG3 | 2.01 | 0.41 |
| 1:J:1710:LEU:HD22 | 1:J:1750:PHE:CE1 | 2.55 | 0.41 |
| 1:J:2278:HIS:N | 1:J:2279:GLN:OE1 | 2.53 | 0.41 |
| 1:J:2617:LYS:HE2 | 1:J:2617:LYS:HB2 | 1.85 | 0.41 |
| 1:J:2919:LYS:HB3 | 1:J:2920:ASP:H | 1.60 | 0.41 |
| 1:K:47:MET:SD | 1:K:47:MET:N | 2.94 | 0.41 |
| 1:K:998:ILE:HD12 | 1:K:998:ILE:H | 1.86 | 0.41 |
| 1:K:1013:THR:O | 1:K:1016:VAL:HG12 | 2.21 | 0.41 |
| 1:K:1133:ILE:HB | 1:K:1134:PRO:HD3 | 2.02 | 0.41 |
| 1:K:1159:ARG:HA | 1:K:1186:ASP:O | 2.21 | 0.41 |
| 1:K:1776:PRO:HD2 | 1:K:1779:PHE:CZ | 2.55 | 0.41 |
| 1:K:1980:ARG:HE | 1:K:1982:PHE:HZ | 1.69 | 0.41 |
| 1:K:2410:PHE:O | 1:K:2422:ALA:HB3 | 2.20 | 0.41 |
| 1:K:3325:LYS:HA | 1:K:3325:LYS:HD2 | 1.84 | 0.41 |
| 1:L:195:ARG:HB2 | 1:S:2200:TYR:CZ | 2.56 | 0.41 |
| 1:L:782:ASP:C | 1:L:783:ARG:HD2 | 2.45 | 0.41 |
| 1:L:806:VAL:HG11 | 1:L:825:HIS:O | 2.20 | 0.41 |
| 1:L:1036:SER:O | 1:L:1042:TYR:HB2 | 2.20 | 0.41 |
| 1:L:1165:THR:O | 1:L:1222:SER:N | 2.51 | 0.41 |
| 1:L:1322:PHE:HB3 | 1:L:1323:PRO:HD3 | 2.02 | 0.41 |
| 1:L:1690:SER:O | 1:L:1693:LEU:HG | 2.21 | 0.41 |
| 1:L:2149:HIS:CD2 | 1:L:2154:PHE:HE2 | 2.38 | 0.41 |
| 1:L:2709:HIS:O | 1:L:2712:VAL:HG22 | 2.20 | 0.41 |
| 1:L:2786:ILE:H | 1:L:2786:ILE:HD12 | 1.85 | 0.41 |
| 1:L:3043:GLN:N | 1:L:3043:GLN:OE1 | 2.53 | 0.41 |
| 1:M:75:VAL:O | 1:M:78:GLU:HG3 | 2.19 | 0.41 |
| 1:M:88:ASP:OD1 | 1:M:89:ILE:N | 2.52 | 0.41 |
| 1:M:158:ASN:HB2 | 1:M:162:PHE:CD2 | 2.55 | 0.41 |
| 1:M:326:ILE:O | 1:M:345:ALA:HB3 | 2.20 | 0.41 |
| 1:M:383:ASP:HB3 | 1:M:672:HIS:CE1 | 2.55 | 0.41 |
| 1:M:2956:ILE:HD12 | 1:M:2959:PHE:CE2 | 2.54 | 0.41 |
| 1:N:755:ILE:HD11 | 1:N:804:TYR:HB2 | 2.02 | 0.41 |
| 1:N:959:GLU:OE2 | 1:N:960:THR:HG23 | 2.20 | 0.41 |
| 1:N:1007:GLU:OE1 | 1:N:1007:GLU:N | 2.53 | 0.41 |
| 1:N:1324:HIS:HE1 | 1:N:1520:PHE:CZ | 2.38 | 0.41 |
| 1:N:1766:TRP:CD1 | 1:N:1766:TRP:C | 2.97 | 0.41 |
| 1:N:2168:ALA:HA | 1:N:2171:LYS:HG2 | 2.02 | 0.41 |
| 1:N:2182:ASP:OD1 | 1:N:2184:THR:OG1 | 2.35 | 0.41 |
| 1:N:2511:ILE:HD12 | 1:N:2773:ASN:HB2 | 2.02 | 0.41 |
| 1:N:2553:TYR:HA | 1:N:2554:PRO:HA | 1.81 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:N:2874:VAL:O | 1:N:2886:SER:OG | 2.39 | 0.41 |
| 1:O:958:PRO:HA | 1:O:961:ASN:HA | 2.02 | 0.41 |
| 1:O:1619:ARG:HD2 | 1:P:2775:GLN:HE21 | 1.86 | 0.41 |
| 1:O:2157:TRP:HZ3 | 1:O:2158:HIS:CE1 | 2.39 | 0.41 |
| 1:O:2387:HIS:O | 1:O:2392:ARG:NH1 | 2.50 | 0.41 |
| 1:O:2940:ALA:HA | 1:O:3002:LYS:HE2 | 2.02 | 0.41 |
| 1:O:3089:ASN:HD21 | 1:O:3247:ILE:HD12 | 1.85 | 0.41 |
| 1:P:122:LYS:HE3 | 1:P:122:LYS:HB3 | 1.89 | 0.41 |
| 1:P:562:LEU:HD23 | 1:P:562:LEU:HA | 1.91 | 0.41 |
| 1:P:860:GLN:NE2 | 1:P:864:GLU:OE2 | 2.54 | 0.41 |
| 1:P:1283:LEU:HD23 | 1:P:1284:ARG:HH12 | 1.85 | 0.41 |
| 1:P:1679:SER:OG | 1:P:1680:VAL:N | 2.54 | 0.41 |
| 1:P:2397:PHE:HD2 | 1:P:2425:ILE:HD13 | 1.86 | 0.41 |
| 1:P:2668:CYS:SG | 1:P:2849:ARG:NH2 | 2.93 | 0.41 |
| 1:P:3163:ASN:O | 1:P:3169:ARG:NH2 | 2.54 | 0.41 |
| 1:Q:639:LEU:O | 1:Q:642:SER:OG | 2.29 | 0.41 |
| 1:Q:767:LYS:HD3 | 1:Q:768:LEU:N | 2.35 | 0.41 |
| 1:Q:1133:ILE:HB | 1:Q:1134:PRO:HD3 | 2.02 | 0.41 |
| 1:Q:2085:GLN:HE21 | 1:Q:2366:ARG:NE | 2.19 | 0.41 |
| 1:Q:2096:ILE:HG12 | 1:Q:2180:TYR:O | 2.20 | 0.41 |
| 1:Q:2218:LYS:HE2 | 1:Q:2218:LYS:HB2 | 1.88 | 0.41 |
| 1:Q:2821:LEU:HB3 | 1:Q:2872:PHE:CE1 | 2.56 | 0.41 |
| 1:Q:3089:ASN:HD21 | 1:Q:3247:ILE:HA | 1.85 | 0.41 |
| 1:R:378:LYS:HE2 | 1:R:382:GLY:HA3 | 2.03 | 0.41 |
| 1:R:845:LEU:HB3 | 1:R:926:ARG:NH1 | 2.34 | 0.41 |
| 1:R:970:HIS:CG | 1:R:977:LYS:HB3 | 2.56 | 0.41 |
| 1:R:994:ARG:HE | 1:R:995:LEU:N | 2.05 | 0.41 |
| 1:R:1229:LYS:HB3 | 1:R:1229:LYS:HE3 | 1.83 | 0.41 |
| 1:R:1325:TRP:HD1 | 1:R:1326:HIS:ND1 | 2.18 | 0.41 |
| 1:R:1364:GLU:O | 1:R:1378:ASN:ND2 | 2.33 | 0.41 |
| 1:R:1385:ILE:HG23 | 1:R:1453:PHE:CE2 | 2.56 | 0.41 |
| 1:R:1917:ARG:O | 1:R:1940:LYS:NZ | 2.47 | 0.41 |
| 1:S:288:LEU:HD23 | 1:S:289:ASN:OD1 | 2.21 | 0.41 |
| 1:S:718:MET:HE1 | 1:S:723:LEU:HG | 2.02 | 0.41 |
| 1:S:889:ASN:HB3 | 1:S:900:PHE:O | 2.21 | 0.41 |
| 1:S:1349:TRP:CE2 | 1:S:1359:PRO:HG3 | 2.55 | 0.41 |
| 1:S:2108:LYS:HA | 1:S:2111:LEU:HG | 2.03 | 0.41 |
| 1:S:2746:PRO:O | 1:S:2749:TRP:HB2 | 2.21 | 0.41 |
| 1:S:2960:HIS:HE1 | 1:S:3119:HIS:HE1 | 1.69 | 0.41 |
| 1:S:3334:ARG:NH2 | 1:S:3406:ILE:HA | 2.35 | 0.41 |
| 1:S:3340:PHE:CE2 | 1:S:3351:VAL:HG11 | 2.44 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:T:160:GLN:O | 1:T:164:MET:HG3 | 2.20 | 0.41 |
| 1:T:273:LEU:HD23 | 1:T:278:GLN:HE21 | 1.86 | 0.41 |
| 1:T:845:LEU:HD21 | 1:T:932:ASP:HA | 2.00 | 0.41 |
| 1:T:1166:LEU:HB3 | 1:T:1179:GLY:O | 2.20 | 0.41 |
| 1:T:3234:PRO:HG2 | 1:T:3237:GLY:HA3 | 2.03 | 0.41 |
| 1:A:304:ARG:HG2 | 1:A:304:ARG:HH11 | 1.85 | 0.41 |
| 1:A:580:TYR:OH | 1:A:860:GLN:OE1 | 2.30 | 0.41 |
| 1:A:1518:ASP:OD1 | 1:A:1525:HIS:ND1 | 2.47 | 0.41 |
| 1:A:2053:VAL:HG11 | 1:A:2068:ILE:HG21 | 2.02 | 0.41 |
| 1:A:2286:LEU:HA | 1:A:2289:SER:HB2 | 2.03 | 0.41 |
| 1:A:2308:VAL:O | 1:A:2311:GLU:HG3 | 2.20 | 0.41 |
| 1:A:2654:PHE:HA | 1:A:2657:GLN:HG2 | 2.03 | 0.41 |
| 1:A:2679:ASN:HD21 | 1:A:2836:VAL:C | 2.29 | 0.41 |
| 1:A:3043:GLN:HG3 | 1:A:3044:VAL:H | 1.85 | 0.41 |
| 1:A:3044:VAL:HG13 | 1:A:3102:SER:HA | 2.02 | 0.41 |
| 1:B:210:PRO:HA | 1:B:213:PHE:HD2 | 1.84 | 0.41 |
| 1:B:337:GLN:N | 1:B:337:GLN:OE1 | 2.54 | 0.41 |
| 1:B:598:ASP:OD1 | 1:B:599:PHE:N | 2.53 | 0.41 |
| 1:B:991:LYS:HD2 | 1:B:992:PHE:N | 2.35 | 0.41 |
| 1:B:1056:THR:HA | 1:B:1059:ILE:HD12 | 2.02 | 0.41 |
| 1:B:1280:LYS:O | 1:B:1284:ARG:HG2 | 2.21 | 0.41 |
| 1:B:1641:ASN:HD22 | 3:a:1:NAG:H83 | 1.85 | 0.41 |
| 1:B:1898:LEU:O | 1:B:1901:LEU:HG | 2.21 | 0.41 |
| 1:B:2038:LEU:HD12 | 1:B:2039:GLU:N | 2.35 | 0.41 |
| 1:B:2259:ASP:HA | 1:B:2262:VAL:HG12 | 2.03 | 0.41 |
| 1:B:3124:ARG:HG2 | 1:B:3124:ARG:HH11 | 1.85 | 0.41 |
| 1:C:222:ILE:O | 1:C:225:ILE:HG22 | 2.21 | 0.41 |
| 1:C:1158:ILE:HD12 | 1:C:1158:ILE:HA | 1.91 | 0.41 |
| 1:C:1221:TYR:CE2 | 1:C:1236:PHE:HB2 | 2.56 | 0.41 |
| 1:C:1305:CYS:SG | 1:C:1306:THR:N | 2.94 | 0.41 |
| 1:C:2297:THR:O | 1:C:2300:THR:OG1 | 2.34 | 0.41 |
| 1:C:2529:LYS:HE3 | 1:C:2620:ASN:OD1 | 2.21 | 0.41 |
| 1:D:17:LEU:HA | 1:D:20:GLU:HG2 | 2.03 | 0.41 |
| 1:D:614:HIS:CD2 | 1:D:614:HIS:H | 2.39 | 0.41 |
| 1:D:695:ARG:NH2 | 1:D:696:PRO:HD2 | 2.36 | 0.41 |
| 1:D:1554:ASP:OD1 | 1:D:1554:ASP:N | 2.53 | 0.41 |
| 1:D:1802:ILE:HG22 | 1:D:1877:TYR:CG | 2.55 | 0.41 |
| 1:D:2511:ILE:HD12 | 1:D:2773:ASN:HB2 | 2.02 | 0.41 |
| 1:D:2712:VAL:HA | 1:D:2715:GLN:NE2 | 2.36 | 0.41 |
| 1:D:3106:LEU:HA | 1:D:3109:SER:HB3 | 2.02 | 0.41 |
| 1:D:3254:MET:O | 1:D:3256:TRP:HD1 | 2.04 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:E:197:ASP:OD1 | 1:E:197:ASP:N | 2.53 | 0.41 |
| 1:E:637:PHE:CZ | 1:E:641:HIS:HE1 | 2.39 | 0.41 |
| 1:E:1133:ILE:HD12 | 1:E:1133:ILE:H | 1.84 | 0.41 |
| 1:E:2051:VAL:HB | 1:E:2071:PRO:HG2 | 2.01 | 0.41 |
| 1:E:2100:ASP:O | 1:E:2104:THR:HG23 | 2.21 | 0.41 |
| 1:E:2342:LEU:HA | 1:E:2342:LEU:HD23 | 1.86 | 0.41 |
| 1:F:434:ARG:HB2 | 1:F:710:TYR:CD1 | 2.56 | 0.41 |
| 1:F:914:HIS:O | 1:F:918:THR:HG23 | 2.20 | 0.41 |
| 1:F:3147:LEU:HD23 | 1:F:3150:LEU:HD12 | 2.02 | 0.41 |
| 1:G:408:GLY:N | 1:G:669:THR:OG1 | 2.53 | 0.41 |
| 1:G:613:PRO:HA | 1:G:616:LEU:HB3 | 2.01 | 0.41 |
| 1:G:773:GLY:O | 1:G:776:GLU:HG2 | 2.21 | 0.41 |
| 1:G:949:ILE:HG23 | 1:G:950:VAL:HG13 | 2.01 | 0.41 |
| 1:G:1184:LEU:HD23 | 1:G:1184:LEU:HA | 1.90 | 0.41 |
| 1:G:1378:ASN:ND2 | 1:G:1380:PHE:HB2 | 2.35 | 0.41 |
| 1:G:1397:GLN:HB2 | 1:G:1436:LEU:O | 2.21 | 0.41 |
| 1:G:2245:PHE:HA | 1:G:2248:VAL:HG12 | 2.03 | 0.41 |
| 1:G:2308:VAL:O | 1:G:2311:GLU:HG3 | 2.20 | 0.41 |
| 1:G:2345:ASN:ND2 | 1:G:2348:THR:HG23 | 2.36 | 0.41 |
| 1:G:2368:ASP:N | 1:G:2368:ASP:OD1 | 2.54 | 0.41 |
| 1:G:2679:ASN:HD21 | 1:G:2836:VAL:CA | 2.33 | 0.41 |
| 1:G:2729:ASP:OD1 | 1:G:2729:ASP:N | 2.47 | 0.41 |
| 1:H:1356:ARG:HH12 | 1:H:1402:ASN:ND2 | 2.18 | 0.41 |
| 1:H:1872:LEU:HD23 | 1:H:1872:LEU:HA | 1.95 | 0.41 |
| 1:H:2359:ASN:OD1 | 1:H:2359:ASN:N | 2.53 | 0.41 |
| 1:H:2378:ASP:O | 1:H:2381:GLU:HG2 | 2.21 | 0.41 |
| 1:I:148:ARG:HB2 | 1:I:151:GLN:HE22 | 1.86 | 0.41 |
| 1:I:648:TRP:NE1 | 1:I:652:GLN:HE22 | 2.18 | 0.41 |
| 1:I:995:LEU:HB3 | 1:I:999:ALA:HB3 | 2.03 | 0.41 |
| 1:I:1159:ARG:NE | 1:I:1186:ASP:O | 2.52 | 0.41 |
| 1:I:1162:ALA:HB1 | 1:I:1224:ILE:O | 2.20 | 0.41 |
| 1:I:1231:ILE:H | 1:I:1231:ILE:HD12 | 1.86 | 0.41 |
| 1:I:1284:ARG:NH2 | 1:I:1377:SER:O | 2.52 | 0.41 |
| 1:I:1328:LEU:HD21 | 1:I:1519:VAL:HG22 | 2.01 | 0.41 |
| 1:I:1749:GLN:HE22 | 1:I:1932:ASP:HB3 | 1.86 | 0.41 |
| 1:I:2569:HIS:HA | 1:I:2574:PHE:CE2 | 2.56 | 0.41 |
| 1:J:47:MET:HG3 | 1:J:55:ARG:HH21 | 1.86 | 0.41 |
| 1:J:178:GLU:O | 1:J:182:GLU:HG2 | 2.20 | 0.41 |
| 1:J:676:LYS:HD3 | 1:J:680:PHE:CE2 | 2.56 | 0.41 |
| 1:J:811:LYS:HD2 | 1:J:815:GLY:HA2 | 2.03 | 0.41 |
| 1:J:1303:SER:OG | 1:J:1311:LYS:O | 2.31 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:J:2141:ALA:HB3 | 1:J:2143:LYS:HZ2 | 1.85 | 0.41 |
| 1:J:2511:ILE:HD12 | 1:J:2773:ASN:HB2 | 2.02 | 0.41 |
| 1:J:3395:ARG:NE | 1:J:3398:GLN:OE1 | 2.54 | 0.41 |
| 1:K:704:HIS:HB3 | 1:K:705:GLU:OE1 | 2.21 | 0.41 |
| 1:K:1624:LYS:HD3 | 1:K:1624:LYS:HA | 1.90 | 0.41 |
| 1:K:2108:LYS:O | 1:K:2112:ARG:NH1 | 2.54 | 0.41 |
| 1:K:2679:ASN:HD21 | 1:K:2836:VAL:C | 2.28 | 0.41 |
| 1:K:3036:GLN:HB2 | 1:K:3043:GLN:HE22 | 1.84 | 0.41 |
| 1:K:3338:VAL:HG11 | 1:K:3381:LEU:HG | 2.03 | 0.41 |
| 1:K:3373:TYR:HB3 | 1:K:3379:TYR:CE2 | 2.55 | 0.41 |
| 1:L:703:GLU:OE1 | 1:L:703:GLU:N | 2.54 | 0.41 |
| 1:L:1116:GLU:O | 1:L:1120:GLN:HB3 | 2.21 | 0.41 |
| 1:L:1132:SER:O | 1:L:1135:GLN:HB3 | 2.21 | 0.41 |
| 1:L:1542:GLN:HA | 1:L:1545:GLU:CD | 2.46 | 0.41 |
| 1:L:1706:GLY:O | 1:L:1710:LEU:HG | 2.21 | 0.41 |
| 1:L:1884:HIS:O | 1:L:1888:THR:HG23 | 2.20 | 0.41 |
| 1:L:1902:ARG:HB3 | 1:L:1904:HIS:HE1 | 1.86 | 0.41 |
| 1:L:2656:ARG:O | 1:L:2659:LEU:HG | 2.20 | 0.41 |
| 1:M:583:HIS:HB3 | 1:M:587:PHE:HD2 | 1.86 | 0.41 |
| 1:M:1349:TRP:NE1 | 1:M:1359:PRO:HG3 | 2.36 | 0.41 |
| 1:M:1999:LYS:HG2 | 1:M:2001:CYS:SG | 2.61 | 0.41 |
| 1:M:2624:HIS:HB2 | 1:M:2633:LYS:NZ | 2.36 | 0.41 |
| 1:M:2986:HIS:HB3 | 1:M:3177:ILE:HD13 | 2.02 | 0.41 |
| 1:M:3337:ARG:NH2 | 1:M:3380:SER:HB2 | 2.36 | 0.41 |
| 1:N:5:ARG:HH22 | 1:N:281:TYR:HB2 | 1.84 | 0.41 |
| 1:N:169:LEU:HA | 1:N:177:PHE:HE1 | 1.85 | 0.41 |
| 1:N:253:PRO:O | 1:N:256:ARG:HG2 | 2.21 | 0.41 |
| 1:N:1276:VAL:O | 1:N:1279:LEU:HG | 2.20 | 0.41 |
| 1:N:1878:ASP:OD2 | 1:N:1880:ILE:HB | 2.20 | 0.41 |
| 1:N:2251:VAL:HG21 | 1:N:2267:THR:HG21 | 2.02 | 0.41 |
| 1:N:2269:ASN:HD21 | 1:N:2428:LEU:HB2 | 1.85 | 0.41 |
| 1:O:757:PRO:HB3 | 1:O:798:LEU:HD11 | 2.02 | 0.41 |
| 1:O:850:ASP:O | 1:O:853:SER:OG | 2.37 | 0.41 |
| 1:O:1158:ILE:HD12 | 1:O:1158:ILE:HA | 1.91 | 0.41 |
| 1:O:1448:LEU:HB3 | 1:O:1596:LEU:HD21 | 2.03 | 0.41 |
| 1:O:1827:ASP:HA | 1:O:1831:TRP:CZ3 | 2.55 | 0.41 |
| 1:O:1857:ILE:HD12 | 1:O:1857:ILE:HA | 1.88 | 0.41 |
| 1:O:1858:HIS:HA | 1:O:1869:MET:HE1 | 2.01 | 0.41 |
| 1:O:1958:LEU:H | 1:O:1958:LEU:HD12 | 1.85 | 0.41 |
| 1:O:2601:TRP:CZ2 | 1:O:2603:TRP:HB3 | 2.56 | 0.41 |
| 1:O:2773:ASN:CG | 1:O:3141:ASN:HB2 | 2.46 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:O:3211:ASP:OD2 | 1:O:3309:ALA:N | 2.52 | 0.41 |
| 1:P:188:ILE:HD12 | 1:P:188:ILE:HA | 1.86 | 0.41 |
| 1:P:737:PHE:CD2 | 1:P:786:LYS:HD3 | 2.55 | 0.41 |
| 1:P:1299:HIS:ND1 | 1:P:1299:HIS:O | 2.53 | 0.41 |
| 1:P:1624:LYS:HA | 1:P:1624:LYS:HD2 | 1.84 | 0.41 |
| 1:P:2712:VAL:HA | 1:P:2715:GLN:NE2 | 2.36 | 0.41 |
| 1:P:3183:PHE:HB2 | 1:P:3185:TYR:CD1 | 2.56 | 0.41 |
| 1:Q:188:ILE:HD13 | 1:Q:188:ILE:HA | 1.91 | 0.41 |
| 1:Q:913:TRP:HE3 | 1:Q:914:HIS:HD2 | 1.69 | 0.41 |
| 1:Q:1241:VAL:HG12 | 1:R:2328:ASN:ND2 | 2.35 | 0.41 |
| 1:Q:1574:PHE:HB2 | 1:Q:1634:GLU:HB3 | 2.03 | 0.41 |
| 1:Q:1857:ILE:HD12 | 1:Q:1857:ILE:HA | 1.91 | 0.41 |
| 1:Q:2392:ARG:HE | 1:Q:2447:THR:HG21 | 1.85 | 0.41 |
| 1:Q:2676:VAL:HG11 | 1:Q:2851:PHE:CZ | 2.55 | 0.41 |
| 1:Q:2963:PRO:HG3 | 1:Q:3039:PHE:CG | 2.55 | 0.41 |
| 1:Q:3395:ARG:HD3 | 1:Q:3400:THR:HB | 2.02 | 0.41 |
| 1:R:1283:LEU:HD12 | 1:R:1286:MET:SD | 2.60 | 0.41 |
| 1:R:1557:PHE:CD2 | 1:R:1611:LYS:HD3 | 2.55 | 0.41 |
| 1:R:1743:HIS:O | 1:R:1747:THR:HG23 | 2.20 | 0.41 |
| 1:R:1802:ILE:HG22 | 1:R:1877:TYR:CG | 2.55 | 0.41 |
| 1:R:1852:ILE:HD12 | 1:R:1852:ILE:HA | 1.95 | 0.41 |
| 1:R:1880:ILE:H | 1:R:1880:ILE:HD12 | 1.84 | 0.41 |
| 1:R:2645:ASP:HB3 | 1:R:2649:GLY:O | 2.20 | 0.41 |
| 1:R:2674:TYR:CZ | 1:R:2712:VAL:HG22 | 2.56 | 0.41 |
| 1:R:3114:PHE:CE1 | 1:R:3118:HIS:HB2 | 2.56 | 0.41 |
| 1:S:1013:THR:O | 1:S:1016:VAL:HG12 | 2.20 | 0.41 |
| 1:S:1811:ARG:NH2 | 1:S:1880:ILE:HB | 2.35 | 0.41 |
| 1:S:2130:HIS:HB3 | 1:S:2290:SER:HB3 | 2.02 | 0.41 |
| 1:S:2219:GLU:OE1 | 1:S:2219:GLU:N | 2.54 | 0.41 |
| 1:S:2298:HIS:O | 1:S:2302:VAL:HG23 | 2.21 | 0.41 |
| 1:S:2315:ARG:HH22 | 1:S:2316:ARG:HG3 | 1.84 | 0.41 |
| 1:S:2340:VAL:HG12 | 1:S:2349:ARG:HD3 | 2.03 | 0.41 |
| 1:T:437:VAL:HG22 | 1:T:521:PRO:HG2 | 2.03 | 0.41 |
| 1:T:610:HIS:O | 1:T:613:PRO:HD2 | 2.20 | 0.41 |
| 1:T:1086:LYS:NZ | 1:T:1089:GLN:HE21 | 2.19 | 0.41 |
| 1:T:2422:ALA:HA | 1:T:2449:THR:HG21 | 2.02 | 0.41 |
| 1:T:2980:GLY:HA3 | 1:T:3256:TRP:CZ3 | 2.56 | 0.41 |
| 1:T:3036:GLN:OE1 | 1:T:3042:HIS:N | 2.54 | 0.41 |
| 1:T:3219:LEU:HB2 | 1:T:3258:TYR:CZ | 2.56 | 0.41 |
| 1:A:4:VAL:HG13 | 1:A:6:LYS:NZ | 2.36 | 0.41 |
| 1:A:204:GLU:OE2 | 1:A:354:ALA:N | 2.48 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:444:GLU:HB3 | 1:A:518:PHE:HZ | 1.84 | 0.41 |
| 1:A:750:LEU:HG | 1:A:768:LEU:O | 2.21 | 0.41 |
| 1:A:1017:GLN:O | 1:A:1020:ILE:HG22 | 2.21 | 0.41 |
| 1:A:1169:CYS:HA | 1:A:1175:CYS:HA | 2.03 | 0.41 |
| 1:A:2229:GLN:HB3 | 1:A:2231:GLU:OE1 | 2.21 | 0.41 |
| 1:A:2407:GLU:HB2 | 1:A:2426:PHE:CE2 | 2.56 | 0.41 |
| 1:A:2623:GLU:OE1 | 1:A:2623:GLU:N | 2.36 | 0.41 |
| 1:A:2977:CYS:HA | 1:A:2987:TRP:CH2 | 2.55 | 0.41 |
| 1:A:3086:MET:HG3 | 1:A:3262:TYR:CD1 | 2.56 | 0.41 |
| 1:B:68:GLN:HA | 1:B:71:ARG:HG2 | 2.02 | 0.41 |
| 1:B:72:LEU:HD22 | 1:B:273:LEU:HD13 | 2.02 | 0.41 |
| 1:B:604:VAL:HG21 | 1:B:783:ARG:HB2 | 2.02 | 0.41 |
| 1:B:847:VAL:HA | 1:B:1122:HIS:O | 2.20 | 0.41 |
| 1:B:1020:ILE:HG13 | 1:B:1021:ALA:N | 2.36 | 0.41 |
| 1:B:2099:LEU:HD11 | 1:B:2179:PRO:HG3 | 2.02 | 0.41 |
| 1:B:2235:LEU:HD12 | 1:B:2239:GLY:HA2 | 2.03 | 0.41 |
| 1:B:2515:LYS:HD2 | 1:B:2777:ASP:HB3 | 2.03 | 0.41 |
| 1:B:2954:GLU:CD | 1:B:2954:GLU:H | 2.29 | 0.41 |
| 1:C:24:ARG:HH12 | 1:C:125:TRP:CD1 | 2.39 | 0.41 |
| 1:C:687:ASN:OD1 | 1:C:688:GLU:N | 2.54 | 0.41 |
| 1:C:744:ASN:OD1 | 1:C:744:ASN:N | 2.53 | 0.41 |
| 1:C:938:ASP:HA | 1:C:1055:ASN:HD21 | 1.85 | 0.41 |
| 1:C:2159:ARG:HD2 | 1:C:2306:TRP:CE3 | 2.56 | 0.41 |
| 1:C:2585:LEU:HD13 | 1:C:2706:PHE:HE2 | 1.84 | 0.41 |
| 1:C:2916:THR:C | 1:C:2918:THR:H | 2.28 | 0.41 |
| 1:C:2977:CYS:SG | 1:C:3106:LEU:HD11 | 2.60 | 0.41 |
| 1:D:59:CYS:C | 1:D:61:HIS:HD1 | 2.28 | 0.41 |
| 1:D:178:GLU:O | 1:D:182:GLU:HG2 | 2.20 | 0.41 |
| 1:D:253:PRO:O | 1:D:256:ARG:HG2 | 2.21 | 0.41 |
| 1:D:757:PRO:HG3 | 1:D:796:LYS:HD2 | 2.03 | 0.41 |
| 1:D:946:LEU:HG | 1:D:951:ALA:HB2 | 2.02 | 0.41 |
| 1:D:1060:TRP:CE2 | 1:D:1064:GLN:NE2 | 2.88 | 0.41 |
| 1:D:1085:ARG:HD3 | 1:D:1110:PHE:CE2 | 2.56 | 0.41 |
| 1:D:1270:ASP:OD1 | 1:D:1270:ASP:C | 2.64 | 0.41 |
| 1:D:1608:ARG:HD3 | 1:D:1608:ARG:HA | 1.83 | 0.41 |
| 1:D:2924:TYR:HD1 | 1:D:3188:ASP:HB3 | 1.85 | 0.41 |
| 1:D:3131:THR:HA | 1:D:3134:LYS:HG2 | 2.03 | 0.41 |
| 1:E:72:LEU:HA | 1:E:75:VAL:HG22 | 2.03 | 0.41 |
| 1:E:425:ASP:OD1 | 1:E:425:ASP:N | 2.44 | 0.41 |
| 1:E:489:CYS:C | 1:E:491:HIS:HD1 | 2.28 | 0.41 |
| 1:E:1095:SER:HB3 | 1:E:1104:ARG:NH2 | 2.36 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:E:1355:ILE:HG13 | 1:E:1355:ILE:O | 2.20 | 0.41 |
| 1:E:1357:GLN:OE1 | 1:E:1357:GLN:N | 2.54 | 0.41 |
| 1:E:2158:HIS:O | 1:E:2162:THR:HG23 | 2.21 | 0.41 |
| 1:E:2995:PHE:O | 1:E:2999:LEU:HD23 | 2.20 | 0.41 |
| 1:F:54:LYS:O | 1:F:56:VAL:HG13 | 2.21 | 0.41 |
| 1:F:461:VAL:HG22 | 1:F:1277:GLU:OE2 | 2.21 | 0.41 |
| 1:F:598:ASP:OD1 | 1:F:599:PHE:N | 2.54 | 0.41 |
| 1:F:737:PHE:O | 1:F:829:ILE:N | 2.38 | 0.41 |
| 1:F:1123:TYR:N | 1:F:1123:TYR:CD1 | 2.89 | 0.41 |
| 1:F:1299:HIS:CD2 | 1:F:1457:PHE:HZ | 2.38 | 0.41 |
| 1:F:1433:LEU:HD11 | 1:F:1460:HIS:CE1 | 2.55 | 0.41 |
| 1:F:1630:ASP:N | 1:F:1630:ASP:OD1 | 2.53 | 0.41 |
| 1:F:1985:PHE:O | 1:F:2029:LEU:HD12 | 2.21 | 0.41 |
| 1:F:2714:ARG:HH21 | 1:F:2779:LEU:HA | 1.85 | 0.41 |
| 1:F:2802:VAL:HG22 | 1:F:2856:THR:HA | 2.03 | 0.41 |
| 1:F:3351:VAL:HG23 | 1:F:3390:SER:HA | 2.02 | 0.41 |
| 1:F:3395:ARG:HA | 1:F:3395:ARG:HD2 | 1.72 | 0.41 |
| 1:G:56:VAL:HG22 | 1:G:57:ALA:H | 1.86 | 0.41 |
| 1:G:471:HIS:O | 1:G:471:HIS:ND1 | 2.53 | 0.41 |
| 1:G:998:ILE:H | 1:G:998:ILE:HD12 | 1.86 | 0.41 |
| 1:G:1061:ALA:HA | 1:G:1064:GLN:CD | 2.46 | 0.41 |
| 1:G:1987:LEU:HD13 | 1:G:2068:ILE:HD11 | 2.01 | 0.41 |
| 1:G:1993:SER:HB2 | 1:G:2017:GLY:H | 1.86 | 0.41 |
| 1:G:2251:VAL:HG21 | 1:G:2267:THR:HG21 | 2.02 | 0.41 |
| 1:G:2627:ILE:O | 1:G:2627:ILE:HG13 | 2.19 | 0.41 |
| 1:G:2665:ARG:HG2 | 1:G:2726:ARG:NH1 | 2.36 | 0.41 |
| 1:G:2814:SER:N | 1:G:2838:GLY:O | 2.54 | 0.41 |
| 1:G:2941:LEU:HA | 1:G:2944:LEU:HG | 2.03 | 0.41 |
| 1:G:2941:LEU:HD13 | 1:G:3032:PHE:CE1 | 2.55 | 0.41 |
| 1:G:3200:ILE:HD12 | 1:G:3200:ILE:H | 1.86 | 0.41 |
| 1:H:670:MET:O | 1:H:670:MET:SD | 2.78 | 0.41 |
| 1:H:743:GLN:HB3 | 1:H:780:ASN:ND2 | 2.36 | 0.41 |
| 1:H:1367:TYR:CE2 | 1:H:1369:ASP:HB3 | 2.55 | 0.41 |
| 1:H:2130:HIS:HD2 | 1:H:2157:TRP:CZ3 | 2.39 | 0.41 |
| 1:H:2312:LEU:O | 1:H:2316:ARG:NH1 | 2.54 | 0.41 |
| 1:H:2741:ARG:NH2 | 1:I:2870:TYR:H | 2.19 | 0.41 |
| 1:H:2994:GLN:HG2 | 1:H:3157:PHE:CZ | 2.56 | 0.41 |
| 1:I:18:SER:O | 1:I:22:TYR:HD1 | 2.02 | 0.41 |
| 1:I:414:LYS:HA | 1:I:414:LYS:HD2 | 1.69 | 0.41 |
| 1:I:1432:ALA:HA | 1:I:1594:SER:OG | 2.20 | 0.41 |
| 1:I:1687:GLU:HA | 1:I:1760:LEU:HD21 | 2.02 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:I:1711:ALA:HA | 1:I:1746:TYR:OH | 2.20 | 0.41 |
| 1:I:2256:ASP:OD2 | 1:I:2258:CYS:HB2 | 2.20 | 0.41 |
| 1:I:2408:VAL:HA | 1:I:2472:GLU:O | 2.21 | 0.41 |
| 1:I:2495:PRO:HB2 | 1:I:2500:ARG:HD2 | 2.02 | 0.41 |
| 1:I:2625:GLY:C | 1:I:2633:LYS:HZ2 | 2.28 | 0.41 |
| 1:I:2801:ARG:HD3 | 1:I:2803:PHE:HZ | 1.84 | 0.41 |
| 1:I:2923:ARG:HD3 | 1:I:3187:PHE:CE1 | 2.56 | 0.41 |
| 1:I:3122:ILE:HA | 1:I:3125:ILE:HG22 | 2.02 | 0.41 |
| 1:J:812:ASP:OD1 | 1:J:812:ASP:N | 2.54 | 0.41 |
| 1:J:896:ALA:HB1 | 1:J:899:LYS:HB2 | 2.03 | 0.41 |
| 1:J:1098:ASN:HB2 | 1:J:1104:ARG:HH11 | 1.86 | 0.41 |
| 1:J:1221:TYR:HE1 | 1:J:1238:LYS:HA | 1.85 | 0.41 |
| 1:J:2051:VAL:HG21 | 1:J:2071:PRO:HG2 | 2.03 | 0.41 |
| 1:J:2345:ASN:O | 1:J:2349:ARG:HG2 | 2.20 | 0.41 |
| 1:J:2369:ASP:N | 1:J:2369:ASP:OD1 | 2.54 | 0.41 |
| 1:J:2379:GLU:OE2 | 1:J:2380:LEU:HD12 | 2.21 | 0.41 |
| 1:K:881:ILE:HD12 | 1:K:884:PHE:CE2 | 2.56 | 0.41 |
| 1:K:2301:PHE:O | 1:K:2305:ILE:HG12 | 2.21 | 0.41 |
| 1:K:2773:ASN:CG | 1:K:3141:ASN:HB2 | 2.45 | 0.41 |
| 1:K:3352:LYS:HD3 | 1:K:3366:PRO:HD2 | 2.03 | 0.41 |
| 1:L:69:TRP:CD1 | 1:L:251:LEU:HD22 | 2.56 | 0.41 |
| 1:L:267:TYR:HB3 | 1:L:273:LEU:HD21 | 2.03 | 0.41 |
| 1:L:469:GLU:OE1 | 1:L:469:GLU:N | 2.48 | 0.41 |
| 1:L:1023:ASN:ND2 | 1:L:1184:LEU:HB2 | 2.36 | 0.41 |
| 1:L:1140:ILE:HD13 | 1:L:1140:ILE:HA | 1.96 | 0.41 |
| 1:L:2159:ARG:O | 1:L:2162:THR:OG1 | 2.33 | 0.41 |
| 1:L:2839:GLY:O | 1:L:2842:GLU:HG2 | 2.21 | 0.41 |
| 1:L:3062:ASP:HB3 | 1:L:3065:PHE:HB3 | 2.03 | 0.41 |
| 1:M:69:TRP:HZ3 | 1:M:70:HIS:CE1 | 2.38 | 0.41 |
| 1:M:502:LEU:O | 1:M:505:VAL:HG12 | 2.21 | 0.41 |
| 1:M:1364:GLU:HA | 1:M:1364:GLU:OE2 | 2.21 | 0.41 |
| 1:M:2159:ARG:HD2 | 1:M:2306:TRP:CE3 | 2.56 | 0.41 |
| 1:M:2398:LEU:HB2 | 1:M:2441:LEU:HD22 | 2.02 | 0.41 |
| 1:M:2755:ASP:OD1 | 1:M:2756:PHE:N | 2.49 | 0.41 |
| 1:M:3149:ASN:HA | 1:M:3152:ARG:HH12 | 1.86 | 0.41 |
| 1:N:1437:VAL:HG23 | 1:N:1445:LEU:HD12 | 2.02 | 0.41 |
| 1:N:1497:LYS:HE3 | 1:N:1497:LYS:HB3 | 1.79 | 0.41 |
| 1:N:1539:THR:OG1 | 1:N:1540:ILE:N | 2.54 | 0.41 |
| 1:N:2890:GLU:HG2 | 1:O:2846:HIS:CE1 | 2.56 | 0.41 |
| 1:N:3020:LEU:HD13 | 1:N:3024:LEU:HB2 | 2.02 | 0.41 |
| 1:O:50:LYS:HD3 | 1:O:54:LYS:HG3 | 2.02 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:O:231:LYS:HE3 | 1:O:237:TYR:CE1 | 2.56 | 0.41 |
| 1:O:327:LYS:HE2 | 1:O:342:CYS:SG | 2.61 | 0.41 |
| 1:O:2052:LYS:HD2 | 1:O:2052:LYS:HA | 1.68 | 0.41 |
| 1:O:3114:PHE:HD1 | 1:O:3117:ILE:HD11 | 1.85 | 0.41 |
| 1:O:3133:GLN:NE2 | 1:O:3138:ARG:O | 2.53 | 0.41 |
| 1:O:3325:LYS:HD2 | 1:O:3325:LYS:HA | 1.85 | 0.41 |
| 1:P:749:ALA:HB3 | 1:P:770:VAL:HG12 | 2.01 | 0.41 |
| 1:P:1147:GLU:OE1 | 1:P:1245:PRO:HA | 2.20 | 0.41 |
| 1:P:1273:GLU:CD | 1:P:1273:GLU:H | 2.29 | 0.41 |
| 1:P:2552:GLY:O | 1:P:2555:GLY:N | 2.53 | 0.41 |
| 1:P:2616:ASP:OD1 | 1:P:2617:LYS:N | 2.54 | 0.41 |
| 1:P:2754:ASN:ND2 | 1:P:2757:ILE:HG12 | 2.35 | 0.41 |
| 1:P:2800:ASP:OD1 | 1:P:2899:GLY:N | 2.54 | 0.41 |
| 1:P:2803:PHE:CD1 | 1:P:2852:GLN:HB3 | 2.56 | 0.41 |
| 1:P:2821:LEU:HB2 | 1:P:2872:PHE:CE1 | 2.56 | 0.41 |
| 1:P:2943:LYS:HB3 | 1:P:3002:LYS:HD2 | 2.02 | 0.41 |
| 1:P:2953:TYR:HA | 1:P:2956:ILE:HG12 | 2.03 | 0.41 |
| 1:P:3138:ARG:HA | 1:P:3138:ARG:HD3 | 1.80 | 0.41 |
| 1:Q:436:ASP:HB3 | 1:Q:522:TYR:CE2 | 2.56 | 0.41 |
| 1:Q:855:THR:OG1 | 1:Q:856:ARG:N | 2.54 | 0.41 |
| 1:Q:1868:SER:O | 1:Q:1874:TYR:HB2 | 2.20 | 0.41 |
| 1:Q:1974:LYS:HZ1 | 1:Q:2361:GLN:C | 2.27 | 0.41 |
| 1:Q:2639:ARG:HE | 1:Q:2640:PRO:HD2 | 1.85 | 0.41 |
| 1:Q:2819:PHE:CZ | 1:Q:2832:GLY:HA3 | 2.56 | 0.41 |
| 1:Q:2821:LEU:HB3 | 1:Q:2872:PHE:HE1 | 1.86 | 0.41 |
| 1:Q:3013:TRP:HH2 | 1:Q:3087:LEU:HD21 | 1.85 | 0.41 |
| 1:Q:3022:SER:HA | 1:Q:3025:THR:OG1 | 2.20 | 0.41 |
| 1:R:334:ASP:OD1 | 1:R:334:ASP:N | 2.50 | 0.41 |
| 1:R:599:PHE:O | 1:R:603:GLU:OE1 | 2.38 | 0.41 |
| 1:R:705:GLU:HG2 | 1:R:706:LEU:HD22 | 2.03 | 0.41 |
| 1:R:841:GLU:O | 1:R:843:GLN:N | 2.54 | 0.41 |
| 1:R:1020:ILE:HG13 | 1:R:1021:ALA:N | 2.36 | 0.41 |
| 1:R:1138:ARG:HH22 | 1:R:1259:VAL:HG23 | 1.86 | 0.41 |
| 1:R:1824:HIS:HB2 | 1:R:1827:ASP:CG | 2.45 | 0.41 |
| 1:R:1890:ARG:NH2 | 1:R:1959:GLU:OE2 | 2.48 | 0.41 |
| 1:R:2088:PRO:HA | 1:R:2089:PRO:HD3 | 1.90 | 0.41 |
| 1:R:2504:ALA:O | 1:R:2505:SER:HB3 | 2.20 | 0.41 |
| 1:R:2552:GLY:HA3 | 1:R:2697:GLU:HA | 2.02 | 0.41 |
| 1:R:2754:ASN:HD22 | 1:R:2757:ILE:HG12 | 1.86 | 0.41 |
| 1:R:2972:ASP:OD1 | 1:R:2972:ASP:N | 2.51 | 0.41 |
| 1:R:3388:PHE:HB2 | 1:R:3402:VAL:HG13 | 2.03 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:S:1017:GLN:O | 1:S:1020:ILE:HG22 | 2.21 | 0.41 |
| 1:S:1905:ASP:HB3 | 1:S:1908:GLU:HB2 | 2.02 | 0.41 |
| 1:S:2101:ALA:O | 1:S:2105:MET:HE3 | 2.20 | 0.41 |
| 1:S:2449:THR:HA | 1:S:2452:GLU:CD | 2.46 | 0.41 |
| 1:S:2819:PHE:O | 1:S:2831:ALA:HB3 | 2.20 | 0.41 |
| 1:S:3034:THR:HG23 | 1:S:3044:VAL:HB | 2.03 | 0.41 |
| 1:S:3114:PHE:HD1 | 1:S:3117:ILE:HD11 | 1.86 | 0.41 |
| 1:T:171:GLU:CD | 1:T:176:HIS:HB3 | 2.45 | 0.41 |
| 1:T:597:ARG:HD2 | 1:T:597:ARG:HA | 1.82 | 0.41 |
| 1:T:599:PHE:HD2 | 1:T:600:CYS:SG | 2.43 | 0.41 |
| 1:T:599:PHE:O | 1:T:603:GLU:OE1 | 2.39 | 0.41 |
| 1:T:1111:GLU:OE1 | 1:T:1111:GLU:N | 2.53 | 0.41 |
| 1:T:1313:ALA:H | 1:T:1600:THR:HG22 | 1.85 | 0.41 |
| 1:T:2368:ASP:OD1 | 1:T:2368:ASP:N | 2.54 | 0.41 |
| 1:T:2518:ASN:OD1 | 1:T:2518:ASN:N | 2.51 | 0.41 |
| 3:1:1:NAG:H62 | 3:1:2:NAG:H82 | 2.02 | 0.41 |
| 1:A:81:LEU:HD21 | 1:A:86:LEU:HD23 | 2.03 | 0.41 |
| 1:A:307:GLU:OE1 | 1:A:412:PRO:HA | 2.21 | 0.41 |
| 1:A:330:ASP:OD1 | 1:A:331:HIS:N | 2.54 | 0.41 |
| 1:A:573:GLU:HB3 | 1:A:616:LEU:HD11 | 2.02 | 0.41 |
| 1:A:1928:PRO:HD2 | 1:A:1929:TYR:CE1 | 2.56 | 0.41 |
| 1:A:1943:ASP:OD1 | 1:A:1943:ASP:N | 2.54 | 0.41 |
| 1:A:2021:GLU:N | 1:A:2021:GLU:OE1 | 2.54 | 0.41 |
| 1:A:2159:ARG:NH2 | 1:A:2360:TYR:HB3 | 2.35 | 0.41 |
| 1:A:2770:ASP:N | 1:A:2770:ASP:OD1 | 2.53 | 0.41 |
| 1:A:2821:LEU:O | 1:A:2828:CYS:HB2 | 2.20 | 0.41 |
| 1:A:3351:VAL:O | 1:A:3372:SER:HA | 2.21 | 0.41 |
| 1:B:80:LYS:HE3 | 1:B:261:ILE:HD11 | 2.03 | 0.41 |
| 1:B:596:GLN:NE2 | 1:B:602:PHE:HD1 | 2.19 | 0.41 |
| 1:B:878:PHE:CD1 | 1:B:881:ILE:HD11 | 2.55 | 0.41 |
| 1:B:1475:GLN:NE2 | 1:B:1478:ARG:HD2 | 2.36 | 0.41 |
| 1:B:1636:LYS:HA | 1:B:1636:LYS:HD2 | 1.94 | 0.41 |
| 1:B:1736:MET:N | 1:B:1736:MET:SD | 2.93 | 0.41 |
| 1:B:2392:ARG:HD2 | 1:B:2394:PHE:HE1 | 1.84 | 0.41 |
| 1:B:2671:GLU:OE1 | 1:B:2671:GLU:N | 2.31 | 0.41 |
| 1:B:3351:VAL:HG12 | 1:B:3373:TYR:O | 2.21 | 0.41 |
| 1:C:46:SER:HB3 | 1:C:57:ALA:HA | 2.03 | 0.41 |
| 1:C:71:ARG:NE | 1:C:220:ASP:OD2 | 2.53 | 0.41 |
| 1:C:1508:ASP:HA | 1:C:1512:ARG:HH11 | 1.86 | 0.41 |
| 1:C:1645:LEU:HA | 1:F:483:ARG:HH22 | 1.86 | 0.41 |
| 1:C:1827:ASP:HA | 1:C:1831:TRP:CZ3 | 2.55 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:1860:TRP:HA | 1:C:1860:TRP:CE3 | 2.56 | 0.41 |
| 1:C:1878:ASP:OD1 | 1:C:1880:ILE:HG22 | 2.21 | 0.41 |
| 1:C:1902:ARG:HB3 | 1:C:1904:HIS:CD2 | 2.56 | 0.41 |
| 1:C:1992:THR:C | 1:C:2017:GLY:O | 2.64 | 0.41 |
| 1:C:2273:TYR:OH | 1:C:2278:HIS:NE2 | 2.53 | 0.41 |
| 1:C:2368:ASP:OD1 | 1:C:2369:ASP:N | 2.49 | 0.41 |
| 1:C:2521:THR:HG23 | 1:C:2524:GLU:H | 1.85 | 0.41 |
| 1:C:3105:THR:HG23 | 1:C:3108:TYR:H | 1.86 | 0.41 |
| 1:C:3214:TYR:HB3 | 1:C:3264:TYR:O | 2.21 | 0.41 |
| 1:D:222:ILE:HD12 | 1:D:222:ILE:H | 1.85 | 0.41 |
| 1:D:257:ASP:HA | 1:D:265:ARG:HD3 | 2.03 | 0.41 |
| 1:D:378:LYS:HA | 1:D:378:LYS:HD2 | 1.91 | 0.41 |
| 1:D:727:ILE:HG22 | 1:D:730:ARG:NH2 | 2.30 | 0.41 |
| 1:D:1174:PRO:HG2 | 1:D:1176:HIS:CE1 | 2.55 | 0.41 |
| 1:D:1195:ASP:OD1 | 1:D:1195:ASP:N | 2.43 | 0.41 |
| 1:D:1283:LEU:HD12 | 1:D:1286:MET:SD | 2.61 | 0.41 |
| 1:D:1472:GLN:O | 1:D:1475:GLN:HB2 | 2.21 | 0.41 |
| 1:D:1557:PHE:HD2 | 1:D:1611:LYS:HD3 | 1.86 | 0.41 |
| 1:D:2482:PRO:HA | 1:D:2483:PRO:HD3 | 1.95 | 0.41 |
| 1:D:2529:LYS:HB3 | 1:D:2529:LYS:HE2 | 1.84 | 0.41 |
| 1:D:2568:HIS:HB3 | 1:D:2571:SER:OG | 2.21 | 0.41 |
| 1:D:2602:ASP:HA | 1:D:2711:ASN:HD21 | 1.85 | 0.41 |
| 1:D:2645:ASP:HB3 | 1:D:2649:GLY:O | 2.21 | 0.41 |
| 1:D:2738:GLN:HG2 | 1:E:2894:VAL:HG23 | 2.03 | 0.41 |
| 1:D:2944:LEU:HD23 | 1:D:2999:LEU:HD23 | 2.03 | 0.41 |
| 1:D:3214:TYR:HB2 | 1:D:3305:ILE:HB | 2.03 | 0.41 |
| 1:E:240:ALA:HB2 | 1:E:247:PHE:CE2 | 2.56 | 0.41 |
| 1:E:306:ARG:HH21 | 1:E:308:ARG:HD2 | 1.86 | 0.41 |
| 1:E:706:LEU:O | 1:E:707:GLU:HG2 | 2.21 | 0.41 |
| 1:E:734:ASP:HB3 | 1:E:833:GLY:H | 1.85 | 0.41 |
| 1:E:878:PHE:HA | 1:E:881:ILE:HG22 | 2.02 | 0.41 |
| 1:E:1849:GLN:OE1 | 1:E:1849:GLN:N | 2.53 | 0.41 |
| 1:E:2024:TRP:CD1 | 1:E:2024:TRP:H | 2.38 | 0.41 |
| 1:E:2238:ASP:OD1 | 1:E:2239:GLY:N | 2.54 | 0.41 |
| 1:E:2387:HIS:O | 1:E:2392:ARG:NH1 | 2.49 | 0.41 |
| 1:E:2673:GLN:NE2 | 1:E:2852:GLN:H | 2.11 | 0.41 |
| 1:E:2878:ALA:N | 1:E:2882:THR:O | 2.51 | 0.41 |
| 1:E:3114:PHE:HD1 | 1:E:3117:ILE:HD11 | 1.85 | 0.41 |
| 1:E:3191:ASN:OD1 | 1:E:3195:HIS:N | 2.54 | 0.41 |
| 1:E:3395:ARG:HH21 | 1:E:3398:GLN:HE22 | 1.69 | 0.41 |
| 1:F:158:ASN:HB3 | 1:F:162:PHE:CD2 | 2.56 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:F:245:GLU:H | 1:F:245:GLU:CD | 2.29 | 0.41 |
| 1:F:312:SER:HB3 | 1:F:407:VAL:HG13 | 2.03 | 0.41 |
| 1:F:599:PHE:HA | 1:F:651:TRP:HH2 | 1.86 | 0.41 |
| 1:F:742:LEU:HD23 | 1:F:781:PHE:CE2 | 2.56 | 0.41 |
| 1:F:1142:HIS:HD2 | 1:F:1143:ARG:HH12 | 1.68 | 0.41 |
| 1:F:1769:VAL:HG11 | 1:F:1960:LEU:HD11 | 2.02 | 0.41 |
| 1:F:1865:LYS:HA | 1:F:1865:LYS:HD2 | 1.85 | 0.41 |
| 1:F:2271:ILE:O | 1:F:2275:VAL:HG12 | 2.21 | 0.41 |
| 1:F:3383:PRO:HG3 | 1:F:3408:ASP:HB3 | 2.02 | 0.41 |
| 1:G:77:LEU:HD22 | 1:G:213:PHE:CZ | 2.56 | 0.41 |
| 1:G:612:LEU:HD21 | 1:G:768:LEU:HA | 2.02 | 0.41 |
| 1:G:1118:SER:OG | 1:G:1119:PHE:N | 2.54 | 0.41 |
| 1:G:1159:ARG:O | 1:G:1160:LYS:HD3 | 2.21 | 0.41 |
| 1:G:1399:GLU:OE1 | 1:G:1399:GLU:N | 2.54 | 0.41 |
| 1:G:1756:ARG:HH21 | 1:H:2176:VAL:HG13 | 1.86 | 0.41 |
| 1:G:1776:PRO:HD2 | 1:G:1779:PHE:CZ | 2.56 | 0.41 |
| 1:G:1872:LEU:HD21 | 1:G:2016:LEU:HB2 | 2.03 | 0.41 |
| 1:G:1967:LEU:HB2 | 1:G:2086:GLU:OE2 | 2.20 | 0.41 |
| 1:G:2328:ASN:ND2 | 1:H:1240:THR:HA | 2.35 | 0.41 |
| 1:G:2889:LEU:HD23 | 1:G:2890:GLU:O | 2.21 | 0.41 |
| 1:G:3022:SER:HA | 1:G:3025:THR:OG1 | 2.20 | 0.41 |
| 1:G:3086:MET:HG3 | 1:G:3262:TYR:CD1 | 2.56 | 0.41 |
| 1:G:3200:ILE:O | 1:G:3204:ILE:HG12 | 2.21 | 0.41 |
| 1:H:17:LEU:HA | 1:H:20:GLU:OE2 | 2.21 | 0.41 |
| 1:H:188:ILE:HD13 | 1:H:215:HIS:NE2 | 2.36 | 0.41 |
| 1:H:235:LYS:HE2 | 1:H:235:LYS:HB3 | 1.88 | 0.41 |
| 1:H:329:CYS:SG | 1:H:330:ASP:N | 2.93 | 0.41 |
| 1:H:455:PHE:N | 1:H:514:ARG:HH12 | 2.19 | 0.41 |
| 1:H:501:ARG:HH11 | 1:H:645:ASP:CG | 2.27 | 0.41 |
| 1:H:597:ARG:HH22 | 1:H:655:GLN:HA | 1.86 | 0.41 |
| 1:H:606:PHE:HA | 1:H:609:VAL:HG22 | 2.02 | 0.41 |
| 1:H:614:HIS:CG | 1:H:771:LEU:HD11 | 2.56 | 0.41 |
| 1:H:825:HIS:CD2 | 1:H:825:HIS:H | 2.39 | 0.41 |
| 1:H:864:GLU:HA | 1:H:867:GLN:OE1 | 2.20 | 0.41 |
| 1:H:867:GLN:HA | 1:H:870:GLU:HG3 | 2.01 | 0.41 |
| 1:H:1166:LEU:HB3 | 1:H:1179:GLY:O | 2.21 | 0.41 |
| 1:H:1321:VAL:HG11 | 1:H:1491:ILE:HG21 | 2.03 | 0.41 |
| 1:H:1802:ILE:HG22 | 1:H:1877:TYR:CD1 | 2.56 | 0.41 |
| 1:H:1910:ASN:O | 1:H:1913:LEU:HG | 2.21 | 0.41 |
| 1:H:1915:LEU:HD23 | 1:H:1915:LEU:HA | 1.88 | 0.41 |
| 1:H:2040:LYS:HE3 | 1:H:2040:LYS:HB3 | 1.89 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:H:2387:HIS:HB3 | 1:H:2392:ARG:NH2 | 2.36 | 0.41 |
| 1:H:2521:THR:HG22 | 1:H:2524:GLU:CD | 2.45 | 0.41 |
| 1:H:2585:LEU:HD22 | 1:H:2706:PHE:CE1 | 2.56 | 0.41 |
| 1:H:2822:CYS:HB2 | 1:H:2871:HIS:NE2 | 2.34 | 0.41 |
| 1:H:2982:PRO:HG2 | 1:H:3146:ALA:HB2 | 2.03 | 0.41 |
| 1:H:3011:TRP:CZ3 | 1:H:3013:TRP:HA | 2.56 | 0.41 |
| 1:H:3117:ILE:O | 1:H:3120:SER:OG | 2.30 | 0.41 |
| 1:H:3128:ILE:HD11 | 1:H:3190:LEU:HD22 | 2.03 | 0.41 |
| 1:I:444:GLU:HB3 | 1:I:518:PHE:HZ | 1.85 | 0.41 |
| 1:I:850:ASP:O | 1:I:853:SER:OG | 2.38 | 0.41 |
| 1:I:1178:GLU:HG2 | 1:I:1205:ILE:HG21 | 2.03 | 0.41 |
| 1:I:1447:SER:O | 1:I:1451:SER:OG | 2.34 | 0.41 |
| 1:I:1630:ASP:OD1 | 1:I:1630:ASP:N | 2.42 | 0.41 |
| 1:I:1730:ALA:H | 1:I:2020:ALA:HB1 | 1.86 | 0.41 |
| 1:I:1842:ASN:OD1 | 1:I:1843:TYR:N | 2.53 | 0.41 |
| 1:I:2165:VAL:O | 1:I:2169:LEU:HD23 | 2.21 | 0.41 |
| 1:I:2199:PHE:CE1 | 1:I:2208:LEU:HB3 | 2.55 | 0.41 |
| 1:I:2266:VAL:HG21 | 1:I:2442:TYR:CD1 | 2.56 | 0.41 |
| 1:I:2404:THR:CA | 1:I:2429:GLY:O | 2.68 | 0.41 |
| 1:I:2578:HIS:CG | 1:I:2709:HIS:CE1 | 3.09 | 0.41 |
| 1:I:2817:VAL:O | 1:I:2833:THR:HG23 | 2.21 | 0.41 |
| 1:I:3069:LEU:HA | 1:I:3072:LEU:HD12 | 2.02 | 0.41 |
| 1:I:3238:ASP:OD1 | 1:I:3238:ASP:N | 2.54 | 0.41 |
| 1:J:171:GLU:CD | 1:J:176:HIS:HB3 | 2.45 | 0.41 |
| 1:J:501:ARG:NH2 | 1:J:699:ILE:O | 2.43 | 0.41 |
| 1:J:502:LEU:O | 1:J:506:GLN:HG2 | 2.20 | 0.41 |
| 1:J:744:ASN:HB3 | 1:J:779:TRP:CD1 | 2.56 | 0.41 |
| 1:J:806:VAL:HG11 | 1:J:825:HIS:O | 2.21 | 0.41 |
| 1:J:1230:LYS:HD2 | 1:J:1230:LYS:HA | 1.81 | 0.41 |
| 1:J:1362:ILE:HG22 | 1:J:1380:PHE:HB3 | 2.03 | 0.41 |
| 1:J:1888:THR:HA | 1:J:1891:ILE:HD12 | 2.03 | 0.41 |
| 1:J:2165:VAL:HG11 | 1:J:2296:PHE:CE2 | 2.56 | 0.41 |
| 1:J:2335:GLN:NE2 | 1:J:2338:ASN:HD21 | 2.19 | 0.41 |
| 1:J:2526:GLU:HA | 1:J:2529:LYS:HG2 | 2.03 | 0.41 |
| 1:J:2578:HIS:CD2 | 1:J:2709:HIS:CD2 | 3.09 | 0.41 |
| 1:J:2822:CYS:HB2 | 1:J:2871:HIS:NE2 | 2.35 | 0.41 |
| 1:K:193:GLY:HA3 | 1:K:201:SER:H | 1.86 | 0.41 |
| 1:K:211:LEU:HA | 1:K:214:LEU:HB2 | 2.03 | 0.41 |
| 1:K:299:LEU:O | 1:K:302:GLN:HG3 | 2.21 | 0.41 |
| 1:K:989:LYS:HD2 | 1:K:989:LYS:HA | 1.79 | 0.41 |
| 1:K:1001:MET:O | 1:K:1004:LEU:HG | 2.21 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:K:1561:LEU:HD13 | 1:K:1561:LEU:HA | 1.95 | 0.41 |
| 1:K:1896:GLN:NE2 | 1:K:1906:PRO:O | 2.45 | 0.41 |
| 1:K:1993:SER:HB2 | 1:K:2017:GLY:H | 1.85 | 0.41 |
| 1:K:2021:GLU:OE1 | 1:K:2021:GLU:N | 2.53 | 0.41 |
| 1:K:2183:TRP:O | 1:K:2242:SER:OG | 2.24 | 0.41 |
| 1:K:2246:ASP:OD1 | 1:K:2246:ASP:N | 2.54 | 0.41 |
| 1:K:2515:LYS:HG2 | 1:K:2777:ASP:HB3 | 2.03 | 0.41 |
| 1:K:2603:TRP:HD1 | 1:K:2711:ASN:HD22 | 1.62 | 0.41 |
| 1:K:2665:ARG:HH12 | 1:K:2726:ARG:HD2 | 1.86 | 0.41 |
| 1:K:2676:VAL:HG11 | 1:K:2851:PHE:CZ | 2.56 | 0.41 |
| 1:K:2705:PHE:HD2 | 1:K:2706:PHE:HD1 | 1.68 | 0.41 |
| 1:K:2972:ASP:N | 1:K:2972:ASP:OD1 | 2.53 | 0.41 |
| 1:L:552:ASN:ND2 | 1:L:554:PHE:HB2 | 2.35 | 0.41 |
| 1:L:599:PHE:O | 1:L:603:GLU:OE1 | 2.38 | 0.41 |
| 1:L:938:ASP:HA | 1:L:1055:ASN:ND2 | 2.35 | 0.41 |
| 1:L:1093:GLN:OE1 | 1:L:1093:GLN:N | 2.54 | 0.41 |
| 1:L:1147:GLU:OE2 | 1:L:1247:SER:HB3 | 2.20 | 0.41 |
| 1:L:1148:ARG:HD3 | 1:L:1150:PHE:CZ | 2.55 | 0.41 |
| 1:L:1225:ASP:HB2 | 1:L:1229:LYS:HB2 | 2.02 | 0.41 |
| 1:L:1415:GLU:OE2 | 1:L:1551:ARG:HG2 | 2.21 | 0.41 |
| 1:L:1889:ASP:OD2 | 1:L:1955:TYR:OH | 2.33 | 0.41 |
| 1:L:2254:GLN:HE21 | 1:L:2260:PHE:HA | 1.85 | 0.41 |
| 1:L:2605:GLU:OE2 | 1:L:2605:GLU:N | 2.54 | 0.41 |
| 1:L:2789:LEU:O | 1:L:2793:ILE:HG12 | 2.21 | 0.41 |
| 1:L:2812:LYS:HG2 | 1:L:2840:PRO:HA | 2.03 | 0.41 |
| 1:L:3214:TYR:N | 1:L:3305:ILE:O | 2.34 | 0.41 |
| 1:M:22:TYR:CD1 | 1:M:86:LEU:HD22 | 2.55 | 0.41 |
| 1:M:86:LEU:HD12 | 1:M:86:LEU:HA | 1.86 | 0.41 |
| 1:M:189:HIS:HE1 | 1:M:212:PHE:CE1 | 2.38 | 0.41 |
| 1:M:330:ASP:OD1 | 1:M:331:HIS:N | 2.54 | 0.41 |
| 1:M:502:LEU:HD23 | 1:M:502:LEU:HA | 1.85 | 0.41 |
| 1:M:611:ASN:ND2 | 1:M:771:LEU:H | 2.11 | 0.41 |
| 1:M:724:ASP:O | 1:M:727:ILE:HG12 | 2.21 | 0.41 |
| 1:M:1163:LEU:HG | 1:M:1182:TYR:CD1 | 2.55 | 0.41 |
| 1:M:1362:ILE:HD12 | 1:M:1394:ARG:NH1 | 2.36 | 0.41 |
| 1:M:1384:LYS:HA | 1:M:1391:VAL:HG12 | 2.02 | 0.41 |
| 1:M:1990:ILE:O | 1:M:1991:LYS:HG3 | 2.21 | 0.41 |
| 1:M:2056:ARG:HA | 1:M:2056:ARG:HD2 | 1.81 | 0.41 |
| 1:M:2090:ASN:ND2 | 1:M:2175:THR:O | 2.54 | 0.41 |
| 1:M:2216:TYR:CD1 | 1:M:2223:TYR:HB3 | 2.56 | 0.41 |
| 1:M:2405:SER:HB3 | 1:M:2426:PHE:HE1 | 1.85 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:M:2449:THR:HA | 1:M:2452:GLU:CD | 2.46 | 0.41 |
| 1:M:2693:MET:O | 1:M:2699:SER:OG | 2.32 | 0.41 |
| 1:M:2812:LYS:HA | 1:M:2812:LYS:HD3 | 1.86 | 0.41 |
| 1:M:2954:GLU:OE2 | 1:M:3035:TYR:OH | 2.30 | 0.41 |
| 1:M:3231:LYS:HB2 | 1:M:3284:GLN:HG3 | 2.01 | 0.41 |
| 1:M:3337:ARG:NH1 | 1:M:3380:SER:HB2 | 2.36 | 0.41 |
| 1:M:3352:LYS:HB3 | 1:M:3371:ASN:HB3 | 2.03 | 0.41 |
| 1:N:811:LYS:HD2 | 1:N:815:GLY:HA2 | 2.02 | 0.41 |
| 1:N:1135:GLN:O | 1:N:1139:GLU:OE1 | 2.39 | 0.41 |
| 1:N:1431:ASN:HA | 1:N:1434:HIS:HB2 | 2.02 | 0.41 |
| 1:N:1493:ARG:NH2 | 1:N:1515:ARG:HD2 | 2.35 | 0.41 |
| 1:N:1802:ILE:CD1 | 1:N:1805:GLU:HB2 | 2.50 | 0.41 |
| 1:N:2045:VAL:HG21 | 1:N:2075:TYR:CD1 | 2.56 | 0.41 |
| 1:N:3089:ASN:HB3 | 1:N:3248:LEU:HD13 | 2.03 | 0.41 |
| 1:N:3106:LEU:HD22 | 1:N:3250:GLY:HA3 | 2.03 | 0.41 |
| 1:O:51:ASP:OD1 | 1:O:51:ASP:N | 2.54 | 0.41 |
| 1:O:190:TYR:HB3 | 1:O:349:PHE:CD2 | 2.56 | 0.41 |
| 1:O:706:LEU:O | 1:O:707:GLU:HG2 | 2.21 | 0.41 |
| 1:O:885:HIS:ND1 | 1:O:885:HIS:O | 2.54 | 0.41 |
| 1:O:1137:GLN:O | 1:O:1140:ILE:HG22 | 2.21 | 0.41 |
| 1:O:1301:PHE:CG | 1:O:1302:PRO:HA | 2.55 | 0.41 |
| 1:O:1315:CYS:HA | 1:O:1325:TRP:CH2 | 2.55 | 0.41 |
| 1:O:1327:ARG:NH1 | 1:O:1528:TYR:OH | 2.53 | 0.41 |
| 1:O:1495:PRO:HD2 | 1:O:1500:ASN:HD21 | 1.85 | 0.41 |
| 1:O:2630:LEU:HD22 | 1:O:2632:GLU:HB2 | 2.02 | 0.41 |
| 1:O:3091:ILE:HD11 | 1:O:3118:HIS:NE2 | 2.36 | 0.41 |
| 1:O:3133:GLN:OE1 | 1:O:3140:PHE:HB3 | 2.19 | 0.41 |
| 1:P:80:LYS:O | 1:P:83:LYS:HG2 | 2.20 | 0.41 |
| 1:P:306:ARG:O | 1:P:411:ARG:NH2 | 2.54 | 0.41 |
| 1:P:314:THR:HG21 | 1:P:782:ASP:HB3 | 2.02 | 0.41 |
| 1:P:531:THR:OG1 | 1:P:532:VAL:N | 2.54 | 0.41 |
| 1:P:719:THR:HG22 | 1:P:722:GLN:CD | 2.46 | 0.41 |
| 1:P:947:PRO:HB2 | 1:P:950:VAL:HG22 | 2.03 | 0.41 |
| 1:P:1085:ARG:HA | 1:P:1110:PHE:HE2 | 1.86 | 0.41 |
| 1:P:1152:GLY:HA2 | 1:P:1198:PHE:O | 2.21 | 0.41 |
| 1:P:1294:LYS:O | 1:P:1297:SER:OG | 2.30 | 0.41 |
| 1:P:1602:MET:HA | 1:P:1602:MET:HE2 | 2.03 | 0.41 |
| 1:P:1619:ARG:HH21 | 1:P:1625:LEU:HD13 | 1.86 | 0.41 |
| 1:P:1677:ARG:HD2 | 1:P:1763:ILE:O | 2.20 | 0.41 |
| 1:P:1684:THR:HG23 | 1:P:1687:GLU:H | 1.84 | 0.41 |
| 1:P:1854:HIS:O | 1:P:1884:HIS:HE1 | 2.03 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:P:1884:HIS:O | 1:P:1888:THR:HG23 | 2.21 | 0.41 |
| 1:P:2313:GLN:HA | 1:P:2316:ARG:NH1 | 2.35 | 0.41 |
| 1:P:2328:ASN:OD1 | 1:P:2329:TYR:N | 2.54 | 0.41 |
| 1:P:2543:GLY:HA3 | 1:P:2546:GLU:CD | 2.46 | 0.41 |
| 1:P:2587:ARG:NH2 | 1:P:2754:ASN:HB2 | 2.36 | 0.41 |
| 1:P:2898:PRO:HG2 | 1:Q:2913:PRO:HB2 | 2.03 | 0.41 |
| 1:P:2923:ARG:HE | 1:P:2924:TYR:H | 1.69 | 0.41 |
| 1:Q:44:GLU:HA | 1:Q:45:PRO:HA | 1.89 | 0.41 |
| 1:Q:222:ILE:O | 1:Q:225:ILE:HG22 | 2.21 | 0.41 |
| 1:Q:230:GLN:HA | 1:Q:233:ARG:HG2 | 2.03 | 0.41 |
| 1:Q:506:GLN:HB2 | 1:Q:690:THR:HG21 | 2.03 | 0.41 |
| 1:Q:562:LEU:HD23 | 1:Q:562:LEU:HA | 1.93 | 0.41 |
| 1:Q:596:GLN:OE1 | 1:Q:596:GLN:N | 2.50 | 0.41 |
| 1:Q:792:ALA:O | 1:Q:795:LYS:HG2 | 2.21 | 0.41 |
| 1:Q:1238:LYS:HD2 | 1:Q:1238:LYS:HA | 1.73 | 0.41 |
| 1:Q:1688:ARG:HH12 | 1:Q:1784:TYR:HE1 | 1.69 | 0.41 |
| 1:Q:1802:ILE:HG22 | 1:Q:1877:TYR:HB3 | 2.02 | 0.41 |
| 1:Q:1869:MET:HA | 1:Q:1875:ALA:HA | 2.02 | 0.41 |
| 1:Q:1910:ASN:OD1 | 1:Q:1911:CYS:N | 2.54 | 0.41 |
| 1:Q:1946:ASP:OD2 | 1:Q:1949:SER:OG | 2.34 | 0.41 |
| 1:Q:2056:ARG:HD2 | 1:Q:2056:ARG:HA | 1.84 | 0.41 |
| 1:Q:2194:PHE:CD1 | 1:Q:2212:PHE:HB3 | 2.56 | 0.41 |
| 1:Q:2808:LEU:HB2 | 1:Q:2847:PHE:HD2 | 1.86 | 0.41 |
| 1:Q:3065:PHE:HA | 1:Q:3068:THR:HG22 | 2.01 | 0.41 |
| 1:Q:3142:TYR:CZ | 1:Q:3144:ARG:HD3 | 2.56 | 0.41 |
| 1:Q:3204:ILE:HG13 | 1:Q:3205:GLU:N | 2.36 | 0.41 |
| 1:Q:3334:ARG:HD2 | 1:Q:3409:GLU:HB3 | 2.02 | 0.41 |
| 1:R:5:ARG:HB3 | 1:R:93:TYR:CD1 | 2.55 | 0.41 |
| 1:R:221:ARG:O | 1:R:224:VAL:HG22 | 2.21 | 0.41 |
| 1:R:696:PRO:HA | 1:R:699:ILE:HD13 | 2.03 | 0.41 |
| 1:R:714:GLN:NE2 | 1:R:717:GLY:O | 2.54 | 0.41 |
| 1:R:972:LEU:HD23 | 1:R:972:LEU:HA | 1.87 | 0.41 |
| 1:R:1067:GLN:HG3 | 1:R:1070:ARG:HH21 | 1.86 | 0.41 |
| 1:R:1159:ARG:NH2 | 1:R:1160:LYS:HB3 | 2.35 | 0.41 |
| 1:R:1283:LEU:HD23 | 1:R:1284:ARG:HH12 | 1.85 | 0.41 |
| 1:R:1576:CYS:HB2 | 1:R:1632:ASP:OD1 | 2.19 | 0.41 |
| 1:R:1602:MET:HA | 1:R:1602:MET:HE2 | 2.03 | 0.41 |
| 1:R:1633:LEU:HD23 | 1:R:1633:LEU:H | 1.85 | 0.41 |
| 1:R:1783:ILE:HD13 | 1:R:1794:PRO:HA | 2.02 | 0.41 |
| 1:R:1854:HIS:HE1 | 1:R:1885:HIS:CD2 | 2.39 | 0.41 |
| 1:R:1865:LYS:HA | 1:R:1865:LYS:HD2 | 1.92 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:R:2106:SER:HB2 | 1:R:2175:THR:HG21 | 2.02 | 0.41 |
| 1:R:2209:GLU:H | 1:R:2209:GLU:CD | 2.27 | 0.41 |
| 1:R:2513:VAL:HG21 | 1:R:2777:ASP:HB3 | 2.02 | 0.41 |
| 1:R:2602:ASP:HA | 1:R:2711:ASN:HD21 | 1.86 | 0.41 |
| 1:R:3131:THR:HA | 1:R:3134:LYS:HG2 | 2.03 | 0.41 |
| 1:R:3266:VAL:HG11 | 1:R:3283:PHE:CZ | 2.56 | 0.41 |
| 1:R:3402:VAL:HG13 | 1:R:3404:ILE:HD11 | 2.02 | 0.41 |
| 1:S:646:ARG:NH2 | 1:S:714:GLN:O | 2.34 | 0.41 |
| 1:S:731:ARG:HE | 1:S:836:HIS:HE1 | 1.69 | 0.41 |
| 1:S:903:CYS:C | 1:S:905:HIS:HD1 | 2.24 | 0.41 |
| 1:S:1327:ARG:HG3 | 1:S:1465:ASP:OD2 | 2.21 | 0.41 |
| 1:S:1517:ILE:HD12 | 1:S:1517:ILE:H | 1.85 | 0.41 |
| 1:S:1956:ASP:OD1 | 1:S:1957:THR:N | 2.52 | 0.41 |
| 1:S:2095:GLU:HG3 | 1:S:2098:HIS:HD2 | 1.86 | 0.41 |
| 1:S:2100:ASP:O | 1:S:2104:THR:HG23 | 2.20 | 0.41 |
| 1:S:2267:THR:O | 1:S:2271:ILE:HG12 | 2.20 | 0.41 |
| 1:S:2421:ARG:HH22 | 1:S:2424:ALA:HB2 | 1.85 | 0.41 |
| 1:S:2622:PHE:O | 1:S:2703:PRO:HD2 | 2.20 | 0.41 |
| 1:S:2700:ALA:HA | 1:S:2705:PHE:CD2 | 2.56 | 0.41 |
| 1:S:2714:ARG:NH2 | 1:S:2778:ASP:O | 2.35 | 0.41 |
| 1:S:3128:ILE:HA | 1:S:3131:THR:HG22 | 2.02 | 0.41 |
| 1:T:68:GLN:HA | 1:T:71:ARG:HG2 | 2.02 | 0.41 |
| 1:T:166:LEU:HA | 1:T:169:LEU:HG | 2.02 | 0.41 |
| 1:T:247:PHE:O | 1:T:271:LYS:NZ | 2.36 | 0.41 |
| 1:T:471:HIS:ND1 | 1:T:471:HIS:O | 2.54 | 0.41 |
| 1:T:538:LYS:NZ | 1:T:540:THR:O | 2.35 | 0.41 |
| 1:T:842:HIS:CE1 | 1:T:844:GLU:HB2 | 2.55 | 0.41 |
| 1:T:998:ILE:HD12 | 1:T:998:ILE:H | 1.86 | 0.41 |
| 1:T:1275:GLU:H | 1:T:1275:GLU:CD | 2.29 | 0.41 |
| 1:T:1324:HIS:CD2 | 1:T:1324:HIS:H | 2.39 | 0.41 |
| 1:T:1397:GLN:HB2 | 1:T:1400:LEU:HD23 | 2.02 | 0.41 |
| 1:T:1620:LYS:HD2 | 1:T:1620:LYS:HA | 1.82 | 0.41 |
| 1:T:2038:LEU:HD12 | 1:T:2039:GLU:N | 2.35 | 0.41 |
| 1:T:2252:LEU:HD23 | 1:T:2309:TRP:HD1 | 1.85 | 0.41 |
| 1:T:2430:GLY:N | 1:T:2433:GLU:OE2 | 2.53 | 0.41 |
| 1:T:2432:LEU:N | 1:T:2433:GLU:OE1 | 2.53 | 0.41 |
| 1:T:2622:PHE:CD2 | 1:T:2703:PRO:HB2 | 2.56 | 0.41 |
| 1:T:2709:HIS:O | 1:T:2712:VAL:HG22 | 2.21 | 0.41 |
| 1:T:3012:ASP:OD2 | 1:T:3015:ARG:HG2 | 2.21 | 0.41 |
| 1:T:3049:GLN:CD | 1:T:3050:PRO:HD2 | 2.45 | 0.41 |
| 1:T:3154:LEU:N | 1:T:3172:SER:O | 2.49 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:T:3287:LEU:HB3 | 1:T:3295:LEU:HB3 | 2.01 | 0.41 |
| 1:A:432:VAL:HB | 1:A:519:GLY:N | 2.34 | 0.41 |
| 1:A:471:HIS:O | 1:A:471:HIS:ND1 | 2.54 | 0.41 |
| 1:A:996:THR:HG23 | 1:A:999:ALA:H | 1.86 | 0.41 |
| 1:A:1268:LEU:HB3 | 1:A:1347:PRO:HB2 | 2.02 | 0.41 |
| 1:A:1832:LYS:O | 1:A:1835:LEU:HG | 2.21 | 0.41 |
| 1:A:2157:TRP:HZ3 | 1:A:2158:HIS:CE1 | 2.39 | 0.41 |
| 1:A:3377:VAL:HB | 1:A:3379:TYR:CZ | 2.55 | 0.41 |
| 1:B:599:PHE:O | 1:B:603:GLU:OE1 | 2.39 | 0.41 |
| 1:B:970:HIS:CD2 | 1:B:977:LYS:HB3 | 2.55 | 0.41 |
| 1:B:1408:ASN:O | 1:B:1411:LEU:HG | 2.21 | 0.41 |
| 1:B:2529:LYS:HE2 | 1:B:2529:LYS:HB3 | 1.82 | 0.41 |
| 1:C:328:VAL:HG13 | 1:C:376:LEU:HD11 | 2.02 | 0.41 |
| 1:C:1114:ASP:OD1 | 1:C:1114:ASP:N | 2.50 | 0.41 |
| 1:C:1320:ALA:HA | 1:C:1423:GLU:OE1 | 2.21 | 0.41 |
| 1:C:1415:GLU:OE1 | 1:C:1551:ARG:NH2 | 2.54 | 0.41 |
| 1:C:1416:GLN:OE1 | 1:C:1425:GLN:NE2 | 2.26 | 0.41 |
| 1:C:2409:ARG:HG3 | 1:C:2421:ARG:NH2 | 2.36 | 0.41 |
| 1:C:2627:ILE:O | 1:C:2627:ILE:HG13 | 2.21 | 0.41 |
| 1:C:2964:LYS:HD3 | 1:C:2974:TYR:HA | 2.03 | 0.41 |
| 1:D:81:LEU:HB3 | 1:D:86:LEU:HD22 | 2.02 | 0.41 |
| 1:D:562:LEU:HD23 | 1:D:562:LEU:HA | 1.84 | 0.41 |
| 1:D:841:GLU:N | 1:D:843:GLN:OE1 | 2.54 | 0.41 |
| 1:D:1158:ILE:O | 1:D:1159:ARG:HG2 | 2.21 | 0.41 |
| 1:D:1467:ILE:HD13 | 1:D:1467:ILE:HA | 1.92 | 0.41 |
| 1:D:1521:ASP:HB3 | 1:D:1525:HIS:CD2 | 2.55 | 0.41 |
| 1:D:2397:PHE:CD1 | 1:D:2489:PRO:HB3 | 2.56 | 0.41 |
| 1:D:2817:VAL:O | 1:D:2833:THR:OG1 | 2.33 | 0.41 |
| 1:D:3065:PHE:HZ | 1:D:3195:HIS:HD2 | 1.69 | 0.41 |
| 1:D:3142:TYR:CZ | 1:D:3144:ARG:HB2 | 2.56 | 0.41 |
| 1:E:148:ARG:NH2 | 1:E:191:LEU:HD21 | 2.36 | 0.41 |
| 1:E:1433:LEU:HD11 | 1:E:1460:HIS:CE1 | 2.56 | 0.41 |
| 1:E:2963:PRO:HG3 | 1:E:3039:PHE:HD2 | 1.85 | 0.41 |
| 1:F:670:MET:HE3 | 1:F:670:MET:HB3 | 1.89 | 0.41 |
| 1:F:743:GLN:HB3 | 1:F:780:ASN:ND2 | 2.35 | 0.41 |
| 1:F:867:GLN:HE21 | 1:F:967:PRO:HD2 | 1.85 | 0.41 |
| 1:F:928:LYS:HG3 | 1:F:929:GLY:N | 2.36 | 0.41 |
| 1:F:1496:LEU:HD23 | 1:F:1497:LYS:O | 2.21 | 0.41 |
| 1:F:1501:ASP:CG | 1:F:1504:GLN:H | 2.29 | 0.41 |
| 1:F:1632:ASP:OD1 | 1:F:1632:ASP:N | 2.53 | 0.41 |
| 1:F:2209:GLU:H | 1:F:2209:GLU:CD | 2.28 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:F:2412:VAL:HG21 | 1:F:2450:LEU:HD21 | 2.03 | 0.41 |
| 1:F:2421:ARG:CZ | 1:F:2423:GLY:HA2 | 2.51 | 0.41 |
| 1:F:2583:VAL:HG21 | 1:F:2772:PHE:HD2 | 1.86 | 0.41 |
| 1:F:2656:ARG:O | 1:F:2659:LEU:HG | 2.21 | 0.41 |
| 1:F:2715:GLN:HA | 1:F:2718:ILE:HG12 | 2.03 | 0.41 |
| 1:F:3117:ILE:O | 1:F:3120:SER:OG | 2.29 | 0.41 |
| 1:F:3131:THR:HG23 | 1:F:3134:LYS:HZ3 | 1.86 | 0.41 |
| 1:F:3373:TYR:CE2 | 1:F:3381:LEU:HD11 | 2.56 | 0.41 |
| 1:G:849:SER:HB3 | 1:G:854:LEU:HD21 | 2.02 | 0.41 |
| 1:G:920:GLN:HE22 | 1:G:1100:ASP:HB3 | 1.86 | 0.41 |
| 1:G:1156:HIS:HB3 | 1:G:1193:GLN:NE2 | 2.29 | 0.41 |
| 1:G:1711:ALA:HA | 1:G:1746:TYR:OH | 2.21 | 0.41 |
| 1:G:1745:LEU:HA | 1:G:1748:VAL:HG12 | 2.02 | 0.41 |
| 1:G:2056:ARG:HA | 1:G:2056:ARG:HD2 | 1.93 | 0.41 |
| 1:G:2410:PHE:O | 1:G:2422:ALA:HB3 | 2.21 | 0.41 |
| 1:G:2966:CYS:HB3 | 1:G:2974:TYR:O | 2.20 | 0.41 |
| 1:G:3173:ARG:O | 1:G:3176:GLN:HG3 | 2.21 | 0.41 |
| 1:H:39:ALA:HB1 | 1:H:208:TYR:CZ | 2.56 | 0.41 |
| 1:H:298:ASN:HA | 1:H:301:GLU:OE2 | 2.20 | 0.41 |
| 1:H:505:VAL:HA | 1:H:508:GLU:HG2 | 2.03 | 0.41 |
| 1:H:1078:ASN:HA | 1:H:1081:ILE:HD11 | 2.03 | 0.41 |
| 1:H:1315:CYS:C | 1:H:1317:HIS:HD1 | 2.29 | 0.41 |
| 1:H:1702:SER:O | 1:H:1702:SER:OG | 2.36 | 0.41 |
| 1:I:291:LEU:HA | 1:I:295:GLN:HE21 | 1.86 | 0.41 |
| 1:I:1732:CYS:O | 1:I:1734:HIS:ND1 | 2.54 | 0.41 |
| 1:I:1776:PRO:HD2 | 1:I:1779:PHE:CZ | 2.56 | 0.41 |
| 1:I:2037:VAL:HA | 1:I:2040:LYS:HG2 | 2.03 | 0.41 |
| 1:I:2510:GLY:HA3 | 1:I:2513:VAL:HB | 2.03 | 0.41 |
| 1:I:2678:HIS:CE1 | 1:I:2709:HIS:NE2 | 2.89 | 0.41 |
| 1:J:255:ASP:OD1 | 1:J:255:ASP:N | 2.52 | 0.41 |
| 1:J:469:GLU:OE1 | 1:J:469:GLU:N | 2.48 | 0.41 |
| 1:J:663:LYS:HD2 | 1:J:664:ALA:O | 2.21 | 0.41 |
| 1:J:1291:THR:HA | 1:J:1294:LYS:NZ | 2.35 | 0.41 |
| 1:J:1304:LEU:HD23 | 1:J:1304:LEU:HA | 1.92 | 0.41 |
| 1:J:1666:ASP:O | 1:J:1668:THR:HG23 | 2.21 | 0.41 |
| 1:K:42:HIS:NE2 | 1:K:59:CYS:SG | 2.94 | 0.41 |
| 1:K:750:LEU:HD11 | 1:K:767:LYS:HD2 | 2.02 | 0.41 |
| 1:K:1295:ILE:HG13 | 1:K:1296:ALA:N | 2.35 | 0.41 |
| 1:K:1983:ALA:HB2 | 1:K:2034:ILE:HG21 | 2.02 | 0.41 |
| 1:K:2094:HIS:CD2 | 1:K:2098:HIS:HB3 | 2.46 | 0.41 |
| 1:K:2990:LEU:O | 1:K:2993:VAL:HG12 | 2.21 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:L:1998:ILE:HG13 | 1:L:2010:ALA:HB3 | 2.02 | 0.41 |
| 1:M:183:VAL:HG21 | 1:M:365:TYR:CE1 | 2.56 | 0.41 |
| 1:M:332:ASP:OD1 | 1:M:332:ASP:N | 2.48 | 0.41 |
| 1:M:650:ILE:HG22 | 1:M:713:LEU:HD12 | 2.02 | 0.41 |
| 1:M:674:LEU:HD13 | 1:M:695:ARG:HH21 | 1.86 | 0.41 |
| 1:M:1231:ILE:HG22 | 1:M:1232:SER:N | 2.36 | 0.41 |
| 1:M:1560:PHE:O | 1:M:1561:LEU:HD22 | 2.21 | 0.41 |
| 1:M:1649:VAL:HG13 | 1:M:1650:LEU:CD2 | 2.51 | 0.41 |
| 1:M:2602:ASP:HA | 1:M:2711:ASN:ND2 | 2.36 | 0.41 |
| 1:M:2679:ASN:HD21 | 1:M:2836:VAL:C | 2.29 | 0.41 |
| 1:M:3154:LEU:O | 1:M:3158:ASN:N | 2.54 | 0.41 |
| 1:N:201:SER:OG | 1:N:202:THR:N | 2.53 | 0.41 |
| 1:N:1136:LEU:HA | 1:N:1139:GLU:OE2 | 2.21 | 0.41 |
| 1:N:1542:GLN:HA | 1:N:1545:GLU:CD | 2.46 | 0.41 |
| 1:N:1676:ILE:HG13 | 1:N:1761:VAL:HG23 | 2.03 | 0.41 |
| 1:N:1802:ILE:HG12 | 1:N:1807:THR:O | 2.21 | 0.41 |
| 1:N:1992:THR:CA | 1:N:2017:GLY:O | 2.69 | 0.41 |
| 1:N:2803:PHE:CD1 | 1:N:2852:GLN:HB3 | 2.56 | 0.41 |
| 1:O:22:TYR:HA | 1:O:25:GLU:HG3 | 2.02 | 0.41 |
| 1:O:508:GLU:CD | 1:O:520:ILE:H | 2.28 | 0.41 |
| 1:O:675:LEU:HD11 | 1:O:696:PRO:HG3 | 2.03 | 0.41 |
| 1:O:1413:ALA:HA | 1:O:1425:GLN:HG3 | 2.03 | 0.41 |
| 1:O:1607:ASP:OD1 | 1:O:1607:ASP:N | 2.48 | 0.41 |
| 1:O:2533:ARG:HA | 1:O:2536:GLN:OE1 | 2.20 | 0.41 |
| 1:O:2819:PHE:O | 1:O:2831:ALA:HB3 | 2.21 | 0.41 |
| 1:O:3083:GLN:O | 1:O:3087:LEU:HD13 | 2.21 | 0.41 |
| 1:O:3088:HIS:CD2 | 1:O:3092:HIS:CE1 | 3.09 | 0.41 |
| 1:O:3100:THR:HA | 1:O:3290:TYR:HE2 | 1.86 | 0.41 |
| 1:P:112:PHE:HB3 | 1:P:121:GLN:O | 2.21 | 0.41 |
| 1:P:221:ARG:O | 1:P:224:VAL:HG22 | 2.21 | 0.41 |
| 1:P:735:ARG:NH2 | 1:P:789:ILE:H | 2.19 | 0.41 |
| 1:P:972:LEU:HD23 | 1:P:972:LEU:HA | 1.92 | 0.41 |
| 1:P:1017:GLN:HG2 | 1:P:1018:TYR:N | 2.36 | 0.41 |
| 1:P:1461:HIS:HA | 1:P:1464:VAL:HB | 2.02 | 0.41 |
| 1:P:1688:ARG:HE | 1:P:1778:PHE:HD1 | 1.69 | 0.41 |
| 1:P:2771:GLN:HG2 | 1:P:2772:PHE:HD1 | 1.86 | 0.41 |
| 1:P:2896:PHE:O | 1:Q:2734:ASN:ND2 | 2.54 | 0.41 |
| 1:P:3227:THR:HB | 1:P:3246:TYR:CD2 | 2.55 | 0.41 |
| 1:P:3258:TYR:HB3 | 1:P:3260:ARG:O | 2.20 | 0.41 |
| 1:Q:148:ARG:HH22 | 1:Q:349:PHE:HZ | 1.68 | 0.41 |
| 1:Q:1646:GLU:OE1 | 1:Q:1646:GLU:N | 2.39 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:Q:1721:PRO:HD3 | 1:Q:1729:TYR:CE2 | 2.56 | 0.41 |
| 1:Q:1816:ASN:OD1 | 1:Q:1816:ASN:N | 2.53 | 0.41 |
| 1:Q:2343:ASN:HD22 | 1:Q:2349:ARG:HH22 | 1.67 | 0.41 |
| 1:Q:2576:GLN:HE22 | 1:Q:2767:PHE:HA | 1.85 | 0.41 |
| 1:Q:2679:ASN:HD21 | 1:Q:2836:VAL:CA | 2.34 | 0.41 |
| 1:Q:2696:LEU:H | 1:Q:2696:LEU:HD23 | 1.86 | 0.41 |
| 1:Q:2912:ASP:OD1 | 1:Q:2912:ASP:N | 2.52 | 0.41 |
| 1:Q:2966:CYS:HB3 | 1:Q:2974:TYR:O | 2.21 | 0.41 |
| 1:R:171:GLU:CD | 1:R:176:HIS:HB3 | 2.46 | 0.41 |
| 1:R:480:PRO:C | 1:R:485:ARG:HH12 | 2.29 | 0.41 |
| 1:R:1221:TYR:CE2 | 1:R:1233:SER:HB2 | 2.56 | 0.41 |
| 1:R:2286:LEU:HD21 | 1:R:2428:LEU:HD13 | 2.03 | 0.41 |
| 1:R:2598:ILE:HA | 1:R:2599:PRO:HD3 | 1.97 | 0.41 |
| 1:R:2648:ARG:HG3 | 1:R:2656:ARG:HD2 | 2.03 | 0.41 |
| 1:R:3076:ASN:OD1 | 1:R:3079:ASP:N | 2.54 | 0.41 |
| 1:R:3232:LEU:HD13 | 1:R:3269:ALA:HB3 | 2.01 | 0.41 |
| 1:S:2174:SER:O | 1:T:1757:ARG:NH1 | 2.54 | 0.41 |
| 1:S:2491:ILE:HG22 | 1:T:1082:ALA:H | 1.86 | 0.41 |
| 1:T:418:ASP:OD2 | 1:T:661:PRO:HA | 2.21 | 0.41 |
| 1:T:752:ILE:HD12 | 1:T:767:LYS:HG2 | 2.02 | 0.41 |
| 1:T:1007:GLU:N | 1:T:1007:GLU:OE1 | 2.54 | 0.41 |
| 1:T:1783:ILE:HD13 | 1:T:1794:PRO:HA | 2.03 | 0.41 |
| 1:A:299:LEU:HD23 | 1:A:299:LEU:HA | 1.89 | 0.40 |
| 1:A:704:HIS:HB3 | 1:A:705:GLU:OE1 | 2.20 | 0.40 |
| 1:A:968:PHE:HA | 1:A:1047:PRO:HG3 | 2.02 | 0.40 |
| 1:A:1448:LEU:HA | 1:A:1451:SER:HB2 | 2.03 | 0.40 |
| 1:A:1492:MET:N | 1:A:1492:MET:SD | 2.94 | 0.40 |
| 1:A:1920:LEU:HD21 | 1:A:1941:PRO:HB3 | 2.03 | 0.40 |
| 1:A:2213:ALA:HA | 1:A:2226:ARG:NH2 | 2.36 | 0.40 |
| 1:A:3021:PRO:HD2 | 1:A:3024:LEU:HD21 | 2.03 | 0.40 |
| 1:B:220:ASP:O | 1:B:224:VAL:HG13 | 2.19 | 0.40 |
| 1:B:307:GLU:HG3 | 1:B:413:ALA:HA | 2.03 | 0.40 |
| 1:B:811:LYS:HB2 | 1:B:811:LYS:HE2 | 1.91 | 0.40 |
| 1:B:849:SER:HA | 1:B:1124:ASP:CG | 2.46 | 0.40 |
| 1:B:2137:PRO:HD3 | 1:B:2143:LYS:HB2 | 2.03 | 0.40 |
| 1:B:2162:THR:O | 1:B:2165:VAL:HG22 | 2.20 | 0.40 |
| 1:B:2515:LYS:HA | 1:B:2777:ASP:OD2 | 2.21 | 0.40 |
| 1:B:3358:THR:O | 1:B:3362:LEU:HB2 | 2.21 | 0.40 |
| 1:C:889:ASN:HB2 | 1:C:899:LYS:HB3 | 2.03 | 0.40 |
| 1:C:2027:ASP:OD2 | 1:C:2028:ARG:NH1 | 2.54 | 0.40 |
| 1:C:2755:ASP:OD1 | 1:C:2756:PHE:N | 2.54 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:D:1216:ARG:H | 1:D:1216:ARG:HD3 | 1.86 | 0.40 |
| 1:D:2270:ALA:O | 1:D:2274:LEU:HD23 | 2.21 | 0.40 |
| 1:D:2483:PRO:HD3 | 1:M:895:ASP:OD1 | 2.20 | 0.40 |
| 1:D:2579:ARG:NH1 | 1:D:2766:ALA:O | 2.54 | 0.40 |
| 1:D:2602:ASP:OD1 | 1:D:2603:TRP:N | 2.55 | 0.40 |
| 1:D:3213:VAL:HA | 1:D:3306:SER:HA | 2.03 | 0.40 |
| 1:D:3284:GLN:N | 1:D:3284:GLN:OE1 | 2.54 | 0.40 |
| 1:E:939:TRP:HA | 1:E:943:MET:HE1 | 2.04 | 0.40 |
| 1:E:953:GLU:OE1 | 1:E:969:HIS:ND1 | 2.54 | 0.40 |
| 1:E:1017:GLN:O | 1:E:1020:ILE:HG22 | 2.21 | 0.40 |
| 1:E:1133:ILE:HB | 1:E:1134:PRO:HD3 | 2.01 | 0.40 |
| 1:E:2085:GLN:CD | 1:E:2087:LEU:H | 2.28 | 0.40 |
| 1:E:2416:ASN:OD1 | 1:E:2417:GLY:N | 2.46 | 0.40 |
| 1:E:3046:ARG:NH2 | 1:E:3112:ASP:OD2 | 2.54 | 0.40 |
| 1:F:13:ASP:O | 1:F:17:LEU:HD23 | 2.21 | 0.40 |
| 1:F:24:ARG:HD3 | 1:F:123:ASN:HA | 2.03 | 0.40 |
| 1:F:552:ASN:HD21 | 1:F:554:PHE:HB2 | 1.85 | 0.40 |
| 1:F:599:PHE:O | 1:F:603:GLU:OE1 | 2.39 | 0.40 |
| 1:F:654:LEU:HD11 | 1:F:724:ASP:OD1 | 2.21 | 0.40 |
| 1:F:1813:PHE:C | 1:F:1814:LYS:HD3 | 2.46 | 0.40 |
| 1:F:2273:TYR:HB3 | 1:F:2426:PHE:CD1 | 2.56 | 0.40 |
| 1:F:2477:ASN:ND2 | 1:F:2479:THR:OG1 | 2.55 | 0.40 |
| 1:G:580:TYR:CE1 | 1:G:856:ARG:HD2 | 2.56 | 0.40 |
| 1:G:672:HIS:O | 1:G:695:ARG:NH1 | 2.50 | 0.40 |
| 1:G:1448:LEU:HD22 | 1:G:1596:LEU:HG | 2.03 | 0.40 |
| 1:G:2633:LYS:HE3 | 1:G:2633:LYS:HB3 | 1.84 | 0.40 |
| 1:G:2725:TYR:CE2 | 1:G:2790:GLU:HG2 | 2.56 | 0.40 |
| 1:G:3131:THR:O | 1:G:3134:LYS:HG2 | 2.20 | 0.40 |
| 1:G:3307:ARG:NH2 | 1:G:3314:ASP:OD2 | 2.54 | 0.40 |
| 1:H:225:ILE:O | 1:H:229:LEU:HG | 2.20 | 0.40 |
| 1:H:536:ALA:HB2 | 1:H:554:PHE:HD2 | 1.86 | 0.40 |
| 1:H:1158:ILE:O | 1:H:1159:ARG:HG2 | 2.21 | 0.40 |
| 1:H:1285:ARG:HB3 | 1:H:1340:ARG:HH11 | 1.86 | 0.40 |
| 1:H:1584:ARG:HB3 | 1:H:1586:CYS:SG | 2.60 | 0.40 |
| 1:H:1857:ILE:HD12 | 1:H:1884:HIS:CD2 | 2.57 | 0.40 |
| 1:H:2022:MET:HA | 1:H:2023:PRO:HD3 | 1.97 | 0.40 |
| 1:H:2262:VAL:HG23 | 1:H:2438:PHE:CD1 | 2.56 | 0.40 |
| 1:H:2353:LEU:O | 1:H:2356:GLU:HG2 | 2.20 | 0.40 |
| 1:H:2504:ALA:C | 1:H:2506:TYR:H | 2.29 | 0.40 |
| 1:H:2726:ARG:HA | 1:H:2726:ARG:HD2 | 1.90 | 0.40 |
| 1:H:3320:LEU:H | 1:H:3342:SER:HA | 1.85 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:I:28:ASP:OD1 | 1:I:29:ASP:N | 2.53 | 0.40 |
| 1:I:71:ARG:O | 1:I:75:VAL:HG22 | 2.21 | 0.40 |
| 1:I:80:LYS:O | 1:I:83:LYS:HG2 | 2.21 | 0.40 |
| 1:I:170:GLU:HA | 1:I:300:LEU:HD23 | 2.03 | 0.40 |
| 1:I:1149:VAL:HG11 | 1:I:1206:LEU:HD12 | 2.02 | 0.40 |
| 1:I:2520:LEU:HD21 | 1:I:2525:THR:HG23 | 2.03 | 0.40 |
| 1:J:473:LEU:HG | 1:J:629:HIS:ND1 | 2.36 | 0.40 |
| 1:J:703:GLU:N | 1:J:703:GLU:OE1 | 2.54 | 0.40 |
| 1:J:714:GLN:N | 1:J:714:GLN:OE1 | 2.53 | 0.40 |
| 1:J:2168:ALA:HA | 1:J:2171:LYS:HG2 | 2.04 | 0.40 |
| 1:J:2794:GLU:O | 1:J:2798:SER:CB | 2.69 | 0.40 |
| 1:J:3185:TYR:CD2 | 1:J:3187:PHE:HE1 | 2.38 | 0.40 |
| 1:J:3198:SER:O | 1:J:3201:ASN:HB2 | 2.22 | 0.40 |
| 1:K:514:ARG:NH1 | 1:K:1343:ALA:HA | 2.36 | 0.40 |
| 1:K:885:HIS:ND1 | 1:K:885:HIS:O | 2.54 | 0.40 |
| 1:K:1495:PRO:HD2 | 1:K:1500:ASN:HD21 | 1.86 | 0.40 |
| 1:K:2171:LYS:HE3 | 1:K:2171:LYS:HB3 | 1.93 | 0.40 |
| 1:K:2784:LEU:HD23 | 1:K:2789:LEU:HA | 2.02 | 0.40 |
| 1:K:2938:ARG:HD3 | 1:K:3032:PHE:CE2 | 2.56 | 0.40 |
| 1:L:80:LYS:NZ | 1:L:261:ILE:HG13 | 2.36 | 0.40 |
| 1:L:298:ASN:HA | 1:L:301:GLU:CD | 2.46 | 0.40 |
| 1:L:727:ILE:HG13 | 1:L:728:ASP:N | 2.36 | 0.40 |
| 1:L:973:VAL:O | 1:L:974:GLU:HG3 | 2.20 | 0.40 |
| 1:L:1687:GLU:OE2 | 1:L:1760:LEU:HB2 | 2.21 | 0.40 |
| 1:L:1785:ARG:HH22 | 1:L:1790:ASP:HA | 1.86 | 0.40 |
| 1:L:2068:ILE:HD12 | 1:L:2068:ILE:HA | 1.97 | 0.40 |
| 1:L:2523:ALA:O | 1:L:2526:GLU:HG3 | 2.21 | 0.40 |
| 1:M:299:LEU:O | 1:M:302:GLN:HG3 | 2.21 | 0.40 |
| 1:M:512:LYS:HB3 | 1:M:512:LYS:HE3 | 1.88 | 0.40 |
| 1:M:675:LEU:HD11 | 1:M:696:PRO:HG3 | 2.03 | 0.40 |
| 1:M:2110:ALA:HB1 | 1:M:2172:HIS:HB3 | 2.03 | 0.40 |
| 1:M:2616:ASP:OD1 | 1:M:2616:ASP:N | 2.54 | 0.40 |
| 1:M:2676:VAL:HG11 | 1:M:2851:PHE:CZ | 2.56 | 0.40 |
| 1:N:437:VAL:HG22 | 1:N:521:PRO:HG2 | 2.03 | 0.40 |
| 1:N:495:THR:HG23 | 1:N:670:MET:HE2 | 2.02 | 0.40 |
| 1:N:599:PHE:O | 1:N:603:GLU:OE1 | 2.40 | 0.40 |
| 1:N:752:ILE:HB | 1:N:809:SER:HB3 | 2.03 | 0.40 |
| 1:N:1852:ILE:HA | 1:N:1855:ASN:HD21 | 1.85 | 0.40 |
| 1:N:2210:ASN:ND2 | 1:N:2212:PHE:HB2 | 2.36 | 0.40 |
| 1:N:2786:ILE:N | 1:N:2787:PRO:HD2 | 2.36 | 0.40 |
| 1:N:2800:ASP:HB3 | 1:N:2896:PHE:CE1 | 2.57 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:N:3020:LEU:HD11 | 1:N:3025:THR:HB | 2.03 | 0.40 |
| 1:O:50:LYS:NZ | 1:O:357:MET:HE1 | 2.36 | 0.40 |
| 1:O:376:LEU:HD12 | 1:O:378:LYS:NZ | 2.37 | 0.40 |
| 1:O:1025:ILE:HG21 | 1:O:1052:HIS:CE1 | 2.56 | 0.40 |
| 1:O:1844:CYS:N | 1:O:1911:CYS:SG | 2.95 | 0.40 |
| 1:O:1854:HIS:HD2 | 1:O:1888:THR:HG21 | 1.85 | 0.40 |
| 1:O:3214:TYR:HA | 1:O:3266:VAL:HG12 | 2.02 | 0.40 |
| 1:P:583:HIS:HB3 | 1:P:587:PHE:CG | 2.56 | 0.40 |
| 1:P:978:THR:HB | 1:P:1036:SER:HA | 2.03 | 0.40 |
| 1:P:1055:ASN:HA | 1:P:1058:ARG:HG3 | 2.03 | 0.40 |
| 1:P:1905:ASP:HB3 | 1:P:1908:GLU:HB2 | 2.02 | 0.40 |
| 1:P:2041:LYS:HE2 | 1:P:2043:LEU:HD23 | 2.03 | 0.40 |
| 1:P:2201:ASP:OD1 | 1:P:2201:ASP:N | 2.54 | 0.40 |
| 1:P:2674:TYR:OH | 1:P:2712:VAL:HB | 2.20 | 0.40 |
| 1:P:3165:ASN:HB3 | 1:P:3168:THR:OG1 | 2.21 | 0.40 |
| 1:Q:214:LEU:O | 1:Q:217:SER:OG | 2.39 | 0.40 |
| 1:Q:2371:LYS:HA | 1:Q:2371:LYS:HD2 | 1.87 | 0.40 |
| 1:Q:2382:GLU:O | 1:Q:2386:GLN:HG2 | 2.20 | 0.40 |
| 1:Q:2470:ARG:NH1 | 1:Q:2471:TYR:H | 2.20 | 0.40 |
| 1:R:1159:ARG:O | 1:R:1159:ARG:NH1 | 2.53 | 0.40 |
| 1:R:1165:THR:N | 1:R:1222:SER:O | 2.33 | 0.40 |
| 1:R:1286:MET:SD | 1:R:1292:PHE:HB2 | 2.61 | 0.40 |
| 1:R:1947:TYR:CE1 | 1:R:1948:LYS:HG3 | 2.56 | 0.40 |
| 1:R:2269:ASN:OD1 | 1:R:2428:LEU:HG | 2.22 | 0.40 |
| 1:R:2817:VAL:HG22 | 1:R:2876:ILE:HD12 | 2.02 | 0.40 |
| 1:R:3332:VAL:HG22 | 1:R:3406:ILE:HA | 2.03 | 0.40 |
| 1:S:169:LEU:HD23 | 1:S:222:ILE:HD11 | 2.02 | 0.40 |
| 1:S:479:ARG:HG3 | 1:S:676:LYS:HZ2 | 1.86 | 0.40 |
| 1:S:1424:ILE:HG23 | 1:S:1425:GLN:N | 2.37 | 0.40 |
| 1:S:1998:ILE:HG13 | 1:S:2010:ALA:HB3 | 2.03 | 0.40 |
| 1:S:2371:LYS:HD2 | 1:S:2371:LYS:HA | 1.74 | 0.40 |
| 1:S:2479:THR:HG21 | 2:0A:1:NAG:HN2 | 1.87 | 0.40 |
| 1:S:2602:ASP:HA | 1:S:2711:ASN:HD21 | 1.86 | 0.40 |
| 1:T:48:CYS:HB2 | 1:T:58:CYS:HB2 | 1.84 | 0.40 |
| 1:T:409:VAL:HG13 | 1:T:666:CYS:HA | 2.03 | 0.40 |
| 1:T:426:VAL:HG12 | 1:T:428:SER:H | 1.86 | 0.40 |
| 1:T:473:LEU:HD21 | 1:T:775:LYS:HG3 | 2.03 | 0.40 |
| 1:T:1018:TYR:OH | 1:T:1056:THR:HB | 2.21 | 0.40 |
| 1:T:1767:ASP:OD2 | 1:T:1890:ARG:NH2 | 2.55 | 0.40 |
| 1:T:1865:LYS:HA | 1:T:1865:LYS:HD2 | 1.89 | 0.40 |
| 1:T:1978:LYS:HD2 | 1:T:2078:LYS:HE3 | 2.03 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:T:2155:PRO:HB2 | 1:T:2306:TRP:CZ3 | 2.56 | 0.40 |
| 1:T:2271:ILE:HB | 1:T:2298:HIS:CE1 | 2.56 | 0.40 |
| 1:T:2481:LEU:CD1 | 1:T:2482:PRO:HD2 | 2.51 | 0.40 |
| 1:T:2666:ASP:HB3 | 1:T:2669:ASN:CG | 2.46 | 0.40 |
| 1:A:423:GLU:OE1 | 1:A:423:GLU:N | 2.54 | 0.40 |
| 1:A:973:VAL:O | 1:A:976:LYS:HG3 | 2.21 | 0.40 |
| 1:A:1775:LEU:HD12 | 1:A:1779:PHE:CE2 | 2.56 | 0.40 |
| 1:A:1812:ASP:HB3 | 1:A:1863:GLY:HA3 | 2.03 | 0.40 |
| 1:A:2099:LEU:HD13 | 1:A:2103:ALA:HB3 | 2.02 | 0.40 |
| 1:A:2674:TYR:CZ | 1:A:2716:PHE:HB2 | 2.56 | 0.40 |
| 1:A:2734:ASN:HD21 | 1:J:2896:PHE:HD2 | 1.68 | 0.40 |
| 1:A:2931:LEU:HA | 1:A:2934:VAL:HG12 | 2.03 | 0.40 |
| 1:A:3077:TYR:O | 1:A:3080:PHE:HB2 | 2.21 | 0.40 |
| 1:A:3332:VAL:O | 1:A:3334:ARG:NH2 | 2.51 | 0.40 |
| 1:B:188:ILE:O | 1:B:192:VAL:HG12 | 2.20 | 0.40 |
| 1:B:2533:ARG:O | 1:B:2537:GLN:OE1 | 2.38 | 0.40 |
| 1:B:2823:ASP:N | 1:B:2823:ASP:OD1 | 2.53 | 0.40 |
| 1:B:3319:PRO:HB2 | 1:B:3343:PRO:HD3 | 2.03 | 0.40 |
| 1:B:3332:VAL:HG22 | 1:B:3405:SER:O | 2.22 | 0.40 |
| 1:C:178:GLU:O | 1:C:182:GLU:HG2 | 2.21 | 0.40 |
| 1:C:414:LYS:HE3 | 1:C:414:LYS:HA | 2.03 | 0.40 |
| 1:C:461:VAL:HA | 1:C:1371:ARG:HD3 | 2.03 | 0.40 |
| 1:C:996:THR:HG23 | 1:C:999:ALA:H | 1.86 | 0.40 |
| 1:C:1273:GLU:OE1 | 1:C:1273:GLU:N | 2.42 | 0.40 |
| 1:C:1360:ALA:HA | 1:C:1363:ASN:OD1 | 2.21 | 0.40 |
| 1:C:1508:ASP:CG | 1:C:1509:LEU:N | 2.79 | 0.40 |
| 1:C:1817:ARG:HG3 | 1:C:1860:TRP:CH2 | 2.56 | 0.40 |
| 1:C:2053:VAL:HG11 | 1:C:2068:ILE:HG21 | 2.03 | 0.40 |
| 1:C:2752:ASN:HB3 | 1:C:2758:ARG:HG3 | 2.03 | 0.40 |
| 1:D:35:TYR:OH | 1:D:208:TYR:HA | 2.21 | 0.40 |
| 1:D:502:LEU:CD2 | 1:D:506:GLN:HE21 | 2.34 | 0.40 |
| 1:D:998:ILE:HA | 1:D:1001:MET:HG3 | 2.02 | 0.40 |
| 1:D:1972:ILE:HG13 | 1:D:1973:ASN:N | 2.36 | 0.40 |
| 1:D:2738:GLN:O | 1:D:2742:GLN:NE2 | 2.55 | 0.40 |
| 1:D:2986:HIS:HB3 | 1:D:3177:ILE:HG21 | 2.03 | 0.40 |
| 1:E:77:LEU:HD22 | 1:E:213:PHE:CE1 | 2.56 | 0.40 |
| 1:E:1060:TRP:O | 1:E:1064:GLN:OE1 | 2.40 | 0.40 |
| 1:E:1195:ASP:CG | 1:E:1196:ARG:HE | 2.26 | 0.40 |
| 1:E:1356:ARG:HE | 1:E:1356:ARG:HB3 | 1.68 | 0.40 |
| 1:E:1786:ASP:OD2 | 1:E:1789:LEU:N | 2.28 | 0.40 |
| 1:E:2201:ASP:OD1 | 1:E:2203:TRP:N | 2.33 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:E:2791:GLU:O | 1:E:2794:GLU:HG3 | 2.21 | 0.40 |
| 1:E:2797:ARG:HA | 1:E:2801:ARG:HH22 | 1.86 | 0.40 |
| 1:E:3121:SER:O | 1:E:3125:ILE:HG22 | 2.20 | 0.40 |
| 1:E:3210:HIS:O | 1:E:3212:ARG:NH1 | 2.50 | 0.40 |
| 1:F:663:LYS:HB3 | 1:F:665:HIS:CE1 | 2.57 | 0.40 |
| 1:F:1711:ALA:HA | 1:F:1876:SER:HB2 | 2.03 | 0.40 |
| 1:F:3035:TYR:H | 1:F:3044:VAL:HG22 | 1.86 | 0.40 |
| 1:F:3108:TYR:HB3 | 1:F:3111:PHE:CD2 | 2.56 | 0.40 |
| 1:G:158:ASN:HB2 | 1:G:162:PHE:CD2 | 2.56 | 0.40 |
| 1:G:855:THR:HG22 | 1:G:858:GLN:NE2 | 2.31 | 0.40 |
| 1:G:1490:ASN:ND2 | 1:H:2049:PHE:O | 2.46 | 0.40 |
| 1:G:1750:PHE:CD2 | 1:G:1882:LEU:HD21 | 2.56 | 0.40 |
| 1:G:2575:PRO:O | 1:G:2579:ARG:HB2 | 2.21 | 0.40 |
| 1:G:3214:TYR:CD1 | 1:G:3265:ASP:HA | 2.56 | 0.40 |
| 1:H:172:ASP:OD1 | 1:H:173:ASP:N | 2.54 | 0.40 |
| 1:H:524:ASP:OD2 | 1:H:527:ARG:HG2 | 2.21 | 0.40 |
| 1:H:878:PHE:HZ | 1:H:1050:PHE:HE1 | 1.68 | 0.40 |
| 1:H:934:LEU:HD11 | 1:H:1054:SER:HB3 | 2.02 | 0.40 |
| 1:H:1093:GLN:N | 1:H:1093:GLN:OE1 | 2.54 | 0.40 |
| 1:H:1638:ARG:HG2 | 1:H:1644:TYR:CE1 | 2.56 | 0.40 |
| 1:H:1678:LYS:NZ | 1:H:1683:LEU:HA | 2.36 | 0.40 |
| 1:H:1946:ASP:HB3 | 1:H:1950:HIS:CD2 | 2.56 | 0.40 |
| 1:H:2712:VAL:HA | 1:H:2715:GLN:NE2 | 2.35 | 0.40 |
| 1:H:2987:TRP:CH2 | 1:H:2991:LEU:HD11 | 2.56 | 0.40 |
| 1:I:296:LEU:O | 1:I:300:LEU:HD13 | 2.21 | 0.40 |
| 1:I:884:PHE:HE1 | 1:I:1090:PRO:HG2 | 1.86 | 0.40 |
| 1:I:1858:HIS:HD1 | 1:I:1869:MET:CE | 2.34 | 0.40 |
| 1:I:1865:LYS:HZ2 | 1:I:1867:HIS:H | 1.69 | 0.40 |
| 1:I:1883:LEU:O | 1:I:1886:SER:OG | 2.26 | 0.40 |
| 1:I:2439:ASP:O | 1:J:1196:ARG:HA | 2.21 | 0.40 |
| 1:I:3144:ARG:HA | 1:I:3147:LEU:HD21 | 2.02 | 0.40 |
| 1:I:3212:ARG:HB3 | 1:I:3214:TYR:CZ | 2.57 | 0.40 |
| 1:J:6:LYS:HD2 | 1:J:11:LEU:HA | 2.04 | 0.40 |
| 1:J:42:HIS:HB3 | 1:J:207:ALA:HB1 | 2.03 | 0.40 |
| 1:J:663:LYS:HE3 | 1:J:665:HIS:HE1 | 1.86 | 0.40 |
| 1:J:1852:ILE:HA | 1:J:1855:ASN:HD21 | 1.86 | 0.40 |
| 1:J:2313:GLN:HA | 1:J:2316:ARG:NH1 | 2.35 | 0.40 |
| 1:J:2618:ASP:OD1 | 1:J:2618:ASP:N | 2.54 | 0.40 |
| 1:J:2780:ASN:OD1 | 1:J:2780:ASN:N | 2.52 | 0.40 |
| 1:J:2986:HIS:ND1 | 1:J:3177:ILE:HG23 | 2.36 | 0.40 |
| 1:K:35:TYR:OH | 1:K:208:TYR:O | 2.33 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:K:663:LYS:HB2 | 1:K:665:HIS:CD2 | 2.56 | 0.40 |
| 1:K:1061:ALA:HA | 1:K:1064:GLN:NE2 | 2.36 | 0.40 |
| 1:K:1145:HIS:NE2 | 1:K:1524:ASN:OD1 | 2.54 | 0.40 |
| 1:K:1543:LEU:O | 1:K:1547:LEU:HD23 | 2.21 | 0.40 |
| 1:K:1801:ASP:OD1 | 1:K:1802:ILE:N | 2.55 | 0.40 |
| 1:K:1977:GLU:O | 1:K:2078:LYS:NZ | 2.48 | 0.40 |
| 1:K:2151:VAL:HG12 | 1:K:2153:THR:H | 1.86 | 0.40 |
| 1:K:2569:HIS:HA | 1:K:2574:PHE:CZ | 2.56 | 0.40 |
| 1:K:2750:ASP:HA | 1:K:2758:ARG:HD2 | 2.03 | 0.40 |
| 1:K:3015:ARG:HH11 | 1:K:3016:PRO:HD2 | 1.86 | 0.40 |
| 1:L:337:GLN:HA | 1:S:1585:ASN:C | 2.46 | 0.40 |
| 1:L:365:TYR:CE2 | 1:L:367:PHE:HB2 | 2.55 | 0.40 |
| 1:L:468:ALA:HB1 | 1:L:633:PHE:HA | 2.02 | 0.40 |
| 1:L:728:ASP:HB3 | 1:L:836:HIS:CD2 | 2.56 | 0.40 |
| 1:L:874:SER:O | 1:L:877:GLY:N | 2.53 | 0.40 |
| 1:L:1367:TYR:CE1 | 1:L:1376:GLU:HB3 | 2.56 | 0.40 |
| 1:L:1801:ASP:OD1 | 1:L:1802:ILE:N | 2.55 | 0.40 |
| 1:L:2919:LYS:HB3 | 1:L:2920:ASP:H | 1.55 | 0.40 |
| 1:M:381:ASN:OD1 | 1:M:381:ASN:N | 2.55 | 0.40 |
| 1:M:693:HIS:CE1 | 1:M:705:GLU:HB3 | 2.55 | 0.40 |
| 1:M:827:THR:O | 1:M:828:ILE:HD13 | 2.22 | 0.40 |
| 1:M:922:GLU:O | 1:M:926:ARG:HG2 | 2.21 | 0.40 |
| 1:M:2794:GLU:HA | 1:M:2797:ARG:HG3 | 2.02 | 0.40 |
| 1:M:3047:ASP:HB2 | 1:M:3097:GLY:HA3 | 2.02 | 0.40 |
| 1:M:3204:ILE:O | 1:M:3207:LEU:HG | 2.21 | 0.40 |
| 1:M:3352:LYS:HA | 1:M:3371:ASN:O | 2.22 | 0.40 |
| 1:N:614:HIS:HD1 | 1:N:637:PHE:HE1 | 1.68 | 0.40 |
| 1:N:878:PHE:O | 1:N:881:ILE:HG12 | 2.21 | 0.40 |
| 1:N:1283:LEU:CG | 1:N:1284:ARG:HH12 | 2.34 | 0.40 |
| 1:N:2162:THR:O | 1:N:2165:VAL:HG22 | 2.20 | 0.40 |
| 1:N:3389:VAL:HG23 | 1:N:3401:ARG:NH2 | 2.36 | 0.40 |
| 1:O:371:LYS:HD3 | 1:O:371:LYS:HA | 1.68 | 0.40 |
| 1:O:1564:ASN:HB3 | 1:O:1604:PHE:CE1 | 2.56 | 0.40 |
| 1:O:2008:LYS:H | 1:O:2041:LYS:HE2 | 1.86 | 0.40 |
| 1:O:2181:TRP:H | 1:O:2297:THR:HG22 | 1.86 | 0.40 |
| 1:O:2956:ILE:HD12 | 1:O:2959:PHE:HE2 | 1.84 | 0.40 |
| 1:O:3033:SER:O | 1:O:3046:ARG:NH2 | 2.54 | 0.40 |
| 1:P:113:LYS:HE2 | 1:P:113:LYS:HB2 | 1.86 | 0.40 |
| 1:P:443:GLU:HG2 | 1:P:444:GLU:N | 2.35 | 0.40 |
| 1:P:496:PHE:CE1 | 1:P:500:HIS:CE1 | 3.09 | 0.40 |
| 1:P:656:ILE:HD12 | 1:P:656:ILE:H | 1.85 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:P:673:GLU:C | 1:P:695:ARG:HH12 | 2.28 | 0.40 |
| 1:P:901:ALA:C | 1:P:903:CYS:H | 2.29 | 0.40 |
| 1:P:1543:LEU:O | 1:P:1546:VAL:HG12 | 2.21 | 0.40 |
| 1:P:1878:ASP:OD2 | 1:P:1881:PHE:N | 2.53 | 0.40 |
| 1:P:2738:GLN:HA | 1:P:2741:ARG:HH21 | 1.87 | 0.40 |
| 1:Q:41:PHE:CE1 | 1:Q:253:PRO:HG2 | 2.56 | 0.40 |
| 1:Q:811:LYS:HE2 | 1:Q:811:LYS:HB2 | 1.89 | 0.40 |
| 1:Q:991:LYS:HE3 | 1:Q:994:ARG:HE | 1.86 | 0.40 |
| 1:Q:998:ILE:H | 1:Q:998:ILE:HD12 | 1.85 | 0.40 |
| 1:Q:1315:CYS:HA | 1:Q:1325:TRP:CH2 | 2.56 | 0.40 |
| 1:Q:2214:ARG:HH11 | 1:T:111:ILE:HG13 | 1.86 | 0.40 |
| 1:R:38:LEU:HD21 | 1:R:213:PHE:CZ | 2.57 | 0.40 |
| 1:R:1007:GLU:N | 1:R:1007:GLU:OE1 | 2.54 | 0.40 |
| 1:R:1018:TYR:OH | 1:R:1056:THR:HB | 2.21 | 0.40 |
| 1:R:1106:HIS:HD2 | 1:R:1111:GLU:HG3 | 1.87 | 0.40 |
| 1:R:1560:PHE:HE2 | 1:R:1593:PHE:HE1 | 1.70 | 0.40 |
| 1:R:1677:ARG:HA | 1:R:1677:ARG:HD3 | 1.74 | 0.40 |
| 1:R:1910:ASN:O | 1:R:1913:LEU:HG | 2.21 | 0.40 |
| 1:R:2822:CYS:HB2 | 1:R:2871:HIS:NE2 | 2.36 | 0.40 |
| 1:R:2930:SER:O | 1:R:2934:VAL:HG23 | 2.22 | 0.40 |
| 1:R:2932:GLU:O | 1:R:2935:SER:OG | 2.32 | 0.40 |
| 1:R:3316:LEU:HD23 | 1:R:3338:VAL:HA | 2.04 | 0.40 |
| 1:R:3344:VAL:HG12 | 1:R:3346:SER:H | 1.87 | 0.40 |
| 1:S:5:ARG:HH21 | 1:S:90:GLY:HA3 | 1.86 | 0.40 |
| 1:S:989:LYS:HA | 1:S:989:LYS:HD2 | 1.70 | 0.40 |
| 1:S:1153:PHE:CZ | 1:S:1166:LEU:HD11 | 2.56 | 0.40 |
| 1:S:1212:GLU:CD | 1:S:1214:ASN:H | 2.29 | 0.40 |
| 1:S:1357:GLN:OE1 | 1:S:1357:GLN:N | 2.54 | 0.40 |
| 1:S:1422:PHE:O | 1:S:1425:GLN:NE2 | 2.55 | 0.40 |
| 1:S:1424:ILE:HG13 | 1:S:1606:PHE:CE2 | 2.56 | 0.40 |
| 1:S:1571:VAL:HG22 | 1:S:1593:PHE:O | 2.21 | 0.40 |
| 1:S:2515:LYS:HG2 | 1:S:2777:ASP:HB3 | 2.04 | 0.40 |
| 1:S:2912:ASP:OD1 | 1:S:2912:ASP:N | 2.51 | 0.40 |
| 1:S:3160:GLU:HG2 | 1:S:3169:ARG:NH2 | 2.36 | 0.40 |
| 1:T:562:LEU:HA | 1:T:562:LEU:HD23 | 1.89 | 0.40 |
| 1:T:842:HIS:NE2 | 1:T:844:GLU:HB2 | 2.36 | 0.40 |
| 1:T:1280:LYS:HE2 | 1:T:1280:LYS:HB3 | 1.77 | 0.40 |
| 1:T:1821:ASP:OD1 | 1:T:1821:ASP:N | 2.50 | 0.40 |
| 1:T:2796:ARG:HA | 1:T:2796:ARG:HD2 | 1.75 | 0.40 |
| 1:T:2979:HIS:HA | 1:T:2984:PHE:CD2 | 2.48 | 0.40 |
| 1:A:562:LEU:HD23 | 1:A:562:LEU:HA | 1.88 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:629:HIS:HA | 1:A:775:LYS:NZ | 2.37 | 0.40 |
| 1:A:1060:TRP:O | 1:A:1064:GLN:OE1 | 2.39 | 0.40 |
| 1:A:1745:LEU:O | 1:A:1748:VAL:HG12 | 2.22 | 0.40 |
| 1:A:1760:LEU:H | 1:A:1760:LEU:HD23 | 1.86 | 0.40 |
| 1:A:2741:ARG:NH2 | 1:J:2867:ASP:OD1 | 2.49 | 0.40 |
| 1:A:3138:ARG:HA | 1:A:3138:ARG:HD3 | 1.85 | 0.40 |
| 1:B:461:VAL:HG22 | 1:B:1277:GLU:OE2 | 2.22 | 0.40 |
| 1:B:477:CYS:HA | 1:B:479:ARG:N | 2.36 | 0.40 |
| 1:B:634:ASP:OD1 | 1:B:636:ILE:HG12 | 2.21 | 0.40 |
| 1:B:1419:PHE:HE1 | 1:B:1468:TRP:HE1 | 1.69 | 0.40 |
| 1:B:1560:PHE:O | 1:B:1609:LEU:HD12 | 2.20 | 0.40 |
| 1:B:2345:ASN:O | 1:B:2349:ARG:HG2 | 2.21 | 0.40 |
| 1:B:2527:SER:O | 1:B:2530:LYS:HG3 | 2.21 | 0.40 |
| 1:B:3088:HIS:CE1 | 1:B:3119:HIS:CE1 | 3.07 | 0.40 |
| 1:C:188:ILE:HD13 | 1:C:188:ILE:HA | 1.94 | 0.40 |
| 1:C:612:LEU:HD21 | 1:C:768:LEU:HA | 2.02 | 0.40 |
| 1:C:1204:ASP:OD1 | 1:C:1205:ILE:N | 2.53 | 0.40 |
| 1:C:1265:ARG:HD2 | 1:C:1530:TYR:CE1 | 2.56 | 0.40 |
| 1:C:2742:GLN:HG2 | 1:C:2743:PRO:HD2 | 2.02 | 0.40 |
| 1:C:2811:PHE:HE2 | 1:C:2836:VAL:HG11 | 1.86 | 0.40 |
| 1:D:71:ARG:O | 1:D:74:VAL:HG22 | 2.21 | 0.40 |
| 1:D:135:MET:HG2 | 1:D:137:VAL:HG13 | 2.03 | 0.40 |
| 1:D:348:ILE:HD13 | 1:D:348:ILE:HA | 1.95 | 0.40 |
| 1:D:357:MET:HE3 | 1:D:358:PRO:CD | 2.42 | 0.40 |
| 1:D:509:ASP:OD1 | 1:D:509:ASP:N | 2.53 | 0.40 |
| 1:D:735:ARG:NH2 | 1:D:789:ILE:H | 2.19 | 0.40 |
| 1:D:968:PHE:CD1 | 1:D:1047:PRO:HG2 | 2.55 | 0.40 |
| 1:D:1139:GLU:O | 1:D:1143:ARG:HG2 | 2.21 | 0.40 |
| 1:D:1223:VAL:HG13 | 1:D:1231:ILE:HB | 2.02 | 0.40 |
| 1:D:2530:LYS:HA | 1:D:2533:ARG:NH1 | 2.36 | 0.40 |
| 1:D:2712:VAL:HA | 1:D:2715:GLN:HE21 | 1.85 | 0.40 |
| 1:D:3080:PHE:C | 1:D:3083:GLN:HE22 | 2.30 | 0.40 |
| 1:E:814:SER:C | 1:E:816:LYS:HZ2 | 2.29 | 0.40 |
| 1:E:903:CYS:C | 1:E:905:HIS:HD1 | 2.26 | 0.40 |
| 1:E:1174:PRO:HG2 | 1:E:1176:HIS:CE1 | 2.56 | 0.40 |
| 1:E:1307:HIS:O | 1:E:1308:GLU:HG2 | 2.21 | 0.40 |
| 1:E:2022:MET:SD | 1:E:2022:MET:N | 2.94 | 0.40 |
| 1:E:2392:ARG:HB3 | 1:E:2394:PHE:CE1 | 2.57 | 0.40 |
| 1:E:2876:ILE:HD11 | 1:E:2885:ALA:O | 2.22 | 0.40 |
| 1:E:3037:ILE:HG22 | 1:E:3042:HIS:O | 2.21 | 0.40 |
| 1:E:3144:ARG:HA | 1:E:3147:LEU:HG | 2.03 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:F:1063:TRP:NE1 | 1:F:1067:GLN:HE22 | 2.19 | 0.40 |
| 1:F:1766:TRP:C | 1:F:1766:TRP:CD1 | 2.98 | 0.40 |
| 1:F:2980:GLY:HA2 | 1:F:3085:GLU:CD | 2.47 | 0.40 |
| 1:F:3395:ARG:NE | 1:F:3400:THR:OG1 | 2.42 | 0.40 |
| 1:G:172:ASP:OD2 | 1:G:233:ARG:NH1 | 2.54 | 0.40 |
| 1:G:763:TYR:HE2 | 1:G:792:ALA:HB1 | 1.87 | 0.40 |
| 1:G:885:HIS:ND1 | 1:G:885:HIS:O | 2.54 | 0.40 |
| 1:G:1025:ILE:HG21 | 1:G:1052:HIS:NE2 | 2.37 | 0.40 |
| 1:G:1162:ALA:HB1 | 1:G:1224:ILE:O | 2.22 | 0.40 |
| 1:G:1209:TYR:O | 1:G:1210:LYS:HG2 | 2.21 | 0.40 |
| 1:G:1212:GLU:CD | 1:G:1214:ASN:H | 2.29 | 0.40 |
| 1:G:1541:PRO:HD2 | 1:G:1542:GLN:OE1 | 2.21 | 0.40 |
| 1:G:1905:ASP:HB3 | 1:G:1908:GLU:HB2 | 2.02 | 0.40 |
| 1:G:2088:PRO:HD2 | 1:G:2366:ARG:NH1 | 2.32 | 0.40 |
| 1:G:2790:GLU:HA | 1:G:2793:ILE:HG22 | 2.03 | 0.40 |
| 1:G:2819:PHE:CZ | 1:G:2832:GLY:HA3 | 2.56 | 0.40 |
| 1:G:3204:ILE:O | 1:G:3207:LEU:HG | 2.22 | 0.40 |
| 1:G:3389:VAL:HG22 | 1:G:3401:ARG:HG2 | 2.03 | 0.40 |
| 1:H:12:THR:N | 1:H:15:GLU:OE2 | 2.46 | 0.40 |
| 1:H:729:GLU:O | 1:H:732:THR:HG22 | 2.20 | 0.40 |
| 1:H:742:LEU:HD12 | 1:H:823:PHE:CZ | 2.56 | 0.40 |
| 1:H:1195:ASP:OD1 | 1:H:1195:ASP:N | 2.40 | 0.40 |
| 1:H:1766:TRP:CD1 | 1:H:1766:TRP:C | 3.00 | 0.40 |
| 1:H:2338:ASN:OD1 | 1:H:2338:ASN:N | 2.54 | 0.40 |
| 1:H:3395:ARG:HD2 | 1:H:3395:ARG:HA | 1.70 | 0.40 |
| 1:I:330:ASP:OD1 | 1:I:331:HIS:N | 2.53 | 0.40 |
| 1:I:409:VAL:HG13 | 1:I:666:CYS:HA | 2.02 | 0.40 |
| 1:I:485:ARG:HA | 1:I:485:ARG:HD3 | 1.86 | 0.40 |
| 1:I:950:VAL:HG12 | 1:I:968:PHE:CD2 | 2.56 | 0.40 |
| 1:I:954:THR:HA | 1:I:965:PRO:HA | 2.03 | 0.40 |
| 1:I:1322:PHE:CD2 | 1:I:1426:PHE:HE2 | 2.39 | 0.40 |
| 1:I:1978:LYS:HA | 1:I:2078:LYS:HG2 | 2.02 | 0.40 |
| 1:I:2473:ILE:HG22 | 1:I:2481:LEU:HD13 | 2.04 | 0.40 |
| 1:I:2966:CYS:HB3 | 1:I:2974:TYR:O | 2.22 | 0.40 |
| 1:J:297:TYR:O | 1:J:301:GLU:OE1 | 2.40 | 0.40 |
| 1:J:789:ILE:HG22 | 1:J:793:LEU:HD23 | 2.03 | 0.40 |
| 1:J:900:PHE:HE2 | 1:J:1191:PRO:HD3 | 1.86 | 0.40 |
| 1:J:959:GLU:OE2 | 1:J:960:THR:HG23 | 2.21 | 0.40 |
| 1:J:1223:VAL:C | 1:J:1230:LYS:HZ2 | 2.30 | 0.40 |
| 1:J:1900:ARG:HH22 | 1:J:1901:LEU:HD13 | 1.86 | 0.40 |
| 1:J:1978:LYS:NZ | 1:J:1979:SER:O | 2.55 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:J:1993:SER:O | 1:J:2058:LEU:HG | 2.21 | 0.40 |
| 1:J:2453:LEU:HA | 1:J:2453:LEU:HD23 | 1.85 | 0.40 |
| 1:J:2786:ILE:N | 1:J:2787:PRO:HD2 | 2.36 | 0.40 |
| 1:J:2795:LYS:HE2 | 1:J:2795:LYS:HB2 | 1.79 | 0.40 |
| 1:K:1162:ALA:HB1 | 1:K:1224:ILE:O | 2.21 | 0.40 |
| 1:K:1844:CYS:HB3 | 1:K:2027:ASP:OD2 | 2.22 | 0.40 |
| 1:K:1881:PHE:CE1 | 1:K:1885:HIS:CE1 | 3.10 | 0.40 |
| 1:K:2260:PHE:O | 1:K:2264:PHE:HD2 | 2.04 | 0.40 |
| 1:K:2328:ASN:HD21 | 1:L:1240:THR:HA | 1.86 | 0.40 |
| 1:K:2989:ARG:NH2 | 1:K:3180:ALA:HB2 | 2.36 | 0.40 |
| 1:K:3103:MET:HE2 | 1:K:3115:PHE:HD1 | 1.86 | 0.40 |
| 1:L:473:LEU:HD21 | 1:L:775:LYS:HG3 | 2.03 | 0.40 |
| 1:L:1362:ILE:HG22 | 1:L:1380:PHE:HB3 | 2.02 | 0.40 |
| 1:L:2095:GLU:CD | 1:L:2097:SER:H | 2.28 | 0.40 |
| 1:L:2157:TRP:HD1 | 1:L:2334:MET:SD | 2.44 | 0.40 |
| 1:L:2269:ASN:HD21 | 1:L:2428:LEU:N | 2.18 | 0.40 |
| 1:L:2343:ASN:ND2 | 1:L:2349:ARG:HH21 | 2.19 | 0.40 |
| 1:L:2655:TYR:CD1 | 1:L:2659:LEU:HD23 | 2.56 | 0.40 |
| 1:L:2661:ALA:O | 1:L:2664:GLN:NE2 | 2.54 | 0.40 |
| 1:M:195:ARG:NH2 | 1:M:393:VAL:O | 2.45 | 0.40 |
| 1:M:348:ILE:HD13 | 1:M:348:ILE:HA | 1.94 | 0.40 |
| 1:M:629:HIS:HA | 1:M:775:LYS:HZ3 | 1.86 | 0.40 |
| 1:M:889:ASN:HB3 | 1:M:900:PHE:O | 2.21 | 0.40 |
| 1:M:1169:CYS:HA | 1:M:1175:CYS:HA | 2.03 | 0.40 |
| 1:M:1563:HIS:HB2 | 1:M:1605:ILE:HD13 | 2.03 | 0.40 |
| 1:M:1718:PRO:C | 1:M:1719:LEU:HD12 | 2.46 | 0.40 |
| 1:M:2238:ASP:OD1 | 1:M:2239:GLY:N | 2.54 | 0.40 |
| 1:M:2605:GLU:HA | 1:M:2605:GLU:OE2 | 2.21 | 0.40 |
| 1:M:2714:ARG:NH2 | 1:M:2778:ASP:O | 2.54 | 0.40 |
| 1:M:3188:ASP:OD1 | 1:M:3189:ASN:N | 2.54 | 0.40 |
| 1:N:158:ASN:HB3 | 1:N:162:PHE:CD2 | 2.56 | 0.40 |
| 1:N:363:LEU:HD23 | 1:N:363:LEU:HA | 1.90 | 0.40 |
| 1:N:695:ARG:HG3 | 1:N:697:THR:HG23 | 2.03 | 0.40 |
| 1:N:1356:ARG:HH12 | 1:N:1401:PHE:HB3 | 1.86 | 0.40 |
| 1:N:1777:ALA:HA | 1:N:1780:ASN:HB3 | 2.03 | 0.40 |
| 1:N:1852:ILE:HA | 1:N:1855:ASN:ND2 | 2.37 | 0.40 |
| 1:N:2001:CYS:HB2 | 1:N:2050:THR:OG1 | 2.22 | 0.40 |
| 1:N:2072:SER:OG | 1:N:2073:VAL:N | 2.53 | 0.40 |
| 1:N:3124:ARG:HG2 | 1:N:3124:ARG:HH11 | 1.87 | 0.40 |
| 1:N:3127:GLN:O | 1:N:3130:GLN:HG3 | 2.21 | 0.40 |
| 1:O:1168:VAL:HG12 | 1:O:1178:GLU:CD | 2.46 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:O:1966:GLU:H | 1:O:1966:GLU:CD | 2.27 | 0.40 |
| 1:O:2517:ILE:HG13 | 1:O:2518:ASN:N | 2.37 | 0.40 |
| 1:O:2678:HIS:CE1 | 1:O:2682:HIS:CE1 | 3.09 | 0.40 |
| 1:O:2696:LEU:O | 1:O:2699:SER:OG | 2.29 | 0.40 |
| 1:O:3188:ASP:N | 1:O:3188:ASP:OD1 | 2.54 | 0.40 |
| 1:P:325:ARG:HG2 | 1:P:347:ASP:CG | 2.46 | 0.40 |
| 1:P:428:SER:OG | 1:P:429:ALA:N | 2.54 | 0.40 |
| 1:P:441:THR:HB | 1:P:444:GLU:OE1 | 2.21 | 0.40 |
| 1:P:636:ILE:O | 1:P:639:LEU:HG | 2.20 | 0.40 |
| 1:P:755:ILE:HG21 | 1:P:792:ALA:HB1 | 2.03 | 0.40 |
| 1:P:1733:VAL:HB | 1:P:1736:MET:SD | 2.62 | 0.40 |
| 1:P:2127:ALA:HA | 1:P:2161:TYR:OH | 2.21 | 0.40 |
| 1:P:2576:GLN:HE21 | 1:P:2767:PHE:HE1 | 1.69 | 0.40 |
| 1:Q:771:LEU:HD12 | 1:Q:772:GLY:N | 2.37 | 0.40 |
| 1:Q:958:PRO:HA | 1:Q:961:ASN:HA | 2.02 | 0.40 |
| 1:Q:1272:SER:OG | 1:Q:1275:GLU:OE1 | 2.36 | 0.40 |
| 1:Q:1620:LYS:HE2 | 1:R:2724:ARG:HD3 | 2.04 | 0.40 |
| 1:Q:1632:ASP:OD1 | 1:Q:1632:ASP:N | 2.55 | 0.40 |
| 1:Q:2036:GLU:O | 1:Q:2039:GLU:HG3 | 2.22 | 0.40 |
| 1:Q:2369:ASP:OD1 | 1:Q:2369:ASP:N | 2.54 | 0.40 |
| 1:Q:2602:ASP:OD2 | 1:Q:2603:TRP:N | 2.55 | 0.40 |
| 1:Q:3122:ILE:HA | 1:Q:3125:ILE:HG22 | 2.04 | 0.40 |
| 1:Q:3133:GLN:HE21 | 1:Q:3138:ARG:CB | 2.34 | 0.40 |
| 1:R:878:PHE:CE1 | 1:R:881:ILE:HD11 | 2.56 | 0.40 |
| 1:R:1077:ALA:H | 1:R:1113:PHE:HE2 | 1.69 | 0.40 |
| 1:R:1270:ASP:OD2 | 1:R:1270:ASP:C | 2.64 | 0.40 |
| 1:R:1854:HIS:O | 1:R:1884:HIS:HE1 | 2.04 | 0.40 |
| 1:R:1884:HIS:O | 1:R:1888:THR:HG23 | 2.20 | 0.40 |
| 1:R:2304:LYS:HA | 1:R:2367:TYR:CE2 | 2.55 | 0.40 |
| 1:R:2529:LYS:HE2 | 1:R:2529:LYS:HB3 | 1.89 | 0.40 |
| 1:S:744:ASN:HB3 | 1:S:779:TRP:NE1 | 2.35 | 0.40 |
| 1:S:1420:CYS:HB2 | 1:S:1608:ARG:HH21 | 1.85 | 0.40 |
| 1:S:2088:PRO:HB2 | 1:S:2091:ARG:HH12 | 1.86 | 0.40 |
| 1:S:2149:HIS:HA | 1:S:2154:PHE:HD2 | 1.85 | 0.40 |
| 1:S:2151:VAL:HG12 | 1:S:2153:THR:H | 1.87 | 0.40 |
| 1:S:2517:ILE:HG13 | 1:S:2518:ASN:N | 2.36 | 0.40 |
| 1:S:2931:LEU:HA | 1:S:2934:VAL:HG12 | 2.03 | 0.40 |
| 1:T:297:TYR:O | 1:T:301:GLU:OE1 | 2.39 | 0.40 |
| 1:T:506:GLN:NE2 | 1:T:690:THR:OG1 | 2.53 | 0.40 |
| 1:T:673:GLU:C | 1:T:695:ARG:HH22 | 2.20 | 0.40 |
| 1:T:741:HIS:HE1 | 1:T:780:ASN:HD21 | 1.69 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:T:1356:ARG:NH2 | 1:T:1402:ASN:H | 2.20 | 0.40 |
| 1:T:1457:PHE:CE2 | 1:T:1461:HIS:HE1 | 2.40 | 0.40 |
| 1:T:2266:VAL:HG21 | 1:T:2442:TYR:CZ | 2.56 | 0.40 |
| 1:T:2822:CYS:HB2 | 1:T:2871:HIS:CD2 | 2.56 | 0.40 |
| 1:T:2943:LYS:HB3 | 1:T:3002:LYS:HD2 | 2.04 | 0.40 |
| 1:T:3153:PRO:HB3 | 1:T:3158:ASN:CG | 2.46 | 0.40 |
| 1:T:3225:SER:HB2 | 1:T:3290:TYR:CD1 | 2.57 | 0.40 |
| 1:A:22:TYR:CD1 | 1:A:86:LEU:HD22 | 2.56 | 0.40 |
| 1:A:418:ASP:OD2 | 1:A:663:LYS:N | 2.44 | 0.40 |
| 1:A:657:LYS:NZ | 1:A:720:ILE:O | 2.50 | 0.40 |
| 1:A:744:ASN:HB3 | 1:A:779:TRP:NE1 | 2.37 | 0.40 |
| 1:A:792:ALA:HA | 1:A:795:LYS:HG2 | 2.02 | 0.40 |
| 1:A:1390:LYS:HE3 | 1:A:1390:LYS:HB3 | 1.94 | 0.40 |
| 1:A:1677:ARG:O | 1:A:1678:LYS:HD3 | 2.21 | 0.40 |
| 1:A:1845:ASP:OD1 | 1:A:2028:ARG:HD2 | 2.21 | 0.40 |
| 1:A:2093:ARG:NH1 | 1:A:2177:ALA:O | 2.55 | 0.40 |
| 1:A:2415:GLU:CD | 1:A:2466:PRO:HA | 2.46 | 0.40 |
| 1:A:2454:HIS:O | 1:A:2456:ARG:NH1 | 2.55 | 0.40 |
| 1:A:3047:ASP:CB | 1:A:3097:GLY:HA3 | 2.51 | 0.40 |
| 1:A:3338:VAL:HG11 | 1:A:3381:LEU:CD1 | 2.51 | 0.40 |
| 1:B:24:ARG:HA | 1:B:24:ARG:HD2 | 1.90 | 0.40 |
| 1:B:867:GLN:HA | 1:B:870:GLU:HG3 | 2.03 | 0.40 |
| 1:B:1204:ASP:OD1 | 1:B:1204:ASP:N | 2.54 | 0.40 |
| 1:B:1270:ASP:OD1 | 1:B:1271:LEU:N | 2.55 | 0.40 |
| 1:B:1325:TRP:HD1 | 1:B:1326:HIS:ND1 | 2.18 | 0.40 |
| 1:B:1602:MET:HA | 1:B:1602:MET:HE2 | 2.03 | 0.40 |
| 1:B:2264:PHE:CZ | 1:B:2302:VAL:HG13 | 2.56 | 0.40 |
| 1:B:2504:ALA:O | 1:B:2505:SER:HB3 | 2.21 | 0.40 |
| 1:B:2966:CYS:O | 1:B:2973:ARG:HB3 | 2.21 | 0.40 |
| 1:C:131:ASN:HA | 1:C:138:HIS:HA | 2.04 | 0.40 |
| 1:C:742:LEU:HB2 | 1:C:781:PHE:CE2 | 2.57 | 0.40 |
| 1:C:1587:ASN:H | 1:F:337:GLN:N | 2.19 | 0.40 |
| 1:C:1982:PHE:HB2 | 1:C:2074:LEU:HB2 | 2.03 | 0.40 |
| 1:C:2328:ASN:HD21 | 1:D:1240:THR:HA | 1.86 | 0.40 |
| 1:C:2339:SER:OG | 1:C:2340:VAL:N | 2.54 | 0.40 |
| 1:C:2425:ILE:HG13 | 1:C:2442:TYR:HE2 | 1.87 | 0.40 |
| 1:C:2585:LEU:HD13 | 1:C:2706:PHE:CZ | 2.56 | 0.40 |
| 1:C:3049:GLN:HG2 | 1:C:3050:PRO:HD2 | 2.02 | 0.40 |
| 1:C:3217:PHE:HE1 | 1:C:3302:PRO:HB3 | 1.87 | 0.40 |
| 1:C:3352:LYS:HD3 | 1:C:3366:PRO:HD2 | 2.03 | 0.40 |
| 1:D:756:LYS:HB3 | 1:D:805:ASP:HB2 | 2.03 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:D:848:ARG:O | 1:D:1124:ASP:N | 2.45 | 0.40 |
| 1:D:1098:ASN:HB2 | 1:D:1104:ARG:HH11 | 1.86 | 0.40 |
| 1:D:1205:ILE:HD12 | 1:D:1208:LYS:HE3 | 2.04 | 0.40 |
| 1:D:2404:THR:OG1 | 1:D:2405:SER:N | 2.54 | 0.40 |
| 1:D:2676:VAL:HA | 1:D:2679:ASN:HD21 | 1.86 | 0.40 |
| 1:D:2923:ARG:HD3 | 1:D:3008:ILE:C | 2.46 | 0.40 |
| 1:E:1013:THR:O | 1:E:1016:VAL:HG12 | 2.22 | 0.40 |
| 1:E:1709:ALA:O | 1:E:1712:SER:OG | 2.26 | 0.40 |
| 1:E:1824:HIS:H | 1:E:1827:ASP:CG | 2.29 | 0.40 |
| 1:E:2091:ARG:HH21 | 1:E:2364:ASN:HD21 | 1.70 | 0.40 |
| 1:E:2390:LYS:HB2 | 1:E:2390:LYS:HE2 | 1.87 | 0.40 |
| 1:E:2639:ARG:HG2 | 1:E:2684:TRP:HZ3 | 1.86 | 0.40 |
| 1:E:2698:TYR:HA | 1:E:2701:TYR:HE2 | 1.87 | 0.40 |
| 1:E:2820:ASP:OD1 | 1:E:2831:ALA:N | 2.43 | 0.40 |
| 1:F:223:PHE:HZ | 1:F:274:PHE:HD1 | 1.69 | 0.40 |
| 1:F:376:LEU:HD12 | 1:F:376:LEU:HA | 1.87 | 0.40 |
| 1:F:725:HIS:O | 1:F:729:GLU:HG2 | 2.21 | 0.40 |
| 1:F:1275:GLU:OE1 | 1:F:1275:GLU:N | 2.51 | 0.40 |
| 1:F:1472:GLN:O | 1:F:1475:GLN:HB2 | 2.21 | 0.40 |
| 1:F:1724:GLU:O | 1:H:397:SER:N | 2.39 | 0.40 |
| 1:F:2411:SER:OG | 1:F:2420:THR:O | 2.24 | 0.40 |
| 1:F:2477:ASN:OD1 | 1:F:2477:ASN:N | 2.54 | 0.40 |
| 1:F:2665:ARG:HA | 1:F:2723:GLN:HE22 | 1.85 | 0.40 |
| 1:F:3019:ALA:HB2 | 1:F:3053:TYR:CZ | 2.56 | 0.40 |
| 1:F:3227:THR:HB | 1:F:3246:TYR:CD2 | 2.56 | 0.40 |
| 1:G:129:GLU:HG2 | 1:G:139:THR:C | 2.46 | 0.40 |
| 1:G:561:PHE:CD2 | 1:G:562:LEU:HG | 2.56 | 0.40 |
| 1:G:903:CYS:C | 1:G:905:HIS:HD1 | 2.25 | 0.40 |
| 1:G:1111:GLU:N | 1:G:1111:GLU:OE1 | 2.55 | 0.40 |
| 1:G:1159:ARG:HA | 1:G:1186:ASP:O | 2.21 | 0.40 |
| 1:G:2370:MET:SD | 1:G:2370:MET:N | 2.94 | 0.40 |
| 1:G:2624:HIS:HB2 | 1:G:2633:LYS:NZ | 2.36 | 0.40 |
| 1:G:2770:ASP:OD1 | 1:G:2771:GLN:N | 2.55 | 0.40 |
| 1:G:2820:ASP:HA | 1:G:2831:ALA:HB3 | 2.03 | 0.40 |
| 1:G:2943:LYS:HE2 | 1:G:2943:LYS:HA | 2.04 | 0.40 |
| 1:G:3231:LYS:HB2 | 1:G:3284:GLN:HG3 | 2.04 | 0.40 |
| 1:H:106:LEU:HD12 | 1:H:125:TRP:CE3 | 2.57 | 0.40 |
| 1:H:486:TYR:HA | 1:H:775:LYS:HE3 | 2.03 | 0.40 |
| 1:H:676:LYS:HA | 1:H:677:PRO:HA | 1.89 | 0.40 |
| 1:H:866:LEU:HD22 | 1:H:968:PHE:CZ | 2.56 | 0.40 |
| 1:H:1321:VAL:HA | 1:H:1324:HIS:CD2 | 2.56 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:H:1433:LEU:HD21 | 1:H:1460:HIS:CD2 | 2.57 | 0.40 |
| 1:H:1710:LEU:HB3 | 1:H:1750:PHE:CZ | 2.56 | 0.40 |
| 1:H:2072:SER:OG | 1:H:2073:VAL:N | 2.54 | 0.40 |
| 1:H:2152:PRO:O | 1:H:2155:PRO:HD2 | 2.21 | 0.40 |
| 1:H:2158:HIS:HB3 | 1:H:2299:HIS:CD2 | 2.57 | 0.40 |
| 1:H:2794:GLU:OE2 | 1:H:2794:GLU:HA | 2.20 | 0.40 |
| 1:H:2940:ALA:HA | 1:H:3002:LYS:HB3 | 2.02 | 0.40 |
| 1:I:46:SER:HB3 | 1:I:57:ALA:HA | 2.03 | 0.40 |
| 1:I:69:TRP:HZ3 | 1:I:70:HIS:CE1 | 2.39 | 0.40 |
| 1:I:125:TRP:HZ3 | 1:I:214:LEU:HD21 | 1.87 | 0.40 |
| 1:I:193:GLY:HA3 | 1:I:201:SER:H | 1.85 | 0.40 |
| 1:I:248:ARG:NH1 | 1:I:803:GLU:HA | 2.37 | 0.40 |
| 1:I:1221:TYR:HH | 1:I:1236:PHE:H | 1.64 | 0.40 |
| 1:I:1364:GLU:HA | 1:I:1364:GLU:OE2 | 2.22 | 0.40 |
| 1:I:1400:LEU:HD21 | 1:I:1436:LEU:HB3 | 2.03 | 0.40 |
| 1:I:1431:ASN:HB2 | 1:I:1596:LEU:HB2 | 2.03 | 0.40 |
| 1:I:2728:LEU:HD12 | 1:I:2728:LEU:HA | 1.96 | 0.40 |
| 1:I:3395:ARG:HE | 1:I:3398:GLN:CD | 2.27 | 0.40 |
| 1:J:228:GLU:HA | 1:J:231:LYS:CG | 2.50 | 0.40 |
| 1:J:308:ARG:H | 1:J:411:ARG:HB3 | 1.85 | 0.40 |
| 1:J:558:PRO:HA | 1:J:565:THR:HA | 2.03 | 0.40 |
| 1:J:1088:LEU:CD2 | 1:J:1109:PRO:HG3 | 2.51 | 0.40 |
| 1:J:1416:GLN:NE2 | 1:J:1422:PHE:HA | 2.36 | 0.40 |
| 1:J:1828:ASN:ND2 | 1:J:1831:TRP:HB2 | 2.36 | 0.40 |
| 1:J:2072:SER:OG | 1:J:2073:VAL:N | 2.53 | 0.40 |
| 1:J:2324:ASP:OD1 | 1:J:2325:CYS:N | 2.54 | 0.40 |
| 1:J:2988:HIS:HD2 | 1:J:3119:HIS:CD2 | 2.39 | 0.40 |
| 1:J:3214:TYR:HD1 | 1:J:3265:ASP:HA | 1.85 | 0.40 |
| 1:K:23:LEU:HD12 | 1:K:23:LEU:HA | 1.88 | 0.40 |
| 1:K:489:CYS:C | 1:K:491:HIS:HD1 | 2.29 | 0.40 |
| 1:K:584:THR:HG23 | 1:K:587:PHE:H | 1.85 | 0.40 |
| 1:K:844:GLU:O | 1:K:846:HIS:N | 2.55 | 0.40 |
| 1:K:881:ILE:HD11 | 1:K:920:GLN:HG2 | 2.03 | 0.40 |
| 1:K:971:GLY:N | 1:K:978:THR:OG1 | 2.46 | 0.40 |
| 1:K:1061:ALA:HA | 1:K:1064:GLN:CD | 2.46 | 0.40 |
| 1:K:2157:TRP:HD1 | 1:K:2334:MET:HG2 | 1.86 | 0.40 |
| 1:K:2264:PHE:HE1 | 1:K:2302:VAL:HG13 | 1.86 | 0.40 |
| 1:K:2567:CYS:C | 1:K:2569:HIS:HD1 | 2.28 | 0.40 |
| 1:K:2770:ASP:OD1 | 1:K:2771:GLN:N | 2.54 | 0.40 |
| 1:K:2876:ILE:HD11 | 1:K:2885:ALA:O | 2.21 | 0.40 |
| 1:L:308:ARG:H | 1:L:411:ARG:HB3 | 1.85 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:L:327:LYS:HG3 | 1:L:343:GLU:O | 2.20 | 0.40 |
| 1:L:1452:ALA:HA | 1:L:1457:PHE:CD2 | 2.55 | 0.40 |
| 1:L:1854:HIS:O | 1:L:1884:HIS:HE1 | 2.03 | 0.40 |
| 1:L:2330:MET:SD | 1:L:2331:SER:N | 2.94 | 0.40 |
| 1:L:2434:MET:O | 1:L:2436:TRP:HD1 | 2.04 | 0.40 |
| 1:L:2530:LYS:HA | 1:L:2533:ARG:NH1 | 2.36 | 0.40 |
| 1:L:2654:PHE:HD1 | 1:L:2677:THR:HG23 | 1.86 | 0.40 |
| 1:L:2977:CYS:HA | 1:L:2987:TRP:CH2 | 2.57 | 0.40 |
| 1:M:151:GLN:OE1 | 1:M:151:GLN:N | 2.54 | 0.40 |
| 1:M:680:PHE:HB2 | 1:M:684:LEU:HD22 | 2.04 | 0.40 |
| 1:M:920:GLN:HE22 | 1:M:1100:ASP:HB3 | 1.86 | 0.40 |
| 1:M:1159:ARG:O | 1:M:1186:ASP:HA | 2.21 | 0.40 |
| 1:M:1705:THR:OG1 | 1:M:1931:LEU:HD22 | 2.21 | 0.40 |
| 1:M:1849:GLN:HA | 1:M:1852:ILE:HG22 | 2.03 | 0.40 |
| 1:M:2147:CYS:C | 1:M:2149:HIS:HD1 | 2.27 | 0.40 |
| 1:M:2614:LEU:HD12 | 1:M:2636:ARG:NH2 | 2.29 | 0.40 |
| 1:M:3105:THR:O | 1:M:3109:SER:HB3 | 2.21 | 0.40 |
| 1:M:3220:SER:OG | 1:M:3221:GLY:N | 2.53 | 0.40 |
| 1:N:11:LEU:HD11 | 1:N:92:PRO:HG3 | 2.04 | 0.40 |
| 1:N:435:LYS:HG2 | 1:N:436:ASP:N | 2.35 | 0.40 |
| 1:N:587:PHE:O | 1:N:591:LEU:HG | 2.21 | 0.40 |
| 1:N:655:GLN:OE1 | 1:N:660:LEU:HB3 | 2.22 | 0.40 |
| 1:N:788:GLU:CD | 1:N:791:ASP:H | 2.27 | 0.40 |
| 1:N:928:LYS:HG3 | 1:N:929:GLY:N | 2.37 | 0.40 |
| 1:N:1131:PHE:HB3 | 1:N:1136:LEU:CD2 | 2.51 | 0.40 |
| 1:N:3131:THR:HA | 1:N:3134:LYS:HG2 | 2.04 | 0.40 |
| 1:O:20:GLU:HB2 | 1:O:24:ARG:NH1 | 2.36 | 0.40 |
| 1:O:42:HIS:NE2 | 1:O:59:CYS:SG | 2.95 | 0.40 |
| 1:O:1241:VAL:HG12 | 1:P:2328:ASN:ND2 | 2.37 | 0.40 |
| 1:O:1440:ARG:NH2 | 1:R:1368:PHE:HB3 | 2.37 | 0.40 |
| 1:O:1522:TYR:HA | 1:O:1526:PHE:HB2 | 2.02 | 0.40 |
| 1:O:1998:ILE:HG13 | 1:O:2010:ALA:HB3 | 2.03 | 0.40 |
| 1:O:2012:ASP:N | 1:O:2012:ASP:OD1 | 2.54 | 0.40 |
| 1:O:2159:ARG:NH2 | 1:O:2360:TYR:HB3 | 2.37 | 0.40 |
| 1:O:2614:LEU:HD12 | 1:O:2636:ARG:NH1 | 2.31 | 0.40 |
| 1:P:409:VAL:HG13 | 1:P:665:HIS:O | 2.21 | 0.40 |
| 1:P:663:LYS:HE3 | 1:P:665:HIS:HE1 | 1.87 | 0.40 |
| 1:P:1351:TRP:CZ3 | 1:P:1463:ASN:HB3 | 2.56 | 0.40 |
| 1:P:3058:GLN:N | 1:P:3061:LEU:O | 2.44 | 0.40 |
| 1:P:3106:LEU:HA | 1:P:3109:SER:HB3 | 2.04 | 0.40 |
| 1:Q:7:ASN:OD1 | 1:Q:7:ASN:N | 2.55 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:Q:51:ASP:N | 1:Q:51:ASP:OD1 | 2.53 | 0.40 |
| 1:Q:196:HIS:O | 1:Q:199:SER:OG | 2.40 | 0.40 |
| 1:Q:559:VAL:HG22 | 1:Q:633:PHE:HD2 | 1.86 | 0.40 |
| 1:Q:761:ASP:OD1 | 1:Q:761:ASP:N | 2.44 | 0.40 |
| 1:Q:1149:VAL:HG11 | 1:Q:1206:LEU:HD11 | 2.02 | 0.40 |
| 1:Q:1913:LEU:HD11 | 1:R:1628:ALA:HB3 | 2.04 | 0.40 |
| 1:Q:2102:ARG:HG3 | 1:Q:2103:ALA:N | 2.36 | 0.40 |
| 1:Q:2245:PHE:O | 1:Q:2249:LEU:HD23 | 2.20 | 0.40 |
| 1:Q:2313:GLN:CD | 1:Q:2318:LEU:HB2 | 2.46 | 0.40 |
| 1:Q:2654:PHE:O | 1:Q:2657:GLN:HG2 | 2.21 | 0.40 |
| 1:R:536:ALA:HB2 | 1:R:554:PHE:HD2 | 1.87 | 0.40 |
| 1:R:954:THR:HB | 1:R:963:PRO:HB2 | 2.04 | 0.40 |
| 1:R:1133:ILE:H | 1:R:1133:ILE:HD12 | 1.86 | 0.40 |
| 1:R:1283:LEU:HG | 1:R:1284:ARG:HH22 | 1.86 | 0.40 |
| 1:R:1921:LYS:N | 1:R:1921:LYS:HD2 | 2.37 | 0.40 |
| 1:R:2359:ASN:OD1 | 1:R:2359:ASN:N | 2.53 | 0.40 |
| 1:R:2432:LEU:N | 1:R:2433:GLU:OE1 | 2.54 | 0.40 |
| 1:S:328:VAL:HG13 | 1:S:376:LEU:HD11 | 2.03 | 0.40 |
| 1:S:1298:PHE:HZ | 1:S:1504:GLN:HB3 | 1.86 | 0.40 |
| 1:S:1571:VAL:O | 1:S:1592:SER:HB2 | 2.21 | 0.40 |
| 1:S:1969:LEU:HA | 1:S:1972:ILE:HG12 | 2.04 | 0.40 |
| 1:S:2036:GLU:O | 1:S:2039:GLU:HG3 | 2.21 | 0.40 |
| 1:S:3337:ARG:NH2 | 1:S:3378:ASN:HB2 | 2.36 | 0.40 |
| 1:S:3385:ASP:C | 1:T:3148:ARG:HH22 | 2.28 | 0.40 |
| 1:T:509:ASP:OD1 | 1:T:510:ALA:N | 2.52 | 0.40 |
| 1:T:741:HIS:CE1 | 1:T:780:ASN:HD21 | 2.40 | 0.40 |
| 1:T:914:HIS:O | 1:T:918:THR:HG23 | 2.21 | 0.40 |
| 1:T:1225:ASP:HB2 | 1:T:1229:LYS:HB2 | 2.03 | 0.40 |
| 1:T:1865:LYS:NZ | 1:T:1866:GLU:OE2 | 2.46 | 0.40 |
| 1:T:1979:SER:N | 1:T:2078:LYS:HD3 | 2.35 | 0.40 |
| 1:T:2523:ALA:O | 1:T:2526:GLU:HG3 | 2.22 | 0.40 |
| 1:T:2578:HIS:CD2 | 1:T:2709:HIS:CD2 | 3.09 | 0.40 |
| 1:T:2671:GLU:HA | 1:T:2674:TYR:HB3 | 2.03 | 0.40 |
| 1:T:3131:THR:HG23 | 1:T:3134:LYS:HZ1 | 1.87 | 0.40 |
| 1:A:89:ILE:HG22 | 1:A:90:GLY:O | 2.22 | 0.40 |
| 1:A:158:ASN:HB2 | 1:A:162:PHE:CD2 | 2.56 | 0.40 |
| 1:A:176:HIS:CD2 | 1:A:363:LEU:HD21 | 2.57 | 0.40 |
| 1:A:1133:ILE:HB | 1:A:1134:PRO:HD3 | 2.03 | 0.40 |
| 1:A:1448:LEU:HB3 | 1:A:1596:LEU:HD11 | 2.03 | 0.40 |
| 1:A:1564:ASN:HB3 | 1:A:1604:PHE:CE2 | 2.56 | 0.40 |
| 1:A:1649:VAL:HG13 | 1:A:1650:LEU:CD2 | 2.51 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:1723:PRO:HA | 1:A:1728:ARG:HH12 | 1.87 | 0.40 |
| 1:A:2674:TYR:CE1 | 1:A:2716:PHE:HB2 | 2.56 | 0.40 |
| 1:A:2700:ALA:HA | 1:A:2705:PHE:CD2 | 2.56 | 0.40 |
| 1:A:3160:GLU:HG2 | 1:A:3169:ARG:NH2 | 2.36 | 0.40 |
| 1:B:480:PRO:C | 1:B:485:ARG:HH12 | 2.30 | 0.40 |
| 1:B:610:HIS:O | 1:B:613:PRO:HD2 | 2.22 | 0.40 |
| 1:B:928:LYS:HG3 | 1:B:929:GLY:N | 2.36 | 0.40 |
| 1:B:1947:TYR:CZ | 1:B:1948:LYS:HG3 | 2.56 | 0.40 |
| 1:B:2001:CYS:HB2 | 1:B:2050:THR:OG1 | 2.21 | 0.40 |
| 1:B:2273:TYR:HE2 | 1:B:2476:VAL:HG12 | 1.87 | 0.40 |
| 1:B:2712:VAL:HA | 1:B:2715:GLN:NE2 | 2.36 | 0.40 |
| 1:B:3071:THR:HG23 | 1:B:3083:GLN:HE21 | 1.87 | 0.40 |
| 1:C:166:LEU:O | 1:C:169:LEU:HG | 2.21 | 0.40 |
| 1:C:277:ARG:HH22 | 1:K:731:ARG:NH1 | 2.16 | 0.40 |
| 1:C:608:VAL:HG22 | 1:C:768:LEU:HD11 | 2.02 | 0.40 |
| 1:C:910:PHE:CE2 | 1:C:914:HIS:CE1 | 3.09 | 0.40 |
| 1:C:1266:ARG:NH2 | 1:C:1270:ASP:OD2 | 2.54 | 0.40 |
| 1:C:1858:HIS:NE2 | 1:C:1884:HIS:HE1 | 2.19 | 0.40 |
| 1:C:2056:ARG:HD2 | 1:C:2056:ARG:HA | 1.89 | 0.40 |
| 1:C:2102:ARG:HA | 1:C:2105:MET:HE3 | 2.04 | 0.40 |
| 1:C:2729:ASP:OD1 | 1:C:2916:THR:HB | 2.21 | 0.40 |
| 1:C:3055:ARG:HD3 | 1:C:3062:ASP:OD1 | 2.21 | 0.40 |
| 1:C:3100:THR:HA | 1:C:3290:TYR:CE2 | 2.49 | 0.40 |
| 1:D:328:VAL:HG22 | 1:D:386:VAL:HG22 | 2.03 | 0.40 |
| 1:D:501:ARG:HA | 1:D:501:ARG:HD3 | 1.78 | 0.40 |
| 1:D:938:ASP:CG | 1:D:1055:ASN:HD21 | 2.29 | 0.40 |
| 1:D:982:VAL:HG23 | 1:D:986:LEU:HD12 | 2.03 | 0.40 |
| 1:D:1085:ARG:HD3 | 1:D:1110:PHE:CZ | 2.56 | 0.40 |
| 1:D:1295:ILE:HG21 | 1:D:1333:VAL:HG23 | 2.04 | 0.40 |
| 1:D:2922:VAL:HG22 | 1:D:3186:ASN:ND2 | 2.36 | 0.40 |
| 1:E:91:VAL:HA | 1:E:92:PRO:HD3 | 1.94 | 0.40 |
| 1:E:191:LEU:HD23 | 1:E:191:LEU:HA | 1.95 | 0.40 |
| 1:E:471:HIS:CE1 | 1:E:637:PHE:HZ | 2.39 | 0.40 |
| 1:E:596:GLN:O | 1:E:597:ARG:NE | 2.52 | 0.40 |
| 1:E:1153:PHE:CZ | 1:E:1166:LEU:HD11 | 2.56 | 0.40 |
| 1:E:1745:LEU:HD23 | 1:E:1923:PHE:HD2 | 1.86 | 0.40 |
| 1:E:1998:ILE:HG13 | 1:E:2010:ALA:HB3 | 2.02 | 0.40 |
| 1:E:3103:MET:HE2 | 1:E:3115:PHE:HD1 | 1.87 | 0.40 |
| 1:F:714:GLN:NE2 | 1:F:717:GLY:O | 2.51 | 0.40 |
| 1:F:1143:ARG:HB3 | 1:F:1148:ARG:NH2 | 2.35 | 0.40 |
| 1:F:1433:LEU:O | 1:F:1437:VAL:HG22 | 2.22 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:F:1531:ASP:OD1 | 1:F:1532:THR:N | 2.54 | 0.40 |
| 1:F:1824:HIS:HB2 | 1:F:1827:ASP:CG | 2.47 | 0.40 |
| 1:F:1894:LEU:HD11 | 1:F:1965:ALA:HB2 | 2.02 | 0.40 |
| 1:F:2087:LEU:H | 1:F:2366:ARG:NH1 | 2.18 | 0.40 |
| 1:F:2876:ILE:HB | 1:F:2884:LEU:HB2 | 2.03 | 0.40 |
| 1:F:3216:GLY:C | 1:F:3217:PHE:HD1 | 2.30 | 0.40 |
| 1:G:307:GLU:OE1 | 1:G:412:PRO:HA | 2.21 | 0.40 |
| 1:G:371:LYS:HA | 1:G:371:LYS:HD3 | 1.68 | 0.40 |
| 1:G:473:LEU:H | 1:G:775:LYS:HE3 | 1.86 | 0.40 |
| 1:G:569:GLN:HB3 | 1:G:619:GLY:HA3 | 2.02 | 0.40 |
| 1:G:1066:LEU:HD21 | 1:G:1070:ARG:NH2 | 2.36 | 0.40 |
| 1:G:2027:ASP:OD1 | 1:G:2028:ARG:N | 2.54 | 0.40 |
| 1:G:2509:SER:H | 1:G:3138:ARG:NH2 | 2.18 | 0.40 |
| 1:H:408:GLY:HA3 | 1:H:669:THR:HG21 | 2.02 | 0.40 |
| 1:H:587:PHE:O | 1:H:591:LEU:HG | 2.22 | 0.40 |
| 1:H:832:GLU:OE1 | 1:H:832:GLU:N | 2.54 | 0.40 |
| 1:H:1049:PHE:O | 1:H:1053:HIS:ND1 | 2.48 | 0.40 |
| 1:H:1312:VAL:HG23 | 1:H:1600:THR:HG22 | 2.03 | 0.40 |
| 1:H:1521:ASP:HB3 | 1:H:1525:HIS:CD2 | 2.56 | 0.40 |
| 1:H:1824:HIS:H | 1:H:1827:ASP:CG | 2.30 | 0.40 |
| 1:H:1972:ILE:HG13 | 1:H:1973:ASN:N | 2.36 | 0.40 |
| 1:H:2038:LEU:HD12 | 1:H:2039:GLU:N | 2.37 | 0.40 |
| 1:H:2216:TYR:HD1 | 1:H:2218:LYS:HD2 | 1.87 | 0.40 |
| 1:H:2283:LEU:HD21 | 1:H:2292:ASP:HB3 | 2.04 | 0.40 |
| 1:I:189:HIS:HE1 | 1:I:212:PHE:CD1 | 2.40 | 0.40 |
| 1:I:332:ASP:OD1 | 1:I:332:ASP:N | 2.46 | 0.40 |
| 1:I:962:LEU:HD12 | 1:I:962:LEU:HA | 1.95 | 0.40 |
| 1:I:1219:VAL:HG23 | 1:I:1239:VAL:HG13 | 2.02 | 0.40 |
| 1:I:1301:PHE:CG | 1:I:1302:PRO:HA | 2.56 | 0.40 |
| 1:I:1502:LYS:HB3 | 1:I:1511:ASN:HD21 | 1.86 | 0.40 |
| 1:I:2182:ASP:OD1 | 1:I:2183:TRP:N | 2.55 | 0.40 |
| 1:I:2521:THR:O | 1:I:2525:THR:OG1 | 2.33 | 0.40 |
| 1:I:2961:GLY:HA2 | 1:I:3106:LEU:HD23 | 2.04 | 0.40 |
| 1:I:3070:GLU:O | 1:I:3073:GLU:HG2 | 2.21 | 0.40 |
| 1:I:3188:ASP:OD1 | 1:I:3189:ASN:N | 2.53 | 0.40 |
| 1:J:508:GLU:HA | 1:J:511:LEU:HD12 | 2.04 | 0.40 |
| 1:J:525:TRP:CD1 | 1:J:586:LEU:HD13 | 2.57 | 0.40 |
| 1:J:969:HIS:C | 1:J:980:ARG:HH12 | 2.30 | 0.40 |
| 1:J:2155:PRO:HB2 | 1:J:2306:TRP:CE3 | 2.57 | 0.40 |
| 1:J:2421:ARG:CZ | 1:J:2423:GLY:HA2 | 2.52 | 0.40 |
| 1:J:2693:MET:HE1 | 1:J:2705:PHE:N | 2.36 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:J:2704:ILE:HD13 | 1:J:2707:ILE:HD12 | 2.03 | 0.40 |
| 1:J:3010:TYR:OH | 1:J:3188:ASP:OD1 | 2.37 | 0.40 |
| 1:J:3021:PRO:HD2 | 1:J:3024:LEU:HD13 | 2.04 | 0.40 |
| 1:J:3256:TRP:HZ3 | 1:J:3258:TYR:CE1 | 2.39 | 0.40 |
| 1:J:3388:PHE:HB2 | 1:J:3402:VAL:HG13 | 2.04 | 0.40 |
| 1:K:381:ASN:O | 1:K:668:HIS:NE2 | 2.50 | 0.40 |
| 1:K:636:ILE:HA | 1:K:639:LEU:HD12 | 2.04 | 0.40 |
| 1:K:1397:GLN:HG3 | 1:K:1399:GLU:CD | 2.47 | 0.40 |
| 1:K:2313:GLN:CG | 1:K:2320:TYR:HB3 | 2.52 | 0.40 |
| 1:K:3089:ASN:HD21 | 1:K:3247:ILE:HD12 | 1.86 | 0.40 |
| 1:L:506:GLN:HE22 | 1:L:687:ASN:CB | 2.35 | 0.40 |
| 1:L:568:ARG:NH1 | 1:L:634:ASP:OD1 | 2.49 | 0.40 |
| 1:L:645:ASP:OD1 | 1:L:710:TYR:OH | 2.33 | 0.40 |
| 1:L:866:LEU:HD22 | 1:L:968:PHE:CZ | 2.57 | 0.40 |
| 1:L:941:LEU:H | 1:L:941:LEU:HD12 | 1.86 | 0.40 |
| 1:L:959:GLU:OE2 | 1:L:960:THR:HG23 | 2.22 | 0.40 |
| 1:L:1894:LEU:HD13 | 1:L:1958:LEU:HB3 | 2.04 | 0.40 |
| 1:L:1995:HIS:ND1 | 1:L:2013:PHE:O | 2.54 | 0.40 |
| 1:L:2337:PHE:O | 1:L:2349:ARG:NH1 | 2.55 | 0.40 |
| 1:L:2589:LEU:HG | 1:L:2594:ALA:CB | 2.52 | 0.40 |
| 1:M:574:LEU:HB3 | 1:M:616:LEU:HD21 | 2.02 | 0.40 |
| 1:M:1568:SER:N | 1:M:1597:GLY:O | 2.55 | 0.40 |
| 1:M:3289:LYS:HG2 | 1:M:3295:LEU:HD21 | 2.03 | 0.40 |
| 1:N:281:TYR:CE2 | 1:N:283:TYR:HE1 | 2.39 | 0.40 |
| 1:N:914:HIS:O | 1:N:917:LEU:HG | 2.22 | 0.40 |
| 1:N:1291:THR:HA | 1:N:1294:LYS:HZ3 | 1.86 | 0.40 |
| 1:N:1472:GLN:O | 1:N:1475:GLN:HB2 | 2.21 | 0.40 |
| 1:N:2148:LEU:HD21 | 1:N:2153:THR:OG1 | 2.22 | 0.40 |
| 1:N:2580:LEU:O | 1:N:2584:THR:HG23 | 2.21 | 0.40 |
| 1:O:655:GLN:OE1 | 1:O:660:LEU:HB2 | 2.20 | 0.40 |
| 1:O:1082:ALA:HB2 | 1:P:2491:ILE:HG13 | 2.04 | 0.40 |
| 1:O:1153:PHE:HB2 | 1:O:1198:PHE:HD2 | 1.85 | 0.40 |
| 1:O:1204:ASP:OD1 | 1:O:1205:ILE:N | 2.54 | 0.40 |
| 1:O:1364:GLU:OE2 | 1:O:1364:GLU:HA | 2.22 | 0.40 |
| 1:O:1482:ASP:OD1 | 1:O:1483:ASP:N | 2.53 | 0.40 |
| 1:O:1651:ARG:HH11 | 1:P:2025:SER:HB2 | 1.87 | 0.40 |
| 1:O:1802:ILE:HG12 | 1:O:1807:THR:O | 2.21 | 0.40 |
| 1:O:1931:LEU:HB3 | 1:P:2102:ARG:HB2 | 2.04 | 0.40 |
| 1:O:2152:PRO:HD2 | 1:O:2329:TYR:CD2 | 2.56 | 0.40 |
| 1:O:2369:ASP:N | 1:O:2369:ASP:OD1 | 2.54 | 0.40 |
| 1:O:2394:PHE:CD2 | 1:O:2443:LYS:HG2 | 2.56 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:O:2581:PHE:O | 1:O:2584:THR:HG22 | 2.22 | 0.40 |
| 1:O:2648:ARG:HB2 | 1:O:2656:ARG:HH21 | 1.87 | 0.40 |
| 1:O:2926:VAL:HG12 | 1:O:3009:PRO:HB2 | 2.03 | 0.40 |
| 1:P:32:VAL:HA | 1:P:37:ASN:ND2 | 2.36 | 0.40 |
| 1:P:69:TRP:CD1 | 1:P:251:LEU:HD22 | 2.57 | 0.40 |
| 1:P:308:ARG:HB3 | 1:P:310:LEU:HD21 | 2.03 | 0.40 |
| 1:P:1159:ARG:HG2 | 1:P:1186:ASP:C | 2.47 | 0.40 |
| 1:P:1275:GLU:H | 1:P:1275:GLU:CD | 2.27 | 0.40 |
| 1:P:1301:PHE:CG | 1:P:1302:PRO:HA | 2.57 | 0.40 |
| 1:P:1328:LEU:HG | 1:P:1499:PHE:CE2 | 2.56 | 0.40 |
| 1:P:1750:PHE:CD2 | 1:P:1882:LEU:HD11 | 2.53 | 0.40 |
| 1:P:2264:PHE:HZ | 1:P:2302:VAL:HG13 | 1.86 | 0.40 |
| 1:P:2378:ASP:O | 1:P:2381:GLU:HG2 | 2.22 | 0.40 |
| 1:P:2511:ILE:HD12 | 1:P:2772:PHE:O | 2.21 | 0.40 |
| 1:P:2530:LYS:HA | 1:P:2533:ARG:NH1 | 2.37 | 0.40 |
| 1:Q:881:ILE:HA | 1:Q:884:PHE:CD2 | 2.48 | 0.40 |
| 1:Q:915:ARG:HD3 | 1:Q:1060:TRP:CE3 | 2.57 | 0.40 |
| 1:Q:1517:ILE:HD12 | 1:Q:1517:ILE:H | 1.86 | 0.40 |
| 1:Q:1690:SER:O | 1:Q:1693:LEU:HG | 2.22 | 0.40 |
| 1:Q:2775:GLN:N | 1:Q:2775:GLN:OE1 | 2.55 | 0.40 |
| 1:Q:3049:GLN:HG2 | 1:Q:3050:PRO:HD2 | 2.04 | 0.40 |
| 1:Q:3160:GLU:HG2 | 1:Q:3169:ARG:NH2 | 2.37 | 0.40 |
| 1:R:22:TYR:OH | 1:R:85:GLY:O | 2.29 | 0.40 |
| 1:R:480:PRO:O | 1:R:485:ARG:NH1 | 2.52 | 0.40 |
| 1:R:538:LYS:HE3 | 1:R:538:LYS:HB3 | 1.90 | 0.40 |
| 1:R:627:THR:HG21 | 1:R:630:TYR:HD2 | 1.87 | 0.40 |
| 1:R:751:VAL:HG22 | 1:R:810:ILE:HD13 | 2.03 | 0.40 |
| 1:R:946:LEU:HG | 1:R:951:ALA:HB2 | 2.03 | 0.40 |
| 1:R:1295:ILE:HG21 | 1:R:1333:VAL:HG23 | 2.02 | 0.40 |
| 1:R:1426:PHE:CZ | 1:R:1464:VAL:HG13 | 2.57 | 0.40 |
| 1:R:1710:LEU:HD13 | 1:R:1750:PHE:CE1 | 2.56 | 0.40 |
| 1:R:2787:PRO:HA | 1:R:2790:GLU:HG2 | 2.03 | 0.40 |
| 1:R:2980:GLY:HA3 | 1:R:3256:TRP:CZ3 | 2.56 | 0.40 |
| 1:S:704:HIS:ND1 | 1:S:705:GLU:OE2 | 2.54 | 0.40 |
| 1:S:1060:TRP:O | 1:S:1064:GLN:OE1 | 2.39 | 0.40 |
| 1:S:1449:ASP:OD1 | 1:S:1450:TYR:N | 2.54 | 0.40 |
| 1:S:1894:LEU:O | 1:S:1898:LEU:HD23 | 2.21 | 0.40 |
| 1:S:2096:ILE:HG21 | 1:S:2193:LEU:HD22 | 2.03 | 0.40 |
| 1:S:2254:GLN:OE1 | 1:S:2254:GLN:N | 2.46 | 0.40 |
| 1:S:2287:HIS:HE1 | 1:S:2432:LEU:HG | 1.87 | 0.40 |
| 1:S:2639:ARG:HH21 | 1:S:2687:GLY:HA2 | 1.86 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:T:231:LYS:HB3 | 1:T:237:TYR:CE2 | 2.56 | 0.40 |
| 1:T:299:LEU:O | 1:T:302:GLN:HG3 | 2.22 | 0.40 |
| 1:T:1164:VAL:HG12 | 1:T:1181:PHE:H | 1.85 | 0.40 |
| 1:T:2416:ASN:OD1 | 1:T:2417:GLY:N | 2.54 | 0.40 |
| 1:T:2929:LEU:HG | 1:T:2934:VAL:HG23 | 2.04 | 0.40 |
| 1:T:3191:ASN:HA | 1:T:3195:HIS:O | 2.21 | 0.40 |
| 1:T:3322:GLU:OE1 | 1:T:3322:GLU:N | 2.50 | 0.40 |
| 2:lA:1:NAG:H61 | 2:lA:2:NAG:H2 | 2.03 | 0.40 |

There are no symmetry-related clashes.

## 5.3 Torsion angles (i)

### 5.3.1 Protein backbone (i)

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

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|---|---|---|---|---|---|---|---|
| 1 | A | 3377/3408 (99%) | 3136 (93%) | 241 (7%) | 0 | 100 | 100 |
| 1 | B | 3382/3408 (99%) | 3151 (93%) | 231 (7%) | 0 | 100 | 100 |
| 1 | C | 3377/3408 (99%) | 3138 (93%) | 238 (7%) | 1 (0%) | 100 | 100 |
| 1 | D | 3382/3408 (99%) | 3141 (93%) | 241 (7%) | 0 | 100 | 100 |
| 1 | E | 3377/3408 (99%) | 3143 (93%) | 233 (7%) | 1 (0%) | 100 | 100 |
| 1 | F | 3382/3408 (99%) | 3151 (93%) | 231 (7%) | 0 | 100 | 100 |
| 1 | G | 3377/3408 (99%) | 3143 (93%) | 234 (7%) | 0 | 100 | 100 |
| 1 | H | 3382/3408 (99%) | 3135 (93%) | 247 (7%) | 0 | 100 | 100 |
| 1 | I | 3377/3408 (99%) | 3132 (93%) | 244 (7%) | 1 (0%) | 100 | 100 |
| 1 | J | 3381/3408 (99%) | 3128 (92%) | 253 (8%) | 0 | 100 | 100 |
| 1 | K | 3377/3408 (99%) | 3146 (93%) | 231 (7%) | 0 | 100 | 100 |
| 1 | L | 3382/3408 (99%) | 3147 (93%) | 235 (7%) | 0 | 100 | 100 |
| 1 | M | 3377/3408 (99%) | 3130 (93%) | 246 (7%) | 1 (0%) | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|---|---|---|---|---|---|---|---|
| 1 | N | 3382/3408 (99%) | 3140 (93%) | 242 (7%) | 0 | 100 | 100 |
| 1 | O | 3377/3408 (99%) | 3139 (93%) | 238 (7%) | 0 | 100 | 100 |
| 1 | P | 3382/3408 (99%) | 3137 (93%) | 245 (7%) | 0 | 100 | 100 |
| 1 | Q | 3377/3408 (99%) | 3139 (93%) | 237 (7%) | 1 (0%) | 100 | 100 |
| 1 | R | 3382/3408 (99%) | 3143 (93%) | 239 (7%) | 0 | 100 | 100 |
| 1 | S | 3377/3408 (99%) | 3135 (93%) | 241 (7%) | 1 (0%) | 100 | 100 |
| 1 | T | 3381/3408 (99%) | 3159 (93%) | 222 (7%) | 0 | 100 | 100 |
| All | All | 67588/68160 (99%) | 62813 (93%) | 4769 (7%) | 6 (0%) | 100 | 100 |

All (6) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | M | 1509 | LEU |
| 1 | I | 2477 | ASN |
| 1 | E | 2511 | ILE |
| 1 | Q | 2511 | ILE |
| 1 | S | 2511 | ILE |
| 1 | C | 2511 | ILE |

### 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 PDB entries followed by that with respect to all EM entries.

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|---|---|---|---|---|---|---|
| 1 | A | 2965/2981 (100%) | 2965 (100%) | 0 | 100 | 100 |
| 1 | B | 2964/2981 (99%) | 2963 (100%) | 1 (0%) | 100 | 100 |
| 1 | C | 2965/2981 (100%) | 2965 (100%) | 0 | 100 | 100 |
| 1 | D | 2965/2981 (100%) | 2965 (100%) | 0 | 100 | 100 |
| 1 | E | 2965/2981 (100%) | 2965 (100%) | 0 | 100 | 100 |
| 1 | F | 2965/2981 (100%) | 2965 (100%) | 0 | 100 | 100 |
| 1 | G | 2964/2981 (99%) | 2964 (100%) | 0 | 100 | 100 |
| 1 | H | 2965/2981 (100%) | 2965 (100%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|---|---|---|---|---|---|---|
| 1 | I | 2965/2981 (100%) | 2965 (100%) | 0 | 100 | 100 |
| 1 | J | 2964/2981 (99%) | 2964 (100%) | 0 | 100 | 100 |
| 1 | K | 2965/2981 (100%) | 2965 (100%) | 0 | 100 | 100 |
| 1 | L | 2964/2981 (99%) | 2963 (100%) | 1 (0%) | 100 | 100 |
| 1 | M | 2965/2981 (100%) | 2965 (100%) | 0 | 100 | 100 |
| 1 | N | 2965/2981 (100%) | 2965 (100%) | 0 | 100 | 100 |
| 1 | O | 2965/2981 (100%) | 2965 (100%) | 0 | 100 | 100 |
| 1 | P | 2965/2981 (100%) | 2965 (100%) | 0 | 100 | 100 |
| 1 | Q | 2964/2981 (99%) | 2964 (100%) | 0 | 100 | 100 |
| 1 | R | 2965/2981 (100%) | 2965 (100%) | 0 | 100 | 100 |
| 1 | S | 2965/2981 (100%) | 2965 (100%) | 0 | 100 | 100 |
| 1 | T | 2964/2981 (99%) | 2964 (100%) | 0 | 100 | 100 |
| All | All | 59294/59620 (100%) | 59292 (100%) | 2 (0%) | 100 | 100 |

All (2) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | B | 499 | TRP |
| 1 | L | 499 | TRP |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1349) such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 61 | HIS |
| 1 | A | 70 | HIS |
| 1 | A | 187 | HIS |
| 1 | A | 189 | HIS |
| 1 | A | 216 | HIS |
| 1 | A | 331 | HIS |
| 1 | A | 491 | HIS |
| 1 | A | 605 | GLN |
| 1 | A | 610 | HIS |
| 1 | A | 640 | HIS |
| 1 | A | 725 | HIS |
| 1 | A | 876 | ASN |
| 1 | A | 905 | HIS |
| 1 | A | 914 | HIS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 920 | GLN |
| 1 | A | 1026 | HIS |
| 1 | A | 1052 | HIS |
| 1 | A | 1055 | ASN |
| 1 | A | 1067 | GLN |
| 1 | A | 1089 | GLN |
| 1 | A | 1176 | HIS |
| 1 | A | 1317 | HIS |
| 1 | A | 1326 | HIS |
| 1 | A | 1409 | ASN |
| 1 | A | 1430 | HIS |
| 1 | A | 1460 | HIS |
| 1 | A | 1461 | HIS |
| 1 | A | 1494 | GLN |
| 1 | A | 1500 | ASN |
| 1 | A | 1505 | ASN |
| 1 | A | 1572 | GLN |
| 1 | A | 1708 | GLN |
| 1 | A | 1734 | HIS |
| 1 | A | 1743 | HIS |
| 1 | A | 1749 | GLN |
| 1 | A | 1772 | GLN |
| 1 | A | 1854 | HIS |
| 1 | A | 1855 | ASN |
| 1 | A | 1884 | HIS |
| 1 | A | 2085 | GLN |
| 1 | A | 2149 | HIS |
| 1 | A | 2299 | HIS |
| 1 | A | 2345 | ASN |
| 1 | A | 2569 | HIS |
| 1 | A | 2657 | GLN |
| 1 | A | 2664 | GLN |
| 1 | A | 2678 | HIS |
| 1 | A | 2682 | HIS |
| 1 | A | 2708 | HIS |
| 1 | A | 2723 | GLN |
| 1 | A | 2788 | GLN |
| 1 | A | 2809 | GLN |
| 1 | A | 2960 | HIS |
| 1 | A | 2979 | HIS |
| 1 | A | 3043 | GLN |
| 1 | A | 3089 | ASN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 3092 | HIS |
| 1 | A | 3149 | ASN |
| 1 | A | 3189 | ASN |
| 1 | A | 3206 | ASN |
| 1 | A | 3291 | ASN |
| 1 | A | 3294 | GLN |
| 1 | B | 37 | ASN |
| 1 | B | 61 | HIS |
| 1 | B | 70 | HIS |
| 1 | B | 131 | ASN |
| 1 | B | 186 | ASN |
| 1 | B | 331 | HIS |
| 1 | B | 450 | GLN |
| 1 | B | 491 | HIS |
| 1 | B | 545 | ASN |
| 1 | B | 610 | HIS |
| 1 | B | 614 | HIS |
| 1 | B | 643 | ASN |
| 1 | B | 655 | GLN |
| 1 | B | 665 | HIS |
| 1 | B | 741 | HIS |
| 1 | B | 794 | ASN |
| 1 | B | 846 | HIS |
| 1 | B | 858 | GLN |
| 1 | B | 887 | GLN |
| 1 | B | 905 | HIS |
| 1 | B | 914 | HIS |
| 1 | B | 969 | HIS |
| 1 | B | 1052 | HIS |
| 1 | B | 1068 | HIS |
| 1 | B | 1078 | ASN |
| 1 | B | 1089 | GLN |
| 1 | B | 1142 | HIS |
| 1 | B | 1317 | HIS |
| 1 | B | 1326 | HIS |
| 1 | B | 1408 | ASN |
| 1 | B | 1430 | HIS |
| 1 | B | 1431 | ASN |
| 1 | B | 1475 | GLN |
| 1 | B | 1542 | GLN |
| 1 | B | 1665 | GLN |
| 1 | B | 1708 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | B | 1727 | GLN |
| 1 | B | 1734 | HIS |
| 1 | B | 1743 | HIS |
| 1 | B | 1867 | HIS |
| 1 | B | 1884 | HIS |
| 1 | B | 1952 | ASN |
| 1 | B | 1973 | ASN |
| 1 | B | 2149 | HIS |
| 1 | B | 2229 | GLN |
| 1 | B | 2254 | GLN |
| 1 | B | 2263 | GLN |
| 1 | B | 2298 | HIS |
| 1 | B | 2345 | ASN |
| 1 | B | 2454 | HIS |
| 1 | B | 2569 | HIS |
| 1 | B | 2631 | ASN |
| 1 | B | 2679 | ASN |
| 1 | B | 2711 | ASN |
| 1 | B | 2715 | GLN |
| 1 | B | 2752 | ASN |
| 1 | B | 2775 | GLN |
| 1 | B | 2933 | GLN |
| 1 | B | 2951 | ASN |
| 1 | B | 2979 | HIS |
| 1 | B | 2994 | GLN |
| 1 | B | 3088 | HIS |
| 1 | B | 3089 | ASN |
| 1 | B | 3092 | HIS |
| 1 | B | 3206 | ASN |
| 1 | B | 3276 | ASN |
| 1 | B | 3310 | ASN |
| 1 | C | 37 | ASN |
| 1 | C | 61 | HIS |
| 1 | C | 68 | GLN |
| 1 | C | 187 | HIS |
| 1 | C | 331 | HIS |
| 1 | C | 491 | HIS |
| 1 | C | 545 | ASN |
| 1 | C | 611 | ASN |
| 1 | C | 640 | HIS |
| 1 | C | 858 | GLN |
| 1 | C | 876 | ASN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | C | 905 | HIS |
| 1 | C | 914 | HIS |
| 1 | C | 1023 | ASN |
| 1 | C | 1026 | HIS |
| 1 | C | 1053 | HIS |
| 1 | C | 1055 | ASN |
| 1 | C | 1106 | HIS |
| 1 | C | 1129 | ASN |
| 1 | C | 1263 | HIS |
| 1 | C | 1317 | HIS |
| 1 | C | 1373 | GLN |
| 1 | C | 1430 | HIS |
| 1 | C | 1476 | GLN |
| 1 | C | 1505 | ASN |
| 1 | C | 1708 | GLN |
| 1 | C | 1734 | HIS |
| 1 | C | 1741 | GLN |
| 1 | C | 1743 | HIS |
| 1 | C | 1884 | HIS |
| 1 | C | 1952 | ASN |
| 1 | C | 2085 | GLN |
| 1 | C | 2149 | HIS |
| 1 | C | 2345 | ASN |
| 1 | C | 2451 | ASN |
| 1 | C | 2454 | HIS |
| 1 | C | 2538 | GLN |
| 1 | C | 2569 | HIS |
| 1 | C | 2578 | HIS |
| 1 | C | 2673 | GLN |
| 1 | C | 2678 | HIS |
| 1 | C | 2679 | ASN |
| 1 | C | 2682 | HIS |
| 1 | C | 2708 | HIS |
| 1 | C | 2711 | ASN |
| 1 | C | 2723 | GLN |
| 1 | C | 2788 | GLN |
| 1 | C | 2805 | ASN |
| 1 | C | 2852 | GLN |
| 1 | C | 2960 | HIS |
| 1 | C | 2979 | HIS |
| 1 | C | 2988 | HIS |
| 1 | C | 3043 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | C | 3088 | HIS |
| 1 | C | 3089 | ASN |
| 1 | C | 3092 | HIS |
| 1 | C | 3176 | GLN |
| 1 | C | 3284 | GLN |
| 1 | C | 3291 | ASN |
| 1 | D | 37 | ASN |
| 1 | D | 42 | HIS |
| 1 | D | 61 | HIS |
| 1 | D | 70 | HIS |
| 1 | D | 123 | ASN |
| 1 | D | 158 | ASN |
| 1 | D | 381 | ASN |
| 1 | D | 450 | GLN |
| 1 | D | 462 | ASN |
| 1 | D | 491 | HIS |
| 1 | D | 498 | HIS |
| 1 | D | 500 | HIS |
| 1 | D | 506 | GLN |
| 1 | D | 610 | HIS |
| 1 | D | 611 | ASN |
| 1 | D | 687 | ASN |
| 1 | D | 693 | HIS |
| 1 | D | 741 | HIS |
| 1 | D | 794 | ASN |
| 1 | D | 858 | GLN |
| 1 | D | 905 | HIS |
| 1 | D | 914 | HIS |
| 1 | D | 1023 | ASN |
| 1 | D | 1055 | ASN |
| 1 | D | 1089 | GLN |
| 1 | D | 1106 | HIS |
| 1 | D | 1199 | GLN |
| 1 | D | 1317 | HIS |
| 1 | D | 1430 | HIS |
| 1 | D | 1431 | ASN |
| 1 | D | 1461 | HIS |
| 1 | D | 1463 | ASN |
| 1 | D | 1475 | GLN |
| 1 | D | 1494 | GLN |
| 1 | D | 1665 | GLN |
| 1 | D | 1727 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | D | 1734 | HIS |
| 1 | D | 1743 | HIS |
| 1 | D | 1849 | GLN |
| 1 | D | 1854 | HIS |
| 1 | D | 1867 | HIS |
| 1 | D | 1871 | HIS |
| 1 | D | 1907 | ASN |
| 1 | D | 1952 | ASN |
| 1 | D | 1973 | ASN |
| 1 | D | 2149 | HIS |
| 1 | D | 2158 | HIS |
| 1 | D | 2164 | GLN |
| 1 | D | 2263 | GLN |
| 1 | D | 2299 | HIS |
| 1 | D | 2345 | ASN |
| 1 | D | 2551 | HIS |
| 1 | D | 2569 | HIS |
| 1 | D | 2669 | ASN |
| 1 | D | 2679 | ASN |
| 1 | D | 2682 | HIS |
| 1 | D | 2708 | HIS |
| 1 | D | 2709 | HIS |
| 1 | D | 2715 | GLN |
| 1 | D | 2720 | GLN |
| 1 | D | 2752 | ASN |
| 1 | D | 2863 | HIS |
| 1 | D | 2960 | HIS |
| 1 | D | 2979 | HIS |
| 1 | D | 3067 | GLN |
| 1 | D | 3088 | HIS |
| 1 | D | 3089 | ASN |
| 1 | D | 3133 | GLN |
| 1 | D | 3149 | ASN |
| 1 | D | 3184 | HIS |
| 1 | D | 3206 | ASN |
| 1 | D | 3276 | ASN |
| 1 | D | 3310 | ASN |
| 1 | E | 37 | ASN |
| 1 | E | 61 | HIS |
| 1 | E | 70 | HIS |
| 1 | E | 138 | HIS |
| 1 | E | 158 | ASN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | E | 189 | HIS |
| 1 | E | 227 | GLN |
| 1 | E | 295 | GLN |
| 1 | E | 331 | HIS |
| 1 | E | 375 | HIS |
| 1 | E | 465 | GLN |
| 1 | E | 491 | HIS |
| 1 | E | 640 | HIS |
| 1 | E | 641 | HIS |
| 1 | E | 725 | HIS |
| 1 | E | 876 | ASN |
| 1 | E | 880 | HIS |
| 1 | E | 905 | HIS |
| 1 | E | 914 | HIS |
| 1 | E | 1026 | HIS |
| 1 | E | 1052 | HIS |
| 1 | E | 1055 | ASN |
| 1 | E | 1144 | GLN |
| 1 | E | 1317 | HIS |
| 1 | E | 1460 | HIS |
| 1 | E | 1494 | GLN |
| 1 | E | 1500 | ASN |
| 1 | E | 1734 | HIS |
| 1 | E | 1772 | GLN |
| 1 | E | 1854 | HIS |
| 1 | E | 1884 | HIS |
| 1 | E | 1899 | GLN |
| 1 | E | 1952 | ASN |
| 1 | E | 1973 | ASN |
| 1 | E | 2085 | GLN |
| 1 | E | 2090 | ASN |
| 1 | E | 2098 | HIS |
| 1 | E | 2149 | HIS |
| 1 | E | 2158 | HIS |
| 1 | E | 2278 | HIS |
| 1 | E | 2299 | HIS |
| 1 | E | 2345 | ASN |
| 1 | E | 2538 | GLN |
| 1 | E | 2569 | HIS |
| 1 | E | 2578 | HIS |
| 1 | E | 2592 | GLN |
| 1 | E | 2673 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | E | 2678 | HIS |
| 1 | E | 2679 | ASN |
| 1 | E | 2708 | HIS |
| 1 | E | 2711 | ASN |
| 1 | E | 2723 | GLN |
| 1 | E | 2773 | ASN |
| 1 | E | 2788 | GLN |
| 1 | E | 2805 | ASN |
| 1 | E | 2852 | GLN |
| 1 | E | 2960 | HIS |
| 1 | E | 2979 | HIS |
| 1 | E | 2988 | HIS |
| 1 | E | 3036 | GLN |
| 1 | E | 3043 | GLN |
| 1 | E | 3089 | ASN |
| 1 | E | 3092 | HIS |
| 1 | E | 3176 | GLN |
| 1 | E | 3284 | GLN |
| 1 | E | 3291 | ASN |
| 1 | E | 3294 | GLN |
| 1 | F | 37 | ASN |
| 1 | F | 61 | HIS |
| 1 | F | 131 | ASN |
| 1 | F | 186 | ASN |
| 1 | F | 187 | HIS |
| 1 | F | 295 | GLN |
| 1 | F | 366 | HIS |
| 1 | F | 491 | HIS |
| 1 | F | 545 | ASN |
| 1 | F | 583 | HIS |
| 1 | F | 610 | HIS |
| 1 | F | 611 | ASN |
| 1 | F | 614 | HIS |
| 1 | F | 643 | ASN |
| 1 | F | 714 | GLN |
| 1 | F | 860 | GLN |
| 1 | F | 876 | ASN |
| 1 | F | 905 | HIS |
| 1 | F | 914 | HIS |
| 1 | F | 920 | GLN |
| 1 | F | 969 | HIS |
| 1 | F | 1022 | HIS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | F | 1052 | HIS |
| 1 | F | 1089 | GLN |
| 1 | F | 1098 | ASN |
| 1 | F | 1106 | HIS |
| 1 | F | 1142 | HIS |
| 1 | F | 1317 | HIS |
| 1 | F | 1326 | HIS |
| 1 | F | 1430 | HIS |
| 1 | F | 1494 | GLN |
| 1 | F | 1564 | ASN |
| 1 | F | 1727 | GLN |
| 1 | F | 1734 | HIS |
| 1 | F | 1743 | HIS |
| 1 | F | 1749 | GLN |
| 1 | F | 1772 | GLN |
| 1 | F | 1854 | HIS |
| 1 | F | 1858 | HIS |
| 1 | F | 1884 | HIS |
| 1 | F | 1973 | ASN |
| 1 | F | 2149 | HIS |
| 1 | F | 2164 | GLN |
| 1 | F | 2254 | GLN |
| 1 | F | 2263 | GLN |
| 1 | F | 2387 | HIS |
| 1 | F | 2551 | HIS |
| 1 | F | 2569 | HIS |
| 1 | F | 2679 | ASN |
| 1 | F | 2709 | HIS |
| 1 | F | 2723 | GLN |
| 1 | F | 2752 | ASN |
| 1 | F | 2871 | HIS |
| 1 | F | 2933 | GLN |
| 1 | F | 2979 | HIS |
| 1 | F | 2994 | GLN |
| 1 | F | 3089 | ASN |
| 1 | F | 3119 | HIS |
| 1 | F | 3127 | GLN |
| 1 | F | 3163 | ASN |
| 1 | F | 3206 | ASN |
| 1 | F | 3210 | HIS |
| 1 | F | 3276 | ASN |
| 1 | F | 3280 | ASN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | F | 3341 | HIS |
| 1 | G | 37 | ASN |
| 1 | G | 61 | HIS |
| 1 | G | 180 | GLN |
| 1 | G | 186 | ASN |
| 1 | G | 187 | HIS |
| 1 | G | 259 | ASN |
| 1 | G | 331 | HIS |
| 1 | G | 465 | GLN |
| 1 | G | 491 | HIS |
| 1 | G | 551 | HIS |
| 1 | G | 611 | ASN |
| 1 | G | 640 | HIS |
| 1 | G | 672 | HIS |
| 1 | G | 741 | HIS |
| 1 | G | 858 | GLN |
| 1 | G | 867 | GLN |
| 1 | G | 876 | ASN |
| 1 | G | 887 | GLN |
| 1 | G | 905 | HIS |
| 1 | G | 914 | HIS |
| 1 | G | 1026 | HIS |
| 1 | G | 1055 | ASN |
| 1 | G | 1214 | ASN |
| 1 | G | 1263 | HIS |
| 1 | G | 1269 | GLN |
| 1 | G | 1307 | HIS |
| 1 | G | 1317 | HIS |
| 1 | G | 1326 | HIS |
| 1 | G | 1408 | ASN |
| 1 | G | 1431 | ASN |
| 1 | G | 1460 | HIS |
| 1 | G | 1461 | HIS |
| 1 | G | 1563 | HIS |
| 1 | G | 1572 | GLN |
| 1 | G | 1708 | GLN |
| 1 | G | 1734 | HIS |
| 1 | G | 1743 | HIS |
| 1 | G | 1833 | GLN |
| 1 | G | 1854 | HIS |
| 1 | G | 1884 | HIS |
| 1 | G | 1885 | HIS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | G | 1899 | GLN |
| 1 | G | 1904 | HIS |
| 1 | G | 2149 | HIS |
| 1 | G | 2197 | GLN |
| 1 | G | 2345 | ASN |
| 1 | G | 2364 | ASN |
| 1 | G | 2386 | GLN |
| 1 | G | 2454 | HIS |
| 1 | G | 2518 | ASN |
| 1 | G | 2551 | HIS |
| 1 | G | 2569 | HIS |
| 1 | G | 2576 | GLN |
| 1 | G | 2592 | GLN |
| 1 | G | 2664 | GLN |
| 1 | G | 2673 | GLN |
| 1 | G | 2679 | ASN |
| 1 | G | 2708 | HIS |
| 1 | G | 2736 | ASN |
| 1 | G | 2773 | ASN |
| 1 | G | 2805 | ASN |
| 1 | G | 2826 | ASN |
| 1 | G | 2852 | GLN |
| 1 | G | 2936 | ASN |
| 1 | G | 2939 | ASN |
| 1 | G | 2960 | HIS |
| 1 | G | 2979 | HIS |
| 1 | G | 2988 | HIS |
| 1 | G | 3089 | ASN |
| 1 | G | 3092 | HIS |
| 1 | G | 3141 | ASN |
| 1 | G | 3201 | ASN |
| 1 | G | 3206 | ASN |
| 1 | G | 3284 | GLN |
| 1 | G | 3291 | ASN |
| 1 | G | 3294 | GLN |
| 1 | H | 37 | ASN |
| 1 | H | 61 | HIS |
| 1 | H | 70 | HIS |
| 1 | H | 151 | GLN |
| 1 | H | 186 | ASN |
| 1 | H | 218 | ASN |
| 1 | H | 450 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | H | 491 | HIS |
| 1 | H | 545 | ASN |
| 1 | H | 611 | ASN |
| 1 | H | 655 | GLN |
| 1 | H | 722 | GLN |
| 1 | H | 741 | HIS |
| 1 | H | 794 | ASN |
| 1 | H | 858 | GLN |
| 1 | H | 887 | GLN |
| 1 | H | 905 | HIS |
| 1 | H | 914 | HIS |
| 1 | H | 969 | HIS |
| 1 | H | 1023 | ASN |
| 1 | H | 1052 | HIS |
| 1 | H | 1055 | ASN |
| 1 | H | 1089 | GLN |
| 1 | H | 1098 | ASN |
| 1 | H | 1101 | HIS |
| 1 | H | 1142 | HIS |
| 1 | H | 1144 | GLN |
| 1 | H | 1156 | HIS |
| 1 | H | 1317 | HIS |
| 1 | H | 1402 | ASN |
| 1 | H | 1430 | HIS |
| 1 | H | 1460 | HIS |
| 1 | H | 1463 | ASN |
| 1 | H | 1494 | GLN |
| 1 | H | 1564 | ASN |
| 1 | H | 1727 | GLN |
| 1 | H | 1734 | HIS |
| 1 | H | 1743 | HIS |
| 1 | H | 1854 | HIS |
| 1 | H | 1858 | HIS |
| 1 | H | 1884 | HIS |
| 1 | H | 1973 | ASN |
| 1 | H | 2085 | GLN |
| 1 | H | 2149 | HIS |
| 1 | H | 2164 | GLN |
| 1 | H | 2172 | HIS |
| 1 | H | 2263 | GLN |
| 1 | H | 2298 | HIS |
| 1 | H | 2335 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | H | 2345 | ASN |
| 1 | H | 2400 | HIS |
| 1 | H | 2569 | HIS |
| 1 | H | 2715 | GLN |
| 1 | H | 2723 | GLN |
| 1 | H | 2752 | ASN |
| 1 | H | 2939 | ASN |
| 1 | H | 2969 | ASN |
| 1 | H | 2979 | HIS |
| 1 | H | 2994 | GLN |
| 1 | H | 3089 | ASN |
| 1 | H | 3184 | HIS |
| 1 | H | 3206 | ASN |
| 1 | H | 3276 | ASN |
| 1 | I | 61 | HIS |
| 1 | I | 180 | GLN |
| 1 | I | 189 | HIS |
| 1 | I | 465 | GLN |
| 1 | I | 491 | HIS |
| 1 | I | 610 | HIS |
| 1 | I | 641 | HIS |
| 1 | I | 665 | HIS |
| 1 | I | 693 | HIS |
| 1 | I | 722 | GLN |
| 1 | I | 836 | HIS |
| 1 | I | 843 | GLN |
| 1 | I | 876 | ASN |
| 1 | I | 887 | GLN |
| 1 | I | 905 | HIS |
| 1 | I | 1026 | HIS |
| 1 | I | 1052 | HIS |
| 1 | I | 1055 | ASN |
| 1 | I | 1106 | HIS |
| 1 | I | 1263 | HIS |
| 1 | I | 1307 | HIS |
| 1 | I | 1317 | HIS |
| 1 | I | 1373 | GLN |
| 1 | I | 1402 | ASN |
| 1 | I | 1408 | ASN |
| 1 | I | 1416 | GLN |
| 1 | I | 1434 | HIS |
| 1 | I | 1494 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | I | 1529 | HIS |
| 1 | I | 1572 | GLN |
| 1 | I | 1708 | GLN |
| 1 | I | 1734 | HIS |
| 1 | I | 1743 | HIS |
| 1 | I | 1833 | GLN |
| 1 | I | 1854 | HIS |
| 1 | I | 1885 | HIS |
| 1 | I | 2085 | GLN |
| 1 | I | 2094 | HIS |
| 1 | I | 2098 | HIS |
| 1 | I | 2115 | GLN |
| 1 | I | 2149 | HIS |
| 1 | I | 2158 | HIS |
| 1 | I | 2164 | GLN |
| 1 | I | 2167 | GLN |
| 1 | I | 2197 | GLN |
| 1 | I | 2268 | HIS |
| 1 | I | 2272 | HIS |
| 1 | I | 2287 | HIS |
| 1 | I | 2299 | HIS |
| 1 | I | 2345 | ASN |
| 1 | I | 2414 | GLN |
| 1 | I | 2518 | ASN |
| 1 | I | 2569 | HIS |
| 1 | I | 2673 | GLN |
| 1 | I | 2678 | HIS |
| 1 | I | 2682 | HIS |
| 1 | I | 2708 | HIS |
| 1 | I | 2711 | ASN |
| 1 | I | 2752 | ASN |
| 1 | I | 2760 | ASN |
| 1 | I | 2773 | ASN |
| 1 | I | 2788 | GLN |
| 1 | I | 2936 | ASN |
| 1 | I | 2960 | HIS |
| 1 | I | 2979 | HIS |
| 1 | I | 3036 | GLN |
| 1 | I | 3043 | GLN |
| 1 | I | 3076 | ASN |
| 1 | I | 3089 | ASN |
| 1 | I | 3119 | HIS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | I | 3141 | ASN |
| 1 | I | 3206 | ASN |
| 1 | I | 3210 | HIS |
| 1 | I | 3284 | GLN |
| 1 | J | 61 | HIS |
| 1 | J | 186 | ASN |
| 1 | J | 259 | ASN |
| 1 | J | 341 | HIS |
| 1 | J | 491 | HIS |
| 1 | J | 498 | HIS |
| 1 | J | 610 | HIS |
| 1 | J | 614 | HIS |
| 1 | J | 643 | ASN |
| 1 | J | 652 | GLN |
| 1 | J | 665 | HIS |
| 1 | J | 741 | HIS |
| 1 | J | 887 | GLN |
| 1 | J | 905 | HIS |
| 1 | J | 1026 | HIS |
| 1 | J | 1068 | HIS |
| 1 | J | 1078 | ASN |
| 1 | J | 1089 | GLN |
| 1 | J | 1098 | ASN |
| 1 | J | 1142 | HIS |
| 1 | J | 1317 | HIS |
| 1 | J | 1324 | HIS |
| 1 | J | 1326 | HIS |
| 1 | J | 1353 | GLN |
| 1 | J | 1408 | ASN |
| 1 | J | 1430 | HIS |
| 1 | J | 1431 | ASN |
| 1 | J | 1476 | GLN |
| 1 | J | 1494 | GLN |
| 1 | J | 1511 | ASN |
| 1 | J | 1524 | ASN |
| 1 | J | 1564 | ASN |
| 1 | J | 1581 | ASN |
| 1 | J | 1665 | GLN |
| 1 | J | 1727 | GLN |
| 1 | J | 1734 | HIS |
| 1 | J | 1743 | HIS |
| 1 | J | 1854 | HIS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | J | 1884 | HIS |
| 1 | J | 1973 | ASN |
| 1 | J | 2090 | ASN |
| 1 | J | 2149 | HIS |
| 1 | J | 2172 | HIS |
| 1 | J | 2263 | GLN |
| 1 | J | 2313 | GLN |
| 1 | J | 2335 | GLN |
| 1 | J | 2451 | ASN |
| 1 | J | 2569 | HIS |
| 1 | J | 2578 | HIS |
| 1 | J | 2624 | HIS |
| 1 | J | 2631 | ASN |
| 1 | J | 2679 | ASN |
| 1 | J | 2682 | HIS |
| 1 | J | 2723 | GLN |
| 1 | J | 2752 | ASN |
| 1 | J | 2863 | HIS |
| 1 | J | 2939 | ASN |
| 1 | J | 2960 | HIS |
| 1 | J | 2979 | HIS |
| 1 | J | 3163 | ASN |
| 1 | J | 3184 | HIS |
| 1 | J | 3189 | ASN |
| 1 | J | 3206 | ASN |
| 1 | J | 3276 | ASN |
| 1 | K | 37 | ASN |
| 1 | K | 61 | HIS |
| 1 | K | 187 | HIS |
| 1 | K | 298 | ASN |
| 1 | K | 331 | HIS |
| 1 | K | 375 | HIS |
| 1 | K | 465 | GLN |
| 1 | K | 491 | HIS |
| 1 | K | 610 | HIS |
| 1 | K | 611 | ASN |
| 1 | K | 640 | HIS |
| 1 | K | 643 | ASN |
| 1 | K | 672 | HIS |
| 1 | K | 741 | HIS |
| 1 | K | 836 | HIS |
| 1 | K | 876 | ASN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | K | 905 | HIS |
| 1 | K | 914 | HIS |
| 1 | K | 1026 | HIS |
| 1 | K | 1137 | GLN |
| 1 | K | 1193 | GLN |
| 1 | K | 1317 | HIS |
| 1 | K | 1402 | ASN |
| 1 | K | 1460 | HIS |
| 1 | K | 1461 | HIS |
| 1 | K | 1529 | HIS |
| 1 | K | 1572 | GLN |
| 1 | K | 1708 | GLN |
| 1 | K | 1727 | GLN |
| 1 | K | 1734 | HIS |
| 1 | K | 1743 | HIS |
| 1 | K | 1749 | GLN |
| 1 | K | 1833 | GLN |
| 1 | K | 1842 | ASN |
| 1 | K | 1854 | HIS |
| 1 | K | 1855 | ASN |
| 1 | K | 1884 | HIS |
| 1 | K | 1885 | HIS |
| 1 | K | 1904 | HIS |
| 1 | K | 2085 | GLN |
| 1 | K | 2149 | HIS |
| 1 | K | 2172 | HIS |
| 1 | K | 2189 | GLN |
| 1 | K | 2197 | GLN |
| 1 | K | 2299 | HIS |
| 1 | K | 2345 | ASN |
| 1 | K | 2414 | GLN |
| 1 | K | 2454 | HIS |
| 1 | K | 2518 | ASN |
| 1 | K | 2569 | HIS |
| 1 | K | 2578 | HIS |
| 1 | K | 2657 | GLN |
| 1 | K | 2679 | ASN |
| 1 | K | 2682 | HIS |
| 1 | K | 2708 | HIS |
| 1 | K | 2736 | ASN |
| 1 | K | 2788 | GLN |
| 1 | K | 2805 | ASN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | K | 2826 | ASN |
| 1 | K | 2827 | HIS |
| 1 | K | 2852 | GLN |
| 1 | K | 2863 | HIS |
| 1 | K | 2979 | HIS |
| 1 | K | 2988 | HIS |
| 1 | K | 3043 | GLN |
| 1 | K | 3089 | ASN |
| 1 | K | 3119 | HIS |
| 1 | K | 3149 | ASN |
| 1 | K | 3201 | ASN |
| 1 | K | 3206 | ASN |
| 1 | K | 3291 | ASN |
| 1 | K | 3294 | GLN |
| 1 | L | 37 | ASN |
| 1 | L | 61 | HIS |
| 1 | L | 70 | HIS |
| 1 | L | 186 | ASN |
| 1 | L | 491 | HIS |
| 1 | L | 506 | GLN |
| 1 | L | 545 | ASN |
| 1 | L | 614 | HIS |
| 1 | L | 643 | ASN |
| 1 | L | 655 | GLN |
| 1 | L | 714 | GLN |
| 1 | L | 741 | HIS |
| 1 | L | 794 | ASN |
| 1 | L | 858 | GLN |
| 1 | L | 887 | GLN |
| 1 | L | 905 | HIS |
| 1 | L | 914 | HIS |
| 1 | L | 969 | HIS |
| 1 | L | 1023 | ASN |
| 1 | L | 1026 | HIS |
| 1 | L | 1055 | ASN |
| 1 | L | 1089 | GLN |
| 1 | L | 1098 | ASN |
| 1 | L | 1106 | HIS |
| 1 | L | 1142 | HIS |
| 1 | L | 1257 | ASN |
| 1 | L | 1317 | HIS |
| 1 | L | 1326 | HIS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | L | 1353 | GLN |
| 1 | L | 1408 | ASN |
| 1 | L | 1430 | HIS |
| 1 | L | 1494 | GLN |
| 1 | L | 1663 | ASN |
| 1 | L | 1727 | GLN |
| 1 | L | 1734 | HIS |
| 1 | L | 1743 | HIS |
| 1 | L | 1749 | GLN |
| 1 | L | 1770 | ASN |
| 1 | L | 1884 | HIS |
| 1 | L | 1973 | ASN |
| 1 | L | 2085 | GLN |
| 1 | L | 2149 | HIS |
| 1 | L | 2164 | GLN |
| 1 | L | 2263 | GLN |
| 1 | L | 2345 | ASN |
| 1 | L | 2569 | HIS |
| 1 | L | 2620 | ASN |
| 1 | L | 2679 | ASN |
| 1 | L | 2709 | HIS |
| 1 | L | 2752 | ASN |
| 1 | L | 2773 | ASN |
| 1 | L | 2775 | GLN |
| 1 | L | 2863 | HIS |
| 1 | L | 2871 | HIS |
| 1 | L | 2875 | HIS |
| 1 | L | 2939 | ASN |
| 1 | L | 2946 | ASN |
| 1 | L | 2951 | ASN |
| 1 | L | 2960 | HIS |
| 1 | L | 2979 | HIS |
| 1 | L | 3089 | ASN |
| 1 | L | 3118 | HIS |
| 1 | L | 3119 | HIS |
| 1 | L | 3137 | HIS |
| 1 | L | 3206 | ASN |
| 1 | L | 3276 | ASN |
| 1 | M | 61 | HIS |
| 1 | M | 70 | HIS |
| 1 | M | 186 | ASN |
| 1 | M | 465 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | M | 491 | HIS |
| 1 | M | 611 | ASN |
| 1 | M | 629 | HIS |
| 1 | M | 722 | GLN |
| 1 | M | 744 | ASN |
| 1 | M | 843 | GLN |
| 1 | M | 860 | GLN |
| 1 | M | 876 | ASN |
| 1 | M | 905 | HIS |
| 1 | M | 914 | HIS |
| 1 | M | 931 | GLN |
| 1 | M | 1026 | HIS |
| 1 | M | 1055 | ASN |
| 1 | M | 1078 | ASN |
| 1 | M | 1106 | HIS |
| 1 | M | 1137 | GLN |
| 1 | M | 1263 | HIS |
| 1 | M | 1307 | HIS |
| 1 | M | 1317 | HIS |
| 1 | M | 1402 | ASN |
| 1 | M | 1430 | HIS |
| 1 | M | 1460 | HIS |
| 1 | M | 1494 | GLN |
| 1 | M | 1529 | HIS |
| 1 | M | 1708 | GLN |
| 1 | M | 1727 | GLN |
| 1 | M | 1734 | HIS |
| 1 | M | 1743 | HIS |
| 1 | M | 2085 | GLN |
| 1 | M | 2098 | HIS |
| 1 | M | 2149 | HIS |
| 1 | M | 2278 | HIS |
| 1 | M | 2345 | ASN |
| 1 | M | 2569 | HIS |
| 1 | M | 2578 | HIS |
| 1 | M | 2673 | GLN |
| 1 | M | 2678 | HIS |
| 1 | M | 2679 | ASN |
| 1 | M | 2682 | HIS |
| 1 | M | 2711 | ASN |
| 1 | M | 2723 | GLN |
| 1 | M | 2760 | ASN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | M | 2788 | GLN |
| 1 | M | 2861 | GLN |
| 1 | M | 2863 | HIS |
| 1 | M | 2914 | GLN |
| 1 | M | 2979 | HIS |
| 1 | M | 3043 | GLN |
| 1 | M | 3076 | ASN |
| 1 | M | 3089 | ASN |
| 1 | M | 3092 | HIS |
| 1 | M | 3119 | HIS |
| 1 | M | 3284 | GLN |
| 1 | M | 3291 | ASN |
| 1 | N | 37 | ASN |
| 1 | N | 42 | HIS |
| 1 | N | 61 | HIS |
| 1 | N | 70 | HIS |
| 1 | N | 160 | GLN |
| 1 | N | 186 | ASN |
| 1 | N | 187 | HIS |
| 1 | N | 491 | HIS |
| 1 | N | 605 | GLN |
| 1 | N | 610 | HIS |
| 1 | N | 665 | HIS |
| 1 | N | 741 | HIS |
| 1 | N | 794 | ASN |
| 1 | N | 860 | GLN |
| 1 | N | 887 | GLN |
| 1 | N | 905 | HIS |
| 1 | N | 920 | GLN |
| 1 | N | 1023 | ASN |
| 1 | N | 1026 | HIS |
| 1 | N | 1052 | HIS |
| 1 | N | 1068 | HIS |
| 1 | N | 1078 | ASN |
| 1 | N | 1089 | GLN |
| 1 | N | 1098 | ASN |
| 1 | N | 1106 | HIS |
| 1 | N | 1142 | HIS |
| 1 | N | 1144 | GLN |
| 1 | N | 1317 | HIS |
| 1 | N | 1324 | HIS |
| 1 | N | 1353 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | N | 1408 | ASN |
| 1 | N | 1430 | HIS |
| 1 | N | 1431 | ASN |
| 1 | N | 1434 | HIS |
| 1 | N | 1463 | ASN |
| 1 | N | 1494 | GLN |
| 1 | N | 1564 | ASN |
| 1 | N | 1727 | GLN |
| 1 | N | 1734 | HIS |
| 1 | N | 1743 | HIS |
| 1 | N | 1749 | GLN |
| 1 | N | 1854 | HIS |
| 1 | N | 1858 | HIS |
| 1 | N | 1907 | ASN |
| 1 | N | 1973 | ASN |
| 1 | N | 2124 | GLN |
| 1 | N | 2149 | HIS |
| 1 | N | 2172 | HIS |
| 1 | N | 2263 | GLN |
| 1 | N | 2272 | HIS |
| 1 | N | 2299 | HIS |
| 1 | N | 2387 | HIS |
| 1 | N | 2551 | HIS |
| 1 | N | 2569 | HIS |
| 1 | N | 2624 | HIS |
| 1 | N | 2631 | ASN |
| 1 | N | 2679 | ASN |
| 1 | N | 2682 | HIS |
| 1 | N | 2709 | HIS |
| 1 | N | 2720 | GLN |
| 1 | N | 2752 | ASN |
| 1 | N | 2875 | HIS |
| 1 | N | 2883 | GLN |
| 1 | N | 2939 | ASN |
| 1 | N | 2960 | HIS |
| 1 | N | 2979 | HIS |
| 1 | N | 3067 | GLN |
| 1 | N | 3089 | ASN |
| 1 | N | 3127 | GLN |
| 1 | N | 3163 | ASN |
| 1 | N | 3206 | ASN |
| 1 | N | 3276 | ASN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | O | 37 | ASN |
| 1 | O | 61 | HIS |
| 1 | O | 138 | HIS |
| 1 | O | 158 | ASN |
| 1 | O | 331 | HIS |
| 1 | O | 465 | GLN |
| 1 | O | 491 | HIS |
| 1 | O | 498 | HIS |
| 1 | O | 500 | HIS |
| 1 | O | 605 | GLN |
| 1 | O | 640 | HIS |
| 1 | O | 836 | HIS |
| 1 | O | 867 | GLN |
| 1 | O | 889 | ASN |
| 1 | O | 905 | HIS |
| 1 | O | 914 | HIS |
| 1 | O | 1026 | HIS |
| 1 | O | 1053 | HIS |
| 1 | O | 1055 | ASN |
| 1 | O | 1067 | GLN |
| 1 | O | 1129 | ASN |
| 1 | O | 1137 | GLN |
| 1 | O | 1176 | HIS |
| 1 | O | 1317 | HIS |
| 1 | O | 1408 | ASN |
| 1 | O | 1476 | GLN |
| 1 | O | 1494 | GLN |
| 1 | O | 1500 | ASN |
| 1 | O | 1708 | GLN |
| 1 | O | 1734 | HIS |
| 1 | O | 1743 | HIS |
| 1 | O | 1855 | ASN |
| 1 | O | 1884 | HIS |
| 1 | O | 1952 | ASN |
| 1 | O | 1975 | GLN |
| 1 | O | 2085 | GLN |
| 1 | O | 2149 | HIS |
| 1 | O | 2197 | GLN |
| 1 | O | 2278 | HIS |
| 1 | O | 2299 | HIS |
| 1 | O | 2345 | ASN |
| 1 | O | 2569 | HIS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | O | 2592 | GLN |
| 1 | O | 2624 | HIS |
| 1 | O | 2657 | GLN |
| 1 | O | 2678 | HIS |
| 1 | O | 2679 | ASN |
| 1 | O | 2682 | HIS |
| 1 | O | 2708 | HIS |
| 1 | O | 2711 | ASN |
| 1 | O | 2736 | ASN |
| 1 | O | 2788 | GLN |
| 1 | O | 2809 | GLN |
| 1 | O | 2969 | ASN |
| 1 | O | 2979 | HIS |
| 1 | O | 2988 | HIS |
| 1 | O | 2994 | GLN |
| 1 | O | 3043 | GLN |
| 1 | O | 3089 | ASN |
| 1 | O | 3092 | HIS |
| 1 | O | 3119 | HIS |
| 1 | O | 3137 | HIS |
| 1 | O | 3165 | ASN |
| 1 | O | 3206 | ASN |
| 1 | O | 3291 | ASN |
| 1 | O | 3294 | GLN |
| 1 | P | 37 | ASN |
| 1 | P | 42 | HIS |
| 1 | P | 61 | HIS |
| 1 | P | 186 | ASN |
| 1 | P | 295 | GLN |
| 1 | P | 302 | GLN |
| 1 | P | 381 | ASN |
| 1 | P | 399 | ASN |
| 1 | P | 450 | GLN |
| 1 | P | 491 | HIS |
| 1 | P | 506 | GLN |
| 1 | P | 545 | ASN |
| 1 | P | 583 | HIS |
| 1 | P | 611 | ASN |
| 1 | P | 614 | HIS |
| 1 | P | 643 | ASN |
| 1 | P | 698 | ASN |
| 1 | P | 722 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | P | 744 | ASN |
| 1 | P | 858 | GLN |
| 1 | P | 860 | GLN |
| 1 | P | 887 | GLN |
| 1 | P | 905 | HIS |
| 1 | P | 920 | GLN |
| 1 | P | 1022 | HIS |
| 1 | P | 1023 | ASN |
| 1 | P | 1055 | ASN |
| 1 | P | 1068 | HIS |
| 1 | P | 1078 | ASN |
| 1 | P | 1089 | GLN |
| 1 | P | 1142 | HIS |
| 1 | P | 1317 | HIS |
| 1 | P | 1324 | HIS |
| 1 | P | 1408 | ASN |
| 1 | P | 1430 | HIS |
| 1 | P | 1475 | GLN |
| 1 | P | 1490 | ASN |
| 1 | P | 1665 | GLN |
| 1 | P | 1727 | GLN |
| 1 | P | 1734 | HIS |
| 1 | P | 1743 | HIS |
| 1 | P | 1749 | GLN |
| 1 | P | 1854 | HIS |
| 1 | P | 1867 | HIS |
| 1 | P | 1884 | HIS |
| 1 | P | 1973 | ASN |
| 1 | P | 2149 | HIS |
| 1 | P | 2229 | GLN |
| 1 | P | 2263 | GLN |
| 1 | P | 2272 | HIS |
| 1 | P | 2298 | HIS |
| 1 | P | 2387 | HIS |
| 1 | P | 2451 | ASN |
| 1 | P | 2454 | HIS |
| 1 | P | 2569 | HIS |
| 1 | P | 2631 | ASN |
| 1 | P | 2679 | ASN |
| 1 | P | 2709 | HIS |
| 1 | P | 2711 | ASN |
| 1 | P | 2734 | ASN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | P | 2846 | HIS |
| 1 | P | 2883 | GLN |
| 1 | P | 2951 | ASN |
| 1 | P | 2960 | HIS |
| 1 | P | 2979 | HIS |
| 1 | P | 2994 | GLN |
| 1 | P | 3089 | ASN |
| 1 | P | 3137 | HIS |
| 1 | P | 3163 | ASN |
| 1 | P | 3206 | ASN |
| 1 | P | 3276 | ASN |
| 1 | P | 3280 | ASN |
| 1 | P | 3341 | HIS |
| 1 | P | 3398 | GLN |
| 1 | Q | 37 | ASN |
| 1 | Q | 61 | HIS |
| 1 | Q | 186 | ASN |
| 1 | Q | 187 | HIS |
| 1 | Q | 189 | HIS |
| 1 | Q | 331 | HIS |
| 1 | Q | 465 | GLN |
| 1 | Q | 491 | HIS |
| 1 | Q | 545 | ASN |
| 1 | Q | 610 | HIS |
| 1 | Q | 611 | ASN |
| 1 | Q | 629 | HIS |
| 1 | Q | 640 | HIS |
| 1 | Q | 858 | GLN |
| 1 | Q | 860 | GLN |
| 1 | Q | 876 | ASN |
| 1 | Q | 905 | HIS |
| 1 | Q | 914 | HIS |
| 1 | Q | 1026 | HIS |
| 1 | Q | 1106 | HIS |
| 1 | Q | 1129 | ASN |
| 1 | Q | 1137 | GLN |
| 1 | Q | 1193 | GLN |
| 1 | Q | 1317 | HIS |
| 1 | Q | 1326 | HIS |
| 1 | Q | 1408 | ASN |
| 1 | Q | 1409 | ASN |
| 1 | Q | 1461 | HIS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | Q | 1476 | GLN |
| 1 | Q | 1505 | ASN |
| 1 | Q | 1529 | HIS |
| 1 | Q | 1708 | GLN |
| 1 | Q | 1734 | HIS |
| 1 | Q | 1743 | HIS |
| 1 | Q | 1833 | GLN |
| 1 | Q | 1867 | HIS |
| 1 | Q | 1884 | HIS |
| 1 | Q | 1975 | GLN |
| 1 | Q | 2085 | GLN |
| 1 | Q | 2149 | HIS |
| 1 | Q | 2268 | HIS |
| 1 | Q | 2272 | HIS |
| 1 | Q | 2343 | ASN |
| 1 | Q | 2345 | ASN |
| 1 | Q | 2386 | GLN |
| 1 | Q | 2414 | GLN |
| 1 | Q | 2454 | HIS |
| 1 | Q | 2569 | HIS |
| 1 | Q | 2592 | GLN |
| 1 | Q | 2679 | ASN |
| 1 | Q | 2708 | HIS |
| 1 | Q | 2711 | ASN |
| 1 | Q | 2788 | GLN |
| 1 | Q | 2805 | ASN |
| 1 | Q | 2852 | GLN |
| 1 | Q | 2861 | GLN |
| 1 | Q | 2914 | GLN |
| 1 | Q | 2979 | HIS |
| 1 | Q | 2988 | HIS |
| 1 | Q | 3089 | ASN |
| 1 | Q | 3092 | HIS |
| 1 | Q | 3137 | HIS |
| 1 | Q | 3206 | ASN |
| 1 | Q | 3284 | GLN |
| 1 | Q | 3291 | ASN |
| 1 | Q | 3294 | GLN |
| 1 | Q | 3310 | ASN |
| 1 | R | 37 | ASN |
| 1 | R | 61 | HIS |
| 1 | R | 70 | HIS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | R | 341 | HIS |
| 1 | R | 366 | HIS |
| 1 | R | 381 | ASN |
| 1 | R | 491 | HIS |
| 1 | R | 545 | ASN |
| 1 | R | 610 | HIS |
| 1 | R | 611 | ASN |
| 1 | R | 614 | HIS |
| 1 | R | 714 | GLN |
| 1 | R | 722 | GLN |
| 1 | R | 741 | HIS |
| 1 | R | 794 | ASN |
| 1 | R | 858 | GLN |
| 1 | R | 880 | HIS |
| 1 | R | 887 | GLN |
| 1 | R | 905 | HIS |
| 1 | R | 914 | HIS |
| 1 | R | 969 | HIS |
| 1 | R | 1089 | GLN |
| 1 | R | 1101 | HIS |
| 1 | R | 1137 | GLN |
| 1 | R | 1145 | HIS |
| 1 | R | 1317 | HIS |
| 1 | R | 1408 | ASN |
| 1 | R | 1430 | HIS |
| 1 | R | 1431 | ASN |
| 1 | R | 1461 | HIS |
| 1 | R | 1494 | GLN |
| 1 | R | 1524 | ASN |
| 1 | R | 1727 | GLN |
| 1 | R | 1734 | HIS |
| 1 | R | 1743 | HIS |
| 1 | R | 1854 | HIS |
| 1 | R | 1858 | HIS |
| 1 | R | 1867 | HIS |
| 1 | R | 1884 | HIS |
| 1 | R | 2085 | GLN |
| 1 | R | 2149 | HIS |
| 1 | R | 2158 | HIS |
| 1 | R | 2164 | GLN |
| 1 | R | 2254 | GLN |
| 1 | R | 2263 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | R | 2299 | HIS |
| 1 | R | 2313 | GLN |
| 1 | R | 2345 | ASN |
| 1 | R | 2551 | HIS |
| 1 | R | 2569 | HIS |
| 1 | R | 2669 | ASN |
| 1 | R | 2679 | ASN |
| 1 | R | 2682 | HIS |
| 1 | R | 2709 | HIS |
| 1 | R | 2715 | GLN |
| 1 | R | 2723 | GLN |
| 1 | R | 2871 | HIS |
| 1 | R | 2933 | GLN |
| 1 | R | 2979 | HIS |
| 1 | R | 3067 | GLN |
| 1 | R | 3163 | ASN |
| 1 | R | 3195 | HIS |
| 1 | R | 3201 | ASN |
| 1 | R | 3206 | ASN |
| 1 | R | 3276 | ASN |
| 1 | R | 3310 | ASN |
| 1 | S | 36 | GLN |
| 1 | S | 61 | HIS |
| 1 | S | 138 | HIS |
| 1 | S | 187 | HIS |
| 1 | S | 189 | HIS |
| 1 | S | 295 | GLN |
| 1 | S | 331 | HIS |
| 1 | S | 366 | HIS |
| 1 | S | 491 | HIS |
| 1 | S | 610 | HIS |
| 1 | S | 611 | ASN |
| 1 | S | 614 | HIS |
| 1 | S | 641 | HIS |
| 1 | S | 722 | GLN |
| 1 | S | 741 | HIS |
| 1 | S | 843 | GLN |
| 1 | S | 887 | GLN |
| 1 | S | 905 | HIS |
| 1 | S | 1026 | HIS |
| 1 | S | 1055 | ASN |
| 1 | S | 1137 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | S | 1257 | ASN |
| 1 | S | 1317 | HIS |
| 1 | S | 1326 | HIS |
| 1 | S | 1373 | GLN |
| 1 | S | 1408 | ASN |
| 1 | S | 1434 | HIS |
| 1 | S | 1460 | HIS |
| 1 | S | 1500 | ASN |
| 1 | S | 1708 | GLN |
| 1 | S | 1714 | HIS |
| 1 | S | 1734 | HIS |
| 1 | S | 1743 | HIS |
| 1 | S | 1772 | GLN |
| 1 | S | 1833 | GLN |
| 1 | S | 1884 | HIS |
| 1 | S | 1899 | GLN |
| 1 | S | 2090 | ASN |
| 1 | S | 2098 | HIS |
| 1 | S | 2149 | HIS |
| 1 | S | 2189 | GLN |
| 1 | S | 2268 | HIS |
| 1 | S | 2272 | HIS |
| 1 | S | 2299 | HIS |
| 1 | S | 2345 | ASN |
| 1 | S | 2569 | HIS |
| 1 | S | 2576 | GLN |
| 1 | S | 2592 | GLN |
| 1 | S | 2657 | GLN |
| 1 | S | 2673 | GLN |
| 1 | S | 2678 | HIS |
| 1 | S | 2679 | ASN |
| 1 | S | 2682 | HIS |
| 1 | S | 2708 | HIS |
| 1 | S | 2711 | ASN |
| 1 | S | 2723 | GLN |
| 1 | S | 2788 | GLN |
| 1 | S | 2861 | GLN |
| 1 | S | 2914 | GLN |
| 1 | S | 2979 | HIS |
| 1 | S | 3043 | GLN |
| 1 | S | 3089 | ASN |
| 1 | S | 3092 | HIS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | S | 3119 | HIS |
| 1 | S | 3149 | ASN |
| 1 | S | 3176 | GLN |
| 1 | S | 3206 | ASN |
| 1 | S | 3284 | GLN |
| 1 | S | 3291 | ASN |
| 1 | S | 3403 | GLN |
| 1 | T | 42 | HIS |
| 1 | T | 61 | HIS |
| 1 | T | 131 | ASN |
| 1 | T | 186 | ASN |
| 1 | T | 187 | HIS |
| 1 | T | 198 | HIS |
| 1 | T | 259 | ASN |
| 1 | T | 295 | GLN |
| 1 | T | 302 | GLN |
| 1 | T | 341 | HIS |
| 1 | T | 399 | ASN |
| 1 | T | 401 | ASN |
| 1 | T | 450 | GLN |
| 1 | T | 491 | HIS |
| 1 | T | 506 | GLN |
| 1 | T | 545 | ASN |
| 1 | T | 610 | HIS |
| 1 | T | 611 | ASN |
| 1 | T | 643 | ASN |
| 1 | T | 665 | HIS |
| 1 | T | 712 | ASN |
| 1 | T | 741 | HIS |
| 1 | T | 846 | HIS |
| 1 | T | 880 | HIS |
| 1 | T | 905 | HIS |
| 1 | T | 920 | GLN |
| 1 | T | 969 | HIS |
| 1 | T | 1022 | HIS |
| 1 | T | 1023 | ASN |
| 1 | T | 1052 | HIS |
| 1 | T | 1068 | HIS |
| 1 | T | 1089 | GLN |
| 1 | T | 1142 | HIS |
| 1 | T | 1145 | HIS |
| 1 | T | 1317 | HIS |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | T | 1326 | HIS |
| 1 | T | 1430 | HIS |
| 1 | T | 1431 | ASN |
| 1 | T | 1494 | GLN |
| 1 | T | 1524 | ASN |
| 1 | T | 1727 | GLN |
| 1 | T | 1734 | HIS |
| 1 | T | 1743 | HIS |
| 1 | T | 1854 | HIS |
| 1 | T | 1873 | HIS |
| 1 | T | 1884 | HIS |
| 1 | T | 1973 | ASN |
| 1 | T | 2149 | HIS |
| 1 | T | 2164 | GLN |
| 1 | T | 2229 | GLN |
| 1 | T | 2263 | GLN |
| 1 | T | 2335 | GLN |
| 1 | T | 2345 | ASN |
| 1 | T | 2400 | HIS |
| 1 | T | 2551 | HIS |
| 1 | T | 2569 | HIS |
| 1 | T | 2578 | HIS |
| 1 | T | 2708 | HIS |
| 1 | T | 2752 | ASN |
| 1 | T | 2775 | GLN |
| 1 | T | 2846 | HIS |
| 1 | T | 2860 | ASN |
| 1 | T | 2939 | ASN |
| 1 | T | 2979 | HIS |
| 1 | T | 3089 | ASN |
| 1 | T | 3158 | ASN |
| 1 | T | 3206 | ASN |
| 1 | T | 3276 | 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 (i)

260 monosaccharides are modelled in this entry.

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

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\| > 2$ | Counts | RMSZ | $\#\|Z\| > 2$ |
| 2 | NAG | 0 | 1 | 1,2 | 14,14,15 | 1.05 | 1 (7%) | 17,19,21 | 0.99 | 1 (5%) |
| 2 | NAG | 0 | 2 | 2 | 14,14,15 | 0.28 | 0 | 17,19,21 | 0.46 | 0 |
| 2 | NAG | 0A | 1 | 1,2 | 14,14,15 | 0.22 | 0 | 17,19,21 | 0.42 | 0 |
| 2 | NAG | 0A | 2 | 2 | 14,14,15 | 0.20 | 0 | 17,19,21 | 0.45 | 0 |
| 3 | NAG | 1 | 1 | 1,3 | 14,14,15 | 1.06 | 1 (7%) | 17,19,21 | 0.95 | 1 (5%) |
| 3 | NAG | 1 | 2 | 3 | 14,14,15 | 0.22 | 0 | 17,19,21 | 0.57 | 0 |
| 3 | BMA | 1 | 3 | 3 | 11,11,12 | 0.46 | 0 | 15,15,17 | 0.78 | 0 |
| 3 | NAG | 1A | 1 | 1,3 | 14,14,15 | 0.62 | 0 | 17,19,21 | 0.93 | 1 (5%) |
| 3 | NAG | 1A | 2 | 3 | 14,14,15 | 0.27 | 0 | 17,19,21 | 0.44 | 0 |
| 3 | BMA | 1A | 3 | 3 | 11,11,12 | 0.59 | 0 | 15,15,17 | 0.73 | 0 |
| 2 | NAG | 2 | 1 | 1,2 | 14,14,15 | 0.26 | 0 | 17,19,21 | 0.54 | 0 |
| 2 | NAG | 2 | 2 | 2 | 14,14,15 | 0.29 | 0 | 17,19,21 | 0.43 | 0 |
| 3 | NAG | 2A | 1 | 1,3 | 14,14,15 | 0.53 | 0 | 17,19,21 | 0.45 | 0 |
| 3 | NAG | 2A | 2 | 3 | 14,14,15 | 0.29 | 0 | 17,19,21 | 0.49 | 0 |
| 3 | BMA | 2A | 3 | 3 | 11,11,12 | 0.53 | 0 | 15,15,17 | 0.68 | 0 |
| 3 | NAG | 3 | 1 | 1,3 | 14,14,15 | 0.60 | 0 | 17,19,21 | 0.93 | 1 (5%) |
| 3 | NAG | 3 | 2 | 3 | 14,14,15 | 0.23 | 0 | 17,19,21 | 0.49 | 0 |
| 3 | BMA | 3 | 3 | 3 | 11,11,12 | 0.63 | 0 | 15,15,17 | 0.75 | 0 |
| 3 | NAG | 3A | 1 | 1,3 | 14,14,15 | 0.29 | 0 | 17,19,21 | 0.48 | 0 |
| 3 | NAG | 3A | 2 | 3 | 14,14,15 | 0.19 | 0 | 17,19,21 | 0.44 | 0 |
| 3 | BMA | 3A | 3 | 3 | 11,11,12 | 0.55 | 0 | 15,15,17 | 0.78 | 0 |
| 3 | NAG | 4 | 1 | 1,3 | 14,14,15 | 0.45 | 0 | 17,19,21 | 0.43 | 0 |
| 3 | NAG | 4 | 2 | 3 | 14,14,15 | 0.30 | 0 | 17,19,21 | 0.51 | 0 |
| 3 | BMA | 4 | 3 | 3 | 11,11,12 | 0.57 | 0 | 15,15,17 | 0.77 | 0 |
| 3 | NAG | 4A | 1 | 1,3 | 14,14,15 | 0.39 | 0 | 17,19,21 | 0.73 | 1 (5%) |
| 3 | NAG | 4A | 2 | 3 | 14,14,15 | 0.86 | 1 (7%) | 17,19,21 | 0.95 | 1 (5%) |
| 3 | BMA | 4A | 3 | 3 | 11,11,12 | 0.64 | 0 | 15,15,17 | 1.02 | 0 |
| 3 | NAG | 5 | 1 | 1,3 | 14,14,15 | 0.26 | 0 | 17,19,21 | 0.48 | 0 |
| 3 | NAG | 5 | 2 | 3 | 14,14,15 | 0.19 | 0 | 17,19,21 | 0.42 | 0 |
| 3 | BMA | 5 | 3 | 3 | 11,11,12 | 0.57 | 0 | 15,15,17 | 0.79 | 0 |
| 2 | NAG | 5A | 1 | 1,2 | 14,14,15 | 0.19 | 0 | 17,19,21 | 0.43 | 0 |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\|>2$ | Counts | RMSZ | $\#\|Z\|>2$ |
| 2 | NAG | 5A | 2 | 2 | 14,14,15 | 0.51 | 0 | 17,19,21 | 1.25 | 1 (5%) |
| 3 | NAG | 6 | 1 | 1,3 | 14,14,15 | 0.39 | 0 | 17,19,21 | 0.35 | 0 |
| 3 | NAG | 6 | 2 | 3 | 14,14,15 | 0.63 | 1 (7%) | 17,19,21 | 1.41 | 1 (5%) |
| 3 | BMA | 6 | 3 | 3 | 11,11,12 | 0.67 | 0 | 15,15,17 | 0.77 | 0 |
| 2 | NAG | 7 | 1 | 1,2 | 14,14,15 | 0.18 | 0 | 17,19,21 | 0.42 | 0 |
| 2 | NAG | 7 | 2 | 2 | 14,14,15 | 0.50 | 0 | 17,19,21 | 1.26 | 1 (5%) |
| 2 | NAG | 8 | 1 | 1,2 | 14,14,15 | 0.27 | 0 | 17,19,21 | 0.48 | 0 |
| 2 | NAG | 8 | 2 | 2 | 14,14,15 | 0.24 | 0 | 17,19,21 | 0.45 | 0 |
| 3 | NAG | 9 | 1 | 1,3 | 14,14,15 | 0.54 | 0 | 17,19,21 | 0.76 | 1 (5%) |
| 3 | NAG | 9 | 2 | 3 | 14,14,15 | 0.20 | 0 | 17,19,21 | 0.39 | 0 |
| 3 | BMA | 9 | 3 | 3 | 11,11,12 | 0.54 | 0 | 15,15,17 | 0.78 | 0 |
| 2 | NAG | AA | 1 | 1,2 | 14,14,15 | 0.22 | 0 | 17,19,21 | 0.46 | 0 |
| 2 | NAG | AA | 2 | 2 | 14,14,15 | 0.24 | 0 | 17,19,21 | 0.46 | 0 |
| 3 | NAG | BA | 1 | 1,3 | 14,14,15 | 1.07 | 1 (7%) | 17,19,21 | 0.94 | 1 (5%) |
| 3 | NAG | BA | 2 | 3 | 14,14,15 | 0.23 | 0 | 17,19,21 | 0.60 | 0 |
| 3 | BMA | BA | 3 | 3 | 11,11,12 | 0.47 | 0 | 15,15,17 | 0.78 | 0 |
| 2 | NAG | CA | 1 | 1,2 | 14,14,15 | 0.88 | 1 (7%) | 17,19,21 | 1.43 | 1 (5%) |
| 2 | NAG | CA | 2 | 2 | 14,14,15 | 0.28 | 0 | 17,19,21 | 0.48 | 0 |
| 3 | NAG | DA | 1 | 1,3 | 14,14,15 | 0.64 | 0 | 17,19,21 | 0.96 | 1 (5%) |
| 3 | NAG | DA | 2 | 3 | 14,14,15 | 0.24 | 0 | 17,19,21 | 0.47 | 0 |
| 3 | BMA | DA | 3 | 3 | 11,11,12 | 0.59 | 0 | 15,15,17 | 0.81 | 0 |
| 3 | NAG | EA | 1 | 1,3 | 14,14,15 | 0.50 | 0 | 17,19,21 | 0.48 | 0 |
| 3 | NAG | EA | 2 | 3 | 14,14,15 | 0.27 | 0 | 17,19,21 | 0.49 | 0 |
| 3 | BMA | EA | 3 | 3 | 11,11,12 | 0.52 | 0 | 15,15,17 | 0.71 | 0 |
| 3 | NAG | FA | 1 | 1,3 | 14,14,15 | 0.26 | 0 | 17,19,21 | 0.46 | 0 |
| 3 | NAG | FA | 2 | 3 | 14,14,15 | 0.19 | 0 | 17,19,21 | 0.46 | 0 |
| 3 | BMA | FA | 3 | 3 | 11,11,12 | 0.51 | 0 | 15,15,17 | 0.81 | 0 |
| 3 | NAG | GA | 1 | 1,3 | 14,14,15 | 0.34 | 0 | 17,19,21 | 0.35 | 0 |
| 3 | NAG | GA | 2 | 3 | 14,14,15 | 0.60 | 1 (7%) | 17,19,21 | 1.33 | 1 (5%) |
| 3 | BMA | GA | 3 | 3 | 11,11,12 | 0.63 | 0 | 15,15,17 | 0.76 | 0 |
| 2 | NAG | HA | 1 | 1,2 | 14,14,15 | 0.20 | 0 | 17,19,21 | 0.38 | 0 |
| 2 | NAG | HA | 2 | 2 | 14,14,15 | 0.49 | 0 | 17,19,21 | 1.26 | 1 (5%) |
| 2 | NAG | IA | 1 | 1,2 | 14,14,15 | 0.20 | 0 | 17,19,21 | 0.40 | 0 |
| 2 | NAG | IA | 2 | 2 | 14,14,15 | 0.24 | 0 | 17,19,21 | 0.46 | 0 |
| 3 | NAG | JA | 1 | 1,3 | 14,14,15 | 0.19 | 0 | 17,19,21 | 0.36 | 0 |
| 3 | NAG | JA | 2 | 3 | 14,14,15 | 0.20 | 0 | 17,19,21 | 0.42 | 0 |
| 3 | BMA | JA | 3 | 3 | 11,11,12 | 0.49 | 0 | 15,15,17 | 0.78 | 0 |
| 2 | NAG | KA | 1 | 1,2 | 14,14,15 | 0.38 | 0 | 17,19,21 | 0.65 | 1 (5%) |
| 2 | NAG | KA | 2 | 2 | 14,14,15 | 0.27 | 0 | 17,19,21 | 0.47 | 0 |
| 3 | NAG | LA | 1 | 1,3 | 14,14,15 | 0.46 | 0 | 17,19,21 | 0.66 | 0 |
| 3 | NAG | LA | 2 | 3 | 14,14,15 | 0.18 | 0 | 17,19,21 | 0.49 | 0 |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\|>2$ | Counts | RMSZ | $\#\|Z\|>2$ |
| 3 | BMA | LA | 3 | 3 | 11,11,12 | 0.45 | 0 | 15,15,17 | 0.82 | 0 |
| 2 | NAG | MA | 1 | 1,2 | 14,14,15 | 0.26 | 0 | 17,19,21 | 0.53 | 0 |
| 2 | NAG | MA | 2 | 2 | 14,14,15 | 0.27 | 0 | 17,19,21 | 0.42 | 0 |
| 3 | NAG | NA | 1 | 1,3 | 14,14,15 | 0.61 | 0 | 17,19,21 | 0.95 | 1 (5%) |
| 3 | NAG | NA | 2 | 3 | 14,14,15 | 0.22 | 0 | 17,19,21 | 0.45 | 0 |
| 3 | BMA | NA | 3 | 3 | 11,11,12 | 0.61 | 0 | 15,15,17 | 0.75 | 0 |
| 3 | NAG | OA | 1 | 1,3 | 14,14,15 | 0.44 | 0 | 17,19,21 | 0.41 | 0 |
| 3 | NAG | OA | 2 | 3 | 14,14,15 | 0.29 | 0 | 17,19,21 | 0.51 | 0 |
| 3 | BMA | OA | 3 | 3 | 11,11,12 | 0.58 | 0 | 15,15,17 | 0.77 | 0 |
| 3 | NAG | PA | 1 | 1,3 | 14,14,15 | 0.27 | 0 | 17,19,21 | 0.48 | 0 |
| 3 | NAG | PA | 2 | 3 | 14,14,15 | 0.19 | 0 | 17,19,21 | 0.44 | 0 |
| 3 | BMA | PA | 3 | 3 | 11,11,12 | 0.55 | 0 | 15,15,17 | 0.79 | 0 |
| 3 | NAG | QA | 1 | 1,3 | 14,14,15 | 0.28 | 0 | 17,19,21 | 0.40 | 0 |
| 3 | NAG | QA | 2 | 3 | 14,14,15 | 0.55 | 0 | 17,19,21 | 1.34 | 1 (5%) |
| 3 | BMA | QA | 3 | 3 | 11,11,12 | 0.58 | 0 | 15,15,17 | 0.80 | 0 |
| 2 | NAG | RA | 1 | 1,2 | 14,14,15 | 0.19 | 0 | 17,19,21 | 0.42 | 0 |
| 2 | NAG | RA | 2 | 2 | 14,14,15 | 0.50 | 0 | 17,19,21 | 1.25 | 1 (5%) |
| 2 | NAG | SA | 1 | 1,2 | 14,14,15 | 0.23 | 0 | 17,19,21 | 0.46 | 0 |
| 2 | NAG | SA | 2 | 2 | 14,14,15 | 0.24 | 0 | 17,19,21 | 0.43 | 0 |
| 3 | NAG | TA | 1 | 1,3 | 14,14,15 | 0.18 | 0 | 17,19,21 | 0.39 | 0 |
| 3 | NAG | TA | 2 | 3 | 14,14,15 | 0.22 | 0 | 17,19,21 | 0.42 | 0 |
| 3 | BMA | TA | 3 | 3 | 11,11,12 | 0.54 | 0 | 15,15,17 | 0.76 | 0 |
| 2 | NAG | U | 1 | 1,2 | 14,14,15 | 0.20 | 0 | 17,19,21 | 0.38 | 0 |
| 2 | NAG | U | 2 | 2 | 14,14,15 | 0.23 | 0 | 17,19,21 | 0.45 | 0 |
| 2 | NAG | UA | 1 | 1,2 | 14,14,15 | 0.23 | 0 | 17,19,21 | 0.48 | 0 |
| 2 | NAG | UA | 2 | 2 | 14,14,15 | 0.25 | 0 | 17,19,21 | 0.44 | 0 |
| 3 | NAG | V | 1 | 1,3 | 14,14,15 | 0.14 | 0 | 17,19,21 | 0.39 | 0 |
| 3 | NAG | V | 2 | 3 | 14,14,15 | 0.22 | 0 | 17,19,21 | 0.41 | 0 |
| 3 | BMA | V | 3 | 3 | 11,11,12 | 0.49 | 0 | 15,15,17 | 0.78 | 0 |
| 3 | NAG | VA | 1 | 1,3 | 14,14,15 | 0.43 | 0 | 17,19,21 | 0.65 | 0 |
| 3 | NAG | VA | 2 | 3 | 14,14,15 | 0.17 | 0 | 17,19,21 | 0.50 | 0 |
| 3 | BMA | VA | 3 | 3 | 11,11,12 | 0.45 | 0 | 15,15,17 | 0.85 | 1 (6%) |
| 2 | NAG | W | 1 | 1,2 | 14,14,15 | 0.21 | 0 | 17,19,21 | 0.50 | 0 |
| 2 | NAG | W | 2 | 2 | 14,14,15 | 0.25 | 0 | 17,19,21 | 0.44 | 0 |
| 2 | NAG | WA | 1 | 1,2 | 14,14,15 | 0.60 | 1 (7%) | 17,19,21 | 0.69 | 0 |
| 2 | NAG | WA | 2 | 2 | 14,14,15 | 0.21 | 0 | 17,19,21 | 0.49 | 0 |
| 3 | NAG | X | 1 | 1,3 | 14,14,15 | 1.10 | 1 (7%) | 17,19,21 | 0.96 | 1 (5%) |
| 3 | NAG | X | 2 | 3 | 14,14,15 | 0.25 | 0 | 17,19,21 | 0.58 | 0 |
| 3 | BMA | X | 3 | 3 | 11,11,12 | 0.47 | 0 | 15,15,17 | 0.76 | 0 |
| 3 | NAG | XA | 1 | 1,3 | 14,14,15 | 0.62 | 0 | 17,19,21 | 0.93 | 1 (5%) |
| 3 | NAG | XA | 2 | 3 | 14,14,15 | 0.23 | 0 | 17,19,21 | 0.43 | 0 |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\|>2$ | Counts | RMSZ | $\#\|Z\|>2$ |
| 3 | BMA | XA | 3 | 3 | 11,11,12 | 0.56 | 0 | 15,15,17 | 0.79 | 0 |
| 2 | NAG | Y | 1 | 1,2 | 14,14,15 | 0.27 | 0 | 17,19,21 | 0.44 | 0 |
| 2 | NAG | Y | 2 | 2 | 14,14,15 | 0.22 | 0 | 17,19,21 | 0.43 | 0 |
| 3 | NAG | YA | 1 | 1,3 | 14,14,15 | 0.54 | 0 | 17,19,21 | 0.47 | 0 |
| 3 | NAG | YA | 2 | 3 | 14,14,15 | 0.29 | 0 | 17,19,21 | 0.50 | 0 |
| 3 | BMA | YA | 3 | 3 | 11,11,12 | 0.54 | 0 | 15,15,17 | 0.72 | 0 |
| 3 | NAG | Z | 1 | 1,3 | 14,14,15 | 0.19 | 0 | 17,19,21 | 0.46 | 0 |
| 3 | NAG | Z | 2 | 3 | 14,14,15 | 0.25 | 0 | 17,19,21 | 0.45 | 0 |
| 3 | BMA | Z | 3 | 3 | 11,11,12 | 0.61 | 0 | 15,15,17 | 0.74 | 0 |
| 3 | NAG | ZA | 1 | 1,3 | 14,14,15 | 0.27 | 0 | 17,19,21 | 0.46 | 0 |
| 3 | NAG | ZA | 2 | 3 | 14,14,15 | 0.19 | 0 | 17,19,21 | 0.45 | 0 |
| 3 | BMA | ZA | 3 | 3 | 11,11,12 | 0.51 | 0 | 15,15,17 | 0.83 | 0 |
| 3 | NAG | a | 1 | 1,3 | 14,14,15 | 0.42 | 0 | 17,19,21 | 0.42 | 0 |
| 3 | NAG | a | 2 | 3 | 14,14,15 | 0.31 | 0 | 17,19,21 | 0.49 | 0 |
| 3 | BMA | a | 3 | 3 | 11,11,12 | 0.53 | 0 | 15,15,17 | 0.77 | 0 |
| 3 | NAG | aA | 1 | 1,3 | 14,14,15 | 0.36 | 0 | 17,19,21 | 0.37 | 0 |
| 3 | NAG | aA | 2 | 3 | 14,14,15 | 0.64 | 1 (7%) | 17,19,21 | 1.33 | 1 (5%) |
| 3 | BMA | aA | 3 | 3 | 11,11,12 | 0.63 | 0 | 15,15,17 | 0.77 | 0 |
| 3 | NAG | b | 1 | 1,3 | 14,14,15 | 0.32 | 0 | 17,19,21 | 0.48 | 0 |
| 3 | NAG | b | 2 | 3 | 14,14,15 | 0.21 | 0 | 17,19,21 | 0.43 | 0 |
| 3 | BMA | b | 3 | 3 | 11,11,12 | 0.56 | 0 | 15,15,17 | 0.83 | 0 |
| 2 | NAG | bA | 1 | 1,2 | 14,14,15 | 0.20 | 0 | 17,19,21 | 0.38 | 0 |
| 2 | NAG | bA | 2 | 2 | 14,14,15 | 0.51 | 0 | 17,19,21 | 1.27 | 1 (5%) |
| 3 | NAG | c | 1 | 1,3 | 14,14,15 | 0.35 | 0 | 17,19,21 | 0.38 | 0 |
| 3 | NAG | c | 2 | 3 | 14,14,15 | 0.42 | 0 | 17,19,21 | 1.32 | 1 (5%) |
| 3 | BMA | c | 3 | 3 | 11,11,12 | 0.62 | 0 | 15,15,17 | 0.78 | 0 |
| 2 | NAG | cA | 1 | 1,2 | 14,14,15 | 0.22 | 0 | 17,19,21 | 0.48 | 0 |
| 2 | NAG | cA | 2 | 2 | 14,14,15 | 0.26 | 0 | 17,19,21 | 0.47 | 0 |
| 2 | NAG | d | 1 | 1,2 | 14,14,15 | 0.45 | 0 | 17,19,21 | 0.56 | 0 |
| 2 | NAG | d | 2 | 2 | 14,14,15 | 0.25 | 0 | 17,19,21 | 0.47 | 0 |
| 3 | NAG | dA | 1 | 1,3 | 14,14,15 | 0.15 | 0 | 17,19,21 | 0.39 | 0 |
| 3 | NAG | dA | 2 | 3 | 14,14,15 | 0.22 | 0 | 17,19,21 | 0.40 | 0 |
| 3 | BMA | dA | 3 | 3 | 11,11,12 | 0.50 | 0 | 15,15,17 | 0.79 | 0 |
| 2 | NAG | e | 1 | 1,2 | 14,14,15 | 0.24 | 0 | 17,19,21 | 0.46 | 0 |
| 2 | NAG | e | 2 | 2 | 14,14,15 | 0.24 | 0 | 17,19,21 | 0.44 | 0 |
| 2 | NAG | eA | 1 | 1,2 | 14,14,15 | 0.21 | 0 | 17,19,21 | 0.48 | 0 |
| 2 | NAG | eA | 2 | 2 | 14,14,15 | 0.25 | 0 | 17,19,21 | 0.43 | 0 |
| 3 | NAG | f | 1 | 1,3 | 14,14,15 | 0.18 | 0 | 17,19,21 | 0.38 | 0 |
| 3 | NAG | f | 2 | 3 | 14,14,15 | 0.23 | 0 | 17,19,21 | 0.42 | 0 |
| 3 | BMA | f | 3 | 3 | 11,11,12 | 0.52 | 0 | 15,15,17 | 0.77 | 0 |
| 3 | NAG | fA | 1 | 1,3 | 14,14,15 | 0.44 | 0 | 17,19,21 | 0.64 | 0 |
| 3 | NAG | fA | 2 | 3 | 14,14,15 | 0.19 | 0 | 17,19,21 | 0.47 | 0 |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\|>2$ | Counts | RMSZ | $\#\|Z\|>2$ |
| 3 | BMA | fA | 3 | 3 | 11,11,12 | 0.48 | 0 | 15,15,17 | 0.82 | 0 |
| 2 | NAG | g | 1 | 1,2 | 14,14,15 | 0.21 | 0 | 17,19,21 | 0.49 | 0 |
| 2 | NAG | g | 2 | 2 | 14,14,15 | 0.28 | 0 | 17,19,21 | 0.44 | 0 |
| 2 | NAG | gA | 1 | 1,2 | 14,14,15 | 0.25 | 0 | 17,19,21 | 0.43 | 0 |
| 2 | NAG | gA | 2 | 2 | 14,14,15 | 0.21 | 0 | 17,19,21 | 0.45 | 0 |
| 3 | NAG | h | 1 | 1,3 | 14,14,15 | 0.99 | 1 (7%) | 17,19,21 | 0.91 | 1 (5%) |
| 3 | NAG | h | 2 | 3 | 14,14,15 | 0.22 | 0 | 17,19,21 | 0.58 | 0 |
| 3 | BMA | h | 3 | 3 | 11,11,12 | 0.47 | 0 | 15,15,17 | 0.76 | 0 |
| 3 | NAG | hA | 1 | 1,3 | 14,14,15 | 0.18 | 0 | 17,19,21 | 0.48 | 0 |
| 3 | NAG | hA | 2 | 3 | 14,14,15 | 0.24 | 0 | 17,19,21 | 0.44 | 0 |
| 3 | BMA | hA | 3 | 3 | 11,11,12 | 0.62 | 0 | 15,15,17 | 0.74 | 0 |
| 2 | NAG | i | 1 | 1,2 | 14,14,15 | 0.63 | 1 (7%) | 17,19,21 | 0.70 | 0 |
| 2 | NAG | i | 2 | 2 | 14,14,15 | 0.26 | 0 | 17,19,21 | 0.49 | 0 |
| 3 | NAG | iA | 1 | 1,3 | 14,14,15 | 0.43 | 0 | 17,19,21 | 0.41 | 0 |
| 3 | NAG | iA | 2 | 3 | 14,14,15 | 0.29 | 0 | 17,19,21 | 0.49 | 0 |
| 3 | BMA | iA | 3 | 3 | 11,11,12 | 0.53 | 0 | 15,15,17 | 0.78 | 0 |
| 3 | NAG | j | 1 | 1,3 | 14,14,15 | 0.21 | 0 | 17,19,21 | 0.45 | 0 |
| 3 | NAG | j | 2 | 3 | 14,14,15 | 0.26 | 0 | 17,19,21 | 0.44 | 0 |
| 3 | BMA | j | 3 | 3 | 11,11,12 | 0.62 | 0 | 15,15,17 | 0.78 | 0 |
| 3 | NAG | jA | 1 | 1,3 | 14,14,15 | 0.30 | 0 | 17,19,21 | 0.48 | 0 |
| 3 | NAG | jA | 2 | 3 | 14,14,15 | 0.19 | 0 | 17,19,21 | 0.44 | 0 |
| 3 | BMA | jA | 3 | 3 | 11,11,12 | 0.56 | 0 | 15,15,17 | 0.81 | 0 |
| 3 | NAG | k | 1 | 1,3 | 14,14,15 | 0.46 | 0 | 17,19,21 | 0.43 | 0 |
| 3 | NAG | k | 2 | 3 | 14,14,15 | 0.29 | 0 | 17,19,21 | 0.49 | 0 |
| 3 | BMA | k | 3 | 3 | 11,11,12 | 0.53 | 0 | 15,15,17 | 0.74 | 0 |
| 3 | NAG | kA | 1 | 1,3 | 14,14,15 | 0.25 | 0 | 17,19,21 | 0.38 | 0 |
| 3 | NAG | kA | 2 | 3 | 14,14,15 | 0.25 | 0 | 17,19,21 | 0.42 | 0 |
| 3 | BMA | kA | 3 | 3 | 11,11,12 | 0.55 | 0 | 15,15,17 | 0.71 | 0 |
| 3 | NAG | l | 1 | 1,3 | 14,14,15 | 0.32 | 0 | 17,19,21 | 0.50 | 0 |
| 3 | NAG | l | 2 | 3 | 14,14,15 | 0.21 | 0 | 17,19,21 | 0.43 | 0 |
| 3 | BMA | l | 3 | 3 | 11,11,12 | 0.56 | 0 | 15,15,17 | 0.78 | 0 |
| 2 | NAG | lA | 1 | 1,2 | 14,14,15 | 0.44 | 0 | 17,19,21 | 0.65 | 0 |
| 2 | NAG | lA | 2 | 2 | 14,14,15 | 0.59 | 1 (7%) | 17,19,21 | 1.23 | 1 (5%) |
| 3 | NAG | m | 1 | 1,3 | 14,14,15 | 0.28 | 0 | 17,19,21 | 0.37 | 0 |
| 3 | NAG | m | 2 | 3 | 14,14,15 | 0.51 | 0 | 17,19,21 | 1.37 | 1 (5%) |
| 3 | BMA | m | 3 | 3 | 11,11,12 | 0.57 | 0 | 15,15,17 | 0.76 | 0 |
| 2 | NAG | mA | 1 | 1,2 | 14,14,15 | 0.24 | 0 | 17,19,21 | 0.47 | 0 |
| 2 | NAG | mA | 2 | 2 | 14,14,15 | 0.24 | 0 | 17,19,21 | 0.45 | 0 |
| 2 | NAG | n | 1 | 1,2 | 14,14,15 | 0.18 | 0 | 17,19,21 | 0.39 | 0 |
| 2 | NAG | n | 2 | 2 | 14,14,15 | 0.50 | 0 | 17,19,21 | 1.27 | 1 (5%) |
| 3 | NAG | nA | 1 | 1,3 | 14,14,15 | 0.17 | 0 | 17,19,21 | 0.38 | 0 |
| 3 | NAG | nA | 2 | 3 | 14,14,15 | 0.25 | 0 | 17,19,21 | 0.43 | 0 |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\|>2$ | Counts | RMSZ | $\#\|Z\|>2$ |
| 3 | BMA | nA | 3 | 3 | 11,11,12 | 0.53 | 0 | 15,15,17 | 0.78 | 0 |
| 2 | NAG | o | 1 | 1,2 | 14,14,15 | 0.28 | 0 | 17,19,21 | 0.48 | 0 |
| 2 | NAG | o | 2 | 2 | 14,14,15 | 0.25 | 0 | 17,19,21 | 0.48 | 0 |
| 2 | NAG | oA | 1 | 1,2 | 14,14,15 | 0.19 | 0 | 17,19,21 | 0.50 | 0 |
| 2 | NAG | oA | 2 | 2 | 14,14,15 | 0.24 | 0 | 17,19,21 | 0.43 | 0 |
| 3 | NAG | p | 1 | 1,3 | 14,14,15 | 0.15 | 0 | 17,19,21 | 0.42 | 0 |
| 3 | NAG | p | 2 | 3 | 14,14,15 | 0.19 | 0 | 17,19,21 | 0.42 | 0 |
| 3 | BMA | p | 3 | 3 | 11,11,12 | 0.55 | 0 | 15,15,17 | 0.75 | 0 |
| 3 | NAG | pA | 1 | 1,3 | 14,14,15 | 0.46 | 0 | 17,19,21 | 0.66 | 0 |
| 3 | NAG | pA | 2 | 3 | 14,14,15 | 0.19 | 0 | 17,19,21 | 0.48 | 0 |
| 3 | BMA | pA | 3 | 3 | 11,11,12 | 0.47 | 0 | 15,15,17 | 0.88 | 1 (6%) |
| 2 | NAG | q | 1 | 1,2 | 14,14,15 | 0.29 | 0 | 17,19,21 | 0.49 | 0 |
| 2 | NAG | q | 2 | 2 | 14,14,15 | 0.26 | 0 | 17,19,21 | 0.43 | 0 |
| 2 | NAG | qA | 1 | 1,2 | 14,14,15 | 0.28 | 0 | 17,19,21 | 0.55 | 0 |
| 2 | NAG | qA | 2 | 2 | 14,14,15 | 0.25 | 0 | 17,19,21 | 0.43 | 0 |
| 3 | NAG | r | 1 | 1,3 | 14,14,15 | 1.00 | 1 (7%) | 17,19,21 | 0.91 | 1 (5%) |
| 3 | NAG | r | 2 | 3 | 14,14,15 | 0.23 | 0 | 17,19,21 | 0.55 | 0 |
| 3 | BMA | r | 3 | 3 | 11,11,12 | 0.52 | 0 | 15,15,17 | 0.78 | 0 |
| 3 | NAG | rA | 1 | 1,3 | 14,14,15 | 0.21 | 0 | 17,19,21 | 0.49 | 0 |
| 3 | NAG | rA | 2 | 3 | 14,14,15 | 0.22 | 0 | 17,19,21 | 0.46 | 0 |
| 3 | BMA | rA | 3 | 3 | 11,11,12 | 0.56 | 0 | 15,15,17 | 0.84 | 0 |
| 2 | NAG | s | 1 | 1,2 | 14,14,15 | 0.22 | 0 | 17,19,21 | 0.43 | 0 |
| 2 | NAG | s | 2 | 2 | 14,14,15 | 0.21 | 0 | 17,19,21 | 0.45 | 0 |
| 3 | NAG | sA | 1 | 1,3 | 14,14,15 | 0.47 | 0 | 17,19,21 | 0.42 | 0 |
| 3 | NAG | sA | 2 | 3 | 14,14,15 | 0.29 | 0 | 17,19,21 | 0.50 | 0 |
| 3 | BMA | sA | 3 | 3 | 11,11,12 | 0.54 | 0 | 15,15,17 | 0.74 | 0 |
| 3 | NAG | t | 1 | 1,3 | 14,14,15 | 0.21 | 0 | 17,19,21 | 0.48 | 0 |
| 3 | NAG | t | 2 | 3 | 14,14,15 | 0.28 | 0 | 17,19,21 | 0.48 | 0 |
| 3 | BMA | t | 3 | 3 | 11,11,12 | 0.63 | 0 | 15,15,17 | 0.72 | 0 |
| 3 | NAG | tA | 1 | 1,3 | 14,14,15 | 0.33 | 0 | 17,19,21 | 0.49 | 0 |
| 3 | NAG | tA | 2 | 3 | 14,14,15 | 0.21 | 0 | 17,19,21 | 0.44 | 0 |
| 3 | BMA | tA | 3 | 3 | 11,11,12 | 0.58 | 0 | 15,15,17 | 0.79 | 0 |
| 3 | NAG | u | 1 | 1,3 | 14,14,15 | 0.49 | 0 | 17,19,21 | 0.44 | 0 |
| 3 | NAG | u | 2 | 3 | 14,14,15 | 0.31 | 0 | 17,19,21 | 0.50 | 0 |
| 3 | BMA | u | 3 | 3 | 11,11,12 | 0.58 | 0 | 15,15,17 | 0.75 | 0 |
| 3 | NAG | uA | 1 | 1,3 | 14,14,15 | 0.30 | 0 | 17,19,21 | 0.36 | 0 |
| 3 | NAG | uA | 2 | 3 | 14,14,15 | 0.53 | 0 | 17,19,21 | 1.37 | 1 (5%) |
| 3 | BMA | uA | 3 | 3 | 11,11,12 | 0.59 | 0 | 15,15,17 | 0.76 | 0 |
| 3 | NAG | v | 1 | 1,3 | 14,14,15 | 0.30 | 0 | 17,19,21 | 0.47 | 0 |
| 3 | NAG | v | 2 | 3 | 14,14,15 | 0.19 | 0 | 17,19,21 | 0.44 | 0 |
| 3 | BMA | v | 3 | 3 | 11,11,12 | 0.56 | 0 | 15,15,17 | 0.78 | 0 |
| 2 | NAG | vA | 1 | 1,2 | 14,14,15 | 0.18 | 0 | 17,19,21 | 0.43 | 0 |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\|>2$ | Counts | RMSZ | $\#\|Z\|>2$ |
| 2 | NAG | vA | 2 | 2 | 14,14,15 | 0.54 | 0 | 17,19,21 | 1.26 | 1 (5%) |
| 3 | NAG | w | 1 | 1,3 | 14,14,15 | 0.38 | 0 | 17,19,21 | 0.86 | 1 (5%) |
| 3 | NAG | w | 2 | 3 | 14,14,15 | 0.37 | 0 | 17,19,21 | 0.50 | 0 |
| 3 | BMA | w | 3 | 3 | 11,11,12 | 0.54 | 0 | 15,15,17 | 0.76 | 0 |
| 2 | NAG | wA | 1 | 1,2 | 14,14,15 | 0.25 | 0 | 17,19,21 | 0.49 | 0 |
| 2 | NAG | wA | 2 | 2 | 14,14,15 | 0.23 | 0 | 17,19,21 | 0.46 | 0 |
| 2 | NAG | x | 1 | 1,2 | 14,14,15 | 0.19 | 0 | 17,19,21 | 0.41 | 0 |
| 2 | NAG | x | 2 | 2 | 14,14,15 | 0.51 | 0 | 17,19,21 | 1.24 | 1 (5%) |
| 3 | NAG | xA | 1 | 1,3 | 14,14,15 | 0.27 | 0 | 17,19,21 | 0.38 | 0 |
| 3 | NAG | xA | 2 | 3 | 14,14,15 | 0.16 | 0 | 17,19,21 | 0.47 | 0 |
| 3 | BMA | xA | 3 | 3 | 11,11,12 | 0.58 | 0 | 15,15,17 | 0.76 | 0 |
| 2 | NAG | y | 1 | 1,2 | 14,14,15 | 0.25 | 0 | 17,19,21 | 0.45 | 0 |
| 2 | NAG | y | 2 | 2 | 14,14,15 | 0.27 | 0 | 17,19,21 | 0.47 | 0 |
| 2 | NAG | yA | 1 | 1,2 | 14,14,15 | 0.20 | 0 | 17,19,21 | 0.52 | 0 |
| 2 | NAG | yA | 2 | 2 | 14,14,15 | 0.28 | 0 | 17,19,21 | 0.41 | 0 |
| 3 | NAG | z | 1 | 1,3 | 14,14,15 | 0.17 | 0 | 17,19,21 | 0.39 | 0 |
| 3 | NAG | z | 2 | 3 | 14,14,15 | 0.23 | 0 | 17,19,21 | 0.43 | 0 |
| 3 | BMA | z | 3 | 3 | 11,11,12 | 0.51 | 0 | 15,15,17 | 0.75 | 0 |
| 3 | NAG | zA | 1 | 1,3 | 14,14,15 | 1.04 | 1 (7%) | 17,19,21 | 0.94 | 1 (5%) |
| 3 | NAG | zA | 2 | 3 | 14,14,15 | 0.22 | 0 | 17,19,21 | 0.53 | 0 |
| 3 | BMA | zA | 3 | 3 | 11,11,12 | 0.49 | 0 | 15,15,17 | 0.78 | 0 |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 2 | NAG | 0 | 1 | 1,2 | - | 2/6/23/26 | 0/1/1/1 |
| 2 | NAG | 0 | 2 | 2 | - | 2/6/23/26 | 0/1/1/1 |
| 2 | NAG | 0A | 1 | 1,2 | - | 0/6/23/26 | 0/1/1/1 |
| 2 | NAG | 0A | 2 | 2 | - | 2/6/23/26 | 0/1/1/1 |
| 3 | NAG | 1 | 1 | 1,3 | - | 2/6/23/26 | 0/1/1/1 |
| 3 | NAG | 1 | 2 | 3 | - | 2/6/23/26 | 0/1/1/1 |
| 3 | BMA | 1 | 3 | 3 | - | 2/2/19/22 | 0/1/1/1 |
| 3 | NAG | 1A | 1 | 1,3 | - | 4/6/23/26 | 0/1/1/1 |
| 3 | NAG | 1A | 2 | 3 | - | 2/6/23/26 | 0/1/1/1 |
| 3 | BMA | 1A | 3 | 3 | - | 0/2/19/22 | 0/1/1/1 |
| 2 | NAG | 2 | 1 | 1,2 | - | 0/6/23/26 | 0/1/1/1 |
| 2 | NAG | 2 | 2 | 2 | - | 2/6/23/26 | 0/1/1/1 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 3 | NAG | 2A | 1 | 1,3 | - | 2/6/23/26 | 0/1/1/1 |
| 3 | NAG | 2A | 2 | 3 | - | 3/6/23/26 | 0/1/1/1 |
| 3 | BMA | 2A | 3 | 3 | - | 1/2/19/22 | 0/1/1/1 |
| 3 | NAG | 3 | 1 | 1,3 | - | 4/6/23/26 | 0/1/1/1 |
| 3 | NAG | 3 | 2 | 3 | - | 3/6/23/26 | 0/1/1/1 |
| 3 | BMA | 3 | 3 | 3 | - | 0/2/19/22 | 0/1/1/1 |
| 3 | NAG | 3A | 1 | 1,3 | - | 2/6/23/26 | 0/1/1/1 |
| 3 | NAG | 3A | 2 | 3 | - | 2/6/23/26 | 0/1/1/1 |
| 3 | BMA | 3A | 3 | 3 | - | 0/2/19/22 | 0/1/1/1 |
| 3 | NAG | 4 | 1 | 1,3 | - | 4/6/23/26 | 0/1/1/1 |
| 3 | NAG | 4 | 2 | 3 | - | 4/6/23/26 | 0/1/1/1 |
| 3 | BMA | 4 | 3 | 3 | - | 0/2/19/22 | 0/1/1/1 |
| 3 | NAG | 4A | 1 | 1,3 | - | 2/6/23/26 | 0/1/1/1 |
| 3 | NAG | 4A | 2 | 3 | - | 4/6/23/26 | 0/1/1/1 |
| 3 | BMA | 4A | 3 | 3 | - | 2/2/19/22 | 0/1/1/1 |
| 3 | NAG | 5 | 1 | 1,3 | - | 0/6/23/26 | 0/1/1/1 |
| 3 | NAG | 5 | 2 | 3 | - | 2/6/23/26 | 0/1/1/1 |
| 3 | BMA | 5 | 3 | 3 | - | 0/2/19/22 | 0/1/1/1 |
| 2 | NAG | 5A | 1 | 1,2 | - | 1/6/23/26 | 0/1/1/1 |
| 2 | NAG | 5A | 2 | 2 | - | 2/6/23/26 | 0/1/1/1 |
| 3 | NAG | 6 | 1 | 1,3 | - | 2/6/23/26 | 0/1/1/1 |
| 3 | NAG | 6 | 2 | 3 | - | 2/6/23/26 | 0/1/1/1 |
| 3 | BMA | 6 | 3 | 3 | - | 1/2/19/22 | 0/1/1/1 |
| 2 | NAG | 7 | 1 | 1,2 | - | 0/6/23/26 | 0/1/1/1 |
| 2 | NAG | 7 | 2 | 2 | - | 2/6/23/26 | 0/1/1/1 |
| 2 | NAG | 8 | 1 | 1,2 | - | 1/6/23/26 | 0/1/1/1 |
| 2 | NAG | 8 | 2 | 2 | - | 0/6/23/26 | 0/1/1/1 |
| 3 | NAG | 9 | 1 | 1,3 | - | 3/6/23/26 | 0/1/1/1 |
| 3 | NAG | 9 | 2 | 3 | - | 2/6/23/26 | 0/1/1/1 |
| 3 | BMA | 9 | 3 | 3 | - | 0/2/19/22 | 0/1/1/1 |
| 2 | NAG | AA | 1 | 1,2 | - | 1/6/23/26 | 0/1/1/1 |
| 2 | NAG | AA | 2 | 2 | - | 2/6/23/26 | 0/1/1/1 |
| 3 | NAG | BA | 1 | 1,3 | - | 2/6/23/26 | 0/1/1/1 |
| 3 | NAG | BA | 2 | 3 | - | 2/6/23/26 | 0/1/1/1 |
| 3 | BMA | BA | 3 | 3 | - | 0/2/19/22 | 0/1/1/1 |
| 2 | NAG | CA | 1 | 1,2 | - | 3/6/23/26 | 0/1/1/1 |
| 2 | NAG | CA | 2 | 2 | - | 0/6/23/26 | 0/1/1/1 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 3 | NAG | DA | 1 | 1,3 | - | 4/6/23/26 | 0/1/1/1 |
| 3 | NAG | DA | 2 | 3 | - | 2/6/23/26 | 0/1/1/1 |
| 3 | BMA | DA | 3 | 3 | - | 0/2/19/22 | 0/1/1/1 |
| 3 | NAG | EA | 1 | 1,3 | - | 4/6/23/26 | 0/1/1/1 |
| 3 | NAG | EA | 2 | 3 | - | 3/6/23/26 | 0/1/1/1 |
| 3 | BMA | EA | 3 | 3 | - | 1/2/19/22 | 0/1/1/1 |
| 3 | NAG | FA | 1 | 1,3 | - | 2/6/23/26 | 0/1/1/1 |
| 3 | NAG | FA | 2 | 3 | - | 2/6/23/26 | 0/1/1/1 |
| 3 | BMA | FA | 3 | 3 | - | 0/2/19/22 | 0/1/1/1 |
| 3 | NAG | GA | 1 | 1,3 | - | 3/6/23/26 | 0/1/1/1 |
| 3 | NAG | GA | 2 | 3 | - | 2/6/23/26 | 0/1/1/1 |
| 3 | BMA | GA | 3 | 3 | - | 1/2/19/22 | 0/1/1/1 |
| 2 | NAG | HA | 1 | 1,2 | - | 2/6/23/26 | 0/1/1/1 |
| 2 | NAG | HA | 2 | 2 | - | 3/6/23/26 | 0/1/1/1 |
| 2 | NAG | IA | 1 | 1,2 | - | 1/6/23/26 | 0/1/1/1 |
| 2 | NAG | IA | 2 | 2 | - | 0/6/23/26 | 0/1/1/1 |
| 3 | NAG | JA | 1 | 1,3 | - | 4/6/23/26 | 0/1/1/1 |
| 3 | NAG | JA | 2 | 3 | - | 2/6/23/26 | 0/1/1/1 |
| 3 | BMA | JA | 3 | 3 | - | 0/2/19/22 | 0/1/1/1 |
| 2 | NAG | KA | 1 | 1,2 | - | 1/6/23/26 | 0/1/1/1 |
| 2 | NAG | KA | 2 | 2 | - | 2/6/23/26 | 0/1/1/1 |
| 3 | NAG | LA | 1 | 1,3 | - | 0/6/23/26 | 0/1/1/1 |
| 3 | NAG | LA | 2 | 3 | - | 2/6/23/26 | 0/1/1/1 |
| 3 | BMA | LA | 3 | 3 | - | 1/2/19/22 | 0/1/1/1 |
| 2 | NAG | MA | 1 | 1,2 | - | 0/6/23/26 | 0/1/1/1 |
| 2 | NAG | MA | 2 | 2 | - | 2/6/23/26 | 0/1/1/1 |
| 3 | NAG | NA | 1 | 1,3 | - | 4/6/23/26 | 0/1/1/1 |
| 3 | NAG | NA | 2 | 3 | - | 4/6/23/26 | 0/1/1/1 |
| 3 | BMA | NA | 3 | 3 | - | 0/2/19/22 | 0/1/1/1 |
| 3 | NAG | OA | 1 | 1,3 | - | 4/6/23/26 | 0/1/1/1 |
| 3 | NAG | OA | 2 | 3 | - | 4/6/23/26 | 0/1/1/1 |
| 3 | BMA | OA | 3 | 3 | - | 0/2/19/22 | 0/1/1/1 |
| 3 | NAG | PA | 1 | 1,3 | - | 0/6/23/26 | 0/1/1/1 |
| 3 | NAG | PA | 2 | 3 | - | 2/6/23/26 | 0/1/1/1 |
| 3 | BMA | PA | 3 | 3 | - | 0/2/19/22 | 0/1/1/1 |
| 3 | NAG | QA | 1 | 1,3 | - | 2/6/23/26 | 0/1/1/1 |
| 3 | NAG | QA | 2 | 3 | - | 2/6/23/26 | 0/1/1/1 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 3 | BMA | QA | 3 | 3 | - | 1/2/19/22 | 0/1/1/1 |
| 2 | NAG | RA | 1 | 1,2 | - | 2/6/23/26 | 0/1/1/1 |
| 2 | NAG | RA | 2 | 2 | - | 3/6/23/26 | 0/1/1/1 |
| 2 | NAG | SA | 1 | 1,2 | - | 1/6/23/26 | 0/1/1/1 |
| 2 | NAG | SA | 2 | 2 | - | 0/6/23/26 | 0/1/1/1 |
| 3 | NAG | TA | 1 | 1,3 | - | 4/6/23/26 | 0/1/1/1 |
| 3 | NAG | TA | 2 | 3 | - | 0/6/23/26 | 0/1/1/1 |
| 3 | BMA | TA | 3 | 3 | - | 0/2/19/22 | 0/1/1/1 |
| 2 | NAG | U | 1 | 1,2 | - | 1/6/23/26 | 0/1/1/1 |
| 2 | NAG | U | 2 | 2 | - | 1/6/23/26 | 0/1/1/1 |
| 2 | NAG | UA | 1 | 1,2 | - | 0/6/23/26 | 0/1/1/1 |
| 2 | NAG | UA | 2 | 2 | - | 2/6/23/26 | 0/1/1/1 |
| 3 | NAG | V | 1 | 1,3 | - | 4/6/23/26 | 0/1/1/1 |
| 3 | NAG | V | 2 | 3 | - | 2/6/23/26 | 0/1/1/1 |
| 3 | BMA | V | 3 | 3 | - | 0/2/19/22 | 0/1/1/1 |
| 3 | NAG | VA | 1 | 1,3 | - | 1/6/23/26 | 0/1/1/1 |
| 3 | NAG | VA | 2 | 3 | - | 2/6/23/26 | 0/1/1/1 |
| 3 | BMA | VA | 3 | 3 | - | 0/2/19/22 | 0/1/1/1 |
| 2 | NAG | W | 1 | 1,2 | - | 0/6/23/26 | 0/1/1/1 |
| 2 | NAG | W | 2 | 2 | - | 2/6/23/26 | 0/1/1/1 |
| 2 | NAG | WA | 1 | 1,2 | - | 3/6/23/26 | 0/1/1/1 |
| 2 | NAG | WA | 2 | 2 | - | 2/6/23/26 | 0/1/1/1 |
| 3 | NAG | X | 1 | 1,3 | - | 2/6/23/26 | 0/1/1/1 |
| 3 | NAG | X | 2 | 3 | - | 1/6/23/26 | 0/1/1/1 |
| 3 | BMA | X | 3 | 3 | - | 0/2/19/22 | 0/1/1/1 |
| 3 | NAG | XA | 1 | 1,3 | - | 4/6/23/26 | 0/1/1/1 |
| 3 | NAG | XA | 2 | 3 | - | 2/6/23/26 | 0/1/1/1 |
| 3 | BMA | XA | 3 | 3 | - | 0/2/19/22 | 0/1/1/1 |
| 2 | NAG | Y | 1 | 1,2 | - | 0/6/23/26 | 0/1/1/1 |
| 2 | NAG | Y | 2 | 2 | - | 2/6/23/26 | 0/1/1/1 |
| 3 | NAG | YA | 1 | 1,3 | - | 4/6/23/26 | 0/1/1/1 |
| 3 | NAG | YA | 2 | 3 | - | 3/6/23/26 | 0/1/1/1 |
| 3 | BMA | YA | 3 | 3 | - | 0/2/19/22 | 0/1/1/1 |
| 3 | NAG | Z | 1 | 1,3 | - | 3/6/23/26 | 0/1/1/1 |
| 3 | NAG | Z | 2 | 3 | - | 2/6/23/26 | 0/1/1/1 |
| 3 | BMA | Z | 3 | 3 | - | 0/2/19/22 | 0/1/1/1 |
| 3 | NAG | ZA | 1 | 1,3 | - | 2/6/23/26 | 0/1/1/1 |
| 3 | NAG | ZA | 2 | 3 | - | 2/6/23/26 | 0/1/1/1 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 3 | BMA | ZA | 3 | 3 | - | 0/2/19/22 | 0/1/1/1 |
| 3 | NAG | a | 1 | 1,3 | - | 4/6/23/26 | 0/1/1/1 |
| 3 | NAG | a | 2 | 3 | - | 4/6/23/26 | 0/1/1/1 |
| 3 | BMA | a | 3 | 3 | - | 0/2/19/22 | 0/1/1/1 |
| 3 | NAG | aA | 1 | 1,3 | - | 2/6/23/26 | 0/1/1/1 |
| 3 | NAG | aA | 2 | 3 | - | 2/6/23/26 | 0/1/1/1 |
| 3 | BMA | aA | 3 | 3 | - | 1/2/19/22 | 0/1/1/1 |
| 3 | NAG | b | 1 | 1,3 | - | 2/6/23/26 | 0/1/1/1 |
| 3 | NAG | b | 2 | 3 | - | 2/6/23/26 | 0/1/1/1 |
| 3 | BMA | b | 3 | 3 | - | 0/2/19/22 | 0/1/1/1 |
| 2 | NAG | bA | 1 | 1,2 | - | 2/6/23/26 | 0/1/1/1 |
| 2 | NAG | bA | 2 | 2 | - | 2/6/23/26 | 0/1/1/1 |
| 3 | NAG | c | 1 | 1,3 | - | 2/6/23/26 | 0/1/1/1 |
| 3 | NAG | c | 2 | 3 | - | 2/6/23/26 | 0/1/1/1 |
| 3 | BMA | c | 3 | 3 | - | 1/2/19/22 | 0/1/1/1 |
| 2 | NAG | cA | 1 | 1,2 | - | 1/6/23/26 | 0/1/1/1 |
| 2 | NAG | cA | 2 | 2 | - | 1/6/23/26 | 0/1/1/1 |
| 2 | NAG | d | 1 | 1,2 | - | 0/6/23/26 | 0/1/1/1 |
| 2 | NAG | d | 2 | 2 | - | 1/6/23/26 | 0/1/1/1 |
| 3 | NAG | dA | 1 | 1,3 | - | 4/6/23/26 | 0/1/1/1 |
| 3 | NAG | dA | 2 | 3 | - | 2/6/23/26 | 0/1/1/1 |
| 3 | BMA | dA | 3 | 3 | - | 0/2/19/22 | 0/1/1/1 |
| 2 | NAG | e | 1 | 1,2 | - | 1/6/23/26 | 0/1/1/1 |
| 2 | NAG | e | 2 | 2 | - | 0/6/23/26 | 0/1/1/1 |
| 2 | NAG | eA | 1 | 1,2 | - | 0/6/23/26 | 0/1/1/1 |
| 2 | NAG | eA | 2 | 2 | - | 2/6/23/26 | 0/1/1/1 |
| 3 | NAG | f | 1 | 1,3 | - | 3/6/23/26 | 0/1/1/1 |
| 3 | NAG | f | 2 | 3 | - | 2/6/23/26 | 0/1/1/1 |
| 3 | BMA | f | 3 | 3 | - | 0/2/19/22 | 0/1/1/1 |
| 3 | NAG | fA | 1 | 1,3 | - | 2/6/23/26 | 0/1/1/1 |
| 3 | NAG | fA | 2 | 3 | - | 2/6/23/26 | 0/1/1/1 |
| 3 | BMA | fA | 3 | 3 | - | 0/2/19/22 | 0/1/1/1 |
| 2 | NAG | g | 1 | 1,2 | - | 0/6/23/26 | 0/1/1/1 |
| 2 | NAG | g | 2 | 2 | - | 2/6/23/26 | 0/1/1/1 |
| 2 | NAG | gA | 1 | 1,2 | - | 0/6/23/26 | 0/1/1/1 |
| 2 | NAG | gA | 2 | 2 | - | 2/6/23/26 | 0/1/1/1 |
| 3 | NAG | h | 1 | 1,3 | - | 2/6/23/26 | 0/1/1/1 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 3 | NAG | h | 2 | 3 | - | 2/6/23/26 | 0/1/1/1 |
| 3 | BMA | h | 3 | 3 | - | 0/2/19/22 | 0/1/1/1 |
| 3 | NAG | hA | 1 | 1,3 | - | 3/6/23/26 | 0/1/1/1 |
| 3 | NAG | hA | 2 | 3 | - | 2/6/23/26 | 0/1/1/1 |
| 3 | BMA | hA | 3 | 3 | - | 0/2/19/22 | 0/1/1/1 |
| 2 | NAG | i | 1 | 1,2 | - | 1/6/23/26 | 0/1/1/1 |
| 2 | NAG | i | 2 | 2 | - | 2/6/23/26 | 0/1/1/1 |
| 3 | NAG | iA | 1 | 1,3 | - | 4/6/23/26 | 0/1/1/1 |
| 3 | NAG | iA | 2 | 3 | - | 4/6/23/26 | 0/1/1/1 |
| 3 | BMA | iA | 3 | 3 | - | 0/2/19/22 | 0/1/1/1 |
| 3 | NAG | j | 1 | 1,3 | - | 3/6/23/26 | 0/1/1/1 |
| 3 | NAG | j | 2 | 3 | - | 2/6/23/26 | 0/1/1/1 |
| 3 | BMA | j | 3 | 3 | - | 0/2/19/22 | 0/1/1/1 |
| 3 | NAG | jA | 1 | 1,3 | - | 2/6/23/26 | 0/1/1/1 |
| 3 | NAG | jA | 2 | 3 | - | 2/6/23/26 | 0/1/1/1 |
| 3 | BMA | jA | 3 | 3 | - | 0/2/19/22 | 0/1/1/1 |
| 3 | NAG | k | 1 | 1,3 | - | 4/6/23/26 | 0/1/1/1 |
| 3 | NAG | k | 2 | 3 | - | 4/6/23/26 | 0/1/1/1 |
| 3 | BMA | k | 3 | 3 | - | 0/2/19/22 | 0/1/1/1 |
| 3 | NAG | kA | 1 | 1,3 | - | 1/6/23/26 | 0/1/1/1 |
| 3 | NAG | kA | 2 | 3 | - | 2/6/23/26 | 0/1/1/1 |
| 3 | BMA | kA | 3 | 3 | - | 2/2/19/22 | 0/1/1/1 |
| 3 | NAG | l | 1 | 1,3 | - | 0/6/23/26 | 0/1/1/1 |
| 3 | NAG | l | 2 | 3 | - | 2/6/23/26 | 0/1/1/1 |
| 3 | BMA | l | 3 | 3 | - | 2/2/19/22 | 0/1/1/1 |
| 2 | NAG | lA | 1 | 1,2 | - | 2/6/23/26 | 0/1/1/1 |
| 2 | NAG | lA | 2 | 2 | - | 1/6/23/26 | 0/1/1/1 |
| 3 | NAG | m | 1 | 1,3 | - | 2/6/23/26 | 0/1/1/1 |
| 3 | NAG | m | 2 | 3 | - | 2/6/23/26 | 0/1/1/1 |
| 3 | BMA | m | 3 | 3 | - | 1/2/19/22 | 0/1/1/1 |
| 2 | NAG | mA | 1 | 1,2 | - | 1/6/23/26 | 0/1/1/1 |
| 2 | NAG | mA | 2 | 2 | - | 0/6/23/26 | 0/1/1/1 |
| 2 | NAG | n | 1 | 1,2 | - | 2/6/23/26 | 0/1/1/1 |
| 2 | NAG | n | 2 | 2 | - | 2/6/23/26 | 0/1/1/1 |
| 3 | NAG | nA | 1 | 1,3 | - | 3/6/23/26 | 0/1/1/1 |
| 3 | NAG | nA | 2 | 3 | - | 2/6/23/26 | 0/1/1/1 |
| 3 | BMA | nA | 3 | 3 | - | 0/2/19/22 | 0/1/1/1 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 2 | NAG | o | 1 | 1,2 | - | 1/6/23/26 | 0/1/1/1 |
| 2 | NAG | o | 2 | 2 | - | 1/6/23/26 | 0/1/1/1 |
| 2 | NAG | oA | 1 | 1,2 | - | 0/6/23/26 | 0/1/1/1 |
| 2 | NAG | oA | 2 | 2 | - | 2/6/23/26 | 0/1/1/1 |
| 3 | NAG | p | 1 | 1,3 | - | 4/6/23/26 | 0/1/1/1 |
| 3 | NAG | p | 2 | 3 | - | 2/6/23/26 | 0/1/1/1 |
| 3 | BMA | p | 3 | 3 | - | 0/2/19/22 | 0/1/1/1 |
| 3 | NAG | pA | 1 | 1,3 | - | 2/6/23/26 | 0/1/1/1 |
| 3 | NAG | pA | 2 | 3 | - | 2/6/23/26 | 0/1/1/1 |
| 3 | BMA | pA | 3 | 3 | - | 0/2/19/22 | 0/1/1/1 |
| 2 | NAG | q | 1 | 1,2 | - | 0/6/23/26 | 0/1/1/1 |
| 2 | NAG | q | 2 | 2 | - | 2/6/23/26 | 0/1/1/1 |
| 2 | NAG | qA | 1 | 1,2 | - | 0/6/23/26 | 0/1/1/1 |
| 2 | NAG | qA | 2 | 2 | - | 2/6/23/26 | 0/1/1/1 |
| 3 | NAG | r | 1 | 1,3 | - | 2/6/23/26 | 0/1/1/1 |
| 3 | NAG | r | 2 | 3 | - | 2/6/23/26 | 0/1/1/1 |
| 3 | BMA | r | 3 | 3 | - | 0/2/19/22 | 0/1/1/1 |
| 3 | NAG | rA | 1 | 1,3 | - | 3/6/23/26 | 0/1/1/1 |
| 3 | NAG | rA | 2 | 3 | - | 3/6/23/26 | 0/1/1/1 |
| 3 | BMA | rA | 3 | 3 | - | 1/2/19/22 | 0/1/1/1 |
| 2 | NAG | s | 1 | 1,2 | - | 0/6/23/26 | 0/1/1/1 |
| 2 | NAG | s | 2 | 2 | - | 2/6/23/26 | 0/1/1/1 |
| 3 | NAG | sA | 1 | 1,3 | - | 4/6/23/26 | 0/1/1/1 |
| 3 | NAG | sA | 2 | 3 | - | 4/6/23/26 | 0/1/1/1 |
| 3 | BMA | sA | 3 | 3 | - | 0/2/19/22 | 0/1/1/1 |
| 3 | NAG | t | 1 | 1,3 | - | 3/6/23/26 | 0/1/1/1 |
| 3 | NAG | t | 2 | 3 | - | 2/6/23/26 | 0/1/1/1 |
| 3 | BMA | t | 3 | 3 | - | 0/2/19/22 | 0/1/1/1 |
| 3 | NAG | tA | 1 | 1,3 | - | 0/6/23/26 | 0/1/1/1 |
| 3 | NAG | tA | 2 | 3 | - | 2/6/23/26 | 0/1/1/1 |
| 3 | BMA | tA | 3 | 3 | - | 2/2/19/22 | 0/1/1/1 |
| 3 | NAG | u | 1 | 1,3 | - | 3/6/23/26 | 0/1/1/1 |
| 3 | NAG | u | 2 | 3 | - | 4/6/23/26 | 0/1/1/1 |
| 3 | BMA | u | 3 | 3 | - | 0/2/19/22 | 0/1/1/1 |
| 3 | NAG | uA | 1 | 1,3 | - | 2/6/23/26 | 0/1/1/1 |
| 3 | NAG | uA | 2 | 3 | - | 2/6/23/26 | 0/1/1/1 |
| 3 | BMA | uA | 3 | 3 | - | 1/2/19/22 | 0/1/1/1 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 3 | NAG | v | 1 | 1,3 | - | 2/6/23/26 | 0/1/1/1 |
| 3 | NAG | v | 2 | 3 | - | 2/6/23/26 | 0/1/1/1 |
| 3 | BMA | v | 3 | 3 | - | 0/2/19/22 | 0/1/1/1 |
| 2 | NAG | vA | 1 | 1,2 | - | 2/6/23/26 | 0/1/1/1 |
| 2 | NAG | vA | 2 | 2 | - | 4/6/23/26 | 0/1/1/1 |
| 3 | NAG | w | 1 | 1,3 | - | 2/6/23/26 | 0/1/1/1 |
| 3 | NAG | w | 2 | 3 | - | 2/6/23/26 | 0/1/1/1 |
| 3 | BMA | w | 3 | 3 | - | 1/2/19/22 | 0/1/1/1 |
| 2 | NAG | wA | 1 | 1,2 | - | 1/6/23/26 | 0/1/1/1 |
| 2 | NAG | wA | 2 | 2 | - | 1/6/23/26 | 0/1/1/1 |
| 2 | NAG | x | 1 | 1,2 | - | 2/6/23/26 | 0/1/1/1 |
| 2 | NAG | x | 2 | 2 | - | 2/6/23/26 | 0/1/1/1 |
| 3 | NAG | xA | 1 | 1,3 | - | 3/6/23/26 | 0/1/1/1 |
| 3 | NAG | xA | 2 | 3 | - | 2/6/23/26 | 0/1/1/1 |
| 3 | BMA | xA | 3 | 3 | - | 2/2/19/22 | 0/1/1/1 |
| 2 | NAG | y | 1 | 1,2 | - | 1/6/23/26 | 0/1/1/1 |
| 2 | NAG | y | 2 | 2 | - | 0/6/23/26 | 0/1/1/1 |
| 2 | NAG | yA | 1 | 1,2 | - | 0/6/23/26 | 0/1/1/1 |
| 2 | NAG | yA | 2 | 2 | - | 2/6/23/26 | 0/1/1/1 |
| 3 | NAG | z | 1 | 1,3 | - | 4/6/23/26 | 0/1/1/1 |
| 3 | NAG | z | 2 | 3 | - | 2/6/23/26 | 0/1/1/1 |
| 3 | BMA | z | 3 | 3 | - | 0/2/19/22 | 0/1/1/1 |
| 3 | NAG | zA | 1 | 1,3 | - | 2/6/23/26 | 0/1/1/1 |
| 3 | NAG | zA | 2 | 3 | - | 2/6/23/26 | 0/1/1/1 |
| 3 | BMA | zA | 3 | 3 | - | 0/2/19/22 | 0/1/1/1 |

All (15) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 3 | X | 1 | NAG | O5-C1 | -3.78 | 1.37 | 1.43 |
| 3 | 1 | 1 | NAG | O5-C1 | -3.68 | 1.37 | 1.43 |
| 3 | BA | 1 | NAG | O5-C1 | -3.66 | 1.37 | 1.43 |
| 3 | zA | 1 | NAG | O5-C1 | -3.57 | 1.37 | 1.43 |
| 2 | 0 | 1 | NAG | O5-C1 | -3.53 | 1.37 | 1.43 |
| 3 | r | 1 | NAG | O5-C1 | -3.41 | 1.38 | 1.43 |
| 3 | h | 1 | NAG | O5-C1 | -3.39 | 1.38 | 1.43 |
| 3 | 4A | 2 | NAG | C1-C2 | 2.87 | 1.56 | 1.52 |
| 2 | CA | 1 | NAG | C1-C2 | 2.32 | 1.55 | 1.52 |
| 3 | aA | 2 | NAG | O5-C1 | 2.23 | 1.47 | 1.43 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 3 | 6 | 2 | NAG | O5-C1 | 2.15 | 1.47 | 1.43 |
| 2 | i | 1 | NAG | O5-C1 | -2.15 | 1.40 | 1.43 |
| 3 | GA | 2 | NAG | O5-C1 | 2.08 | 1.47 | 1.43 |
| 2 | WA | 1 | NAG | O5-C1 | -2.03 | 1.40 | 1.43 |
| 2 | lA | 2 | NAG | O5-C1 | 2.01 | 1.47 | 1.43 |

All (36) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 3 | 6 | 2 | NAG | C1-O5-C5 | 5.32 | 119.32 | 112.19 |
| 3 | m | 2 | NAG | C1-O5-C5 | 5.16 | 119.10 | 112.19 |
| 2 | CA | 1 | NAG | C1-O5-C5 | 5.15 | 119.09 | 112.19 |
| 3 | uA | 2 | NAG | C1-O5-C5 | 5.14 | 119.08 | 112.19 |
| 3 | QA | 2 | NAG | C1-O5-C5 | 5.12 | 119.04 | 112.19 |
| 3 | c | 2 | NAG | C1-O5-C5 | 5.05 | 118.96 | 112.19 |
| 3 | GA | 2 | NAG | C1-O5-C5 | 5.03 | 118.93 | 112.19 |
| 3 | aA | 2 | NAG | C1-O5-C5 | 5.03 | 118.93 | 112.19 |
| 2 | bA | 2 | NAG | C1-O5-C5 | 4.85 | 118.68 | 112.19 |
| 2 | n | 2 | NAG | C1-O5-C5 | 4.83 | 118.66 | 112.19 |
| 2 | RA | 2 | NAG | C1-O5-C5 | 4.79 | 118.60 | 112.19 |
| 2 | vA | 2 | NAG | C1-O5-C5 | 4.78 | 118.59 | 112.19 |
| 2 | HA | 2 | NAG | C1-O5-C5 | 4.78 | 118.59 | 112.19 |
| 2 | 7 | 2 | NAG | C1-O5-C5 | 4.77 | 118.58 | 112.19 |
| 2 | 5A | 2 | NAG | C1-O5-C5 | 4.76 | 118.56 | 112.19 |
| 2 | lA | 2 | NAG | C1-O5-C5 | 4.72 | 118.51 | 112.19 |
| 2 | x | 2 | NAG | C1-O5-C5 | 4.72 | 118.51 | 112.19 |
| 3 | DA | 1 | NAG | C1-O5-C5 | 3.37 | 116.70 | 112.19 |
| 3 | w | 1 | NAG | C1-O5-C5 | 3.15 | 116.40 | 112.19 |
| 3 | NA | 1 | NAG | C1-O5-C5 | 3.15 | 116.40 | 112.19 |
| 3 | 1A | 1 | NAG | C1-O5-C5 | 3.11 | 116.35 | 112.19 |
| 3 | 3 | 1 | NAG | C1-O5-C5 | 3.07 | 116.31 | 112.19 |
| 3 | XA | 1 | NAG | C1-O5-C5 | 3.06 | 116.28 | 112.19 |
| 3 | 4A | 2 | NAG | C1-O5-C5 | 2.89 | 116.06 | 112.19 |
| 2 | 0 | 1 | NAG | C3-C4-C5 | 2.67 | 115.08 | 110.23 |
| 3 | X | 1 | NAG | C3-C4-C5 | 2.53 | 114.82 | 110.23 |
| 3 | BA | 1 | NAG | C3-C4-C5 | 2.47 | 114.70 | 110.23 |
| 3 | 1 | 1 | NAG | C3-C4-C5 | 2.44 | 114.66 | 110.23 |
| 3 | 9 | 1 | NAG | C1-O5-C5 | 2.42 | 115.44 | 112.19 |
| 3 | zA | 1 | NAG | C3-C4-C5 | 2.42 | 114.62 | 110.23 |
| 3 | h | 1 | NAG | C3-C4-C5 | 2.35 | 114.49 | 110.23 |
| 3 | r | 1 | NAG | C3-C4-C5 | 2.34 | 114.47 | 110.23 |
| 3 | 4A | 1 | NAG | C1-O5-C5 | 2.30 | 115.27 | 112.19 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 2 | KA | 1 | NAG | C1-O5-C5 | 2.22 | 115.16 | 112.19 |
| 3 | VA | 3 | BMA | C1-O5-C5 | 2.06 | 114.95 | 112.19 |
| 3 | pA | 3 | BMA | C1-O5-C5 | 2.04 | 114.92 | 112.19 |

There are no chirality outliers.

All (421) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 3 | pA | 2 | NAG | C4-C5-C6-O6 |
| 2 | Y | 2 | NAG | C4-C5-C6-O6 |
| 2 | i | 2 | NAG | C4-C5-C6-O6 |
| 2 | WA | 2 | NAG | C4-C5-C6-O6 |
| 3 | fA | 2 | NAG | C4-C5-C6-O6 |
| 3 | BA | 1 | NAG | O5-C5-C6-O6 |
| 3 | FA | 2 | NAG | O5-C5-C6-O6 |
| 3 | ZA | 2 | NAG | O5-C5-C6-O6 |
| 3 | tA | 2 | NAG | O5-C5-C6-O6 |
| 2 | s | 2 | NAG | C4-C5-C6-O6 |
| 3 | b | 2 | NAG | O5-C5-C6-O6 |
| 3 | l | 2 | NAG | O5-C5-C6-O6 |
| 3 | GA | 1 | NAG | O5-C5-C6-O6 |
| 3 | PA | 2 | NAG | O5-C5-C6-O6 |
| 3 | QA | 1 | NAG | O5-C5-C6-O6 |
| 2 | 0A | 2 | NAG | C4-C5-C6-O6 |
| 3 | LA | 2 | NAG | C4-C5-C6-O6 |
| 3 | VA | 2 | NAG | C4-C5-C6-O6 |
| 2 | AA | 2 | NAG | O5-C5-C6-O6 |
| 2 | WA | 1 | NAG | C4-C5-C6-O6 |
| 2 | 0 | 2 | NAG | O5-C5-C6-O6 |
| 2 | UA | 2 | NAG | O5-C5-C6-O6 |
| 3 | 5 | 2 | NAG | O5-C5-C6-O6 |
| 3 | aA | 1 | NAG | O5-C5-C6-O6 |
| 3 | jA | 2 | NAG | O5-C5-C6-O6 |
| 2 | i | 2 | NAG | O5-C5-C6-O6 |
| 2 | qA | 2 | NAG | C4-C5-C6-O6 |
| 2 | Y | 2 | NAG | O5-C5-C6-O6 |
| 2 | q | 2 | NAG | O5-C5-C6-O6 |
| 2 | KA | 2 | NAG | O5-C5-C6-O6 |
| 3 | VA | 2 | NAG | O5-C5-C6-O6 |
| 3 | fA | 2 | NAG | O5-C5-C6-O6 |
| 2 | gA | 2 | NAG | C4-C5-C6-O6 |
| 2 | WA | 1 | NAG | O5-C5-C6-O6 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 3 | h | 1 | NAG | O5-C5-C6-O6 |
| 3 | LA | 2 | NAG | O5-C5-C6-O6 |
| 2 | x | 2 | NAG | C4-C5-C6-O6 |
| 2 | 2 | 2 | NAG | C4-C5-C6-O6 |
| 2 | HA | 2 | NAG | C4-C5-C6-O6 |
| 2 | RA | 2 | NAG | C4-C5-C6-O6 |
| 2 | bA | 2 | NAG | C4-C5-C6-O6 |
| 2 | 5A | 2 | NAG | C4-C5-C6-O6 |
| 2 | n | 2 | NAG | O5-C5-C6-O6 |
| 2 | oA | 2 | NAG | O5-C5-C6-O6 |
| 2 | yA | 2 | NAG | O5-C5-C6-O6 |
| 3 | X | 1 | NAG | O5-C5-C6-O6 |
| 3 | c | 1 | NAG | O5-C5-C6-O6 |
| 3 | v | 2 | NAG | O5-C5-C6-O6 |
| 3 | 1 | 1 | NAG | O5-C5-C6-O6 |
| 3 | XA | 1 | NAG | O5-C5-C6-O6 |
| 3 | kA | 2 | NAG | O5-C5-C6-O6 |
| 3 | pA | 2 | NAG | O5-C5-C6-O6 |
| 3 | uA | 1 | NAG | O5-C5-C6-O6 |
| 3 | 3A | 2 | NAG | O5-C5-C6-O6 |
| 2 | 0 | 1 | NAG | C4-C5-C6-O6 |
| 2 | 7 | 2 | NAG | C4-C5-C6-O6 |
| 2 | AA | 2 | NAG | C4-C5-C6-O6 |
| 3 | NA | 2 | NAG | C4-C5-C6-O6 |
| 2 | W | 2 | NAG | O5-C5-C6-O6 |
| 2 | g | 2 | NAG | O5-C5-C6-O6 |
| 2 | eA | 2 | NAG | O5-C5-C6-O6 |
| 3 | f | 2 | NAG | O5-C5-C6-O6 |
| 3 | r | 1 | NAG | O5-C5-C6-O6 |
| 3 | w | 2 | NAG | O5-C5-C6-O6 |
| 3 | zA | 1 | NAG | O5-C5-C6-O6 |
| 3 | 1A | 1 | NAG | O5-C5-C6-O6 |
| 2 | n | 2 | NAG | C4-C5-C6-O6 |
| 2 | UA | 2 | NAG | C4-C5-C6-O6 |
| 3 | BA | 1 | NAG | C4-C5-C6-O6 |
| 3 | QA | 1 | NAG | C4-C5-C6-O6 |
| 2 | 7 | 2 | NAG | O5-C5-C6-O6 |
| 2 | MA | 2 | NAG | O5-C5-C6-O6 |
| 3 | 3 | 1 | NAG | O5-C5-C6-O6 |
| 3 | DA | 1 | NAG | O5-C5-C6-O6 |
| 3 | nA | 2 | NAG | O5-C5-C6-O6 |
| 3 | p | 1 | NAG | C4-C5-C6-O6 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 3 | uA | 1 | NAG | C4-C5-C6-O6 |
| 2 | WA | 2 | NAG | O5-C5-C6-O6 |
| 3 | m | 1 | NAG | O5-C5-C6-O6 |
| 2 | KA | 2 | NAG | C4-C5-C6-O6 |
| 2 | oA | 2 | NAG | C4-C5-C6-O6 |
| 3 | h | 2 | NAG | C4-C5-C6-O6 |
| 3 | FA | 2 | NAG | C4-C5-C6-O6 |
| 3 | ZA | 2 | NAG | C4-C5-C6-O6 |
| 3 | aA | 1 | NAG | C4-C5-C6-O6 |
| 2 | RA | 2 | NAG | O5-C5-C6-O6 |
| 2 | q | 2 | NAG | C4-C5-C6-O6 |
| 2 | yA | 2 | NAG | C4-C5-C6-O6 |
| 3 | f | 2 | NAG | C4-C5-C6-O6 |
| 3 | nA | 2 | NAG | C4-C5-C6-O6 |
| 3 | tA | 2 | NAG | C4-C5-C6-O6 |
| 2 | s | 2 | NAG | O5-C5-C6-O6 |
| 2 | x | 2 | NAG | O5-C5-C6-O6 |
| 2 | HA | 2 | NAG | O5-C5-C6-O6 |
| 2 | bA | 2 | NAG | O5-C5-C6-O6 |
| 2 | gA | 2 | NAG | O5-C5-C6-O6 |
| 2 | 0A | 2 | NAG | O5-C5-C6-O6 |
| 2 | 5A | 2 | NAG | O5-C5-C6-O6 |
| 2 | g | 2 | NAG | C4-C5-C6-O6 |
| 3 | X | 1 | NAG | C4-C5-C6-O6 |
| 3 | c | 1 | NAG | C4-C5-C6-O6 |
| 3 | w | 2 | NAG | C4-C5-C6-O6 |
| 3 | 5 | 2 | NAG | C4-C5-C6-O6 |
| 3 | JA | 1 | NAG | C4-C5-C6-O6 |
| 3 | jA | 2 | NAG | C4-C5-C6-O6 |
| 3 | p | 1 | NAG | O5-C5-C6-O6 |
| 2 | eA | 2 | NAG | C4-C5-C6-O6 |
| 3 | b | 2 | NAG | C4-C5-C6-O6 |
| 3 | GA | 1 | NAG | C4-C5-C6-O6 |
| 3 | PA | 2 | NAG | C4-C5-C6-O6 |
| 2 | 2 | 2 | NAG | O5-C5-C6-O6 |
| 3 | NA | 1 | NAG | O5-C5-C6-O6 |
| 3 | iA | 2 | NAG | O5-C5-C6-O6 |
| 3 | tA | 3 | BMA | O5-C5-C6-O6 |
| 3 | xA | 2 | NAG | O5-C5-C6-O6 |
| 3 | l | 2 | NAG | C4-C5-C6-O6 |
| 2 | qA | 2 | NAG | O5-C5-C6-O6 |
| 2 | 0 | 2 | NAG | C4-C5-C6-O6 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 3 | NA | 1 | NAG | C4-C5-C6-O6 |
| 3 | FA | 1 | NAG | O5-C5-C6-O6 |
| 3 | JA | 1 | NAG | O5-C5-C6-O6 |
| 2 | W | 2 | NAG | C4-C5-C6-O6 |
| 3 | r | 1 | NAG | C4-C5-C6-O6 |
| 3 | z | 1 | NAG | C4-C5-C6-O6 |
| 3 | ZA | 1 | NAG | O5-C5-C6-O6 |
| 3 | v | 2 | NAG | C4-C5-C6-O6 |
| 3 | FA | 1 | NAG | C4-C5-C6-O6 |
| 3 | ZA | 1 | NAG | C4-C5-C6-O6 |
| 3 | kA | 2 | NAG | C4-C5-C6-O6 |
| 3 | 3A | 2 | NAG | C4-C5-C6-O6 |
| 3 | 1 | 1 | NAG | C4-C5-C6-O6 |
| 3 | DA | 1 | NAG | C4-C5-C6-O6 |
| 2 | 0 | 1 | NAG | O5-C5-C6-O6 |
| 3 | NA | 2 | NAG | O5-C5-C6-O6 |
| 3 | 4A | 3 | BMA | O5-C5-C6-O6 |
| 3 | 3 | 1 | NAG | C4-C5-C6-O6 |
| 3 | k | 2 | NAG | O5-C5-C6-O6 |
| 3 | l | 3 | BMA | O5-C5-C6-O6 |
| 3 | v | 1 | NAG | O5-C5-C6-O6 |
| 3 | sA | 2 | NAG | O5-C5-C6-O6 |
| 3 | h | 1 | NAG | C4-C5-C6-O6 |
| 3 | kA | 3 | BMA | C4-C5-C6-O6 |
| 3 | 3A | 1 | NAG | O5-C5-C6-O6 |
| 3 | zA | 2 | NAG | C4-C5-C6-O6 |
| 3 | zA | 1 | NAG | C4-C5-C6-O6 |
| 3 | 3A | 1 | NAG | C4-C5-C6-O6 |
| 2 | vA | 2 | NAG | C8-C7-N2-C2 |
| 2 | vA | 2 | NAG | O7-C7-N2-C2 |
| 3 | V | 1 | NAG | C8-C7-N2-C2 |
| 3 | V | 1 | NAG | O7-C7-N2-C2 |
| 3 | Z | 1 | NAG | C8-C7-N2-C2 |
| 3 | Z | 1 | NAG | O7-C7-N2-C2 |
| 3 | Z | 2 | NAG | C8-C7-N2-C2 |
| 3 | Z | 2 | NAG | O7-C7-N2-C2 |
| 3 | a | 1 | NAG | C8-C7-N2-C2 |
| 3 | a | 1 | NAG | O7-C7-N2-C2 |
| 3 | c | 2 | NAG | C8-C7-N2-C2 |
| 3 | c | 2 | NAG | O7-C7-N2-C2 |
| 3 | f | 1 | NAG | C8-C7-N2-C2 |
| 3 | f | 1 | NAG | O7-C7-N2-C2 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 3 | j | 1 | NAG | C8-C7-N2-C2 |
| 3 | j | 1 | NAG | O7-C7-N2-C2 |
| 3 | j | 2 | NAG | C8-C7-N2-C2 |
| 3 | j | 2 | NAG | O7-C7-N2-C2 |
| 3 | k | 1 | NAG | C8-C7-N2-C2 |
| 3 | k | 1 | NAG | O7-C7-N2-C2 |
| 3 | m | 2 | NAG | C8-C7-N2-C2 |
| 3 | m | 2 | NAG | O7-C7-N2-C2 |
| 3 | p | 1 | NAG | C8-C7-N2-C2 |
| 3 | p | 1 | NAG | O7-C7-N2-C2 |
| 3 | t | 1 | NAG | C8-C7-N2-C2 |
| 3 | t | 1 | NAG | O7-C7-N2-C2 |
| 3 | t | 2 | NAG | C8-C7-N2-C2 |
| 3 | t | 2 | NAG | O7-C7-N2-C2 |
| 3 | u | 1 | NAG | C8-C7-N2-C2 |
| 3 | u | 1 | NAG | O7-C7-N2-C2 |
| 3 | z | 1 | NAG | C8-C7-N2-C2 |
| 3 | z | 1 | NAG | O7-C7-N2-C2 |
| 3 | 3 | 1 | NAG | C8-C7-N2-C2 |
| 3 | 3 | 1 | NAG | O7-C7-N2-C2 |
| 3 | 3 | 2 | NAG | C8-C7-N2-C2 |
| 3 | 3 | 2 | NAG | O7-C7-N2-C2 |
| 3 | 4 | 1 | NAG | C8-C7-N2-C2 |
| 3 | 4 | 1 | NAG | O7-C7-N2-C2 |
| 3 | 6 | 2 | NAG | C8-C7-N2-C2 |
| 3 | 6 | 2 | NAG | O7-C7-N2-C2 |
| 3 | 9 | 1 | NAG | C8-C7-N2-C2 |
| 3 | 9 | 1 | NAG | O7-C7-N2-C2 |
| 3 | DA | 1 | NAG | C8-C7-N2-C2 |
| 3 | DA | 1 | NAG | O7-C7-N2-C2 |
| 3 | DA | 2 | NAG | C8-C7-N2-C2 |
| 3 | DA | 2 | NAG | O7-C7-N2-C2 |
| 3 | EA | 1 | NAG | C8-C7-N2-C2 |
| 3 | EA | 1 | NAG | O7-C7-N2-C2 |
| 3 | GA | 2 | NAG | C8-C7-N2-C2 |
| 3 | GA | 2 | NAG | O7-C7-N2-C2 |
| 3 | JA | 1 | NAG | C8-C7-N2-C2 |
| 3 | JA | 1 | NAG | O7-C7-N2-C2 |
| 3 | NA | 1 | NAG | C8-C7-N2-C2 |
| 3 | NA | 1 | NAG | O7-C7-N2-C2 |
| 3 | NA | 2 | NAG | C8-C7-N2-C2 |
| 3 | NA | 2 | NAG | O7-C7-N2-C2 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 3 | OA | 1 | NAG | C8-C7-N2-C2 |
| 3 | OA | 1 | NAG | O7-C7-N2-C2 |
| 3 | QA | 2 | NAG | C8-C7-N2-C2 |
| 3 | QA | 2 | NAG | O7-C7-N2-C2 |
| 3 | TA | 1 | NAG | C8-C7-N2-C2 |
| 3 | TA | 1 | NAG | O7-C7-N2-C2 |
| 3 | XA | 1 | NAG | C8-C7-N2-C2 |
| 3 | XA | 1 | NAG | O7-C7-N2-C2 |
| 3 | XA | 2 | NAG | C8-C7-N2-C2 |
| 3 | XA | 2 | NAG | O7-C7-N2-C2 |
| 3 | YA | 1 | NAG | C8-C7-N2-C2 |
| 3 | YA | 1 | NAG | O7-C7-N2-C2 |
| 3 | aA | 2 | NAG | C8-C7-N2-C2 |
| 3 | aA | 2 | NAG | O7-C7-N2-C2 |
| 3 | dA | 1 | NAG | C8-C7-N2-C2 |
| 3 | dA | 1 | NAG | O7-C7-N2-C2 |
| 3 | hA | 1 | NAG | C8-C7-N2-C2 |
| 3 | hA | 1 | NAG | O7-C7-N2-C2 |
| 3 | hA | 2 | NAG | C8-C7-N2-C2 |
| 3 | hA | 2 | NAG | O7-C7-N2-C2 |
| 3 | iA | 1 | NAG | C8-C7-N2-C2 |
| 3 | iA | 1 | NAG | O7-C7-N2-C2 |
| 3 | nA | 1 | NAG | C8-C7-N2-C2 |
| 3 | nA | 1 | NAG | O7-C7-N2-C2 |
| 3 | rA | 1 | NAG | C8-C7-N2-C2 |
| 3 | rA | 1 | NAG | O7-C7-N2-C2 |
| 3 | rA | 2 | NAG | C8-C7-N2-C2 |
| 3 | rA | 2 | NAG | O7-C7-N2-C2 |
| 3 | sA | 1 | NAG | C8-C7-N2-C2 |
| 3 | sA | 1 | NAG | O7-C7-N2-C2 |
| 3 | uA | 2 | NAG | C8-C7-N2-C2 |
| 3 | uA | 2 | NAG | O7-C7-N2-C2 |
| 3 | xA | 1 | NAG | C8-C7-N2-C2 |
| 3 | xA | 1 | NAG | O7-C7-N2-C2 |
| 3 | 1A | 1 | NAG | C8-C7-N2-C2 |
| 3 | 1A | 1 | NAG | O7-C7-N2-C2 |
| 3 | 1A | 2 | NAG | C8-C7-N2-C2 |
| 3 | 1A | 2 | NAG | O7-C7-N2-C2 |
| 3 | 2A | 1 | NAG | C8-C7-N2-C2 |
| 3 | 2A | 1 | NAG | O7-C7-N2-C2 |
| 3 | z | 1 | NAG | O5-C5-C6-O6 |
| 3 | v | 1 | NAG | C4-C5-C6-O6 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 3 | XA | 1 | NAG | C4-C5-C6-O6 |
| 3 | tA | 3 | BMA | C4-C5-C6-O6 |
| 3 | a | 2 | NAG | O5-C5-C6-O6 |
| 3 | 4A | 2 | NAG | O5-C5-C6-O6 |
| 3 | m | 1 | NAG | C4-C5-C6-O6 |
| 3 | TA | 1 | NAG | C4-C5-C6-O6 |
| 2 | vA | 2 | NAG | O5-C5-C6-O6 |
| 3 | h | 2 | NAG | O5-C5-C6-O6 |
| 3 | 9 | 2 | NAG | O5-C5-C6-O6 |
| 3 | xA | 3 | BMA | O5-C5-C6-O6 |
| 2 | MA | 2 | NAG | C4-C5-C6-O6 |
| 3 | 1A | 1 | NAG | C4-C5-C6-O6 |
| 3 | p | 2 | NAG | C4-C5-C6-O6 |
| 2 | wA | 1 | NAG | O5-C5-C6-O6 |
| 3 | u | 2 | NAG | O5-C5-C6-O6 |
| 3 | kA | 3 | BMA | O5-C5-C6-O6 |
| 3 | V | 2 | NAG | C4-C5-C6-O6 |
| 3 | xA | 2 | NAG | C4-C5-C6-O6 |
| 2 | d | 2 | NAG | O5-C5-C6-O6 |
| 3 | QA | 3 | BMA | O5-C5-C6-O6 |
| 3 | z | 2 | NAG | C4-C5-C6-O6 |
| 3 | 6 | 3 | BMA | O5-C5-C6-O6 |
| 2 | vA | 1 | NAG | C4-C5-C6-O6 |
| 3 | 4A | 3 | BMA | C4-C5-C6-O6 |
| 2 | CA | 1 | NAG | O5-C5-C6-O6 |
| 3 | OA | 2 | NAG | O5-C5-C6-O6 |
| 3 | xA | 3 | BMA | C4-C5-C6-O6 |
| 3 | dA | 2 | NAG | C4-C5-C6-O6 |
| 3 | 4A | 1 | NAG | O5-C5-C6-O6 |
| 3 | 4 | 2 | NAG | O5-C5-C6-O6 |
| 2 | lA | 1 | NAG | O5-C5-C6-O6 |
| 2 | n | 1 | NAG | C4-C5-C6-O6 |
| 3 | TA | 1 | NAG | O5-C5-C6-O6 |
| 3 | p | 2 | NAG | O5-C5-C6-O6 |
| 3 | l | 3 | BMA | C4-C5-C6-O6 |
| 3 | zA | 2 | NAG | O5-C5-C6-O6 |
| 2 | bA | 1 | NAG | C4-C5-C6-O6 |
| 3 | hA | 1 | NAG | O5-C5-C6-O6 |
| 3 | 1 | 2 | NAG | C4-C5-C6-O6 |
| 3 | V | 2 | NAG | O5-C5-C6-O6 |
| 3 | 4A | 1 | NAG | C4-C5-C6-O6 |
| 3 | z | 2 | NAG | O5-C5-C6-O6 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 3 | 6 | 1 | NAG | O5-C5-C6-O6 |
| 3 | JA | 2 | NAG | C4-C5-C6-O6 |
| 3 | b | 1 | NAG | C4-C5-C6-O6 |
| 2 | vA | 1 | NAG | O5-C5-C6-O6 |
| 2 | lA | 1 | NAG | C4-C5-C6-O6 |
| 2 | o | 1 | NAG | O5-C5-C6-O6 |
| 2 | CA | 1 | NAG | C4-C5-C6-O6 |
| 3 | EA | 1 | NAG | C4-C5-C6-O6 |
| 2 | i | 1 | NAG | O5-C5-C6-O6 |
| 2 | cA | 1 | NAG | O5-C5-C6-O6 |
| 3 | dA | 2 | NAG | O5-C5-C6-O6 |
| 3 | b | 1 | NAG | O5-C5-C6-O6 |
| 3 | pA | 1 | NAG | C4-C5-C6-O6 |
| 3 | 3 | 2 | NAG | O5-C5-C6-O6 |
| 3 | jA | 1 | NAG | C4-C5-C6-O6 |
| 3 | iA | 2 | NAG | C4-C5-C6-O6 |
| 2 | SA | 1 | NAG | O5-C5-C6-O6 |
| 3 | Z | 1 | NAG | O5-C5-C6-O6 |
| 3 | kA | 1 | NAG | O5-C5-C6-O6 |
| 3 | rA | 1 | NAG | O5-C5-C6-O6 |
| 2 | e | 1 | NAG | O5-C5-C6-O6 |
| 2 | n | 1 | NAG | O5-C5-C6-O6 |
| 2 | IA | 1 | NAG | O5-C5-C6-O6 |
| 2 | mA | 1 | NAG | O5-C5-C6-O6 |
| 3 | 2A | 2 | NAG | O5-C5-C6-O6 |
| 3 | V | 1 | NAG | C4-C5-C6-O6 |
| 3 | 4A | 2 | NAG | C4-C5-C6-O6 |
| 2 | 8 | 1 | NAG | O5-C5-C6-O6 |
| 3 | YA | 2 | NAG | O5-C5-C6-O6 |
| 3 | aA | 3 | BMA | O5-C5-C6-O6 |
| 3 | dA | 1 | NAG | C4-C5-C6-O6 |
| 3 | GA | 3 | BMA | O5-C5-C6-O6 |
| 2 | HA | 1 | NAG | C4-C5-C6-O6 |
| 3 | YA | 1 | NAG | C4-C5-C6-O6 |
| 2 | U | 1 | NAG | O5-C5-C6-O6 |
| 2 | lA | 2 | NAG | O5-C5-C6-O6 |
| 3 | j | 1 | NAG | O5-C5-C6-O6 |
| 3 | 1 | 3 | BMA | O5-C5-C6-O6 |
| 3 | EA | 1 | NAG | O5-C5-C6-O6 |
| 3 | fA | 1 | NAG | C4-C5-C6-O6 |
| 2 | bA | 1 | NAG | O5-C5-C6-O6 |
| 3 | 1 | 2 | NAG | O5-C5-C6-O6 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 2 | y | 1 | NAG | O5-C5-C6-O6 |
| 3 | m | 3 | BMA | O5-C5-C6-O6 |
| 3 | EA | 2 | NAG | O5-C5-C6-O6 |
| 3 | uA | 3 | BMA | O5-C5-C6-O6 |
| 3 | c | 3 | BMA | O5-C5-C6-O6 |
| 3 | t | 1 | NAG | O5-C5-C6-O6 |
| 3 | rA | 2 | NAG | O5-C5-C6-O6 |
| 3 | pA | 1 | NAG | O5-C5-C6-O6 |
| 3 | sA | 2 | NAG | C4-C5-C6-O6 |
| 3 | k | 2 | NAG | C4-C5-C6-O6 |
| 3 | jA | 1 | NAG | O5-C5-C6-O6 |
| 2 | vA | 2 | NAG | C4-C5-C6-O6 |
| 3 | JA | 2 | NAG | O5-C5-C6-O6 |
| 3 | 9 | 2 | NAG | C4-C5-C6-O6 |
| 3 | YA | 1 | NAG | O5-C5-C6-O6 |
| 3 | a | 2 | NAG | C4-C5-C6-O6 |
| 3 | 2A | 3 | BMA | O5-C5-C6-O6 |
| 3 | xA | 1 | NAG | O5-C5-C6-O6 |
| 3 | r | 2 | NAG | C4-C5-C6-O6 |
| 3 | w | 1 | NAG | C4-C5-C6-O6 |
| 3 | a | 2 | NAG | C1-C2-N2-C7 |
| 3 | k | 2 | NAG | C1-C2-N2-C7 |
| 3 | 4 | 2 | NAG | C1-C2-N2-C7 |
| 3 | EA | 2 | NAG | C1-C2-N2-C7 |
| 3 | OA | 2 | NAG | C1-C2-N2-C7 |
| 3 | YA | 2 | NAG | C1-C2-N2-C7 |
| 3 | iA | 2 | NAG | C1-C2-N2-C7 |
| 3 | sA | 2 | NAG | C1-C2-N2-C7 |
| 3 | 4A | 2 | NAG | C1-C2-N2-C7 |
| 3 | V | 1 | NAG | O5-C5-C6-O6 |
| 3 | 4 | 1 | NAG | C4-C5-C6-O6 |
| 2 | HA | 1 | NAG | O5-C5-C6-O6 |
| 3 | fA | 1 | NAG | O5-C5-C6-O6 |
| 3 | dA | 1 | NAG | O5-C5-C6-O6 |
| 3 | OA | 1 | NAG | C4-C5-C6-O6 |
| 3 | rA | 3 | BMA | O5-C5-C6-O6 |
| 3 | k | 1 | NAG | C4-C5-C6-O6 |
| 3 | BA | 2 | NAG | C4-C5-C6-O6 |
| 3 | iA | 1 | NAG | C4-C5-C6-O6 |
| 3 | 9 | 1 | NAG | O5-C5-C6-O6 |
| 3 | sA | 1 | NAG | C4-C5-C6-O6 |
| 3 | a | 1 | NAG | C4-C5-C6-O6 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 3 | u | 2 | NAG | C4-C5-C6-O6 |
| 2 | cA | 2 | NAG | O5-C5-C6-O6 |
| 3 | r | 2 | NAG | O5-C5-C6-O6 |
| 2 | CA | 1 | NAG | C3-C2-N2-C7 |
| 3 | a | 2 | NAG | C3-C2-N2-C7 |
| 3 | k | 2 | NAG | C3-C2-N2-C7 |
| 3 | u | 2 | NAG | C3-C2-N2-C7 |
| 3 | 4 | 2 | NAG | C3-C2-N2-C7 |
| 3 | EA | 2 | NAG | C3-C2-N2-C7 |
| 3 | OA | 2 | NAG | C3-C2-N2-C7 |
| 3 | YA | 2 | NAG | C3-C2-N2-C7 |
| 3 | iA | 2 | NAG | C3-C2-N2-C7 |
| 3 | sA | 2 | NAG | C3-C2-N2-C7 |
| 3 | 2A | 2 | NAG | C3-C2-N2-C7 |
| 3 | f | 1 | NAG | C4-C5-C6-O6 |
| 3 | LA | 3 | BMA | O5-C5-C6-O6 |
| 2 | x | 1 | NAG | C4-C5-C6-O6 |
| 2 | RA | 1 | NAG | C4-C5-C6-O6 |
| 3 | 4 | 1 | NAG | O5-C5-C6-O6 |
| 3 | BA | 2 | NAG | O5-C5-C6-O6 |
| 3 | OA | 1 | NAG | O5-C5-C6-O6 |
| 3 | k | 1 | NAG | O5-C5-C6-O6 |
| 2 | U | 2 | NAG | O5-C5-C6-O6 |
| 2 | o | 2 | NAG | O5-C5-C6-O6 |
| 3 | sA | 1 | NAG | O5-C5-C6-O6 |
| 3 | iA | 1 | NAG | O5-C5-C6-O6 |
| 2 | wA | 2 | NAG | O5-C5-C6-O6 |
| 3 | w | 3 | BMA | C4-C5-C6-O6 |
| 3 | w | 1 | NAG | O5-C5-C6-O6 |
| 3 | a | 1 | NAG | O5-C5-C6-O6 |
| 2 | HA | 2 | NAG | C1-C2-N2-C7 |
| 2 | RA | 2 | NAG | C1-C2-N2-C7 |
| 2 | WA | 1 | NAG | C1-C2-N2-C7 |
| 3 | u | 2 | NAG | C1-C2-N2-C7 |
| 3 | GA | 1 | NAG | C1-C2-N2-C7 |
| 3 | 2A | 2 | NAG | C1-C2-N2-C7 |
| 3 | 4A | 2 | NAG | C3-C2-N2-C7 |
| 2 | x | 1 | NAG | O5-C5-C6-O6 |
| 3 | nA | 1 | NAG | C4-C5-C6-O6 |
| 3 | OA | 2 | NAG | C4-C5-C6-O6 |
| 3 | EA | 3 | BMA | O5-C5-C6-O6 |
| 2 | RA | 1 | NAG | O5-C5-C6-O6 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 3 | 6 | 1 | NAG | C4-C5-C6-O6 |
| 3 | X | 2 | NAG | C4-C5-C6-O6 |
| 2 | KA | 1 | NAG | C4-C5-C6-O6 |
| 2 | 5A | 1 | NAG | C4-C5-C6-O6 |
| 3 | 1 | 3 | BMA | C4-C5-C6-O6 |
| 2 | AA | 1 | NAG | C4-C5-C6-O6 |
| 3 | 4 | 2 | NAG | C4-C5-C6-O6 |
| 3 | u | 1 | NAG | C4-C5-C6-O6 |
| 3 | VA | 1 | NAG | C4-C5-C6-O6 |

There are no ring outliers.

66 monomers are involved in 59 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 2 | yA | 1 | NAG | 1 | 0 |
| 3 | c | 2 | NAG | 1 | 0 |
| 3 | 4A | 1 | NAG | 2 | 0 |
| 3 | dA | 1 | NAG | 1 | 0 |
| 3 | t | 3 | BMA | 1 | 0 |
| 3 | pA | 2 | NAG | 1 | 0 |
| 3 | Z | 3 | BMA | 1 | 0 |
| 2 | IA | 1 | NAG | 1 | 0 |
| 3 | GA | 1 | NAG | 1 | 0 |
| 3 | uA | 1 | NAG | 2 | 0 |
| 3 | aA | 1 | NAG | 1 | 0 |
| 3 | rA | 2 | NAG | 1 | 0 |
| 2 | U | 1 | NAG | 2 | 0 |
| 3 | BA | 2 | NAG | 1 | 0 |
| 3 | c | 1 | NAG | 1 | 0 |
| 3 | hA | 2 | NAG | 1 | 0 |
| 3 | VA | 2 | NAG | 2 | 0 |
| 3 | t | 2 | NAG | 1 | 0 |
| 3 | 1A | 3 | BMA | 1 | 0 |
| 3 | p | 1 | NAG | 2 | 0 |
| 2 | q | 1 | NAG | 1 | 0 |
| 3 | 1 | 1 | NAG | 2 | 0 |
| 3 | fA | 2 | NAG | 2 | 0 |
| 2 | lA | 1 | NAG | 2 | 0 |
| 2 | SA | 1 | NAG | 1 | 0 |
| 3 | X | 1 | NAG | 1 | 0 |
| 3 | JA | 1 | NAG | 1 | 0 |
| 3 | nA | 1 | NAG | 1 | 0 |

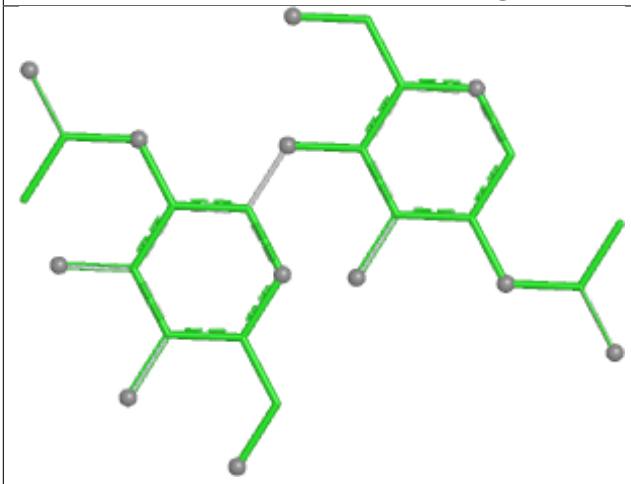
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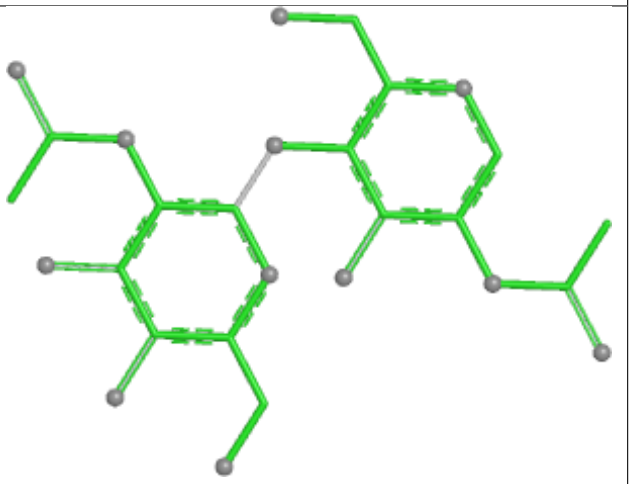
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 3 | z | 1 | NAG | 1 | 0 |
| 3 | uA | 2 | NAG | 1 | 0 |
| 3 | a | 1 | NAG | 1 | 0 |
| 2 | KA | 1 | NAG | 1 | 0 |
| 3 | LA | 2 | NAG | 1 | 0 |
| 3 | LA | 1 | NAG | 1 | 0 |
| 3 | m | 1 | NAG | 2 | 0 |
| 2 | CA | 1 | NAG | 1 | 0 |
| 3 | 6 | 1 | NAG | 1 | 0 |
| 3 | pA | 1 | NAG | 1 | 0 |
| 3 | f | 1 | NAG | 1 | 0 |
| 3 | r | 2 | NAG | 1 | 0 |
| 3 | hA | 3 | BMA | 1 | 0 |
| 3 | zA | 2 | NAG | 1 | 0 |
| 3 | r | 1 | NAG | 3 | 0 |
| 3 | 4A | 2 | NAG | 2 | 0 |
| 2 | 0A | 1 | NAG | 1 | 0 |
| 3 | fA | 1 | NAG | 2 | 0 |
| 3 | m | 2 | NAG | 1 | 0 |
| 3 | YA | 1 | NAG | 1 | 0 |
| 3 | rA | 3 | BMA | 1 | 0 |
| 3 | jA | 2 | NAG | 1 | 0 |
| 3 | EA | 1 | NAG | 1 | 0 |
| 3 | t | 1 | NAG | 1 | 0 |
| 3 | VA | 1 | NAG | 2 | 0 |
| 2 | lA | 2 | NAG | 1 | 0 |
| 3 | BA | 1 | NAG | 1 | 0 |
| 3 | b | 2 | NAG | 1 | 0 |
| 3 | 2A | 1 | NAG | 1 | 0 |
| 3 | Z | 2 | NAG | 1 | 0 |
| 3 | 1 | 2 | NAG | 1 | 0 |
| 3 | 1A | 2 | NAG | 1 | 0 |
| 3 | X | 2 | NAG | 1 | 0 |
| 3 | zA | 1 | NAG | 1 | 0 |
| 3 | w | 1 | NAG | 1 | 0 |
| 3 | rA | 1 | NAG | 1 | 0 |
| 3 | V | 1 | NAG | 1 | 0 |
| 2 | oA | 1 | NAG | 1 | 0 |

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

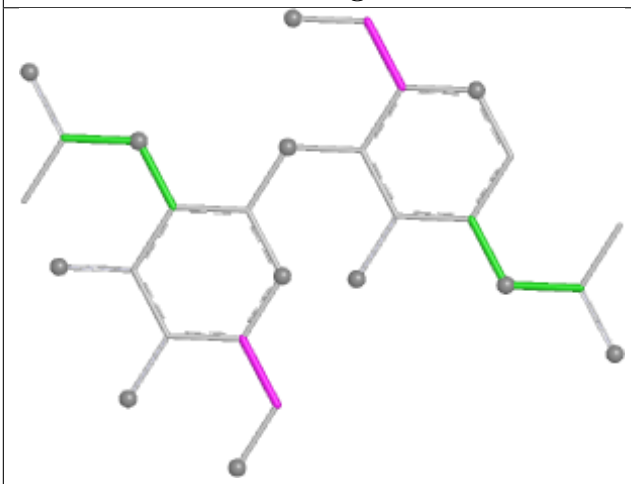
**Oligosaccharide Chain U**



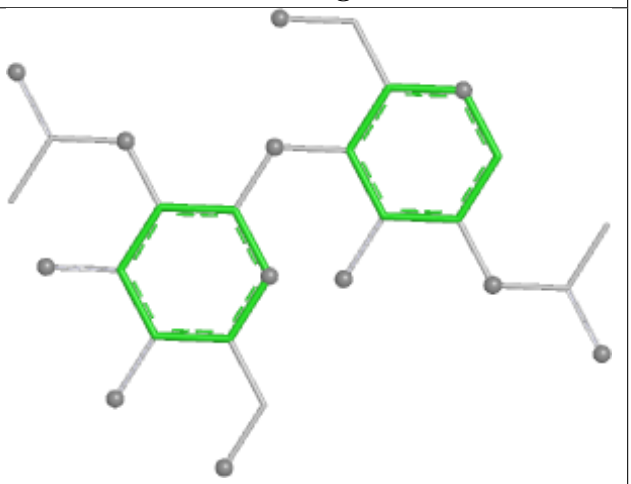
**Bond lengths**



**Bond angles**

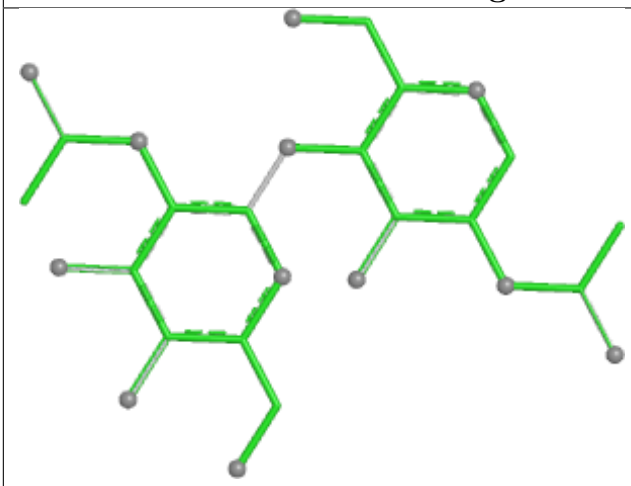


**Torsions**

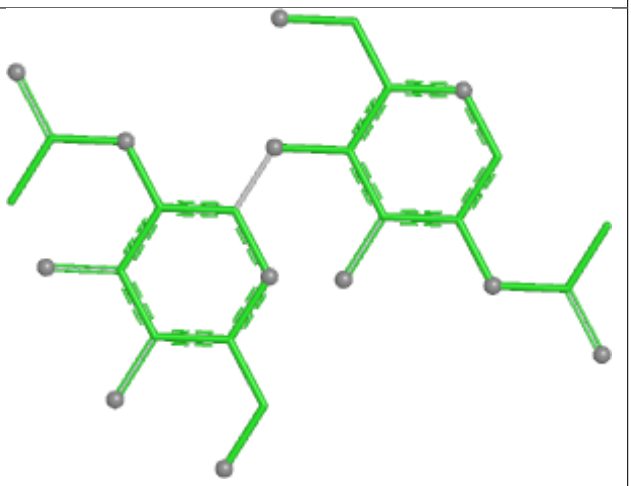


**Rings**

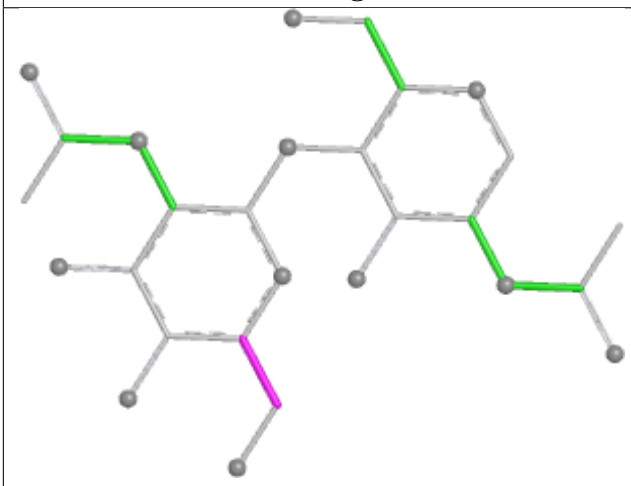
**Oligosaccharide Chain W**



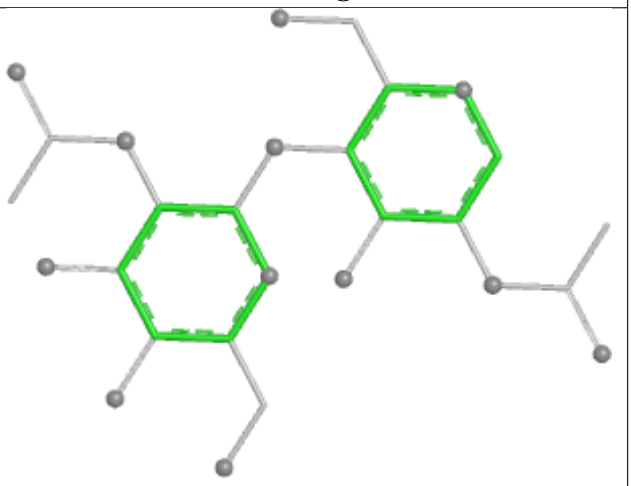
**Bond lengths**



**Bond angles**

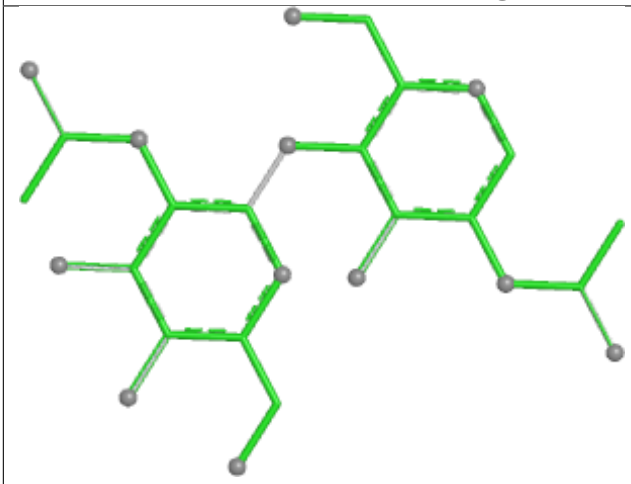


**Torsions**

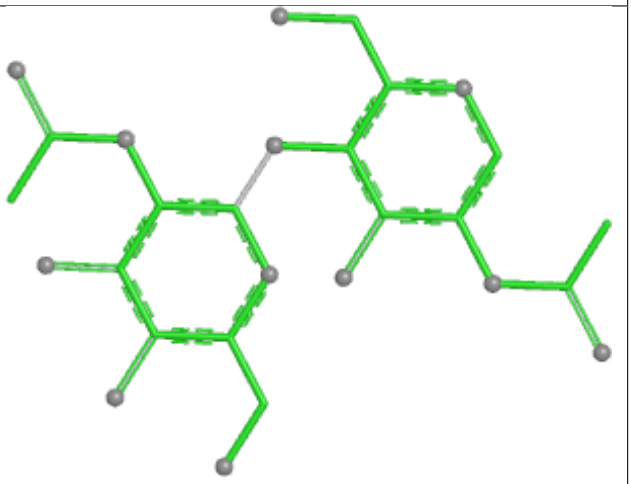


**Rings**

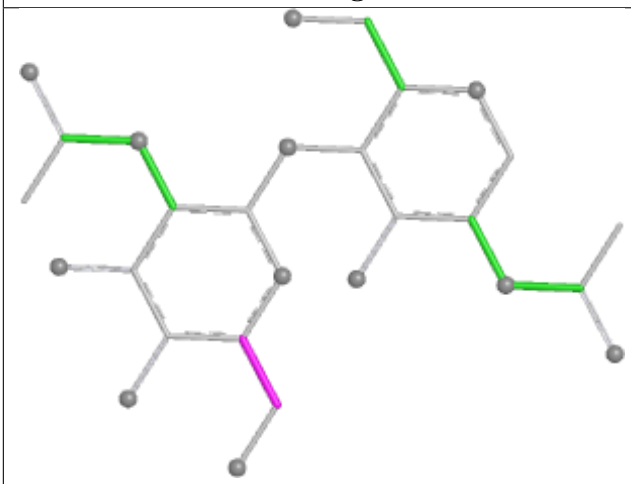
**Oligosaccharide Chain Y**



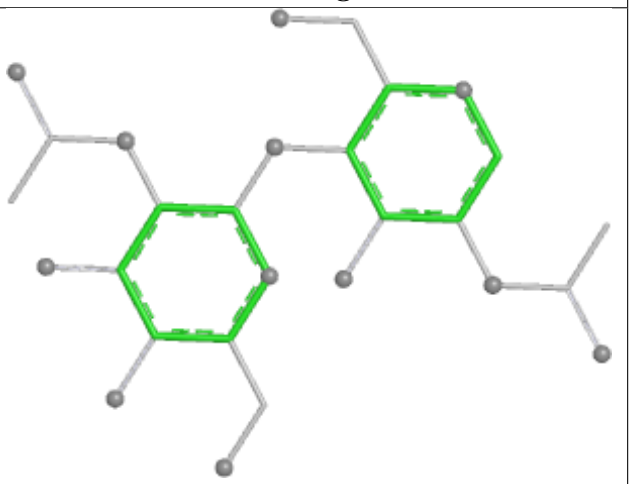
**Bond lengths**



**Bond angles**

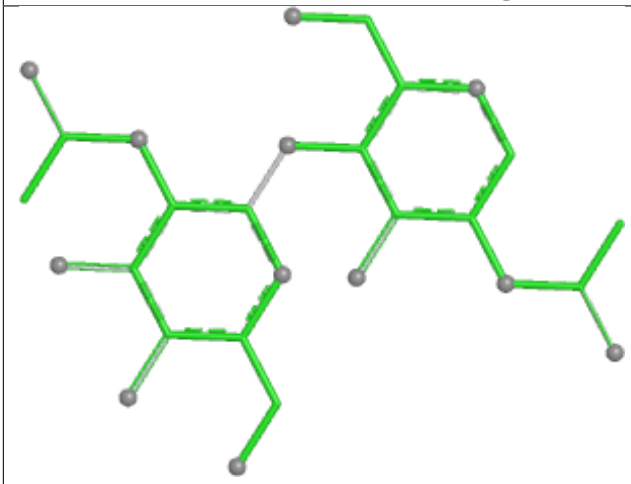


**Torsions**

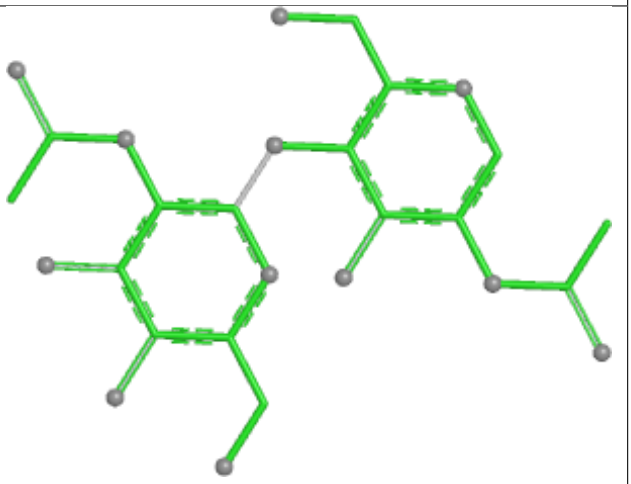


**Rings**

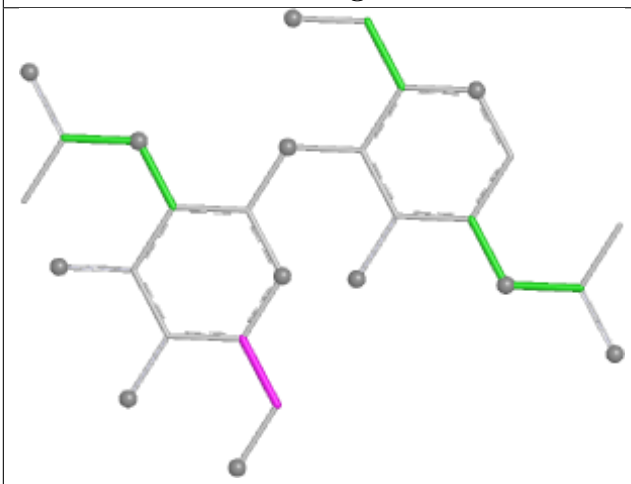
**Oligosaccharide Chain d**



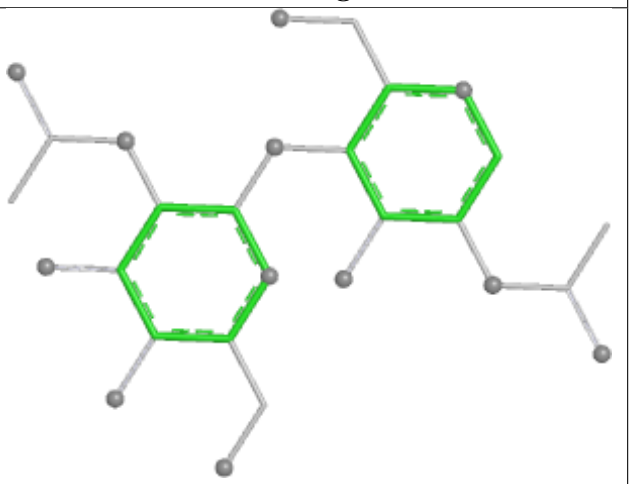
**Bond lengths**



**Bond angles**

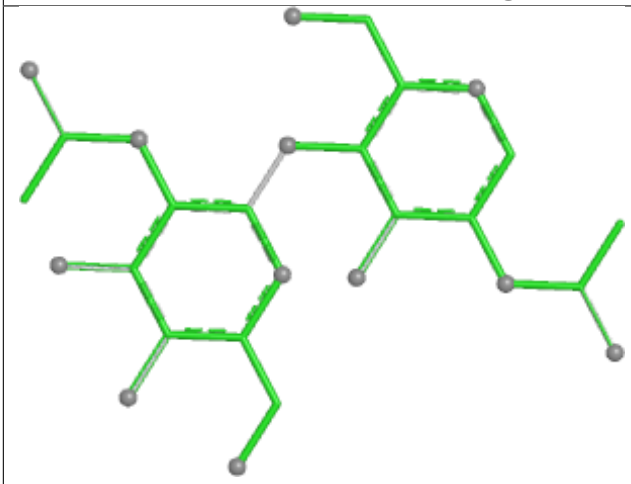


**Torsions**

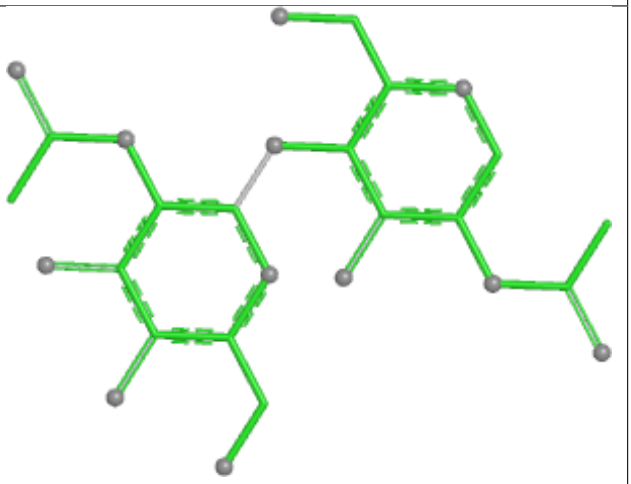


**Rings**

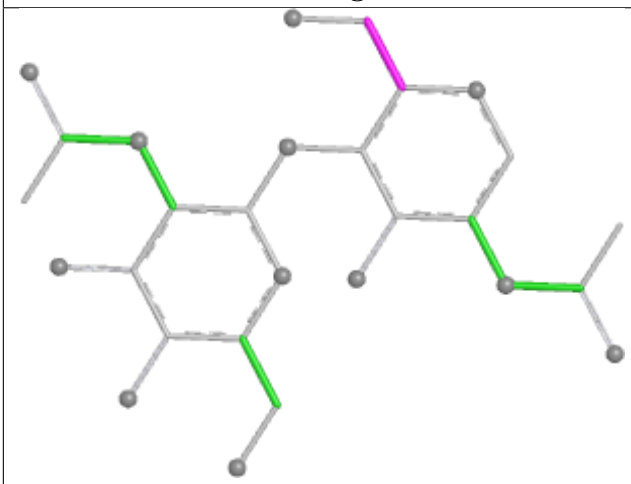
**Oligosaccharide Chain e**



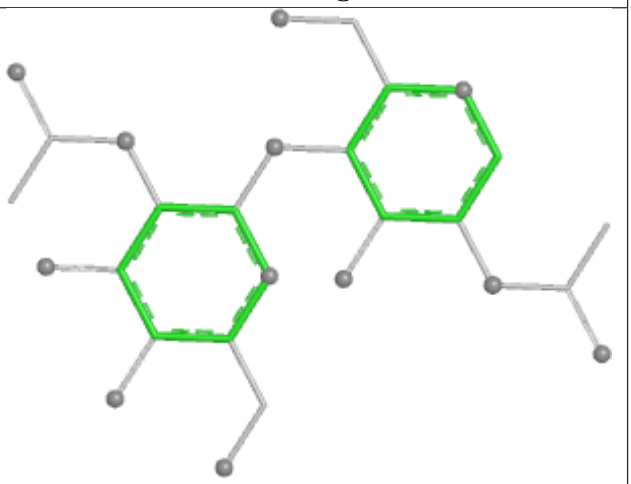
**Bond lengths**



**Bond angles**

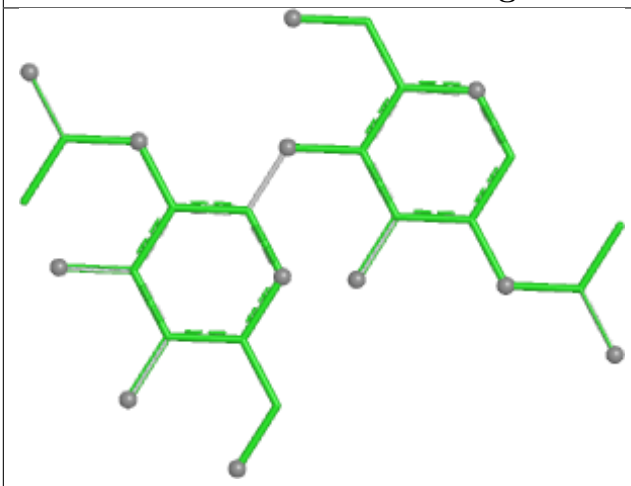


**Torsions**

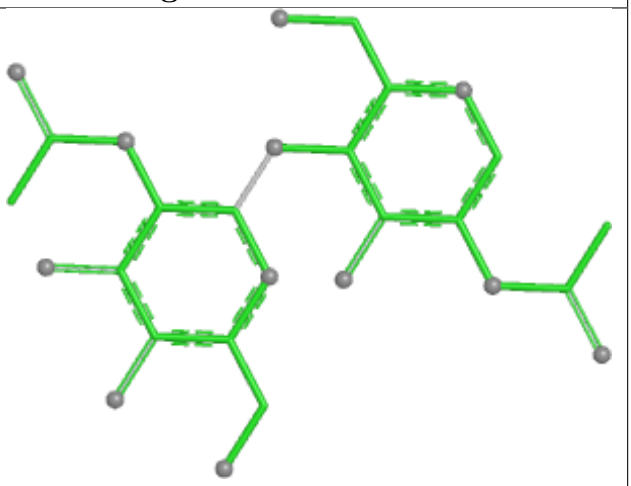


**Rings**

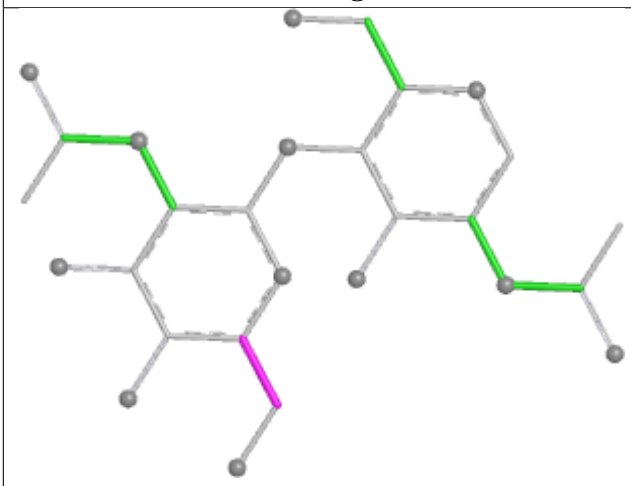
**Oligosaccharide Chain g**



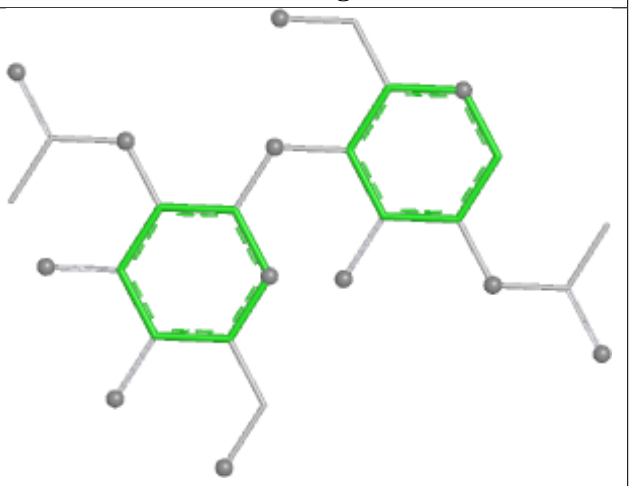
**Bond lengths**



**Bond angles**

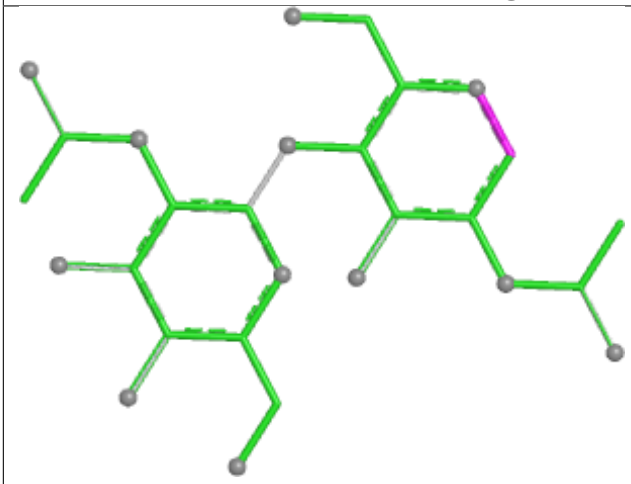


**Torsions**

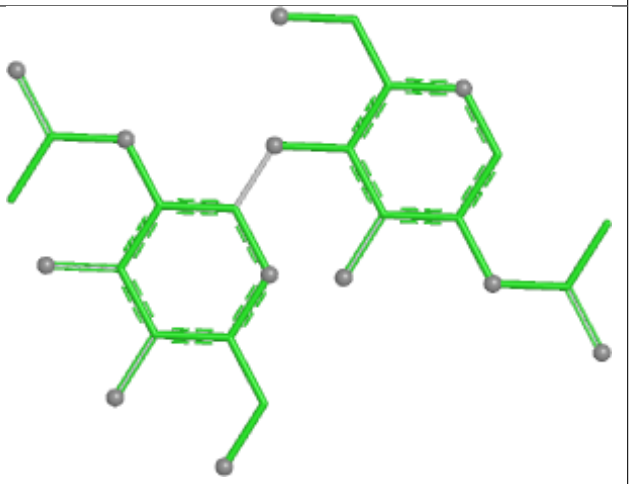


**Rings**

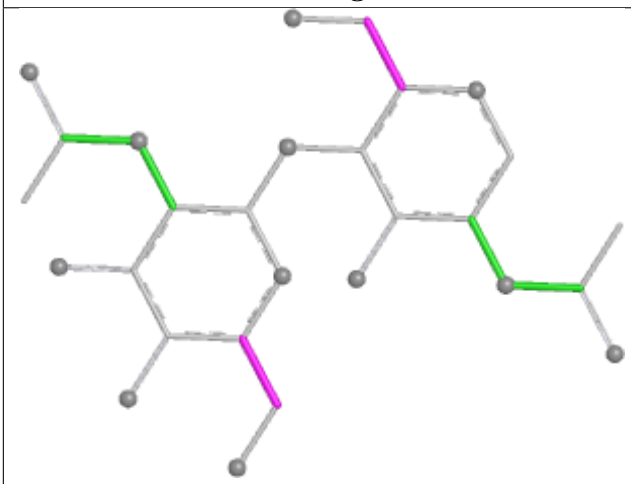
**Oligosaccharide Chain i**



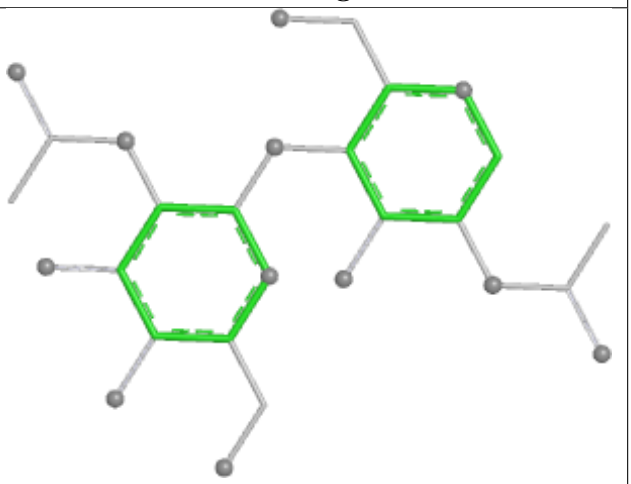
**Bond lengths**



**Bond angles**

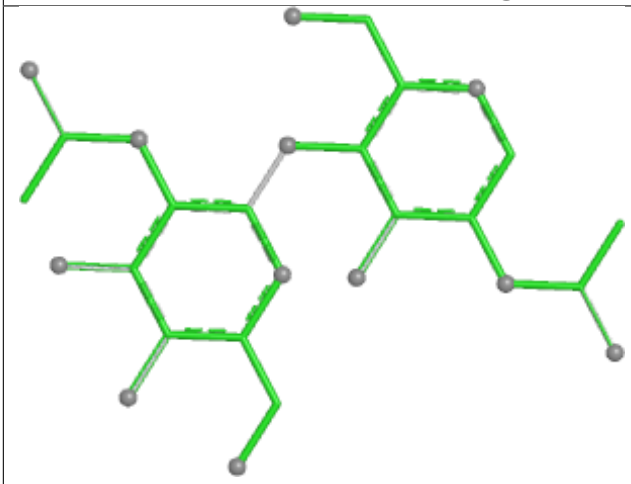


**Torsions**

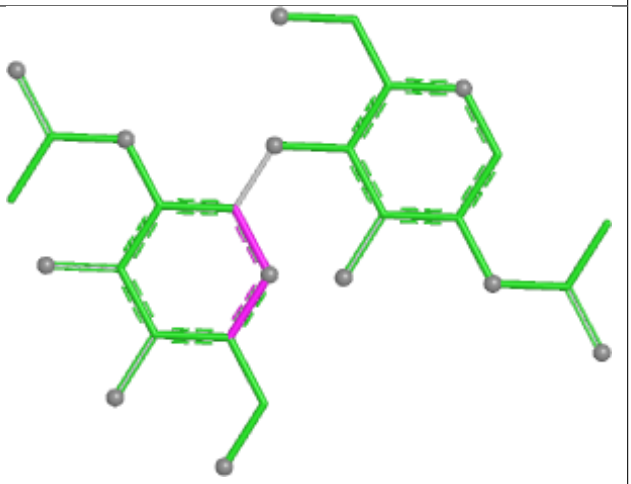


**Rings**

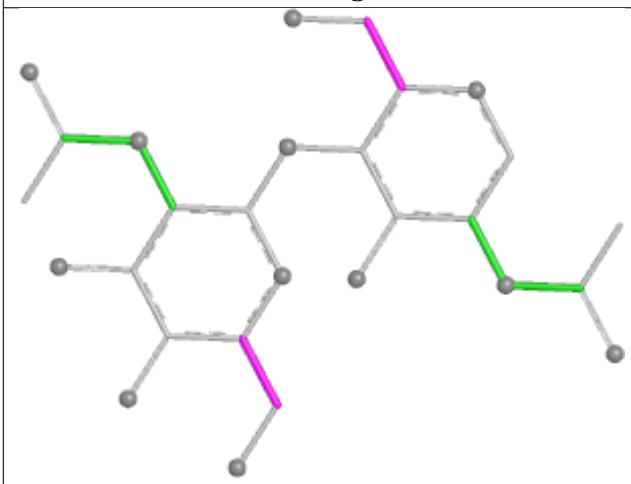
**Oligosaccharide Chain n**



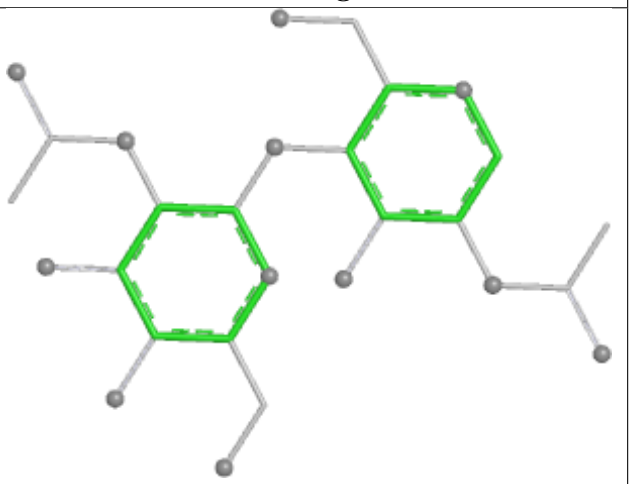
**Bond lengths**



**Bond angles**

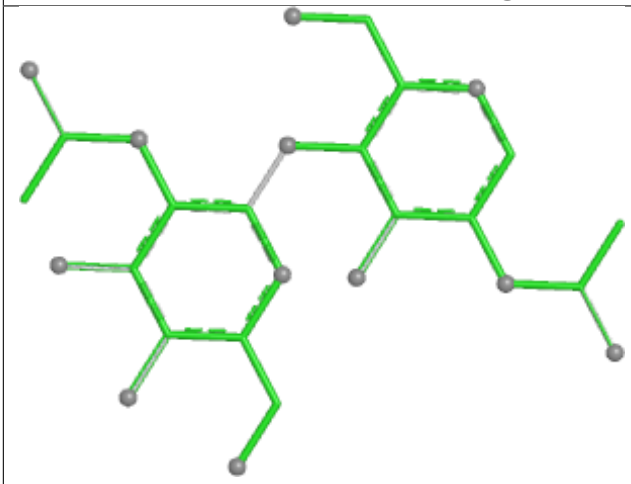


**Torsions**

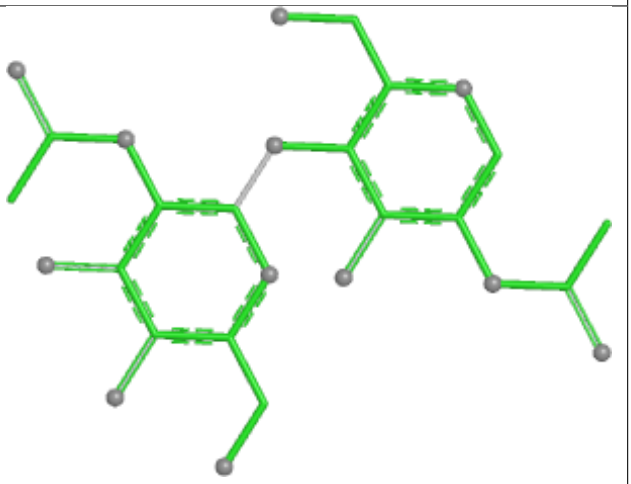


**Rings**

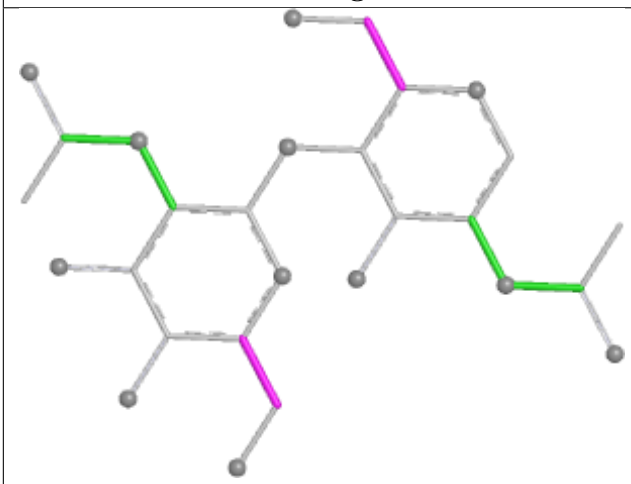
**Oligosaccharide Chain o**



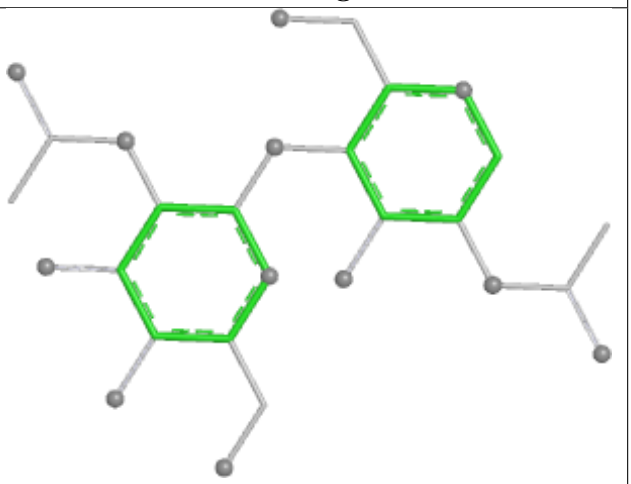
**Bond lengths**



**Bond angles**

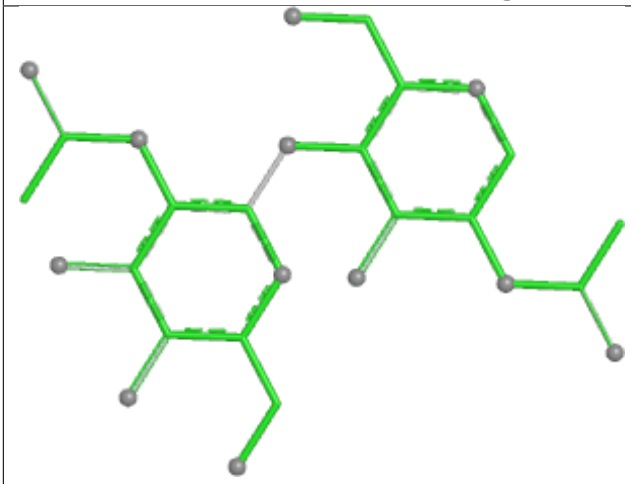


**Torsions**

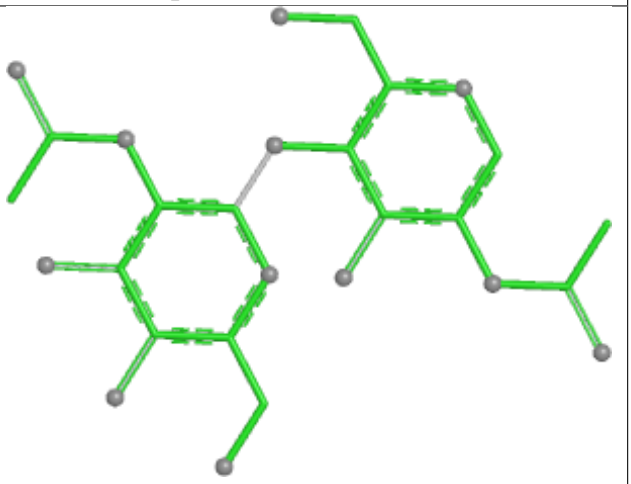


**Rings**

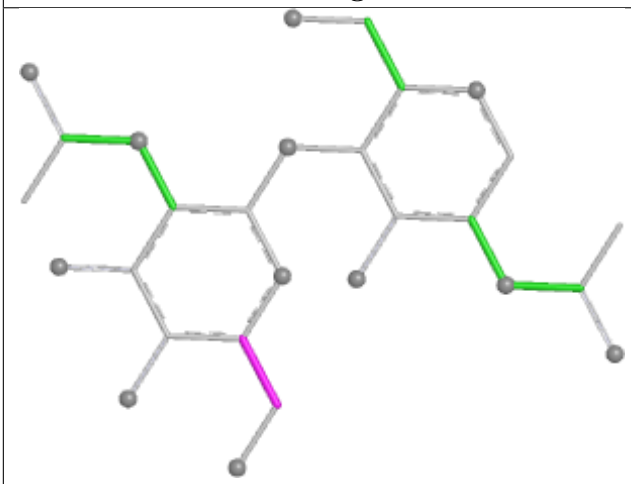
**Oligosaccharide Chain q**



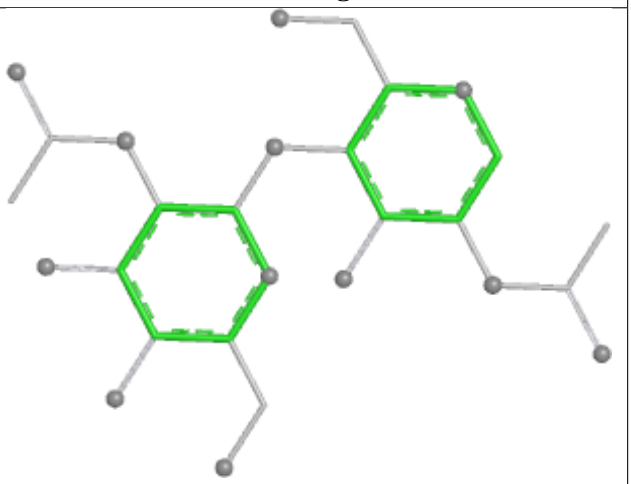
**Bond lengths**



**Bond angles**

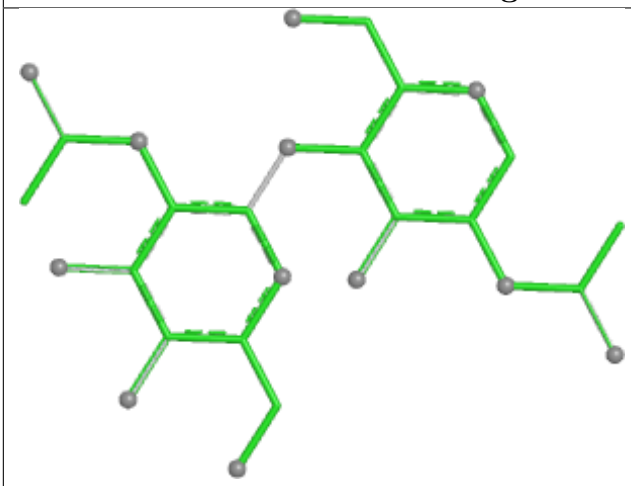


**Torsions**

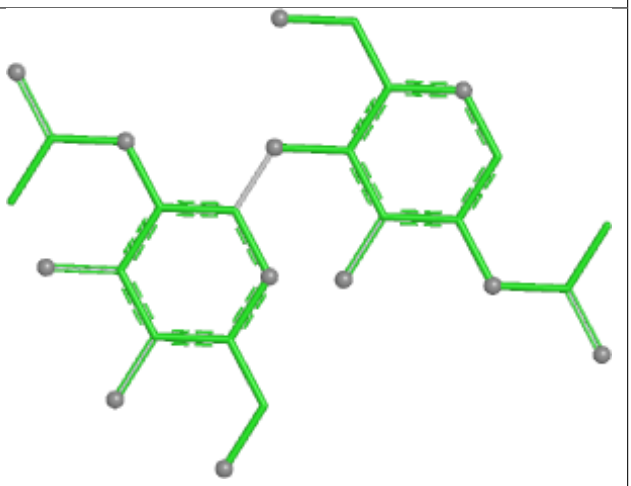


**Rings**

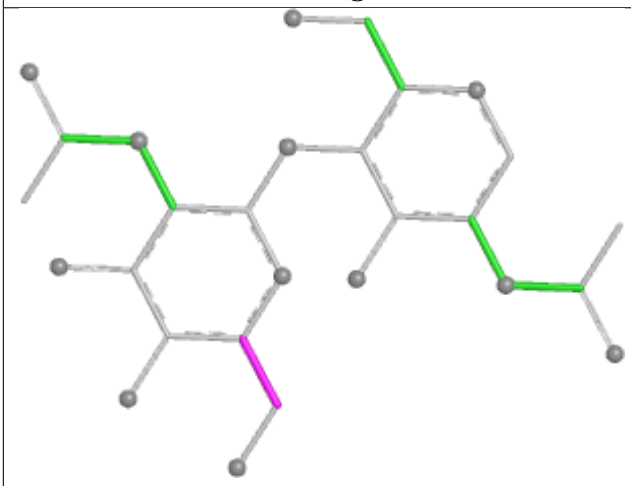
**Oligosaccharide Chain s**



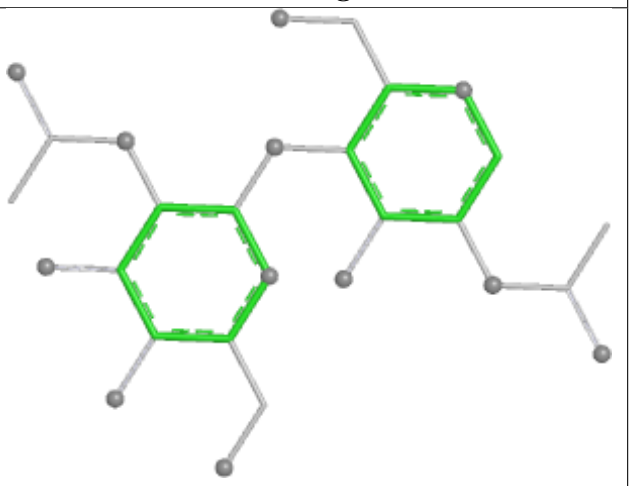
**Bond lengths**



**Bond angles**

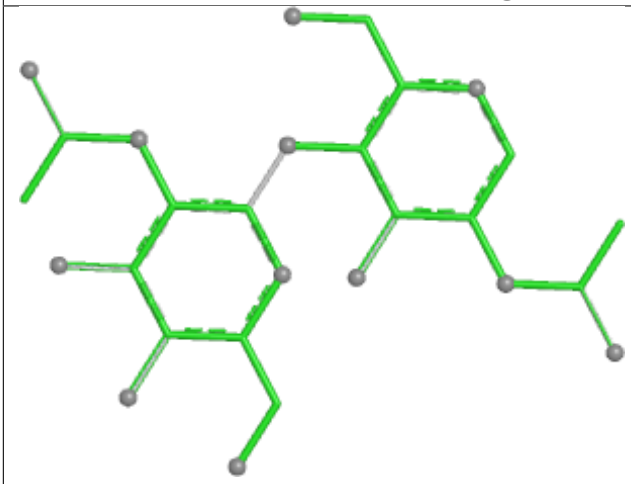


**Torsions**

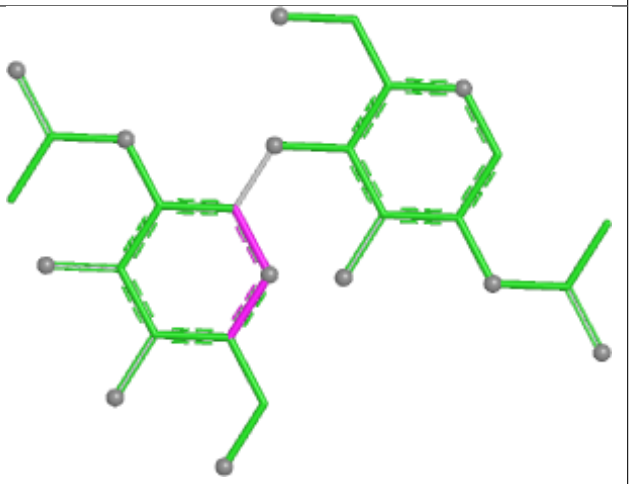


**Rings**

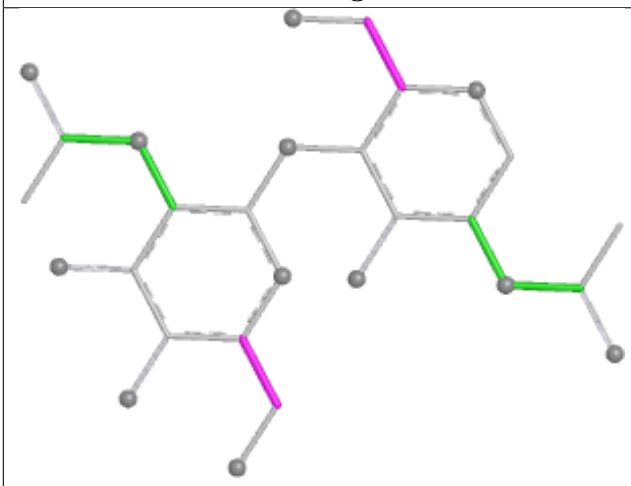
**Oligosaccharide Chain x**



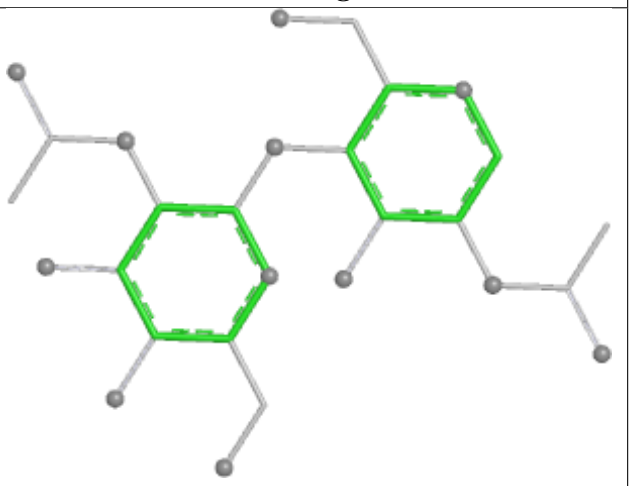
**Bond lengths**



**Bond angles**

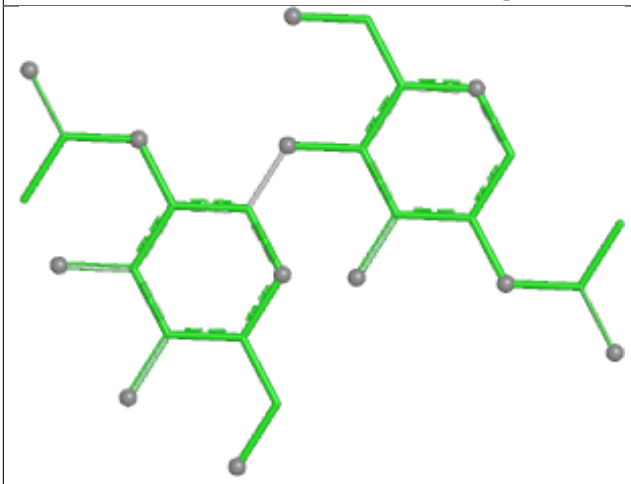


**Torsions**

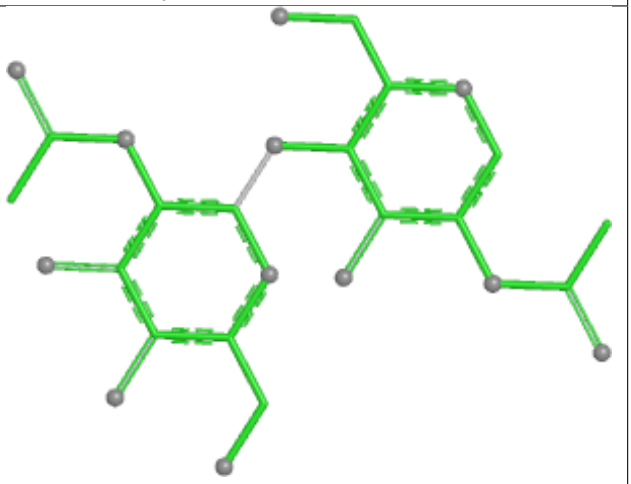


**Rings**

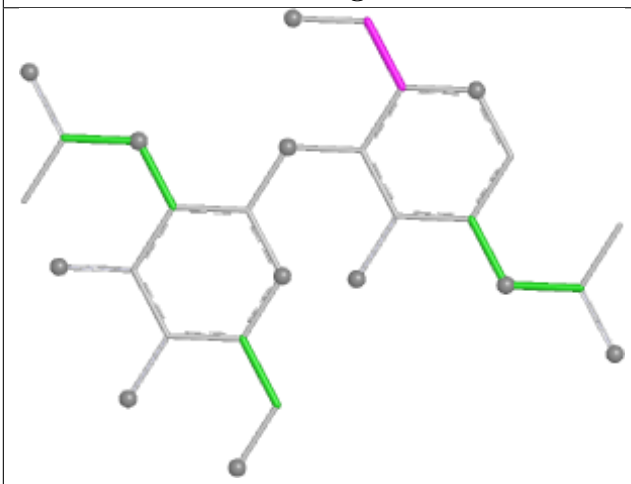
**Oligosaccharide Chain y**



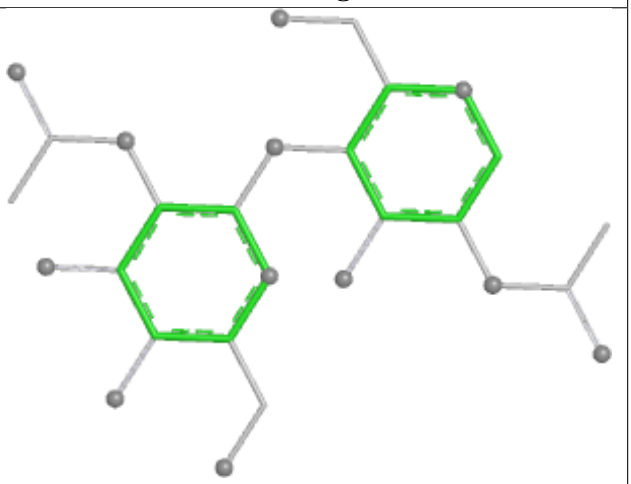
**Bond lengths**



**Bond angles**

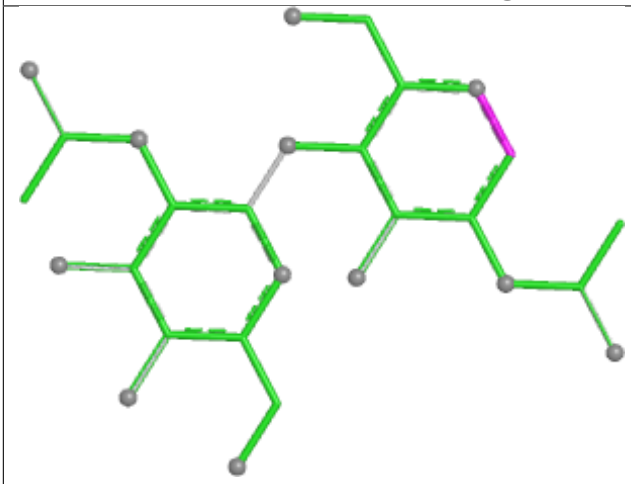


**Torsions**

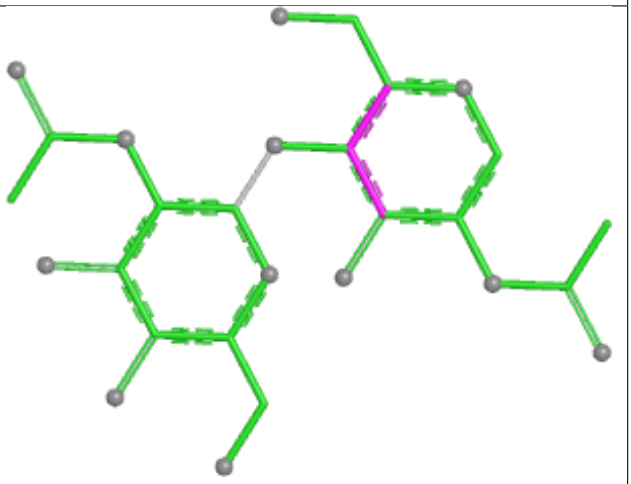


**Rings**

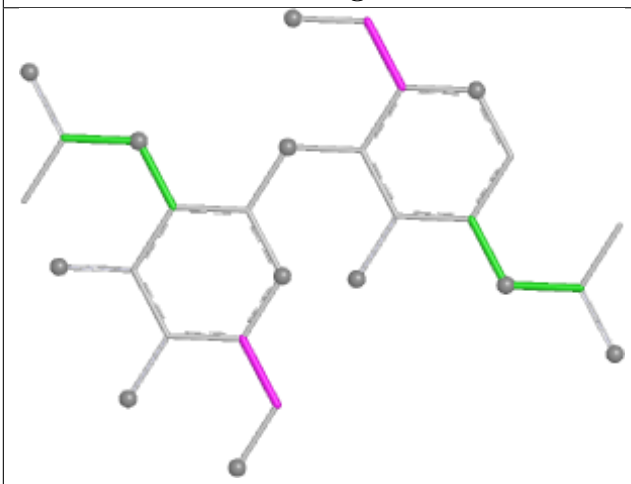
**Oligosaccharide Chain 0**



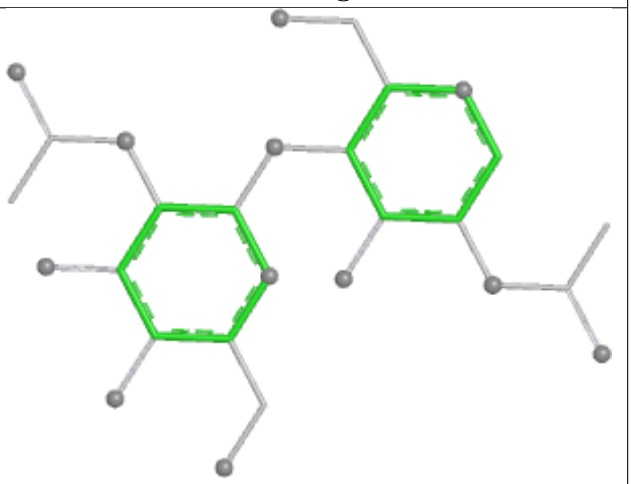
**Bond lengths**



**Bond angles**

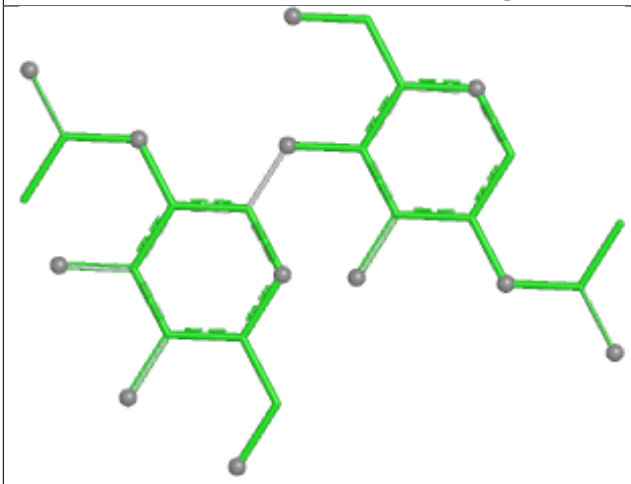


**Torsions**

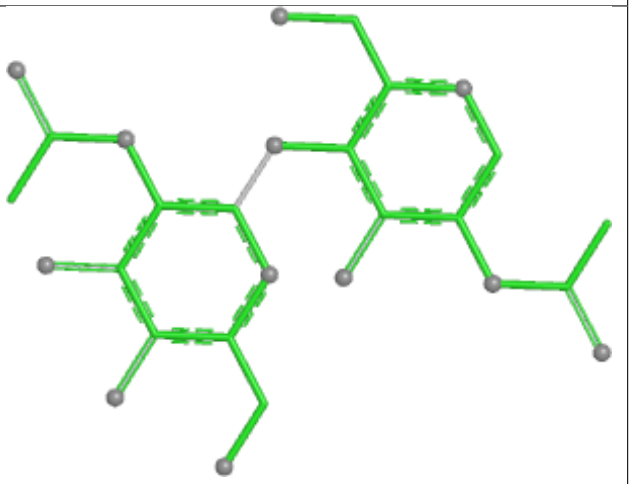


**Rings**

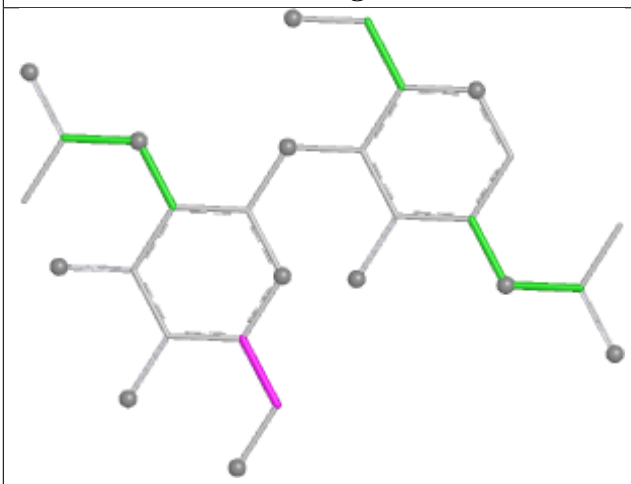
**Oligosaccharide Chain 2**



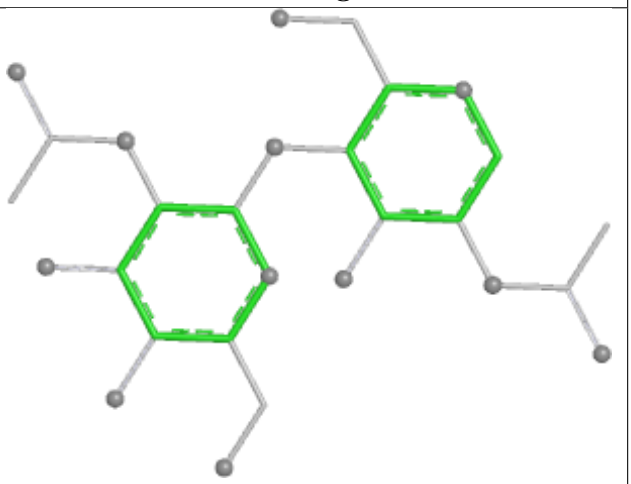
**Bond lengths**



**Bond angles**

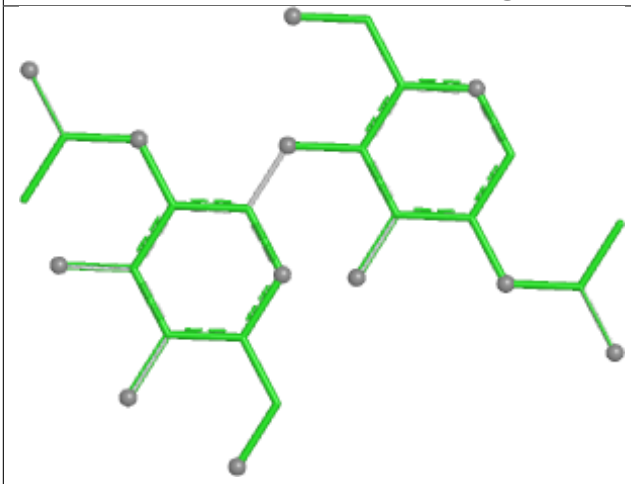


**Torsions**

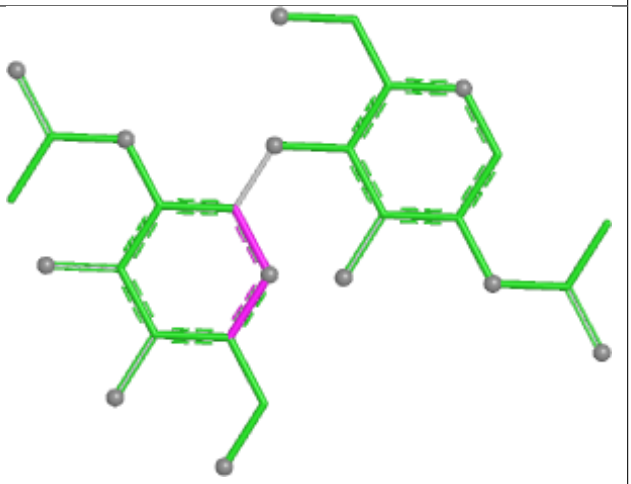


**Rings**

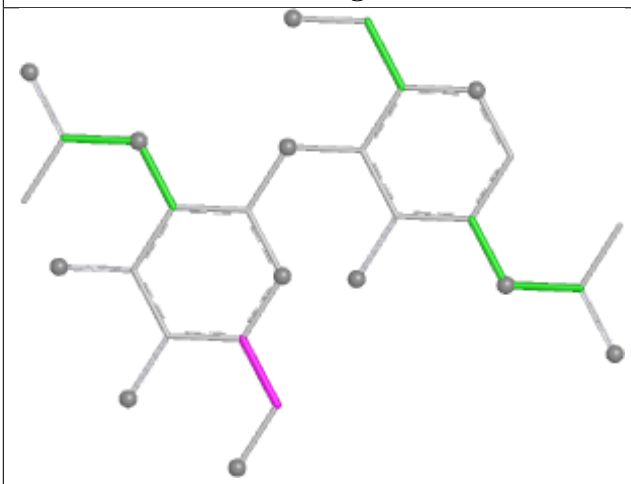
**Oligosaccharide Chain 7**



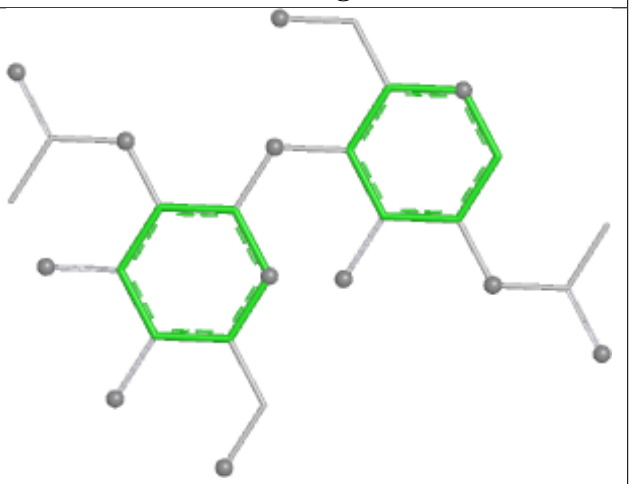
**Bond lengths**



**Bond angles**

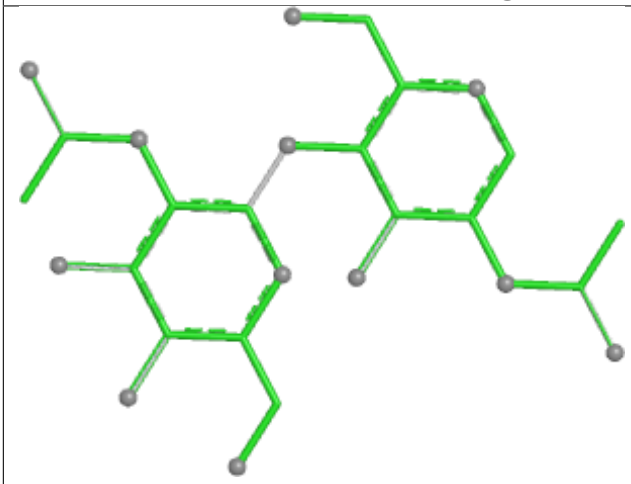


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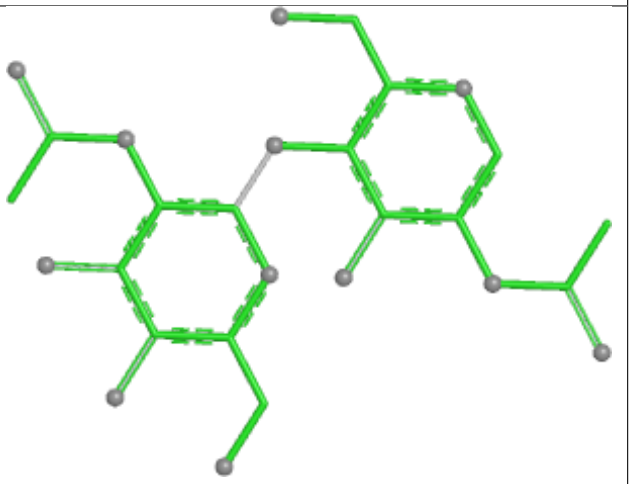


**Rings**

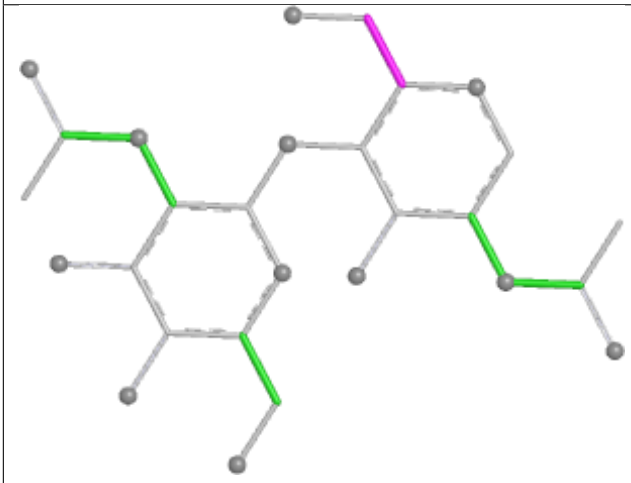
**Oligosaccharide Chain 8**



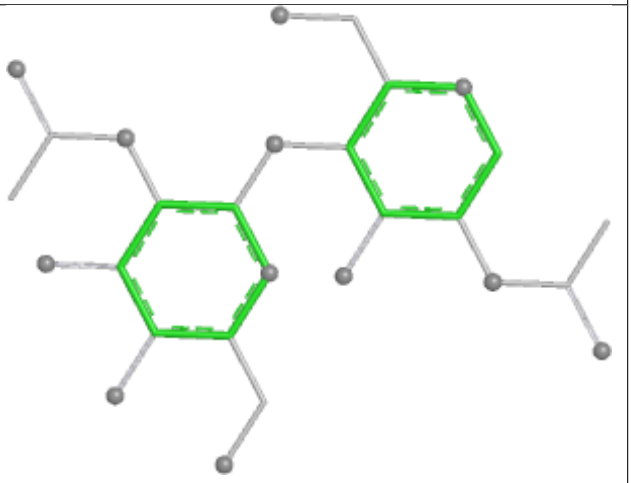
**Bond lengths**



**Bond angles**

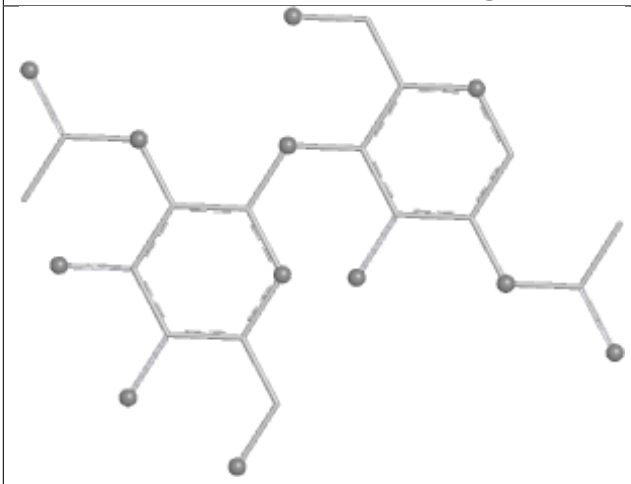


**Torsions**

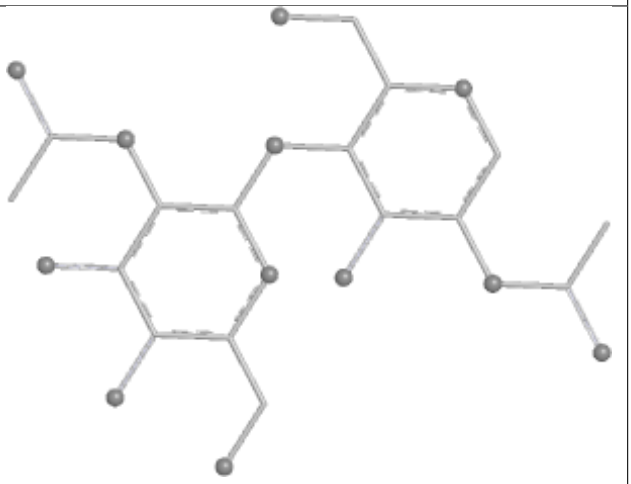


**Rings**

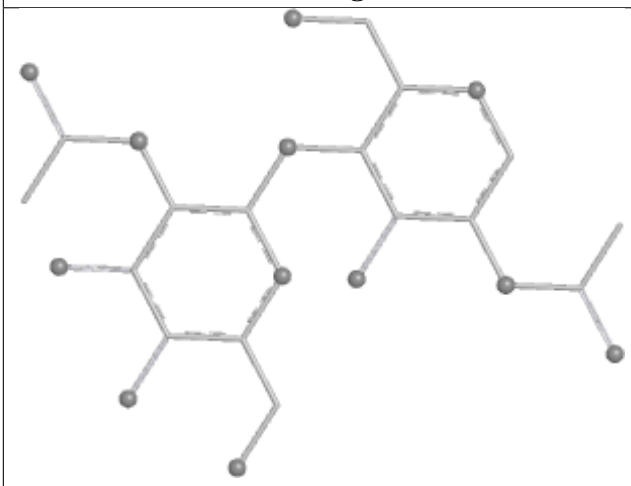
**Oligosaccharide Chain AA**



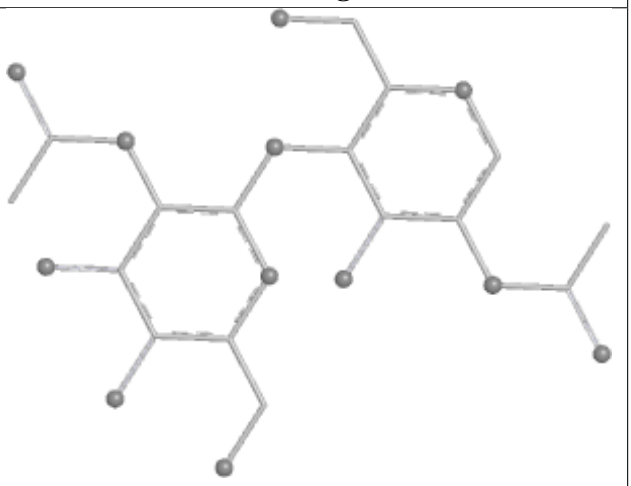
**Bond lengths**



**Bond angles**

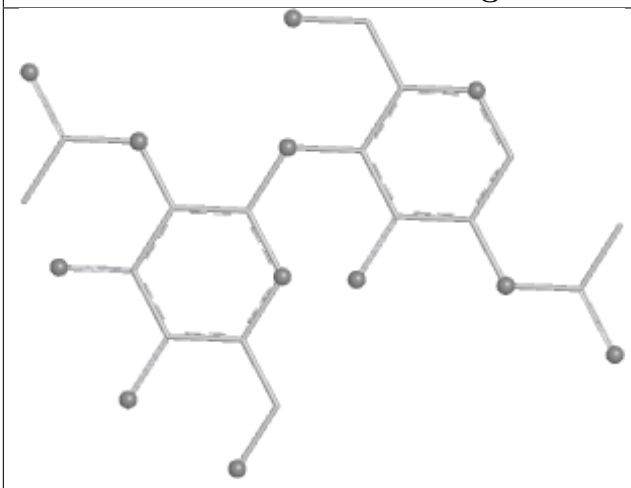


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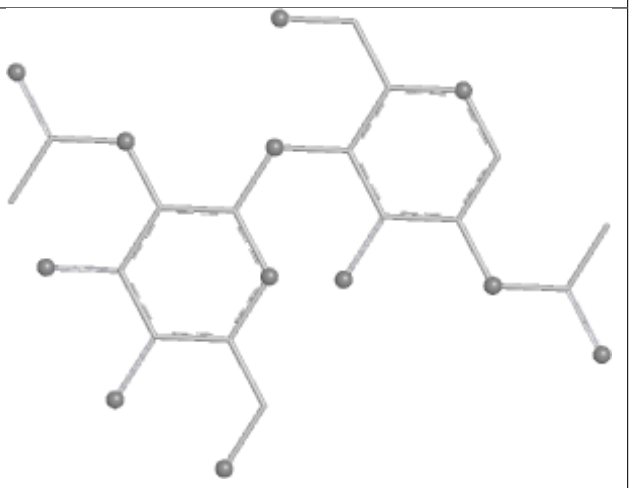


**Rings**

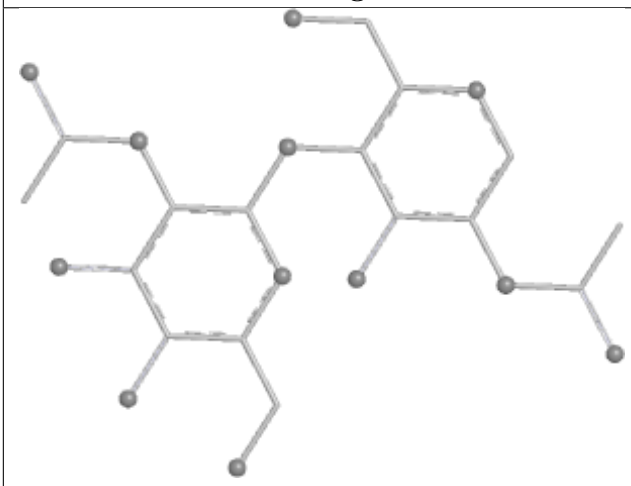
**Oligosaccharide Chain CA**



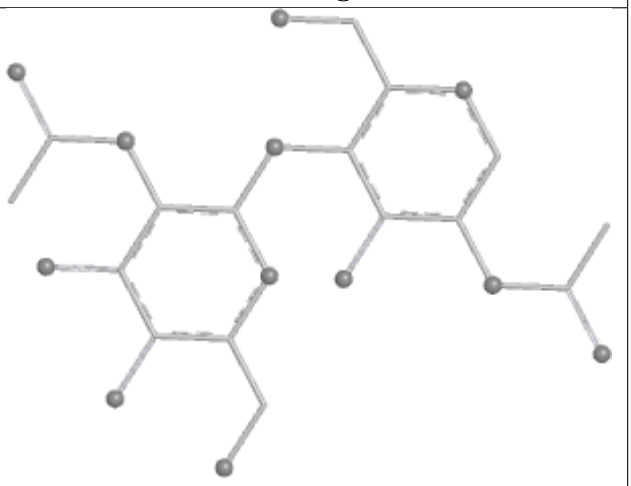
**Bond lengths**



**Bond angles**

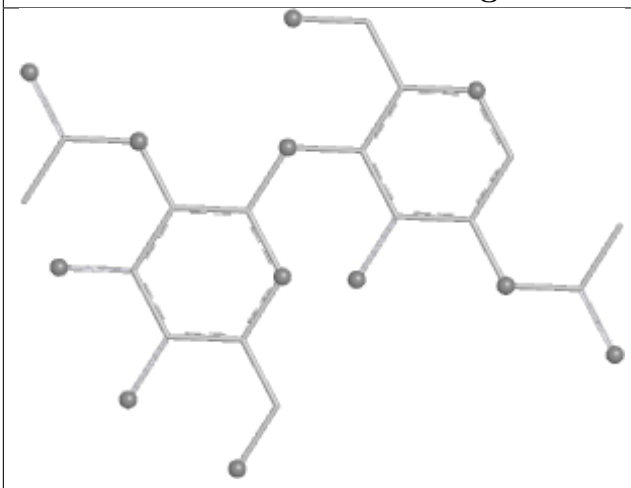


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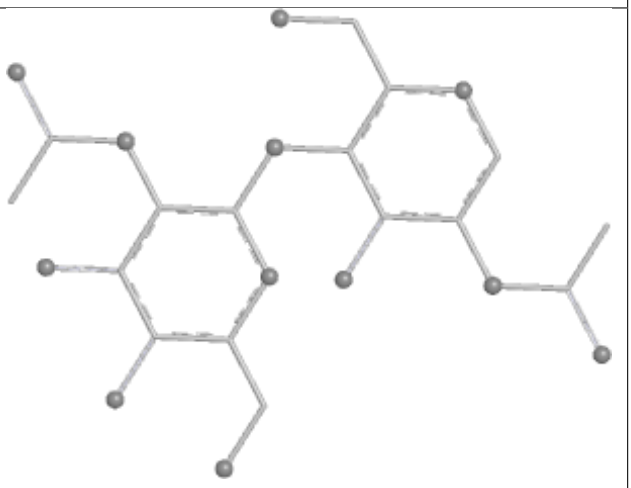


**Rings**

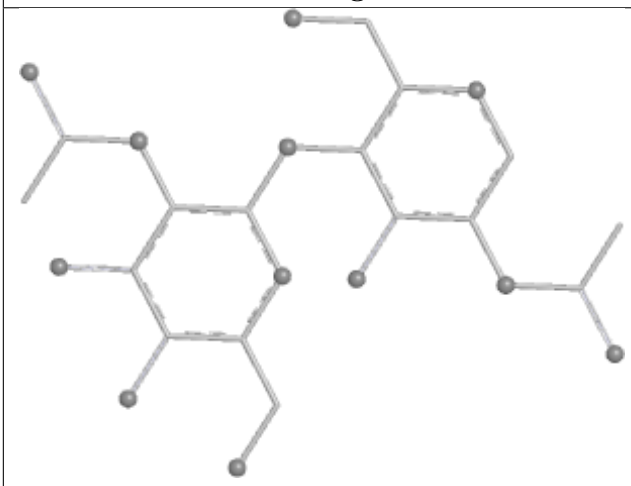
**Oligosaccharide Chain HA**



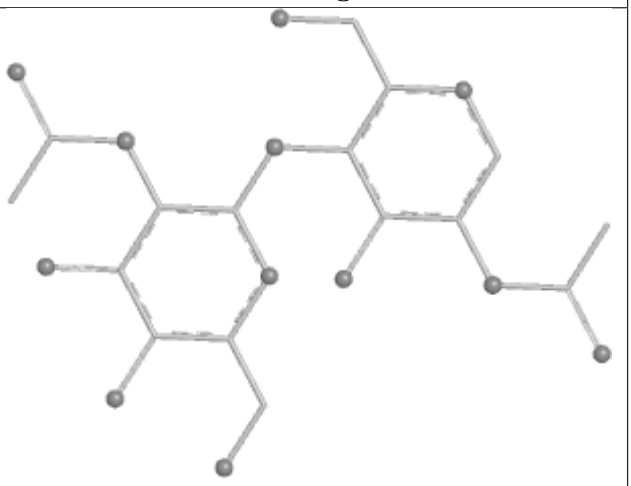
**Bond lengths**



**Bond angles**

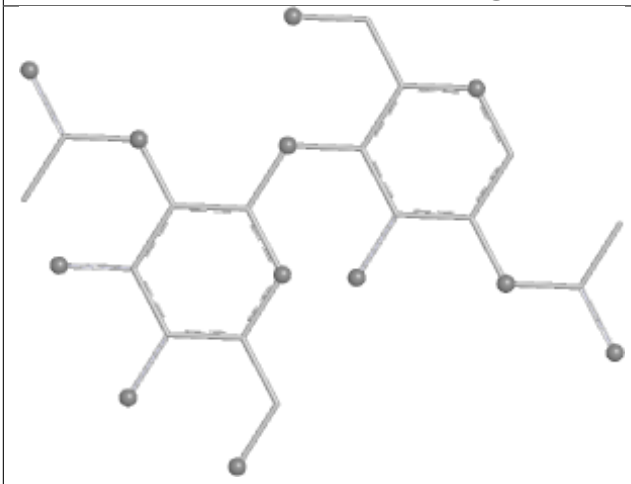


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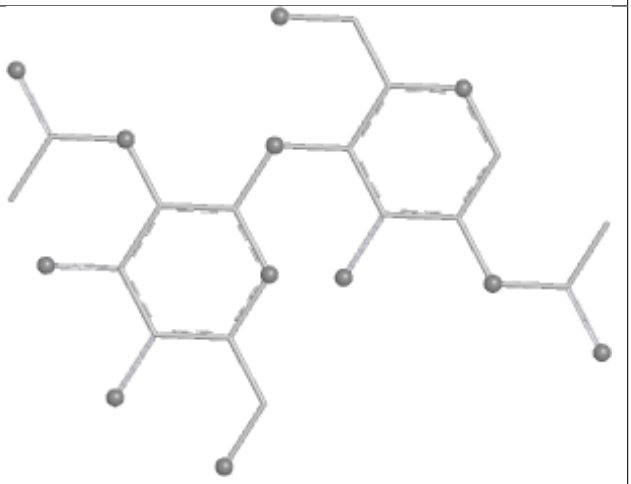


**Rings**

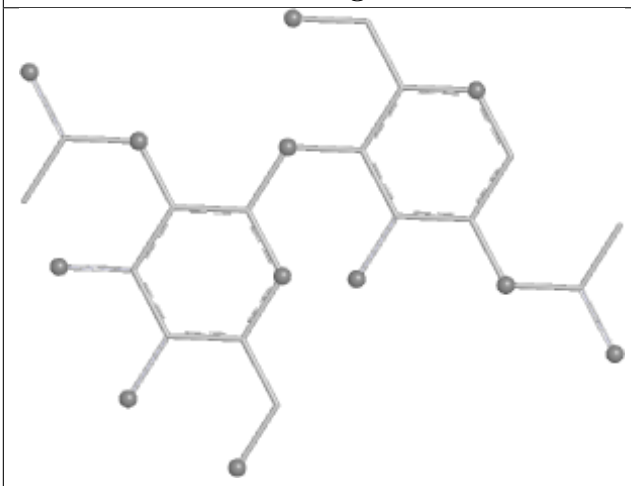
**Oligosaccharide Chain IA**



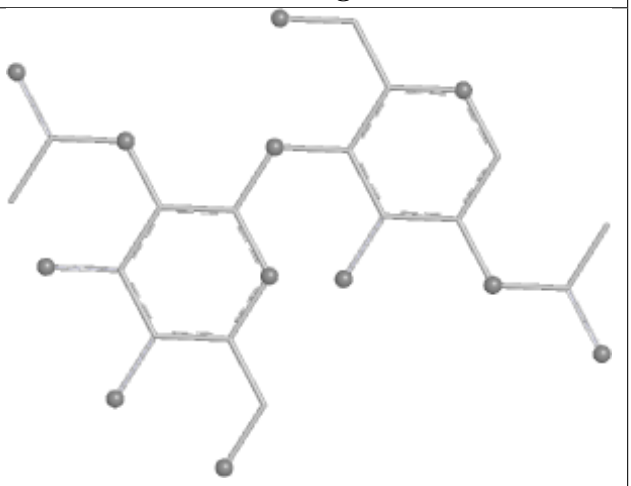
**Bond lengths**



**Bond angles**

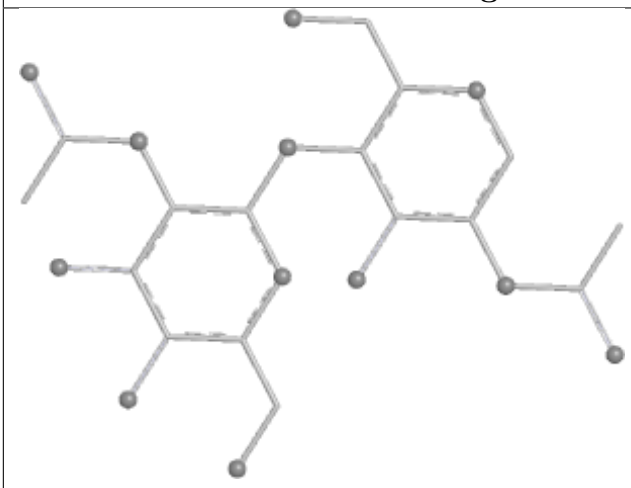


**Torsions**

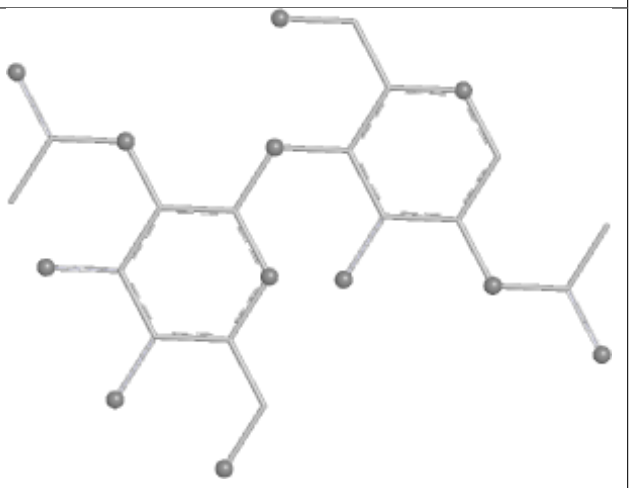


**Rings**

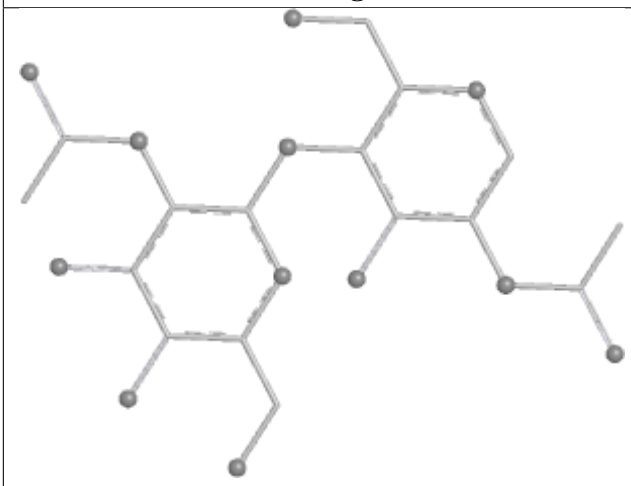
**Oligosaccharide Chain KA**



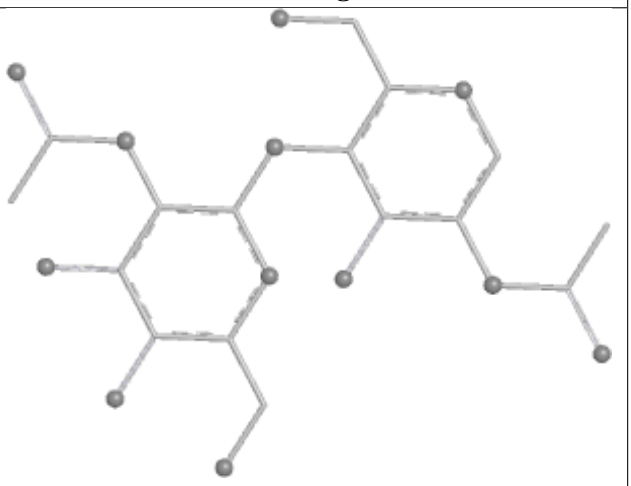
**Bond lengths**



**Bond angles**

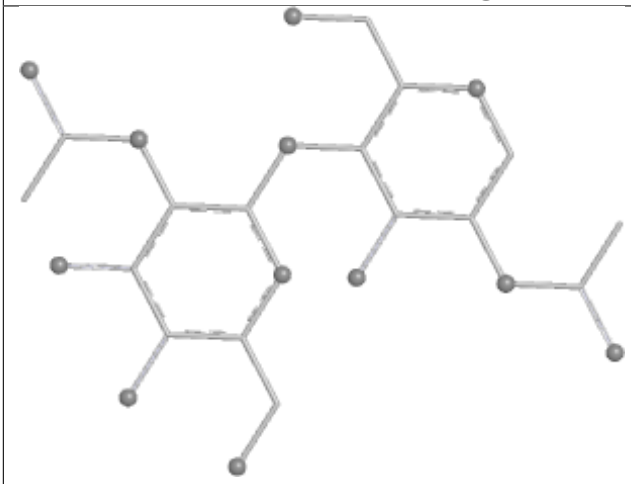


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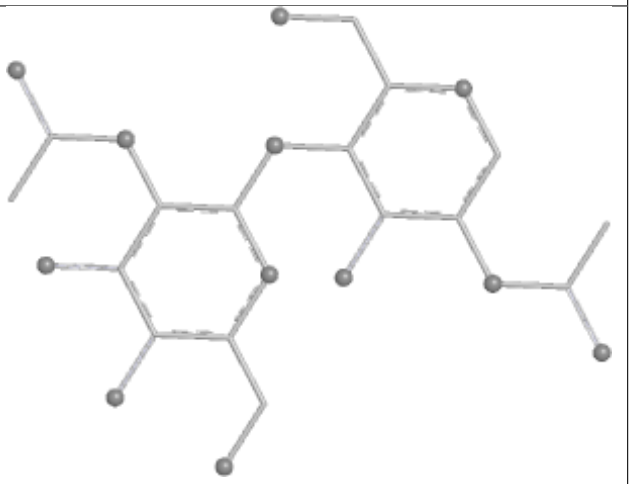


**Rings**

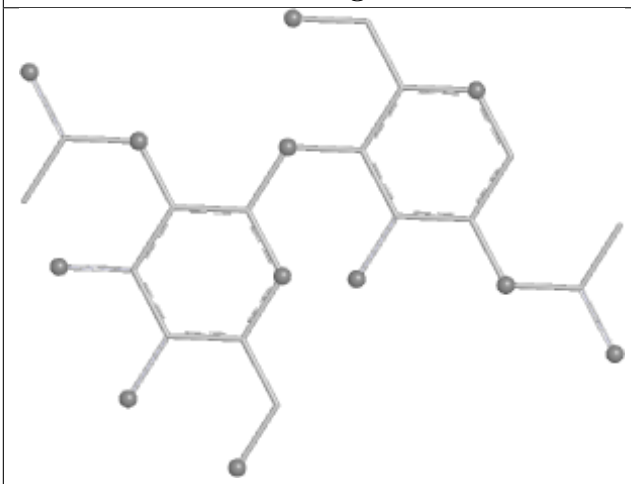
**Oligosaccharide Chain MA**



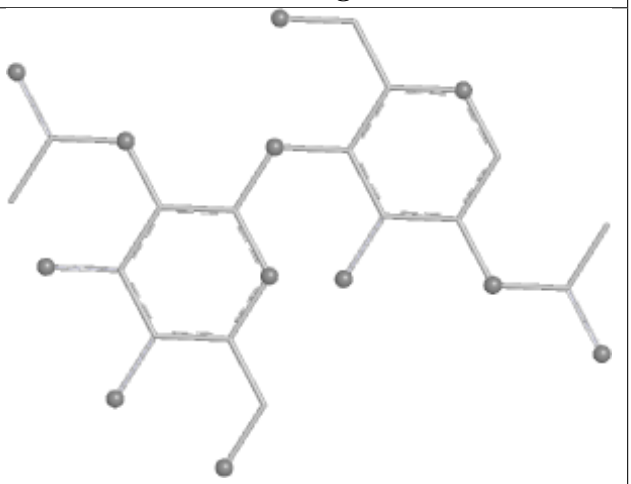
**Bond lengths**



**Bond angles**

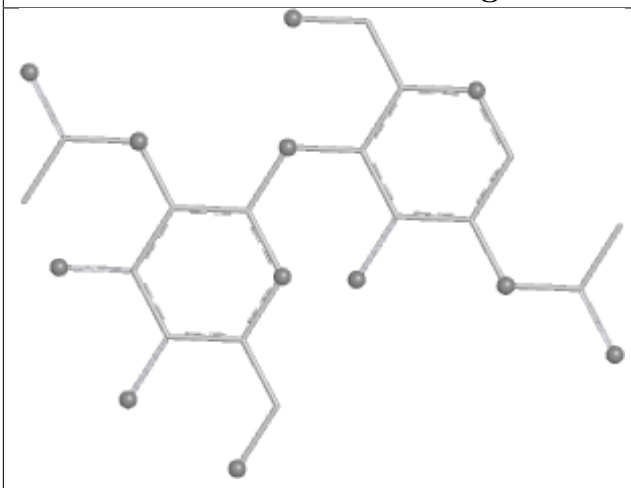


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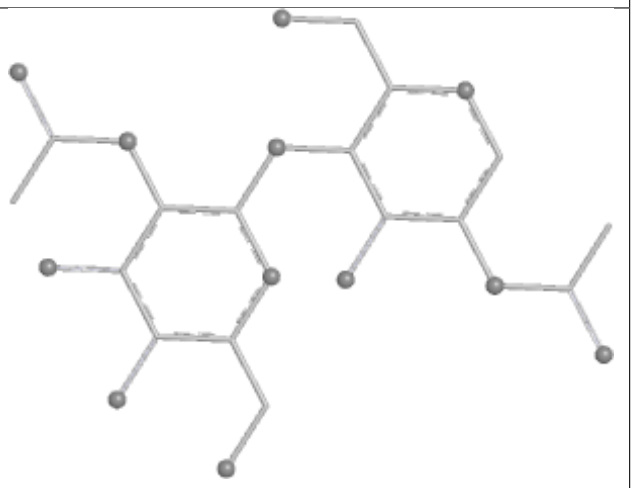


**Rings**

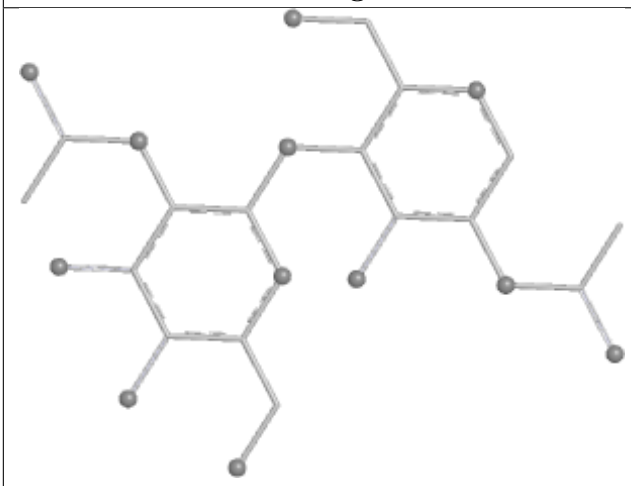
**Oligosaccharide Chain RA**



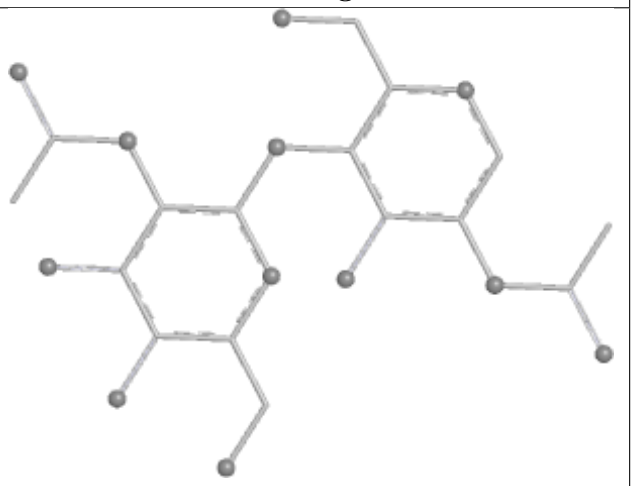
**Bond lengths**



**Bond angles**

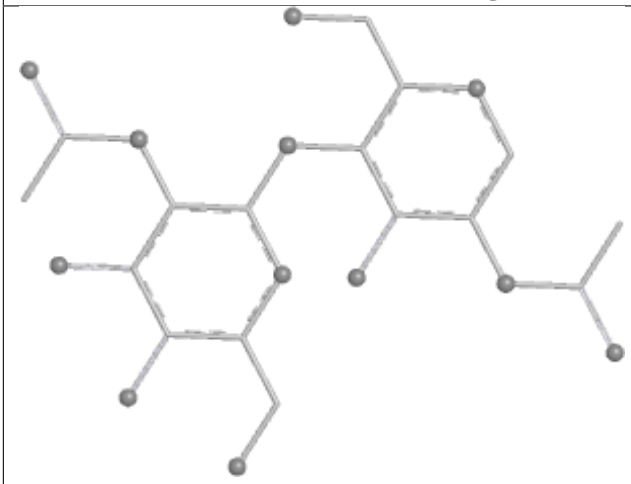


**Torsions**

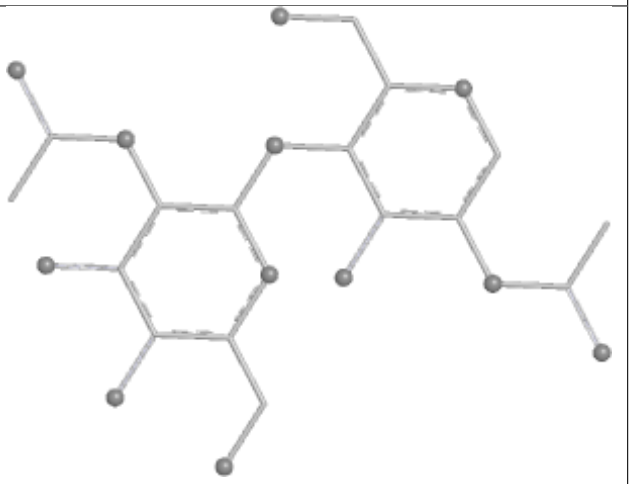


**Rings**

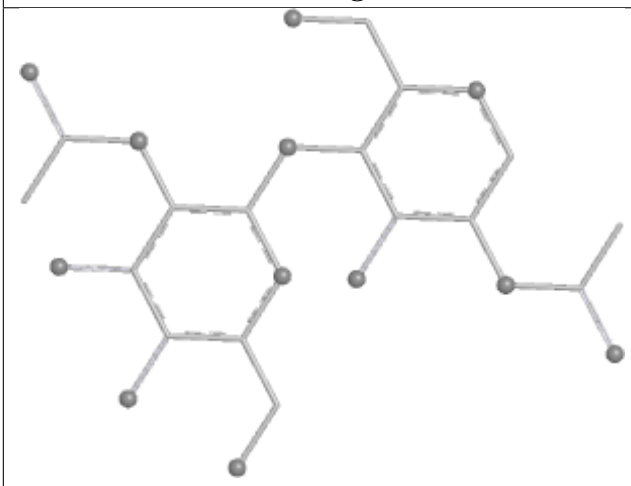
**Oligosaccharide Chain SA**



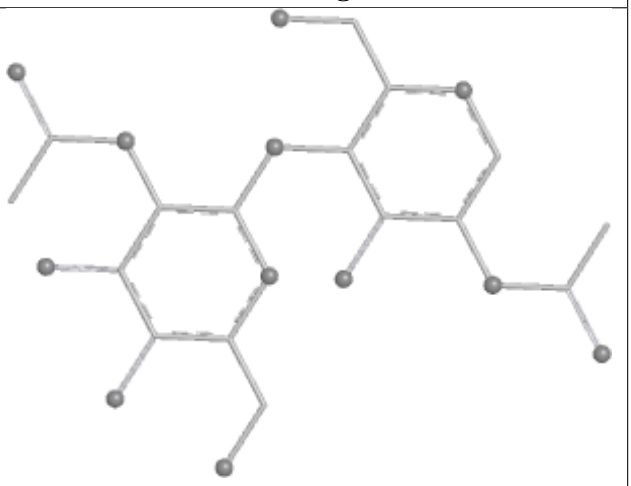
**Bond lengths**



**Bond angles**

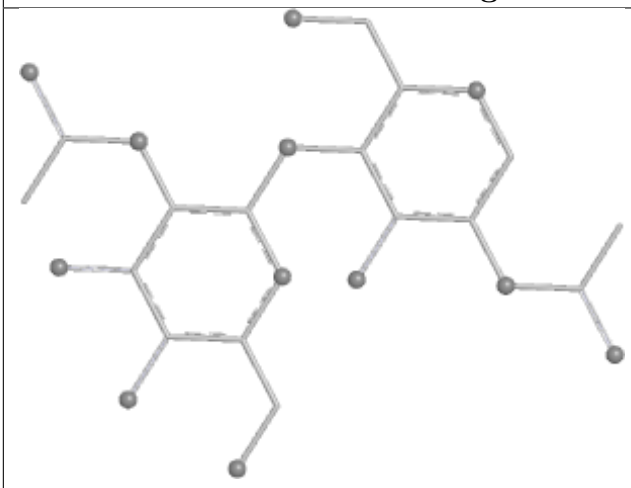


**Torsions**

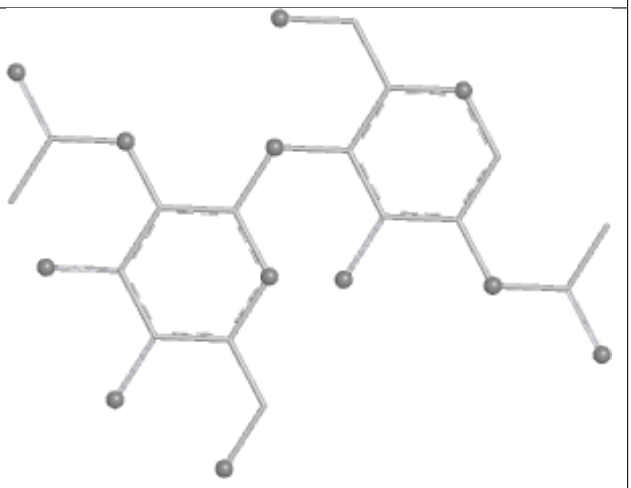


**Rings**

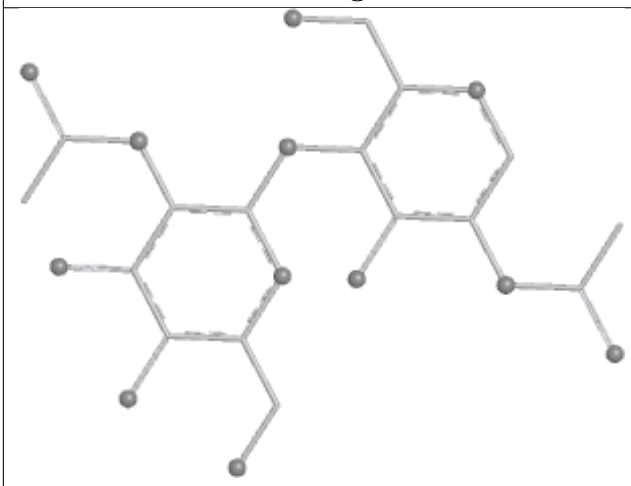
**Oligosaccharide Chain UA**



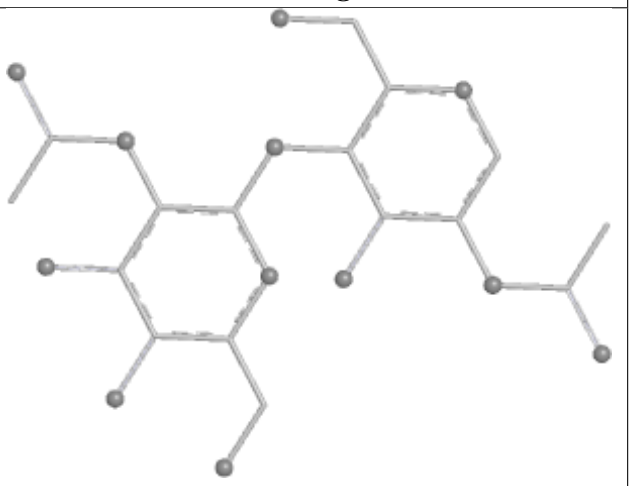
**Bond lengths**



**Bond angles**

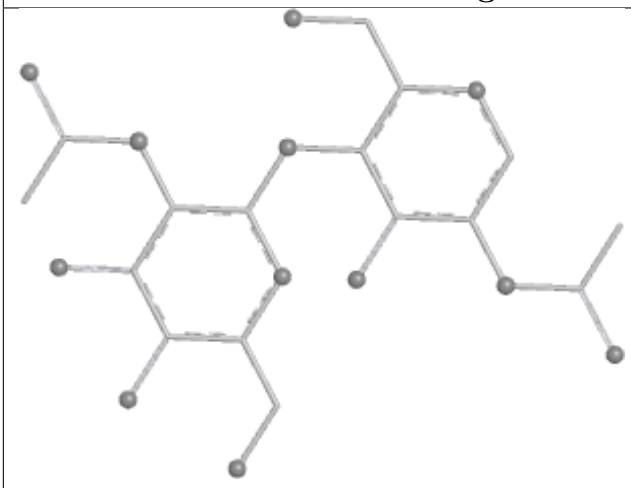


**Torsions**

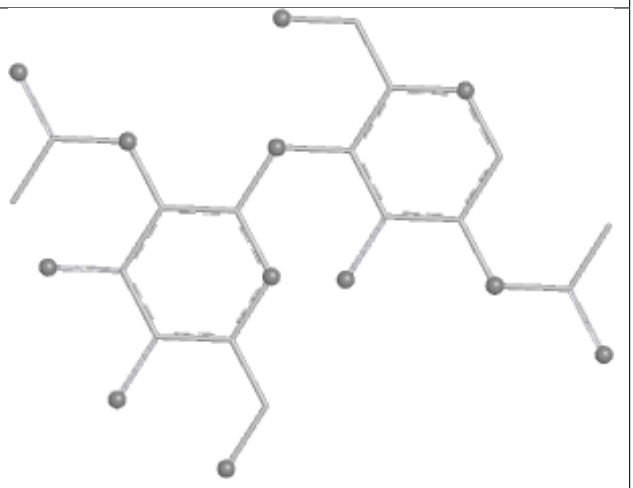


**Rings**

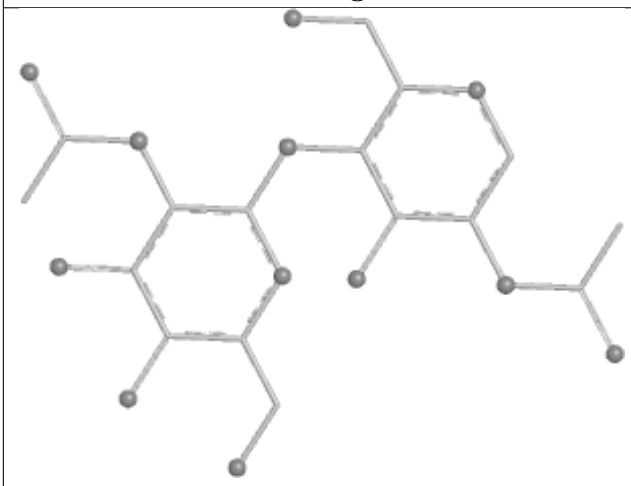
**Oligosaccharide Chain WA**



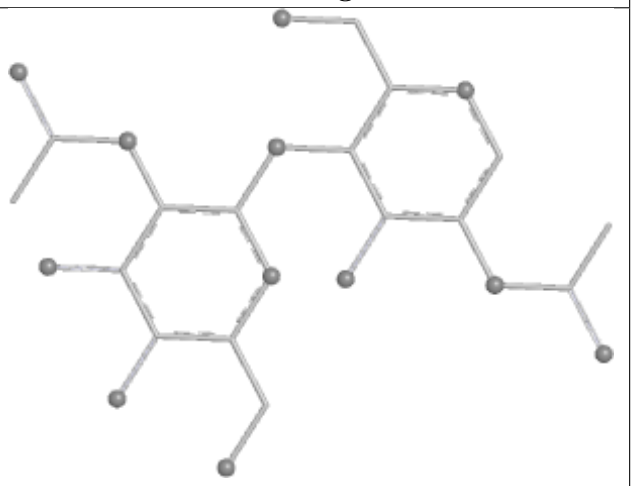
**Bond lengths**



**Bond angles**

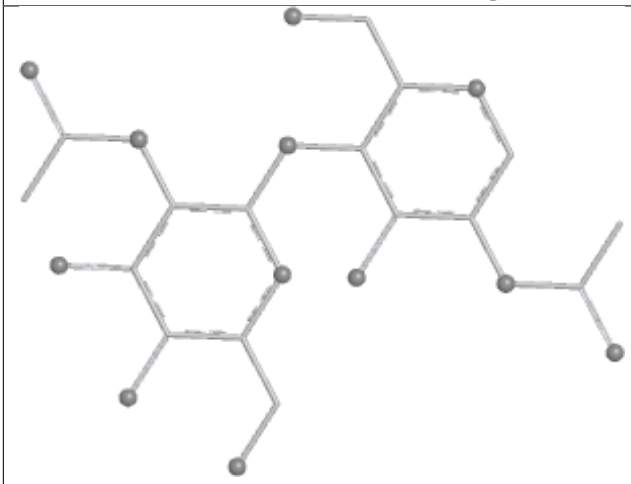


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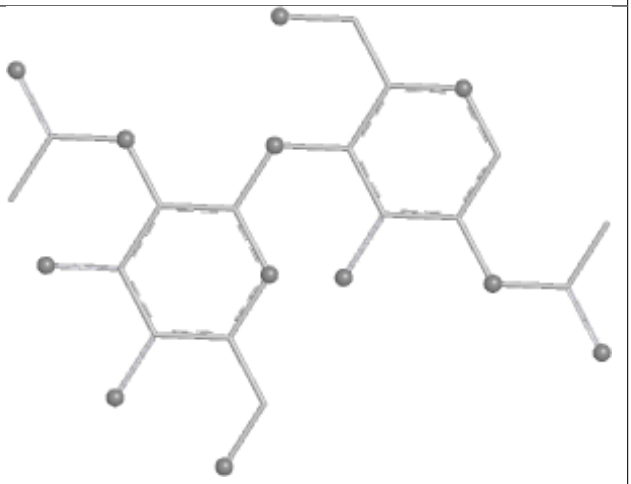


**Rings**

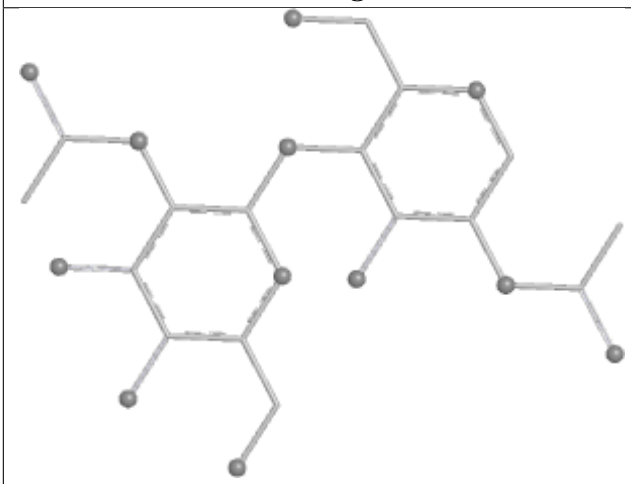
**Oligosaccharide Chain bA**



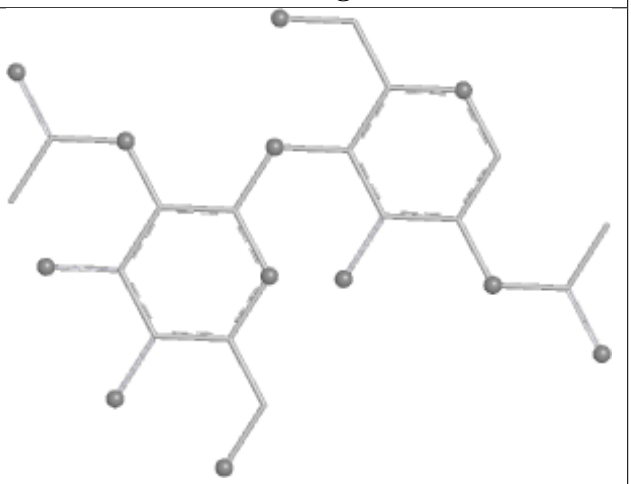
**Bond lengths**



**Bond angles**

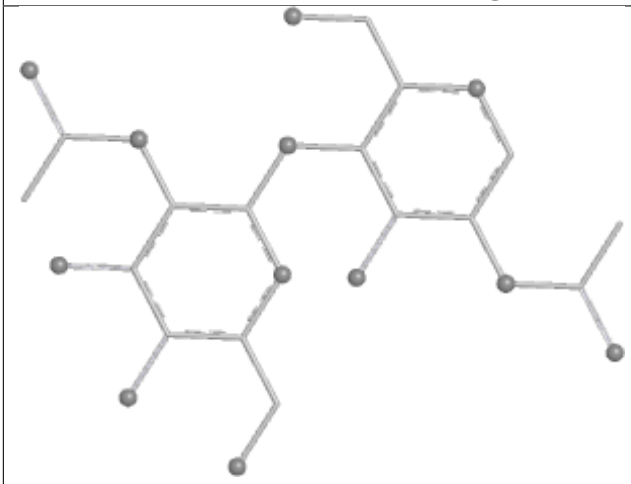


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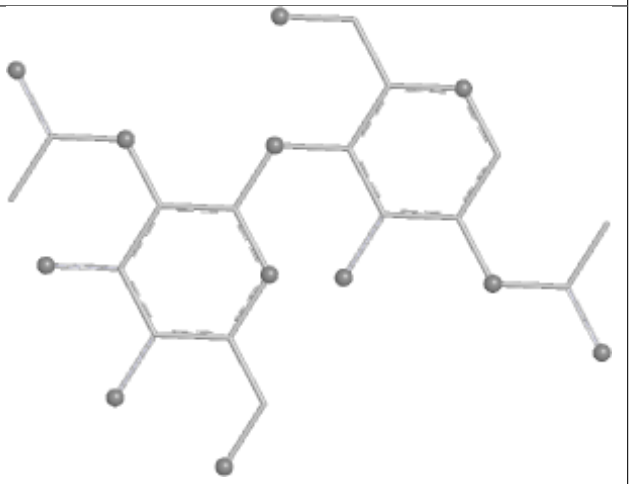


**Rings**

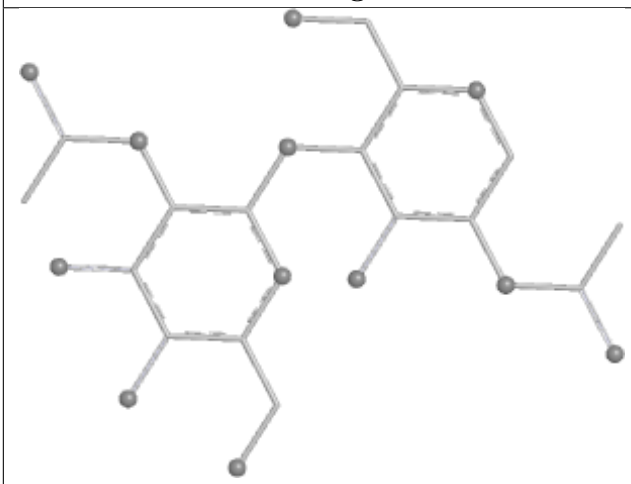
**Oligosaccharide Chain cA**



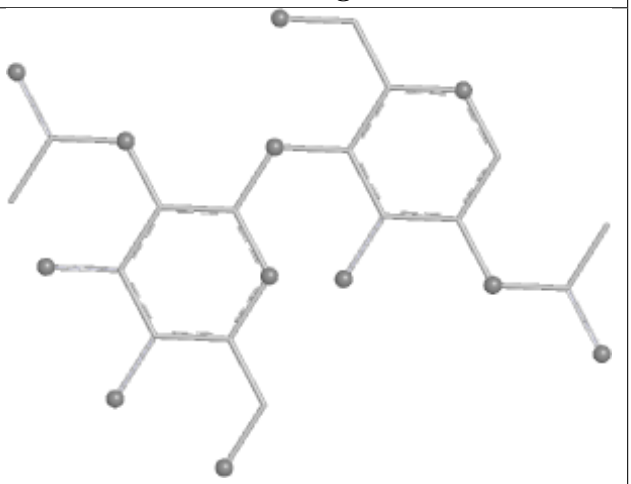
**Bond lengths**



**Bond angles**

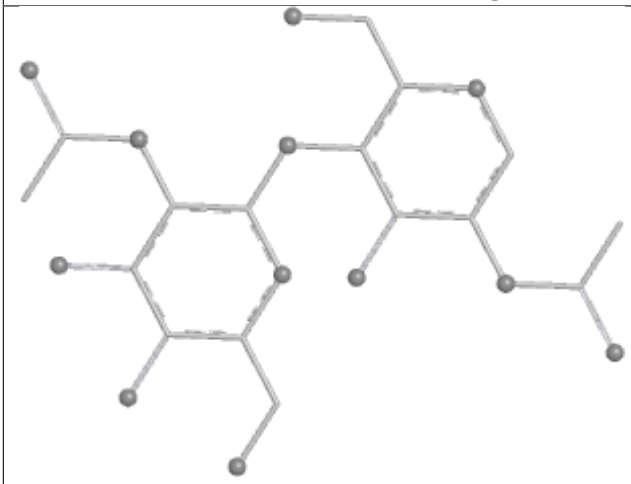


**Torsions**

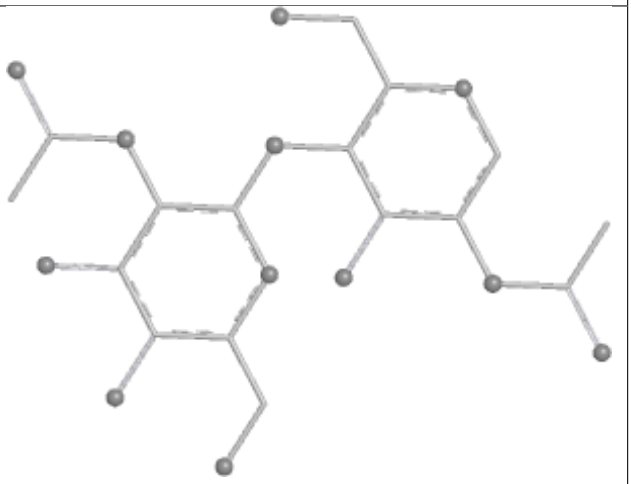


**Rings**

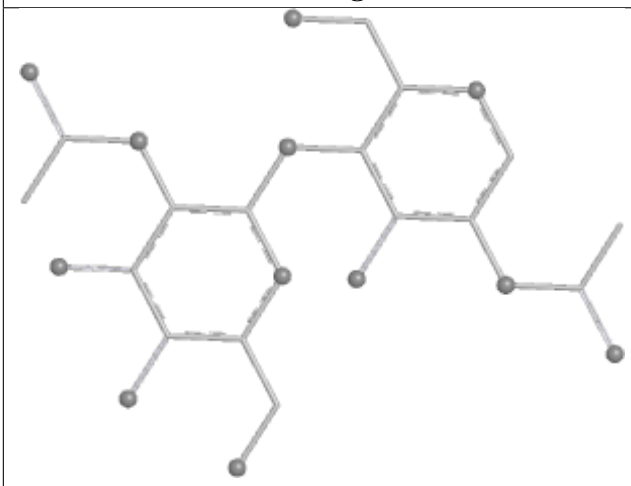
**Oligosaccharide Chain eA**



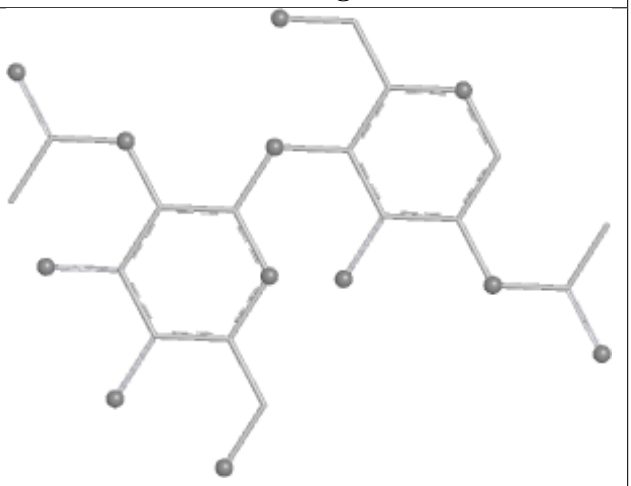
**Bond lengths**



**Bond angles**

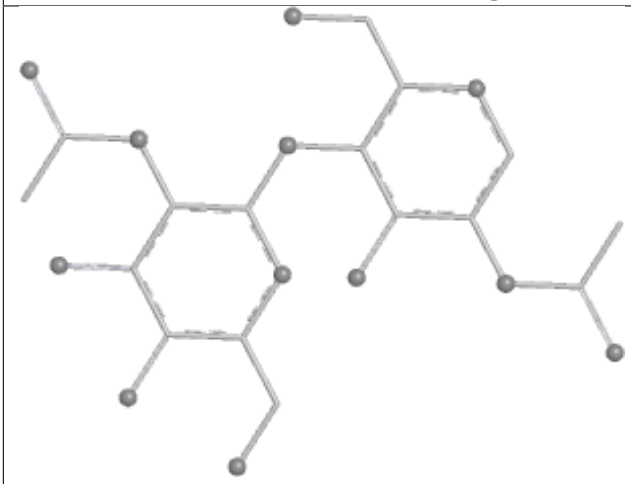


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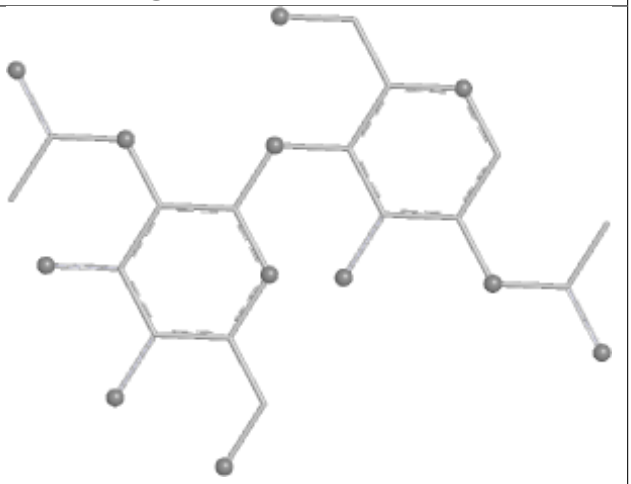


**Rings**

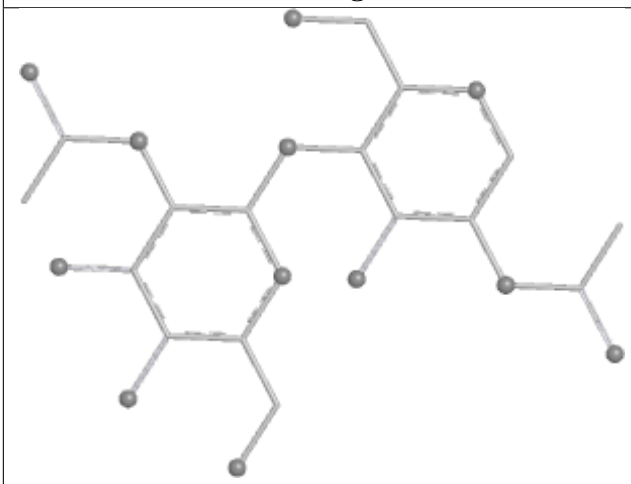
**Oligosaccharide Chain gA**



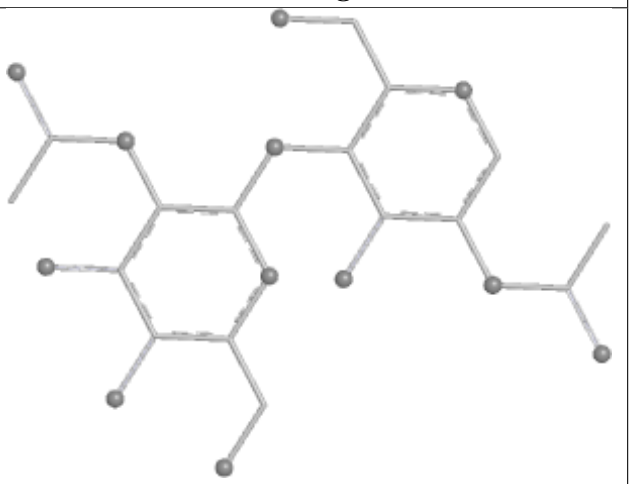
**Bond lengths**



**Bond angles**

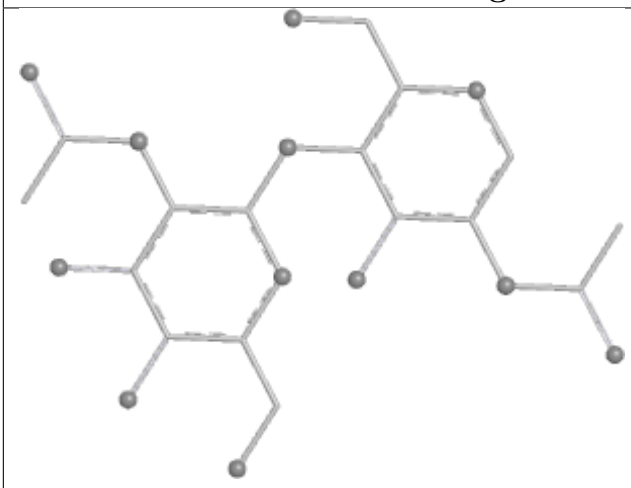


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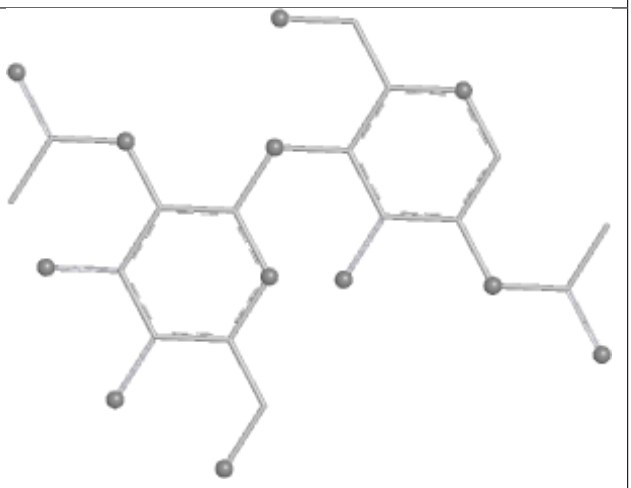


**Rings**

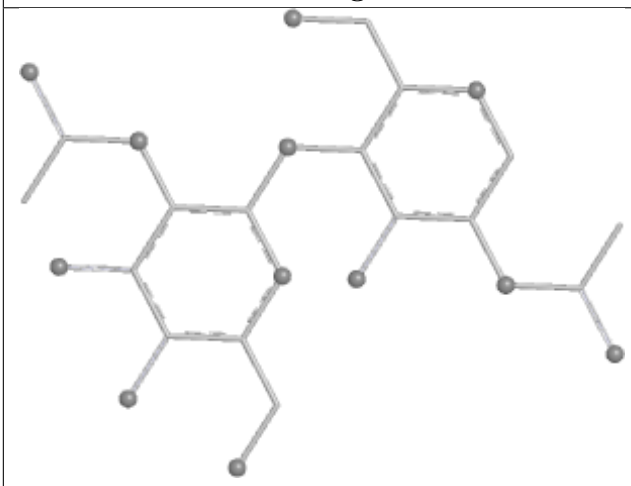
**Oligosaccharide Chain lA**



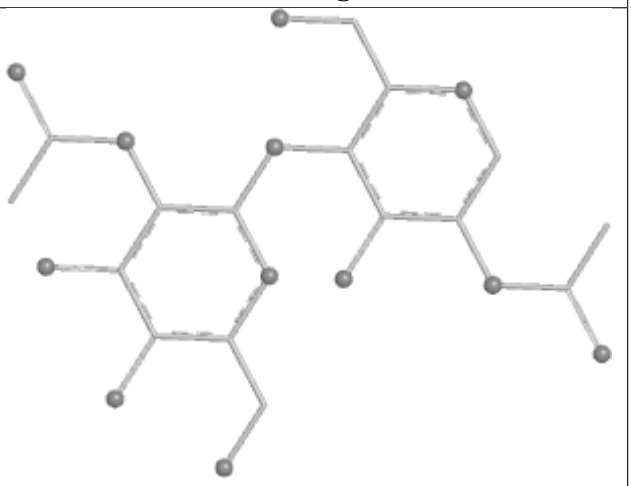
**Bond lengths**



**Bond angles**

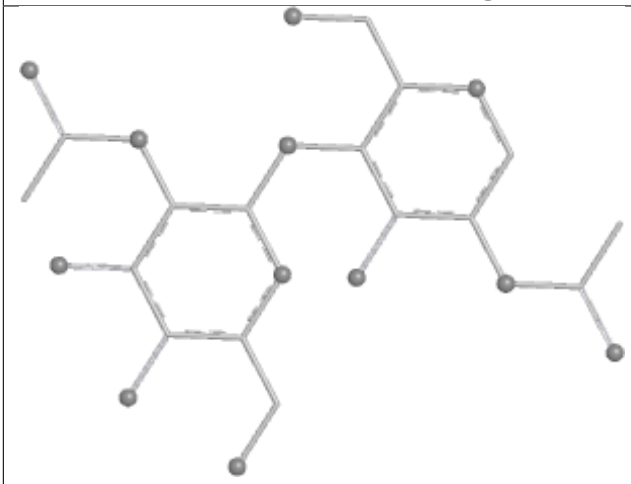


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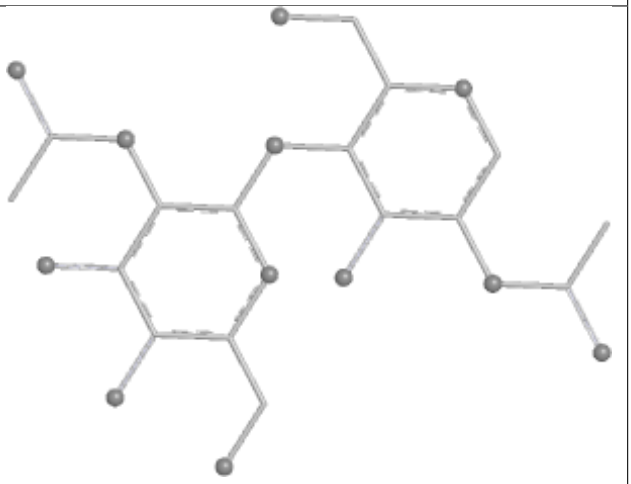


**Rings**

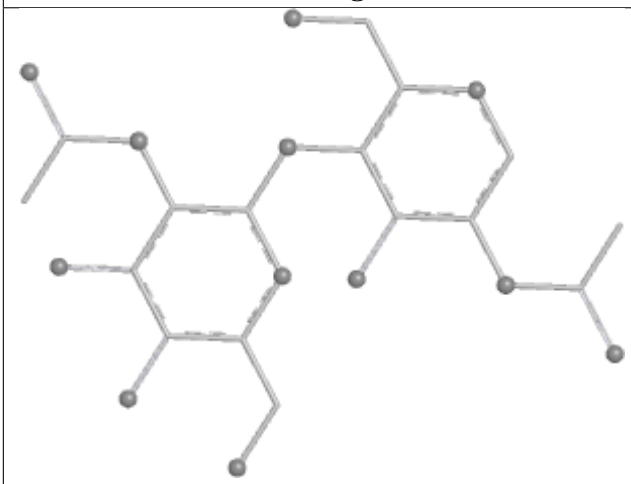
**Oligosaccharide Chain mA**



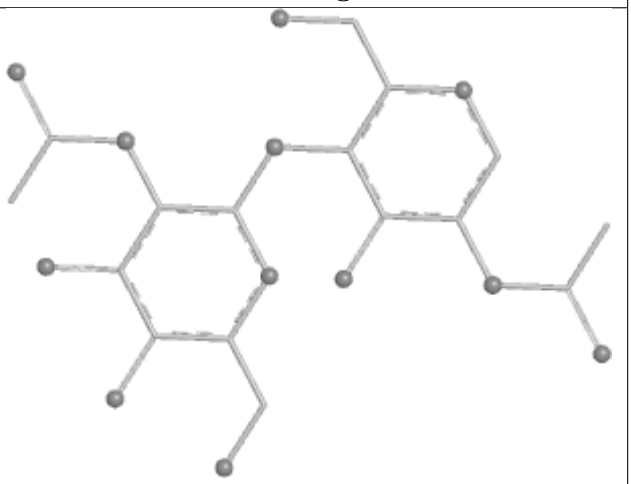
**Bond lengths**



**Bond angles**

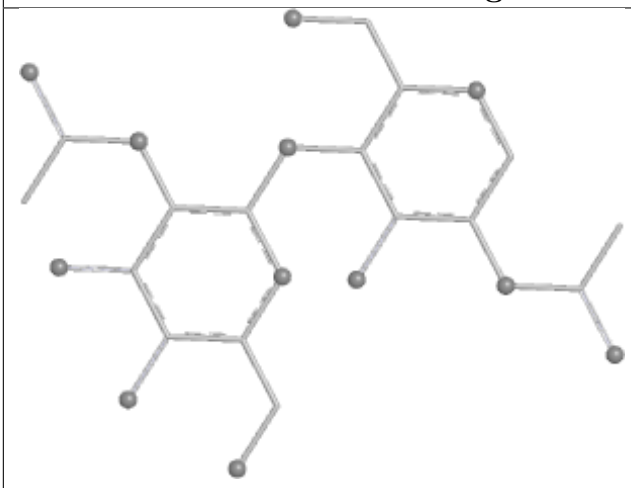


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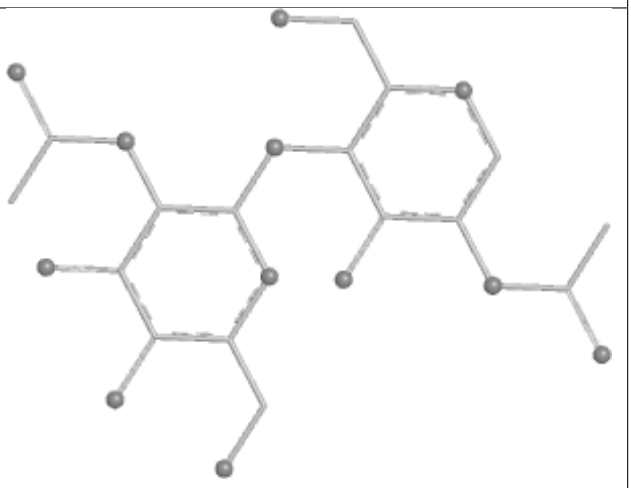


**Rings**

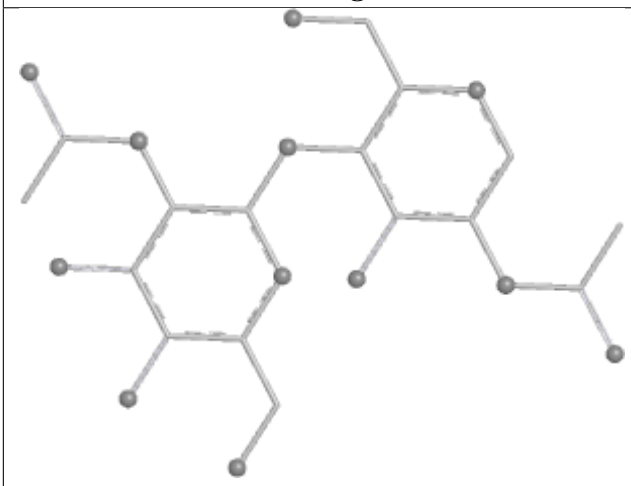
**Oligosaccharide Chain oA**



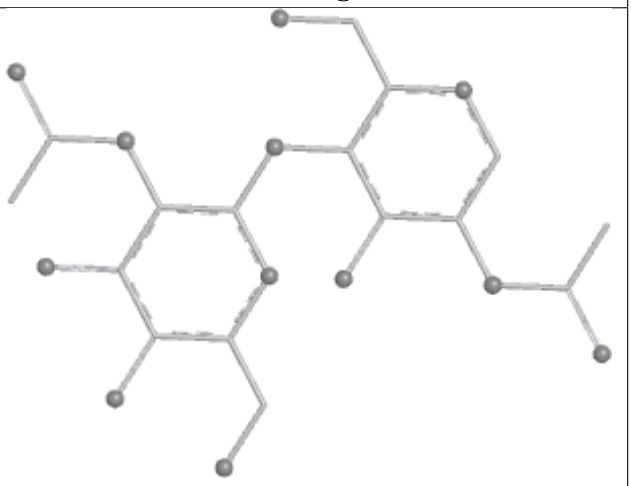
**Bond lengths**



**Bond angles**

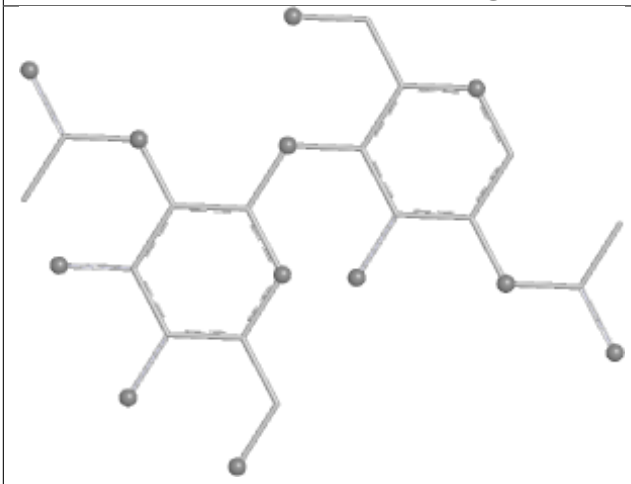


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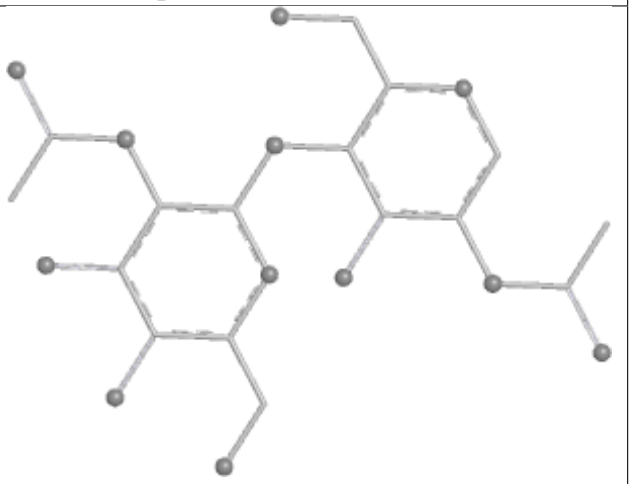


**Rings**

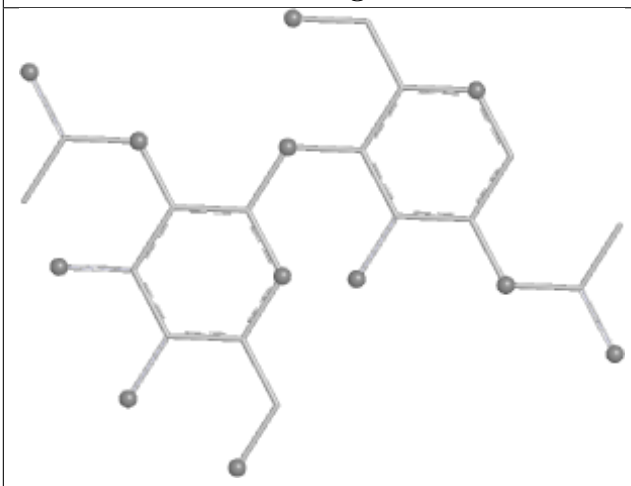
**Oligosaccharide Chain qA**



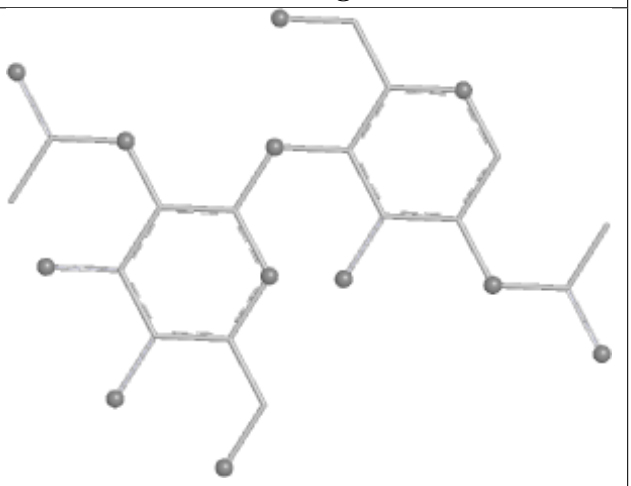
**Bond lengths**



**Bond angles**

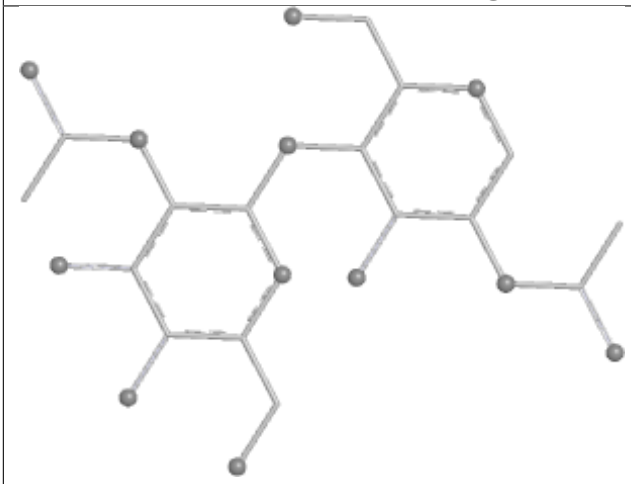


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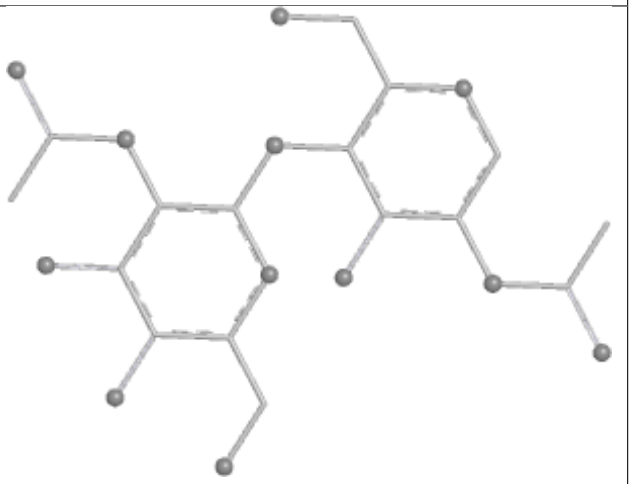


**Rings**

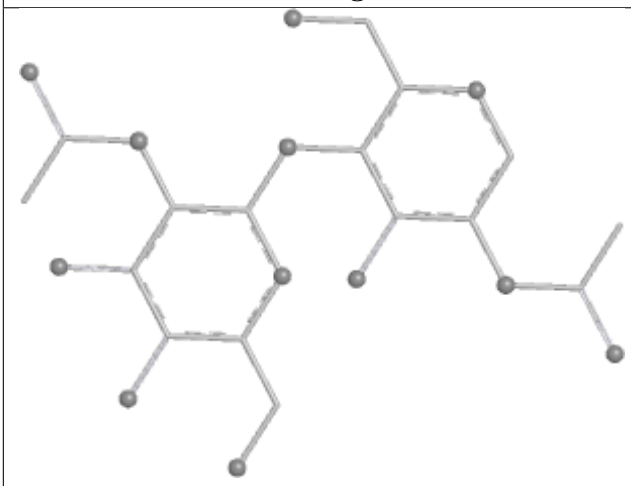
**Oligosaccharide Chain vA**



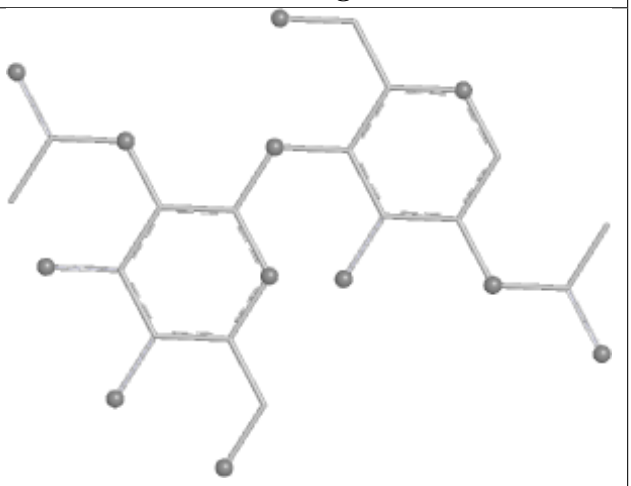
**Bond lengths**



**Bond angles**

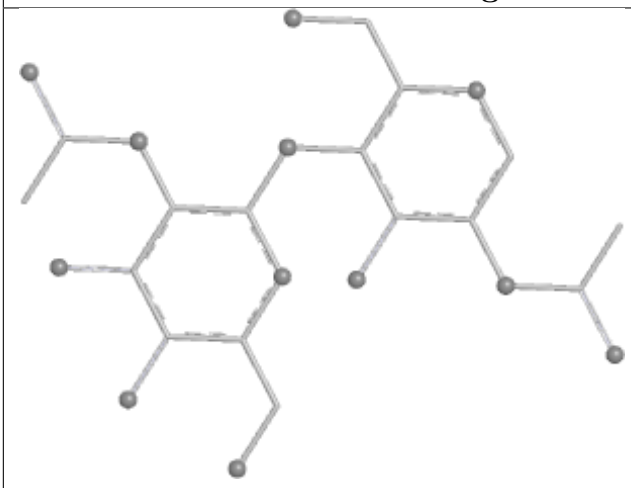


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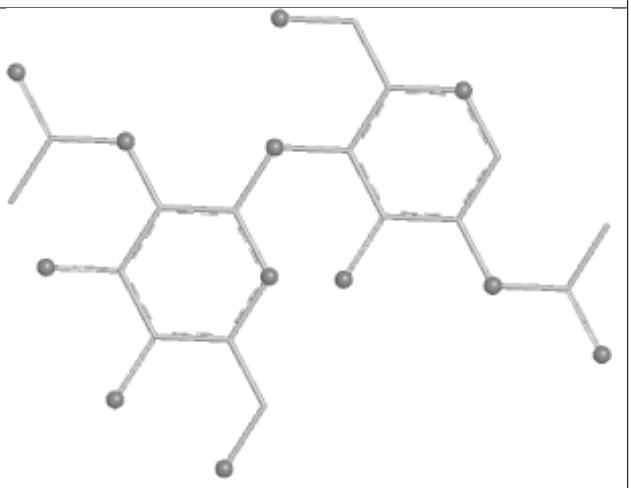


**Rings**

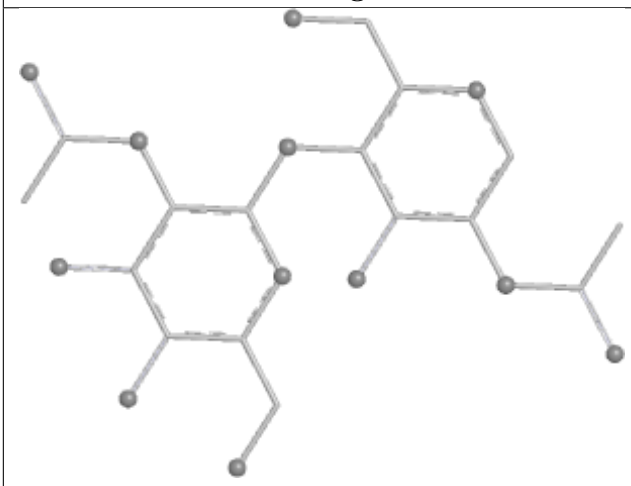
**Oligosaccharide Chain wA**



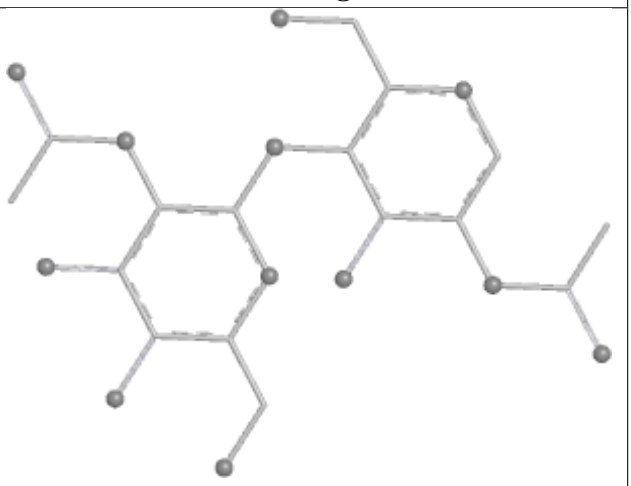
**Bond lengths**



**Bond angles**

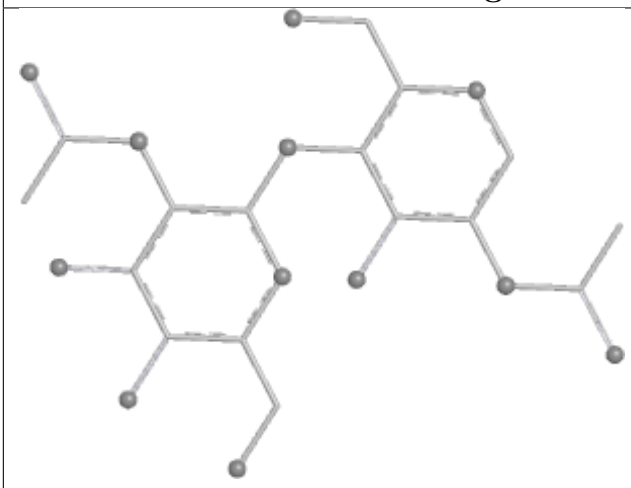


**Torsions**

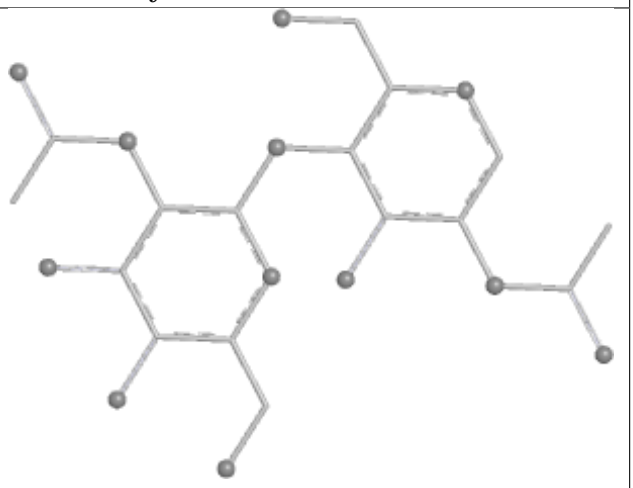


**Rings**

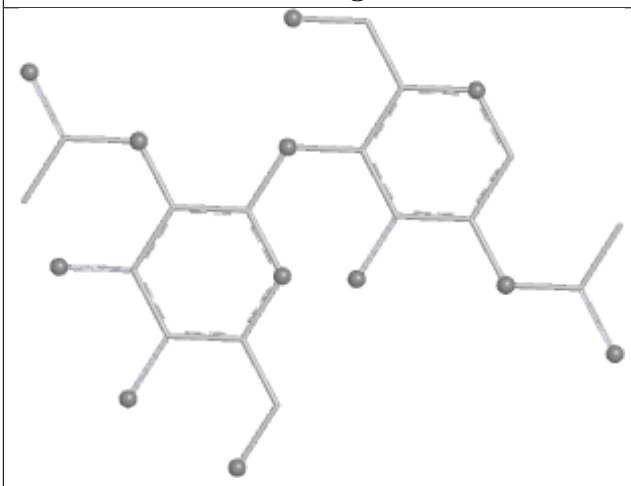
**Oligosaccharide Chain yA**



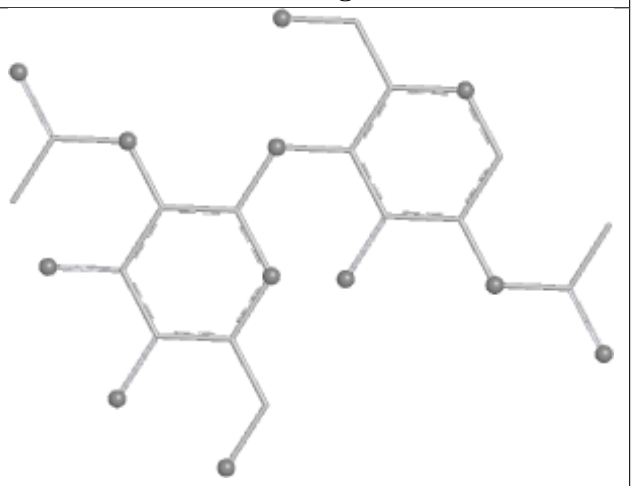
**Bond lengths**



**Bond angles**

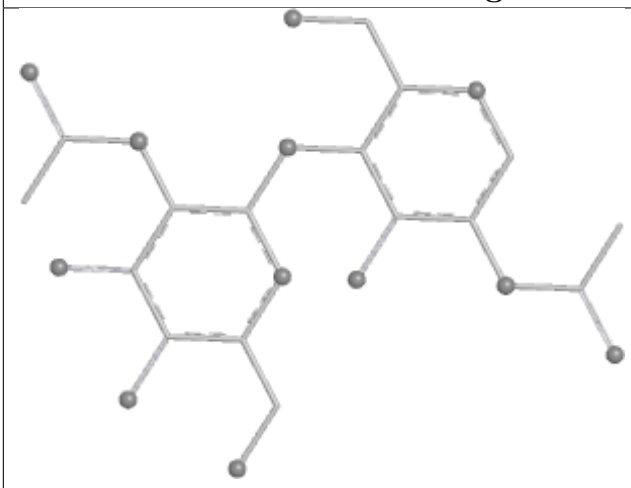


**Torsions**

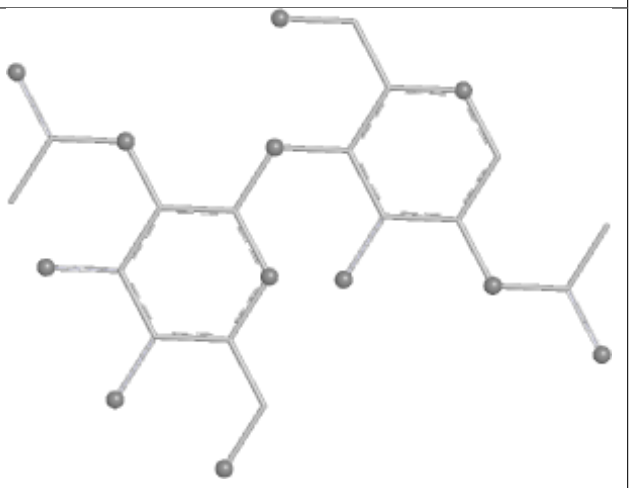


**Rings**

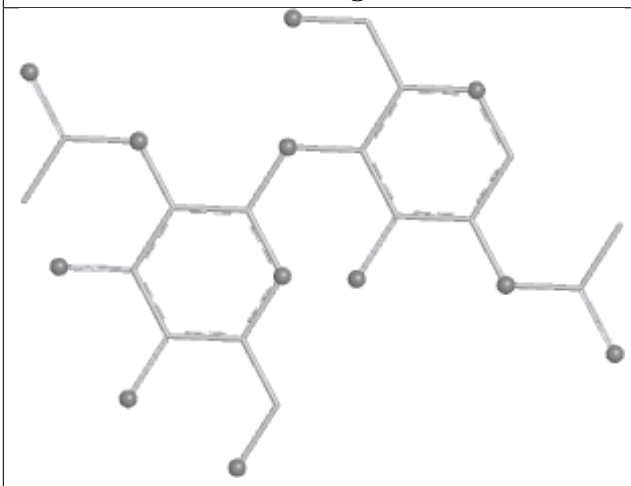
**Oligosaccharide Chain 0A**



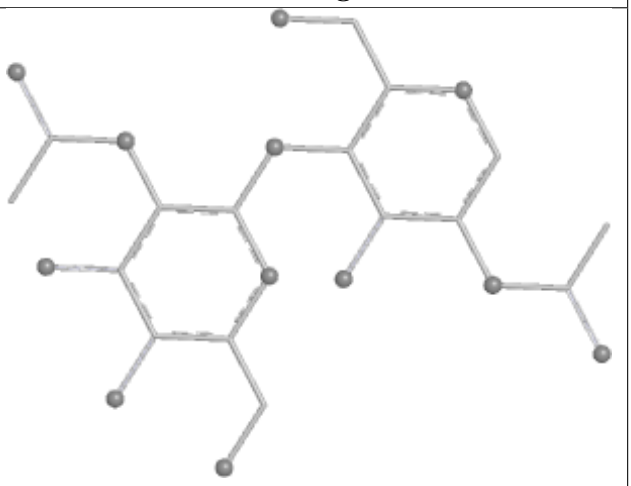
**Bond lengths**



**Bond angles**

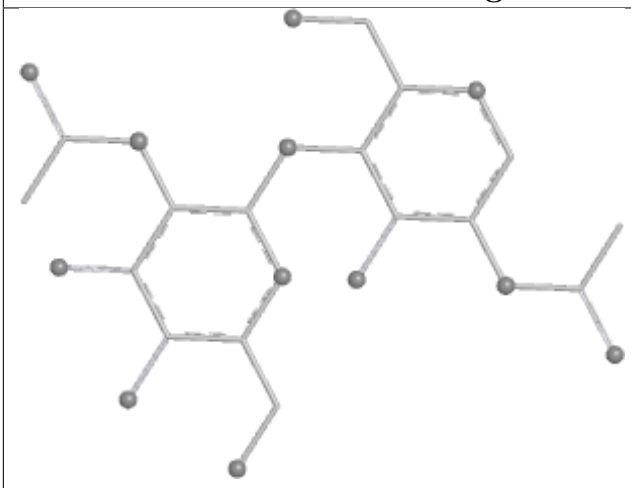


**Torsions**

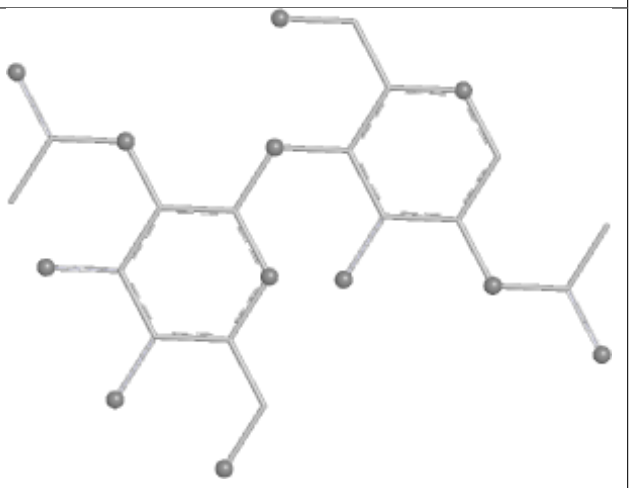


**Rings**

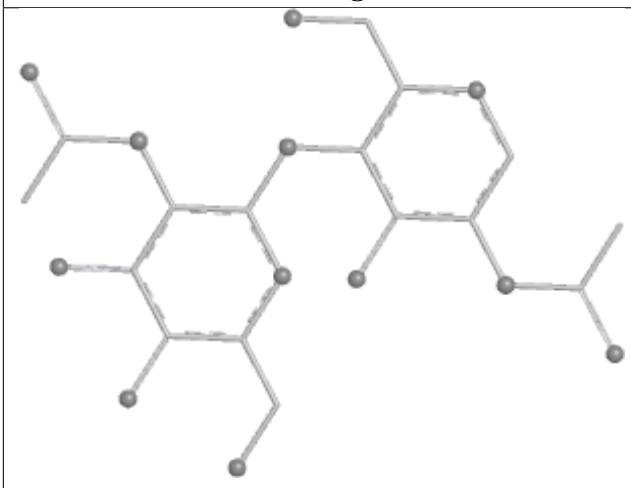
**Oligosaccharide Chain 5A**



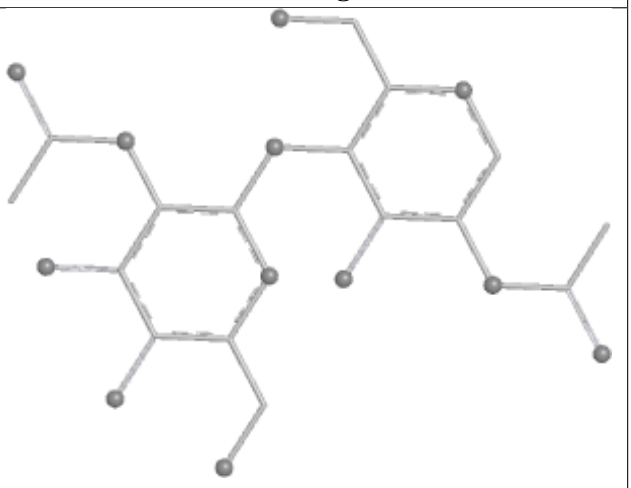
**Bond lengths**



**Bond angles**

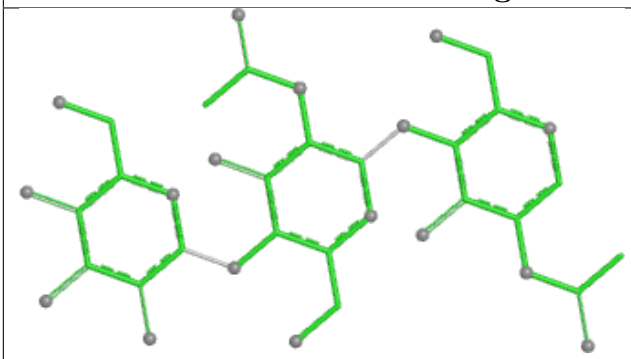


**Torsions**

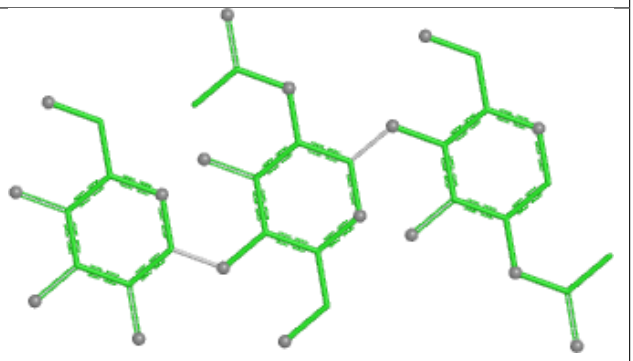


**Rings**

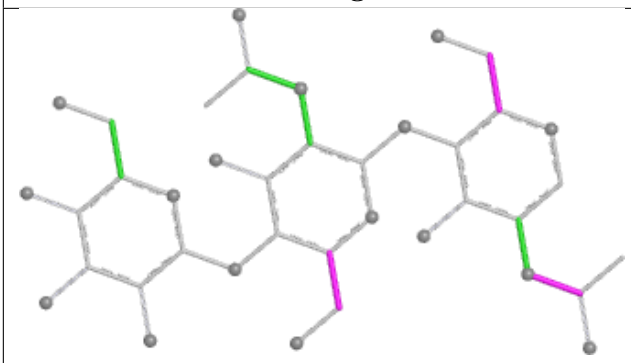
## Oligosaccharide Chain V



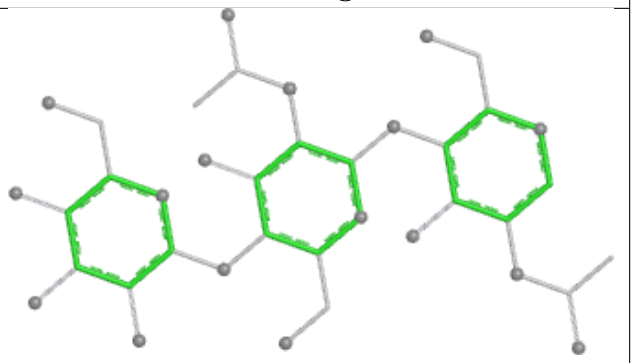
Bond lengths



Bond angles

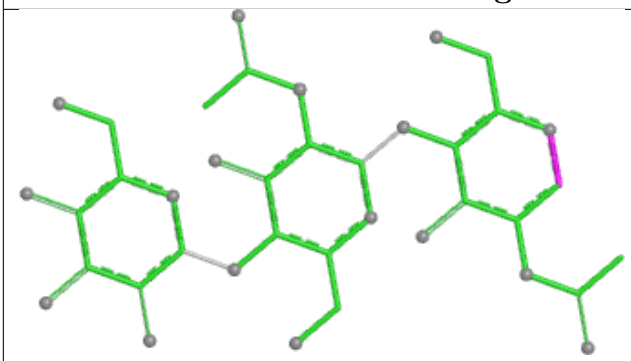


Torsions

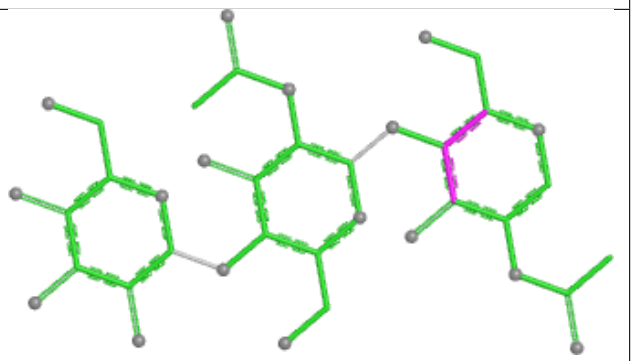


Rings

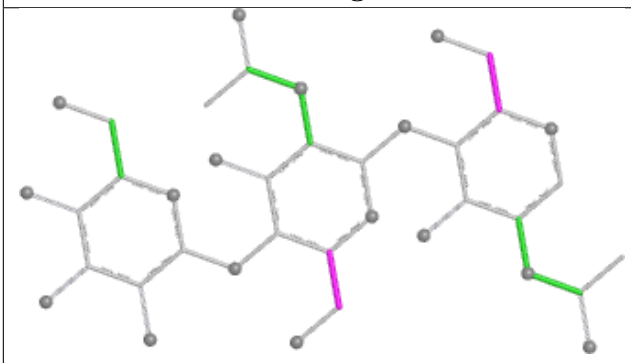
## Oligosaccharide Chain X



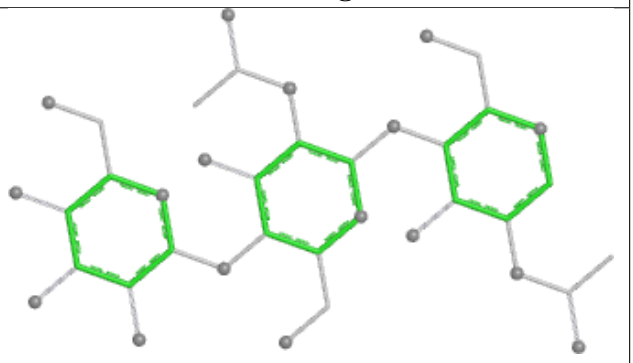
Bond lengths



Bond angles

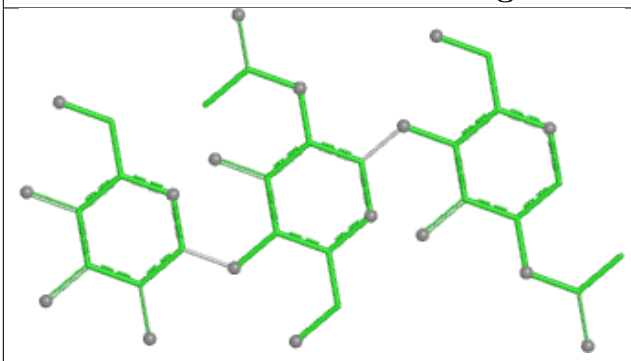


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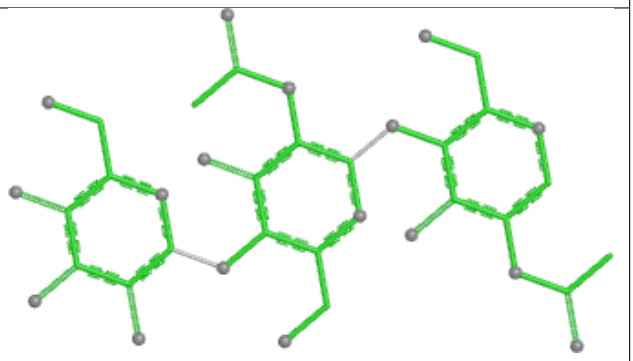


Rings

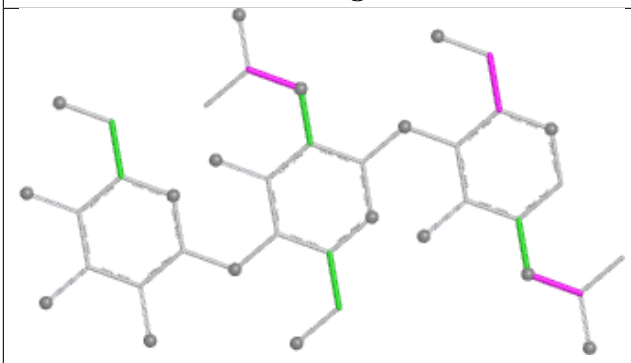
## Oligosaccharide Chain Z



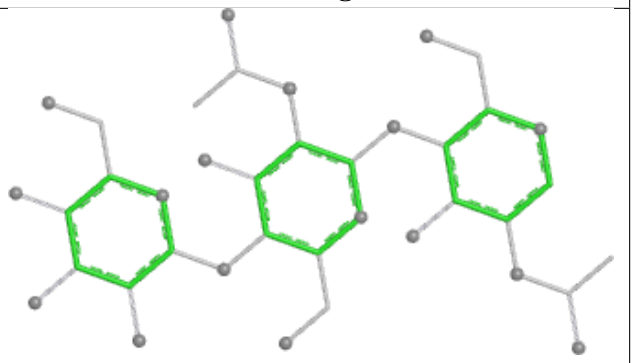
Bond lengths



Bond angles

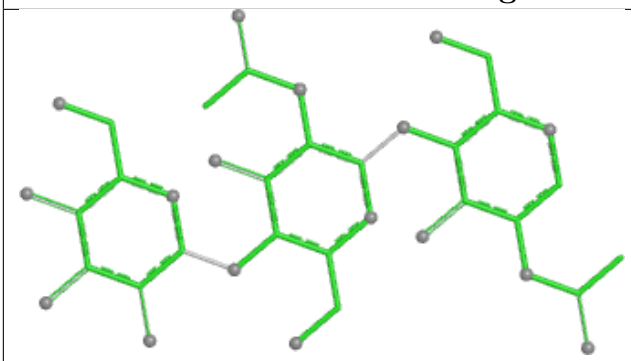


Torsions

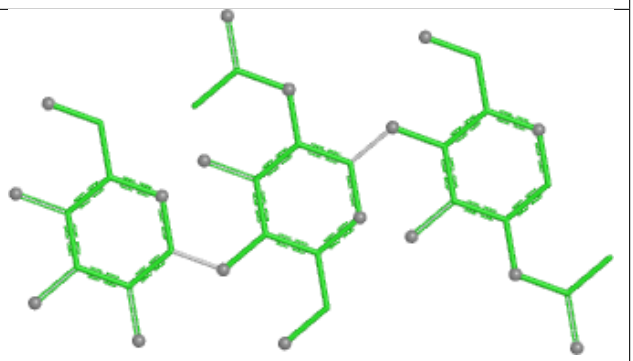


Rings

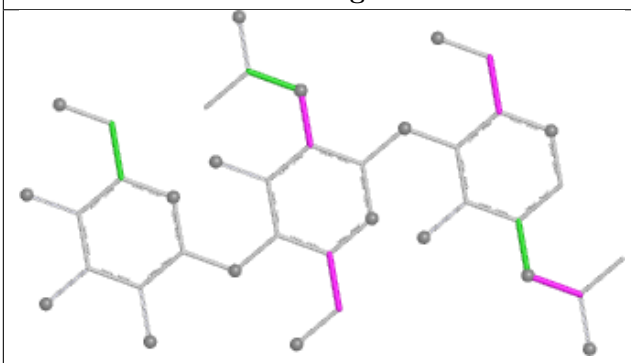
## Oligosaccharide Chain a



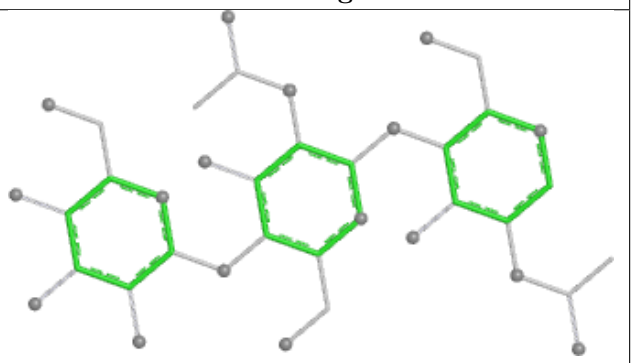
Bond lengths



Bond angles

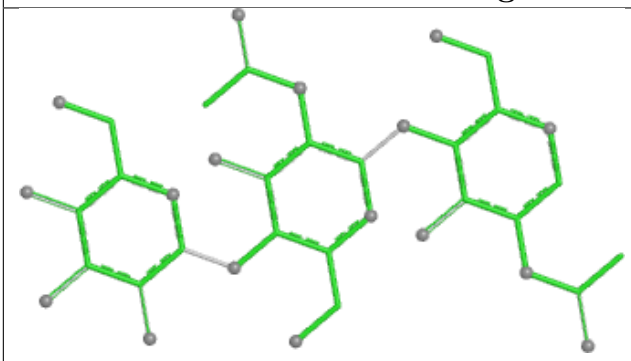


Torsions

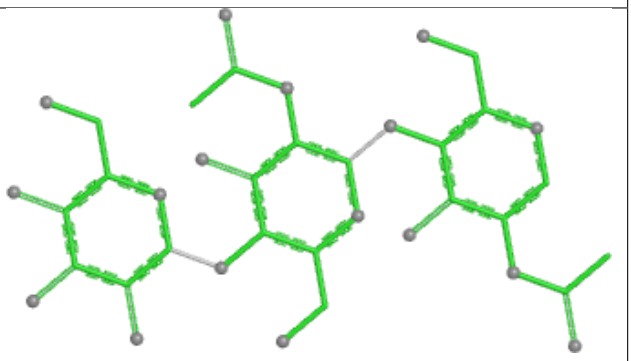


Rings

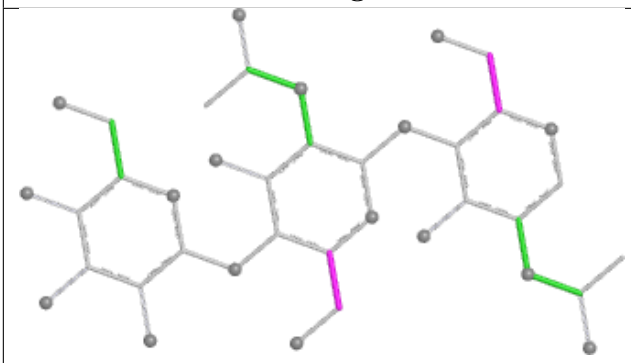
## Oligosaccharide Chain b



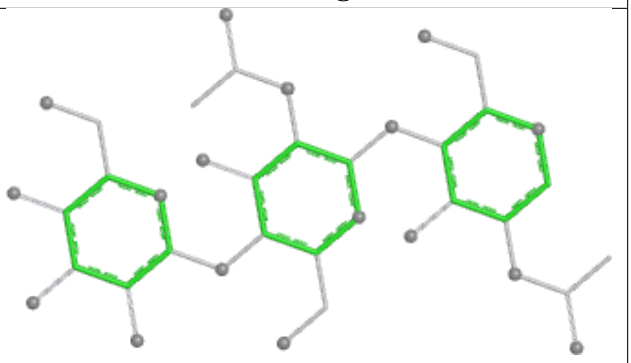
Bond lengths



Bond angles

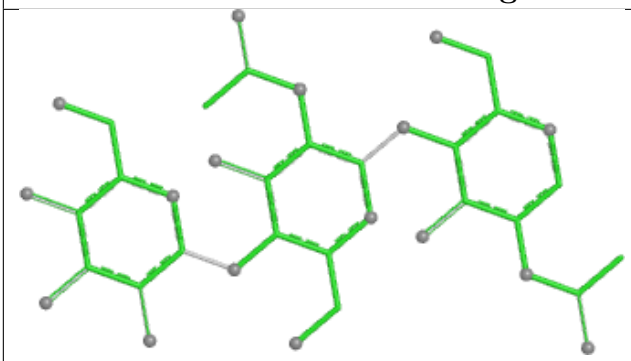


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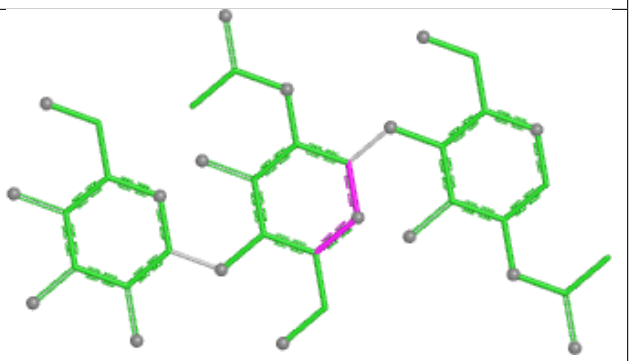


Rings

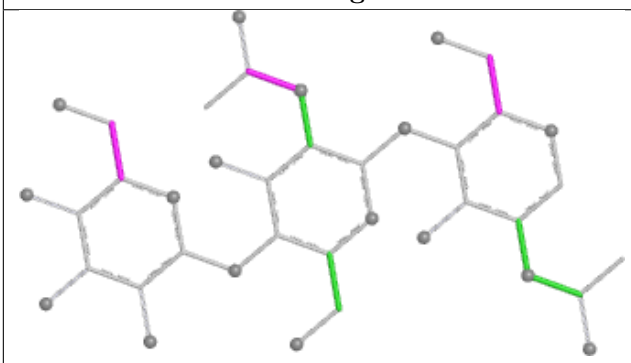
## Oligosaccharide Chain c



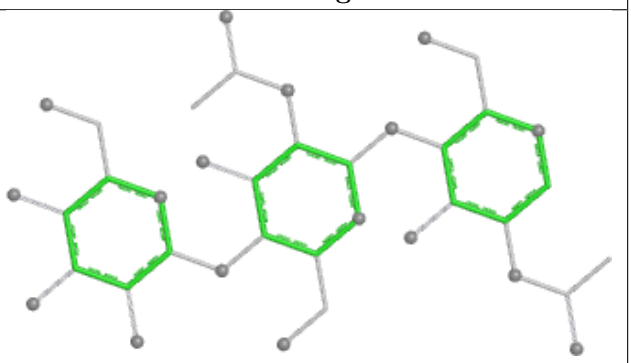
Bond lengths



Bond angles

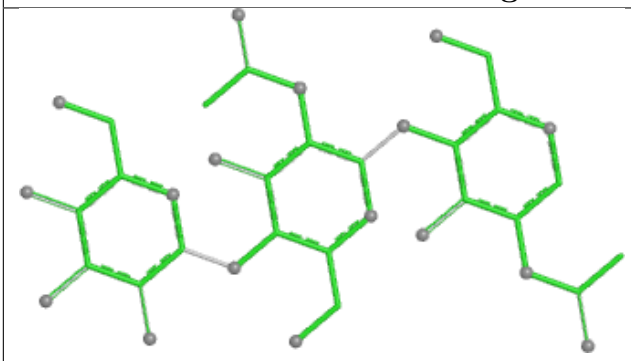


Torsions

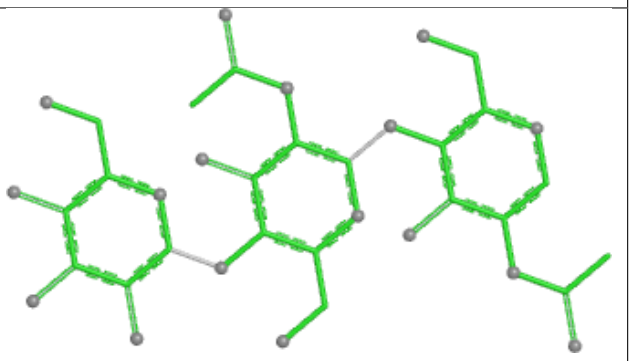


Rings

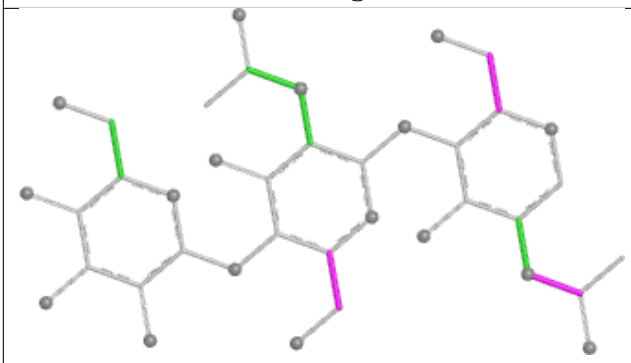
## Oligosaccharide Chain f



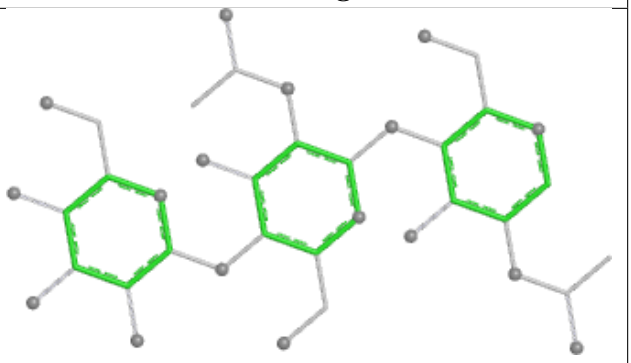
Bond lengths



Bond angles

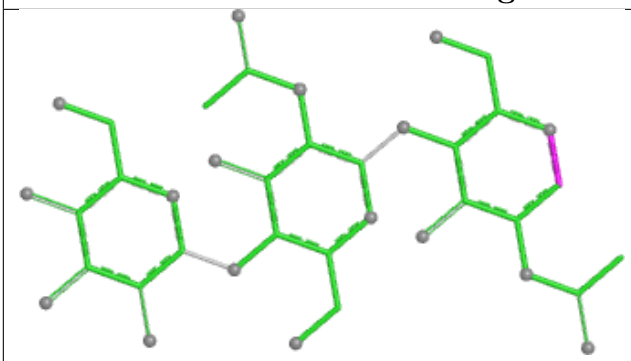


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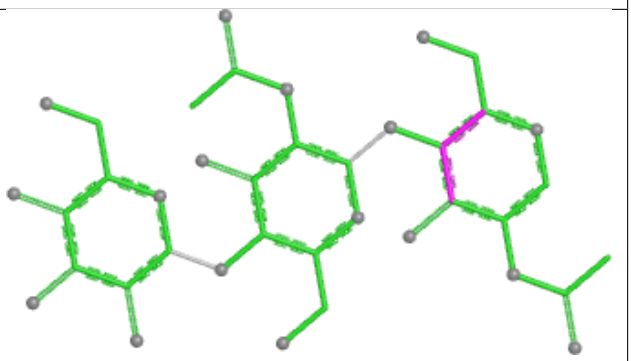


Rings

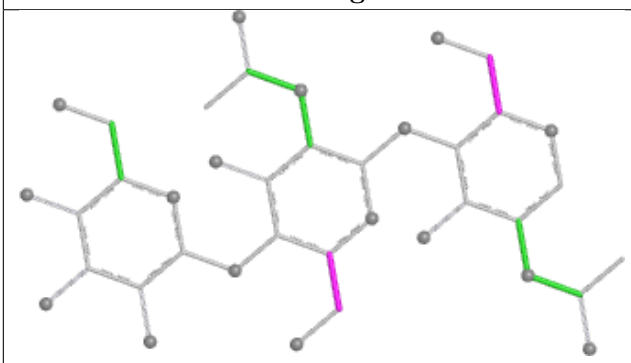
## Oligosaccharide Chain h



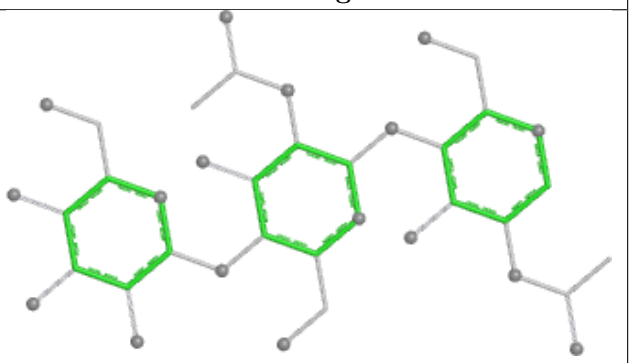
Bond lengths



Bond angles

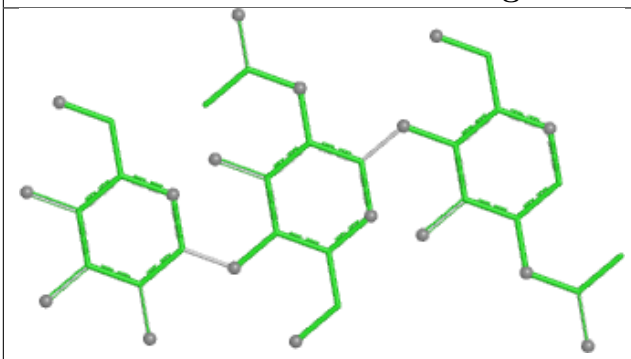


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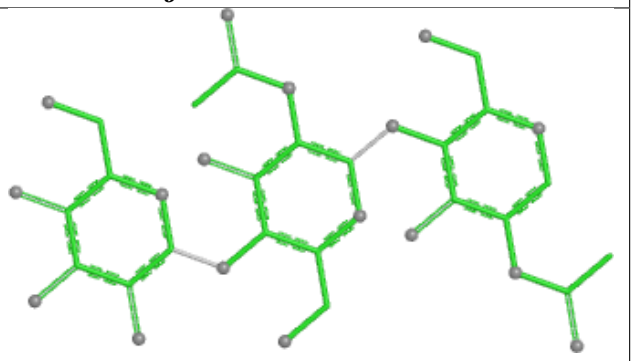


Rings

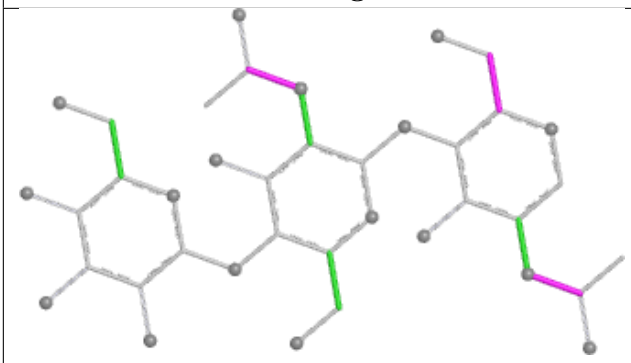
## Oligosaccharide Chain j



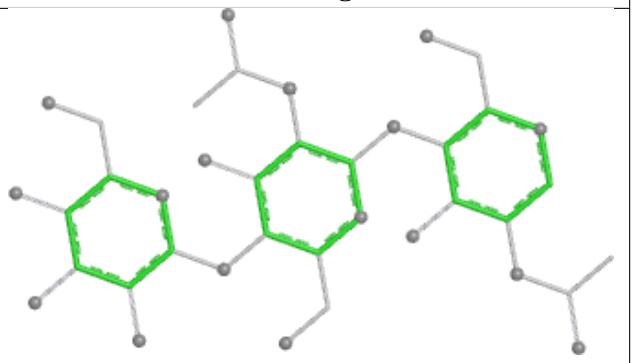
Bond lengths



Bond angles

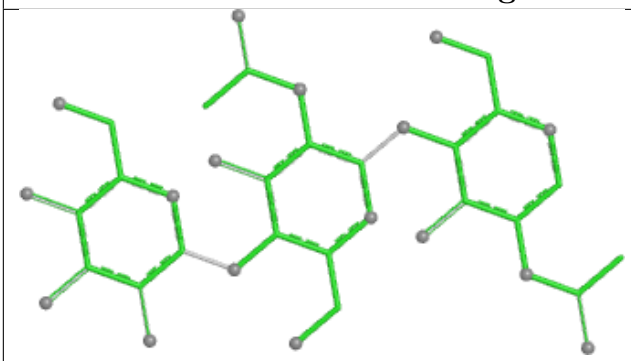


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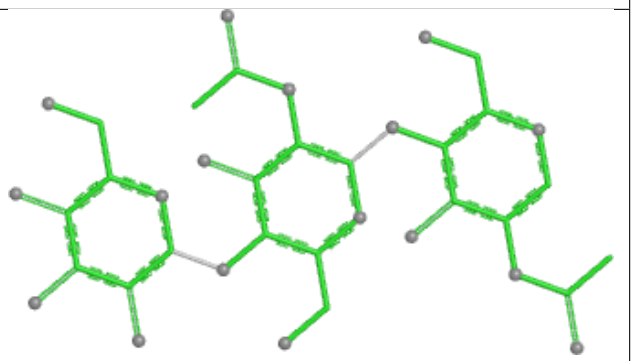


Rings

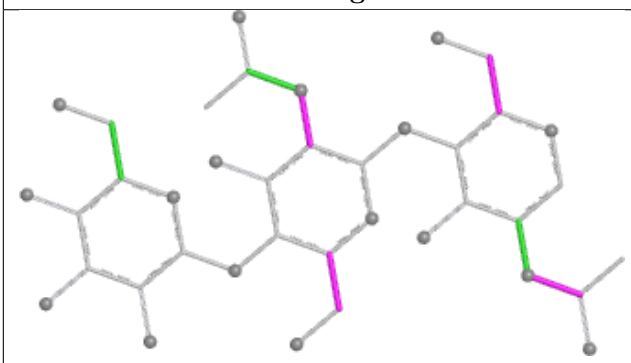
## Oligosaccharide Chain k



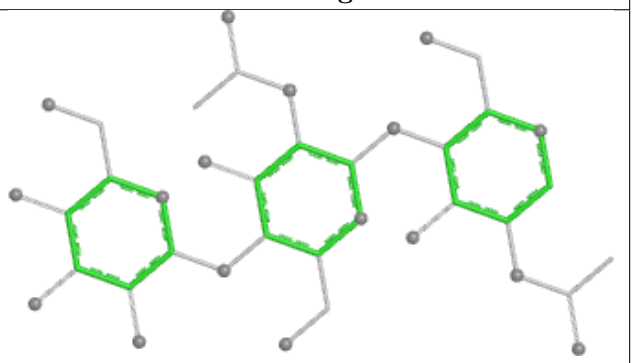
Bond lengths



Bond angles

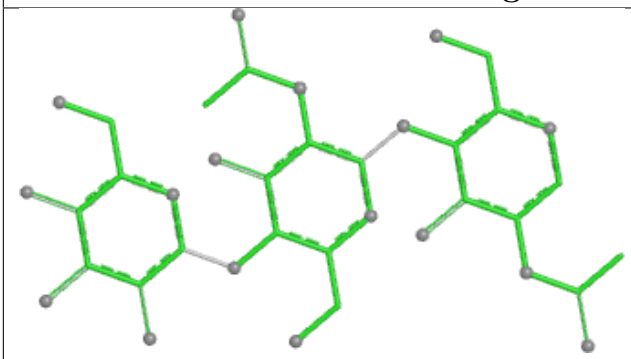


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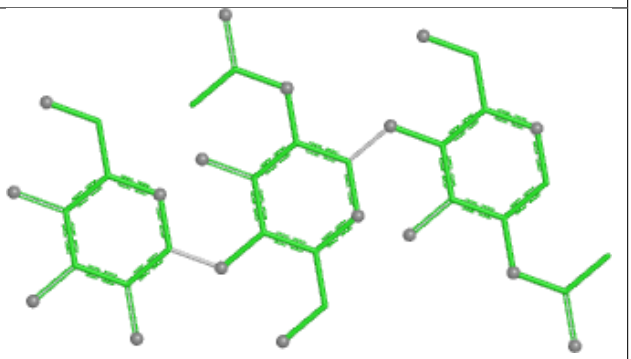


Rings

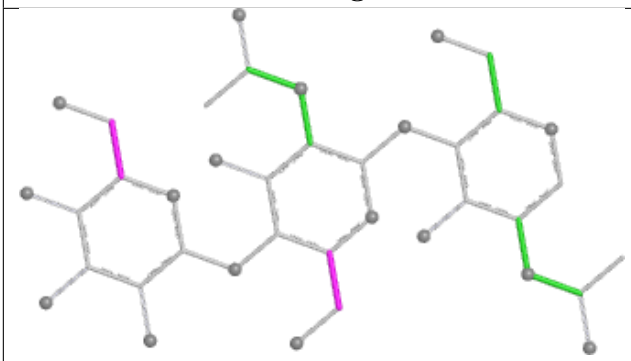
## Oligosaccharide Chain l



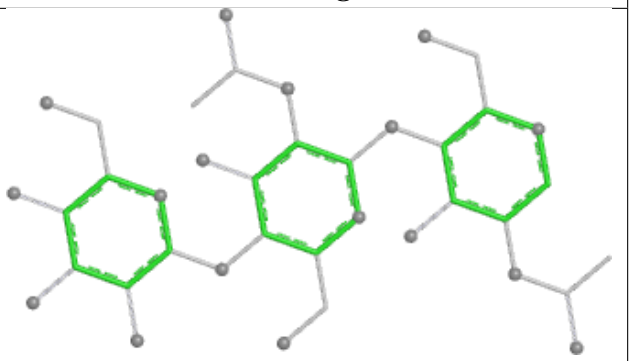
Bond lengths



Bond angles

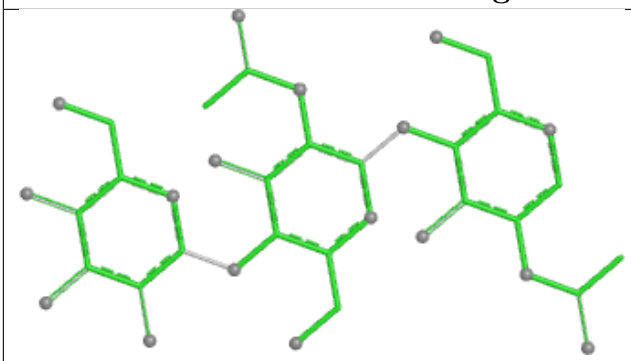


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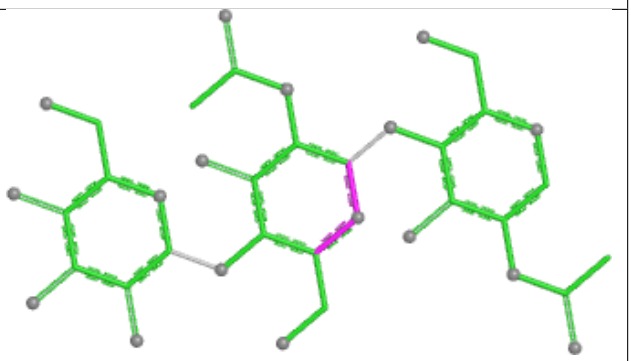


Rings

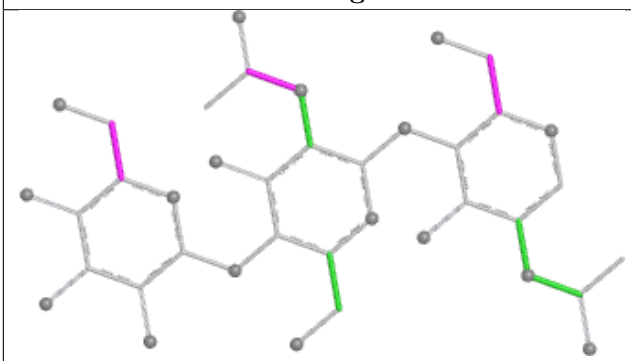
## Oligosaccharide Chain m



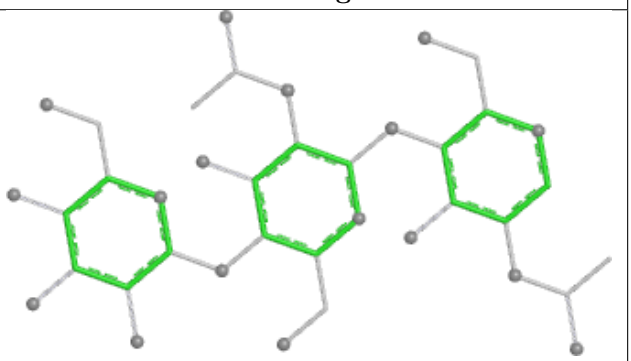
Bond lengths



Bond angles

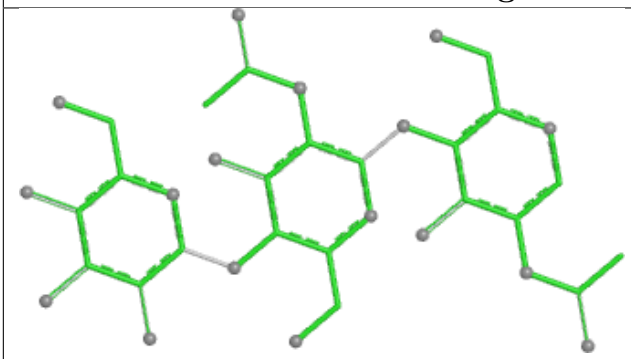


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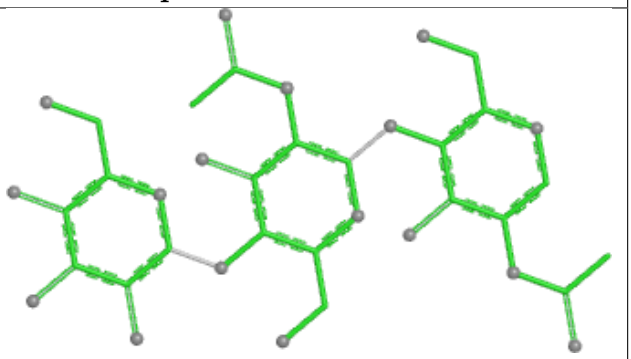


Rings

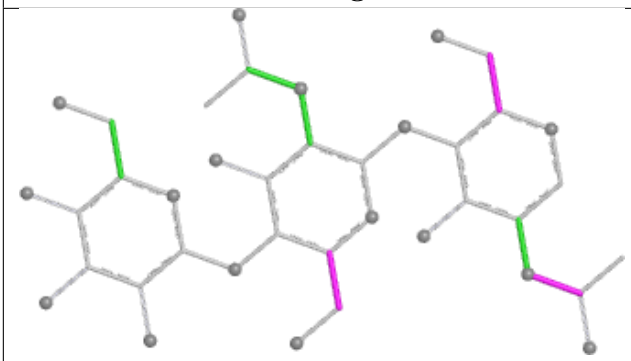
## Oligosaccharide Chain p



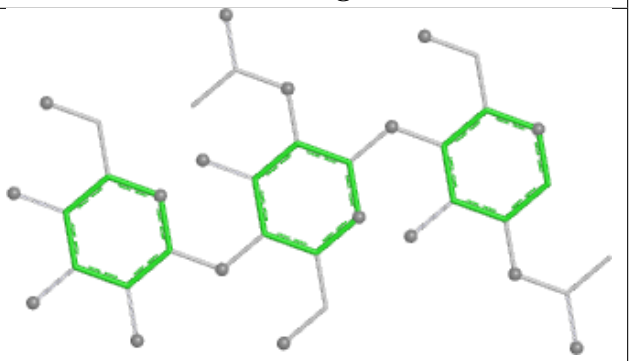
Bond lengths



Bond angles

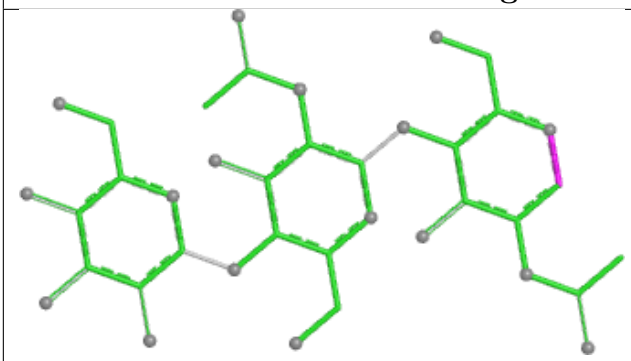


Torsions

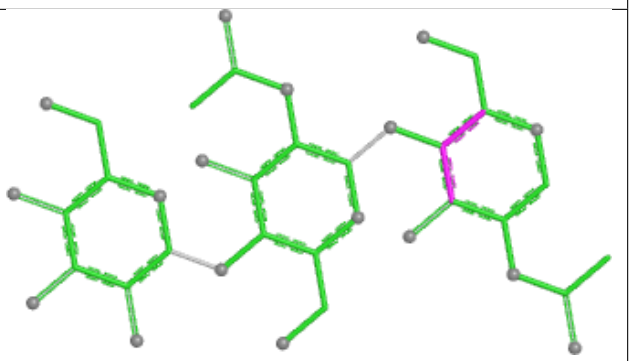


Rings

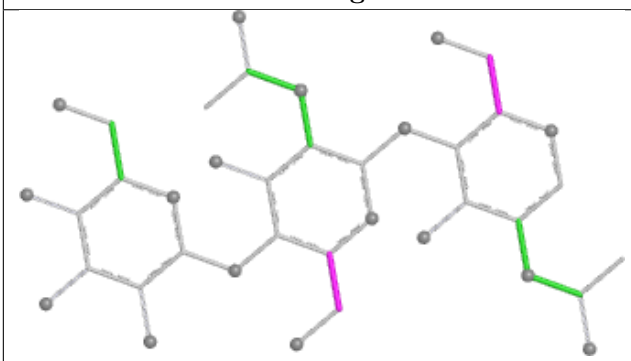
## Oligosaccharide Chain r



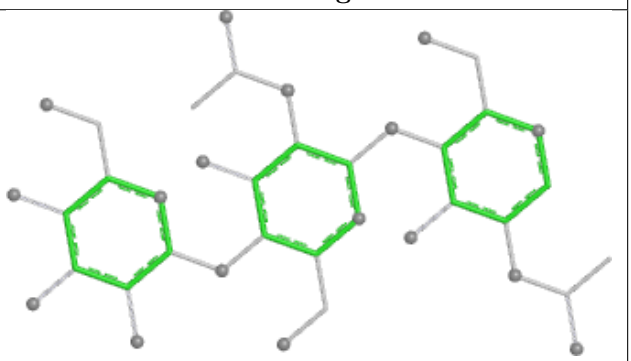
Bond lengths



Bond angles

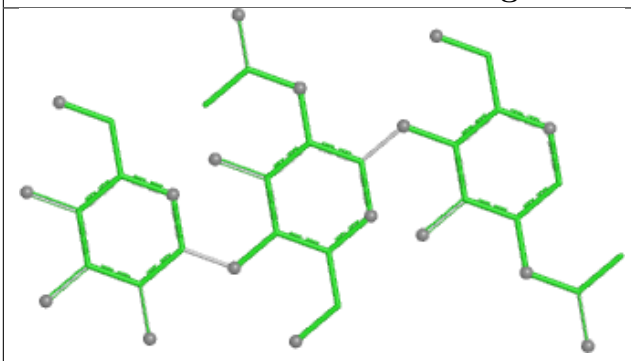


Torsions

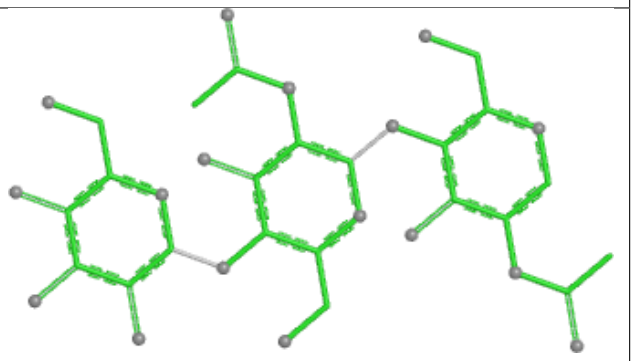


Rings

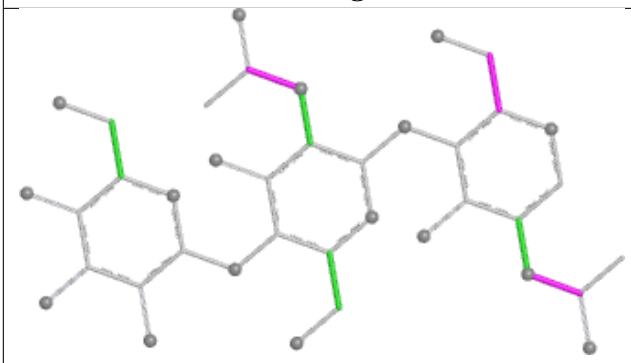
## Oligosaccharide Chain t



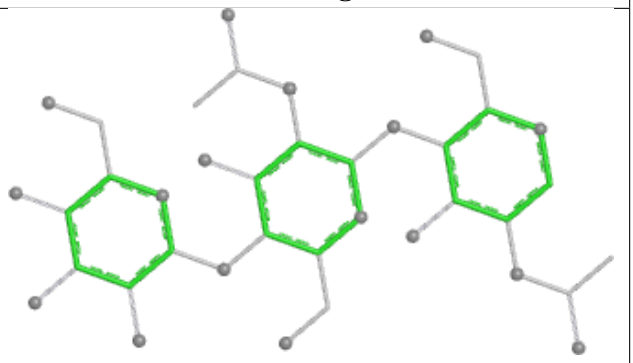
Bond lengths



Bond angles

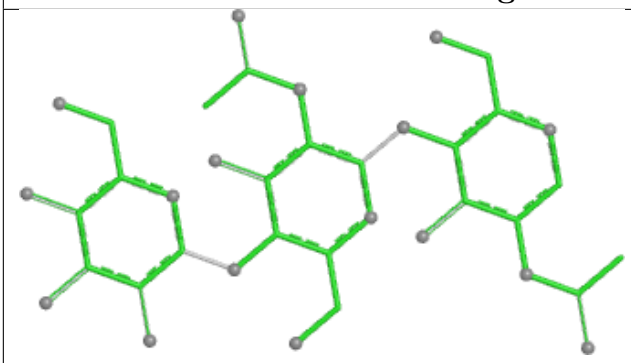


Torsions

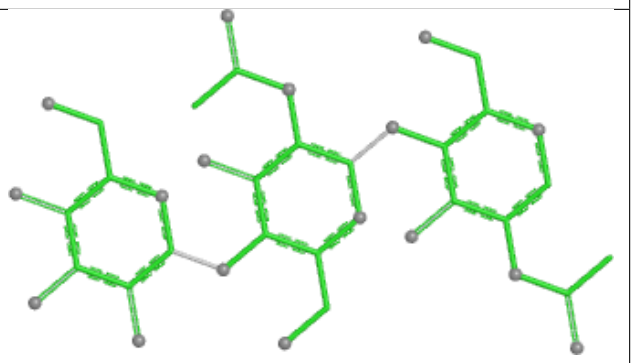


Rings

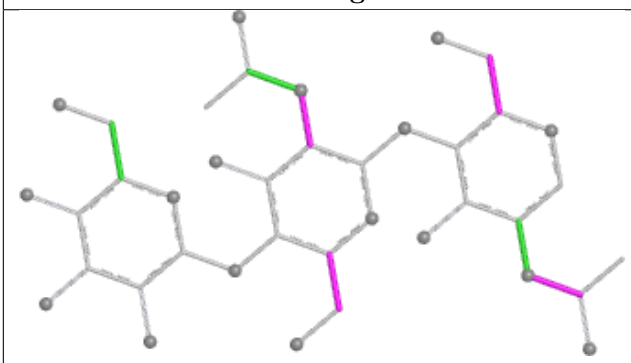
## Oligosaccharide Chain u



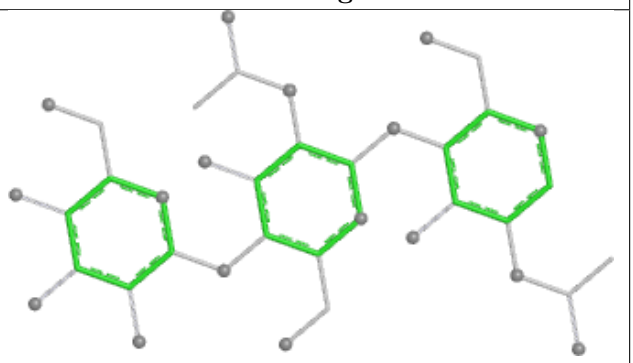
Bond lengths



Bond angles

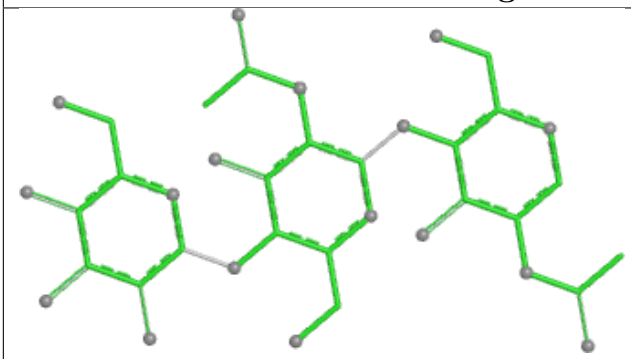


Torsions

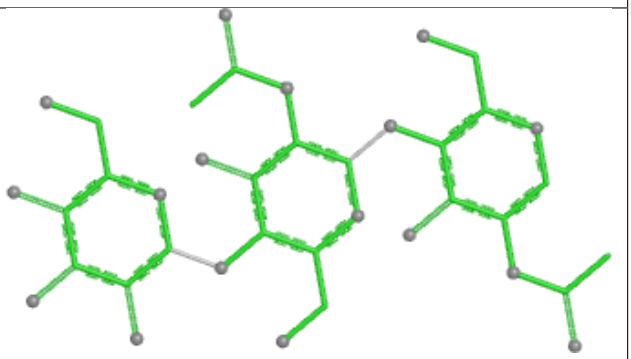


Rings

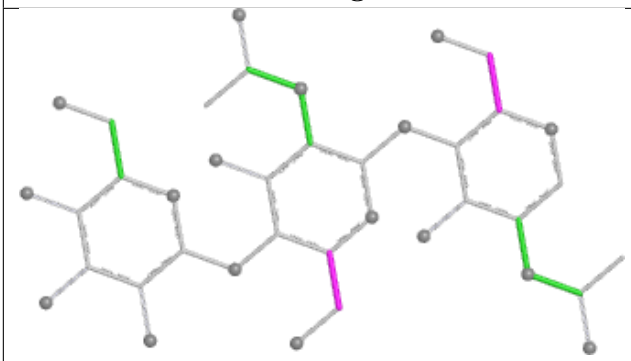
## Oligosaccharide Chain v



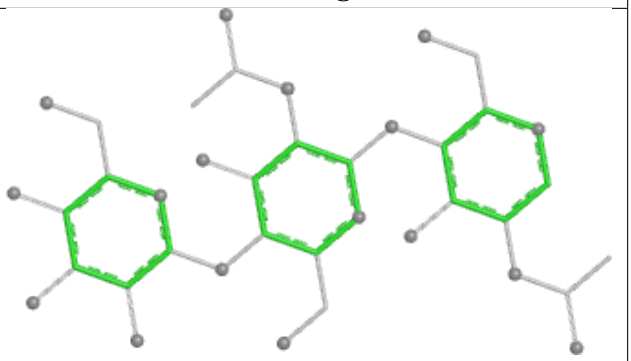
Bond lengths



Bond angles

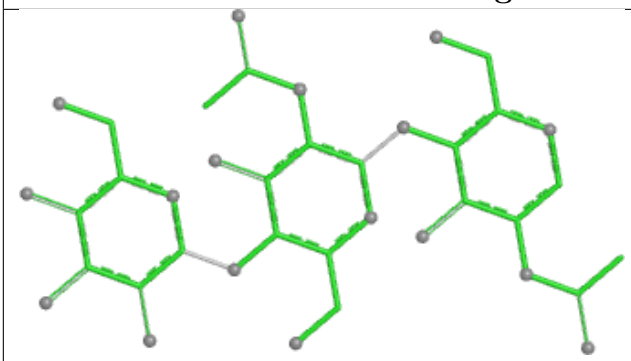


Torsions

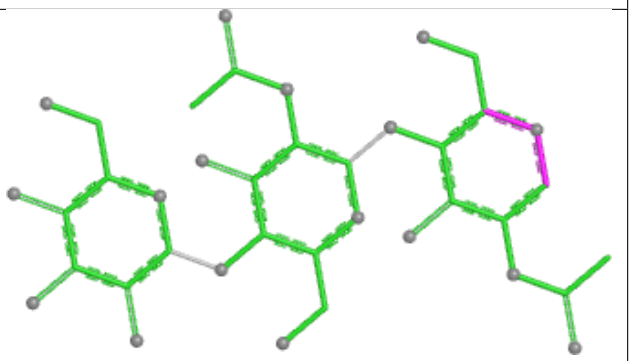


Rings

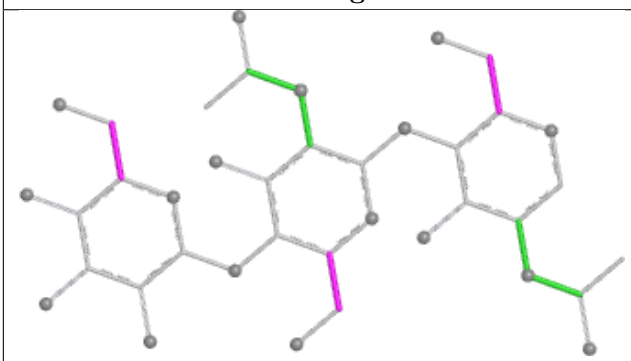
## Oligosaccharide Chain w



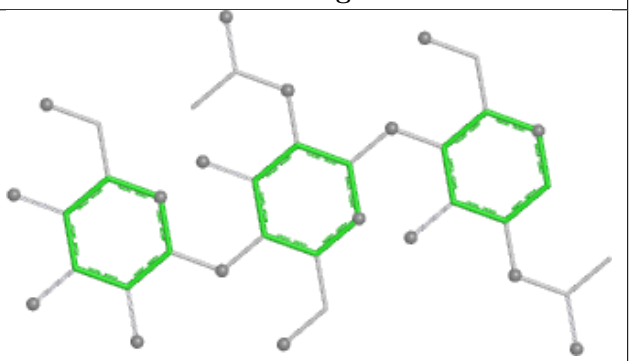
Bond lengths



Bond angles

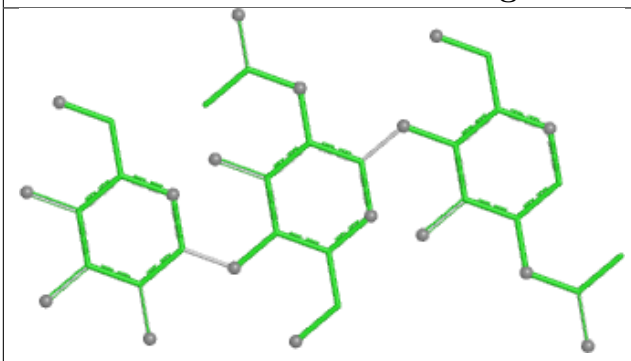


Torsions

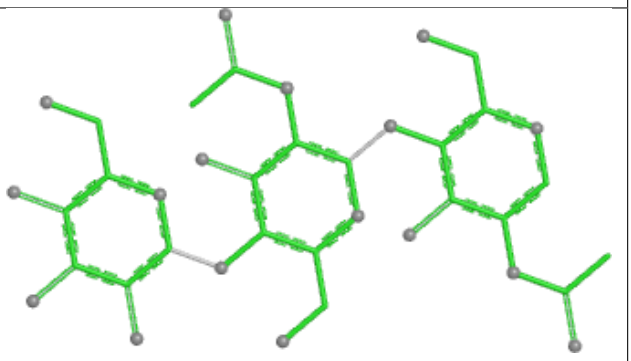


Rings

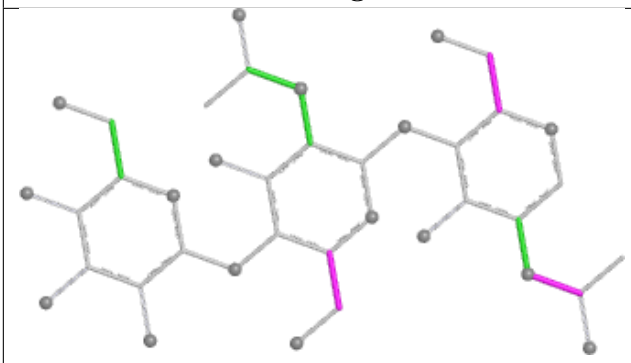
## Oligosaccharide Chain z



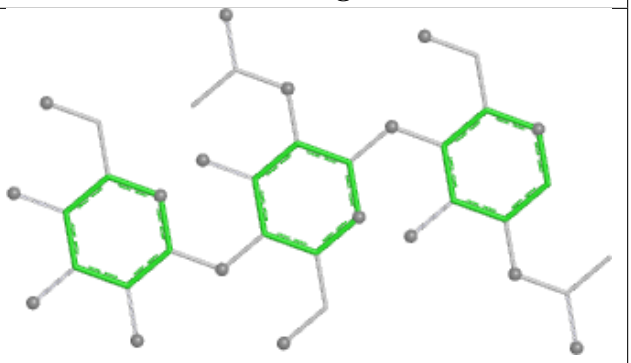
Bond lengths



Bond angles

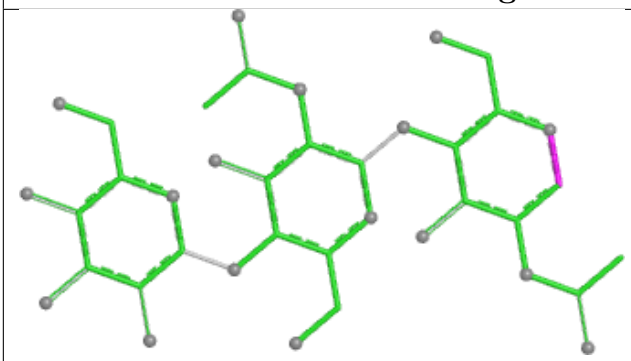


Torsions

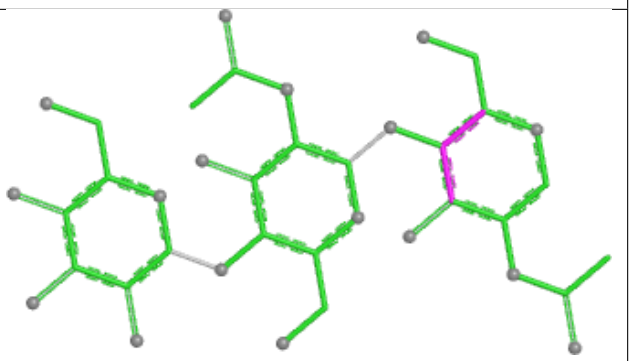


Rings

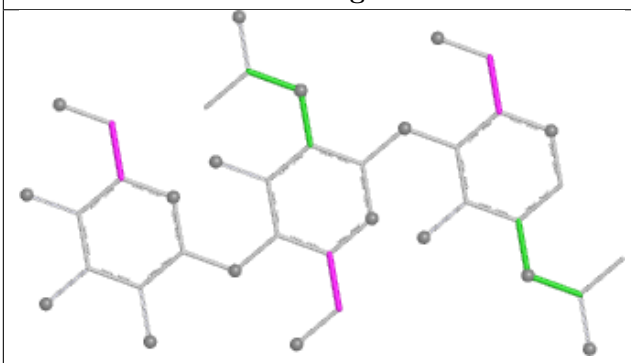
## Oligosaccharide Chain 1



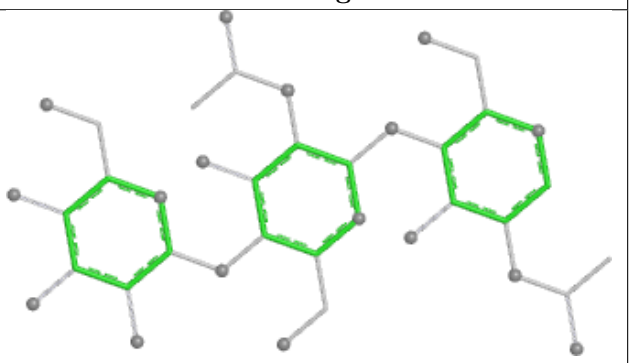
Bond lengths



Bond angles

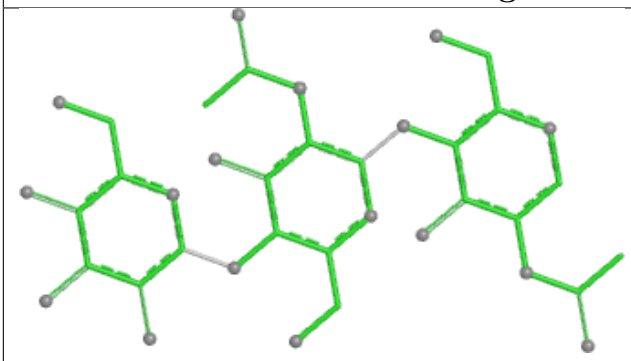


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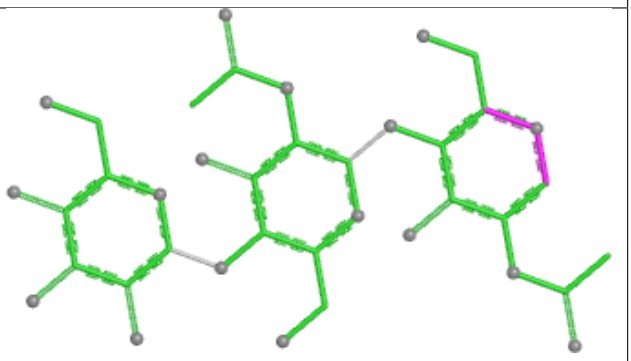


Rings

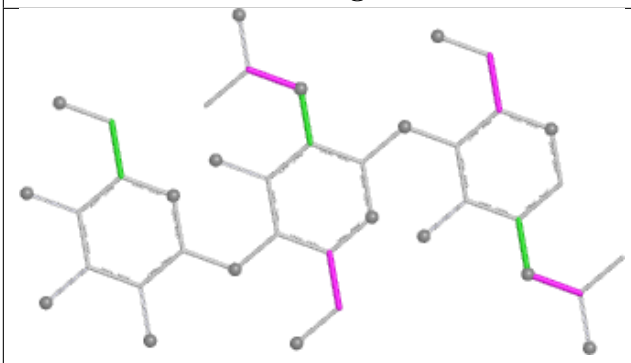
## Oligosaccharide Chain 3



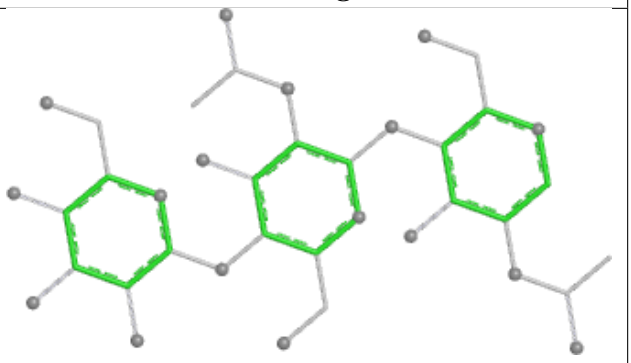
Bond lengths



Bond angles

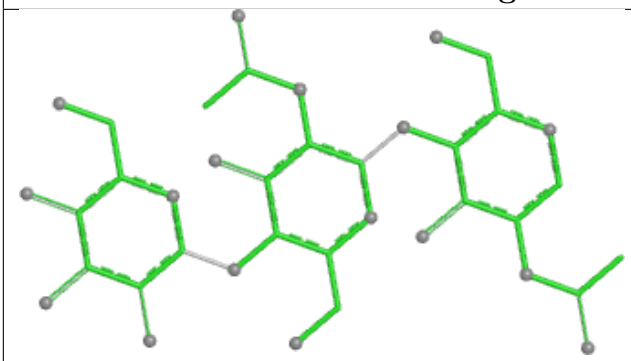


Torsions

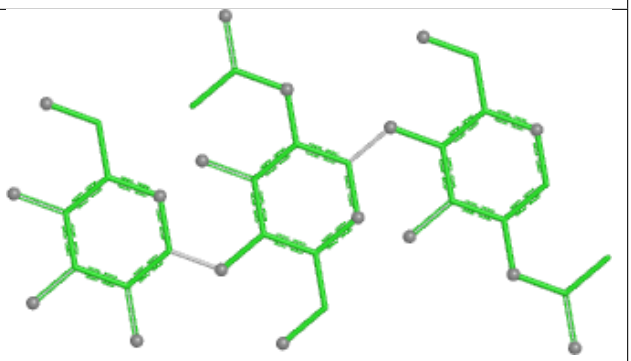


Rings

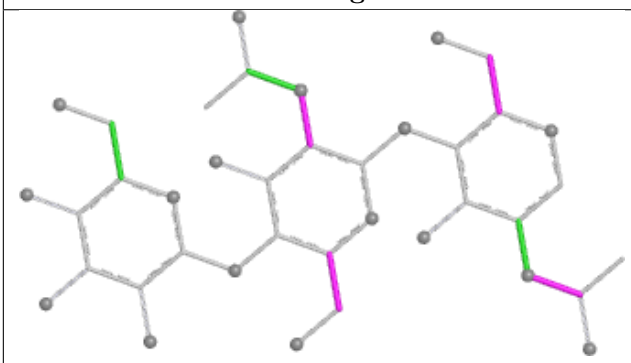
## Oligosaccharide Chain 4



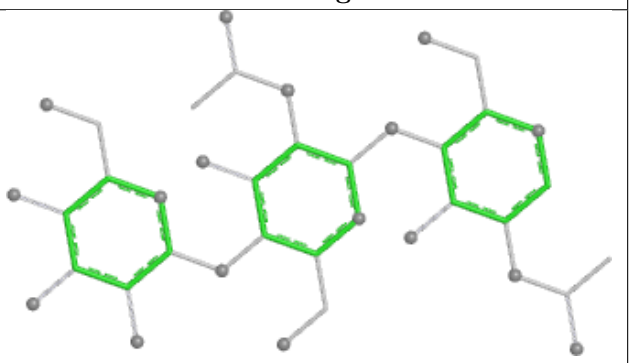
Bond lengths



Bond angles

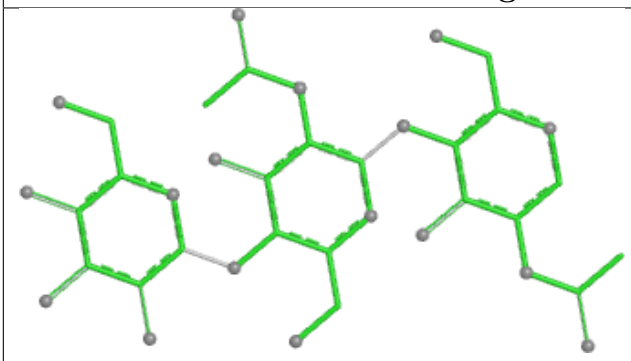


Torsions

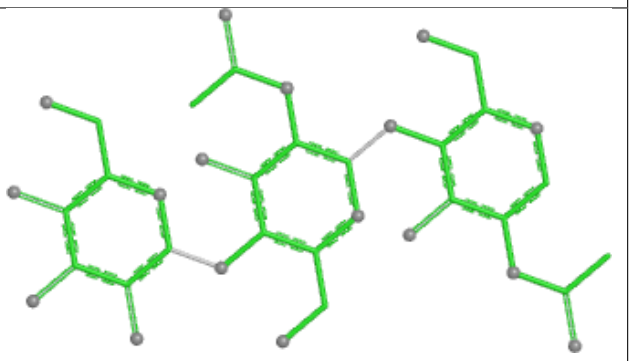


Rings

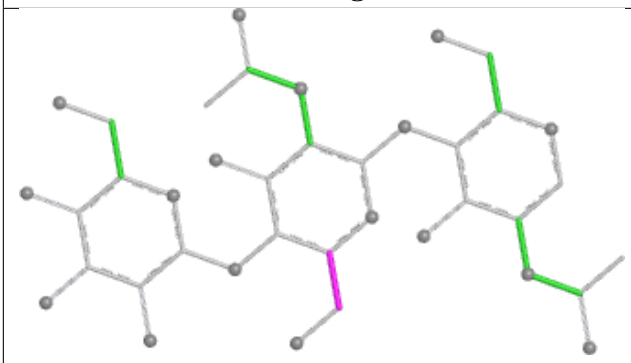
## Oligosaccharide Chain 5



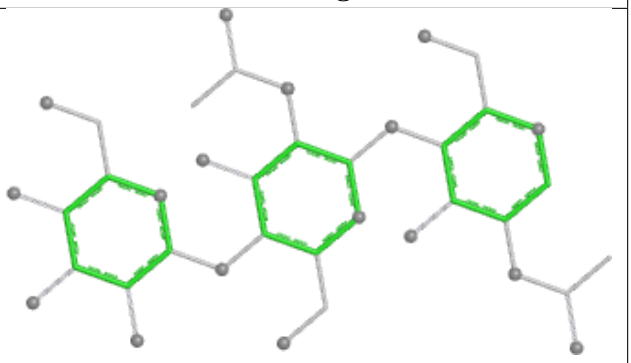
Bond lengths



Bond angles

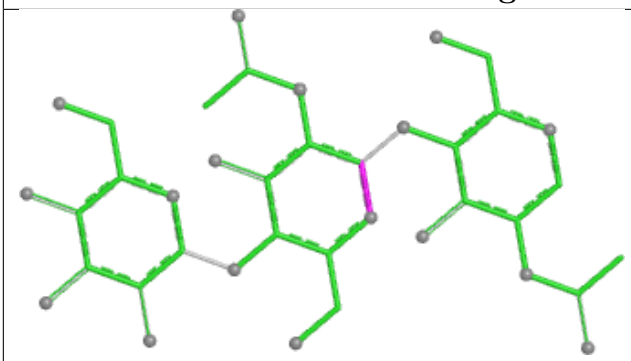


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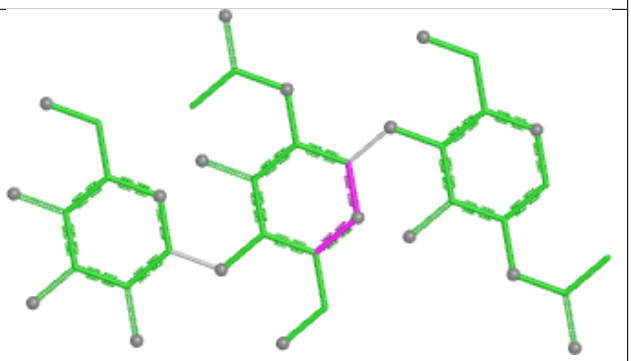


Rings

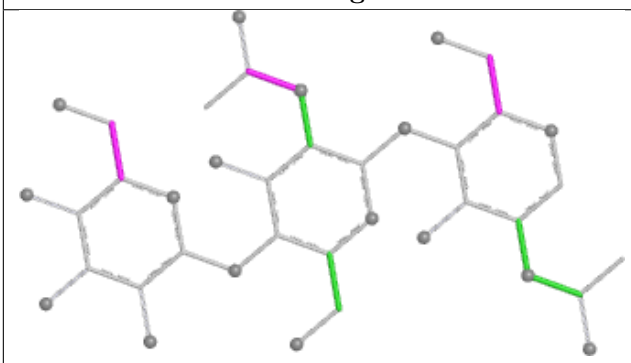
## Oligosaccharide Chain 6



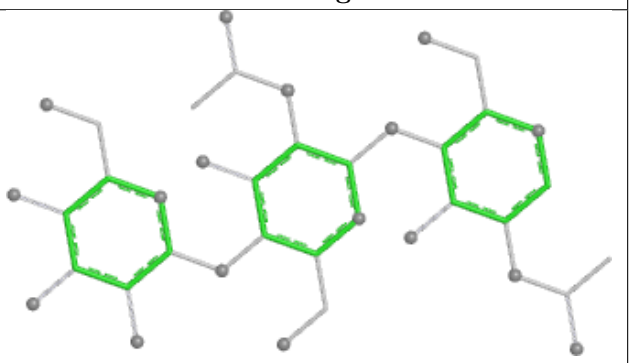
Bond lengths



Bond angles

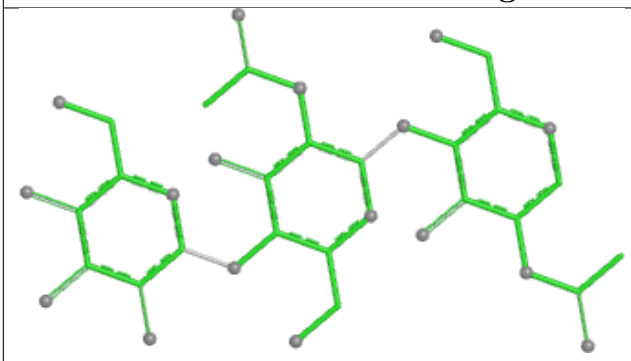


Torsions

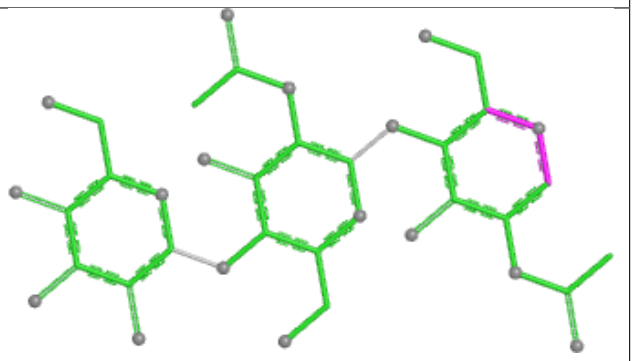


Rings

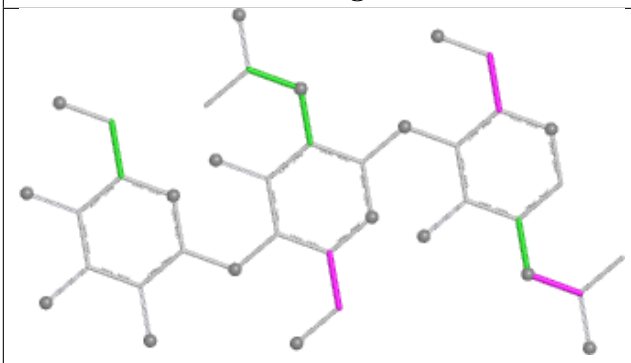
## Oligosaccharide Chain 9



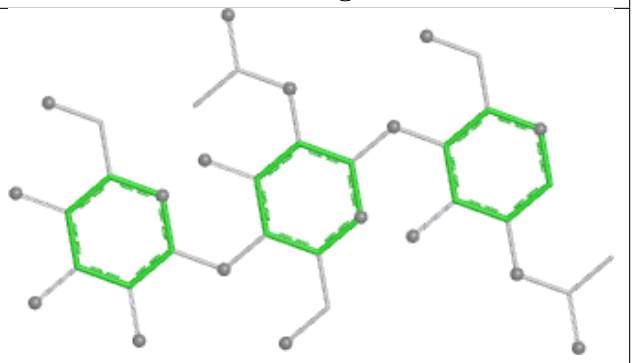
Bond lengths



Bond angles

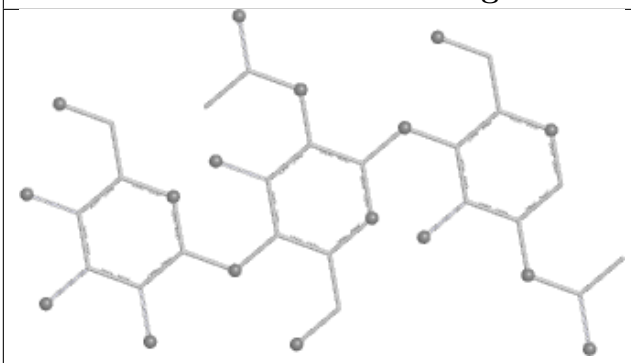


Torsions

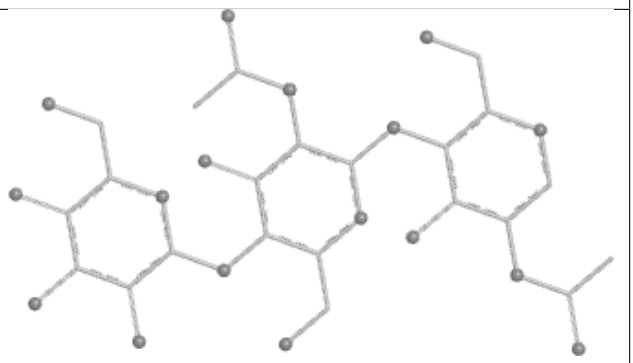


Rings

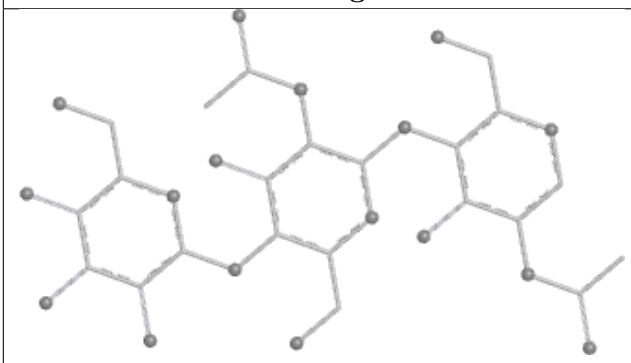
## Oligosaccharide Chain BA



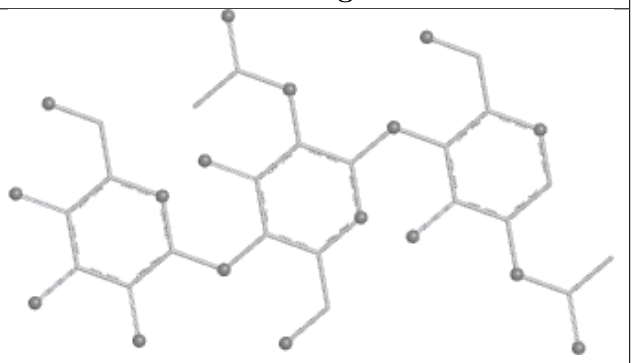
Bond lengths



Bond angles

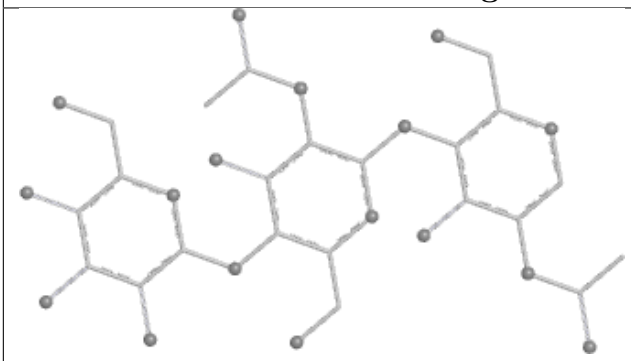


Torsions

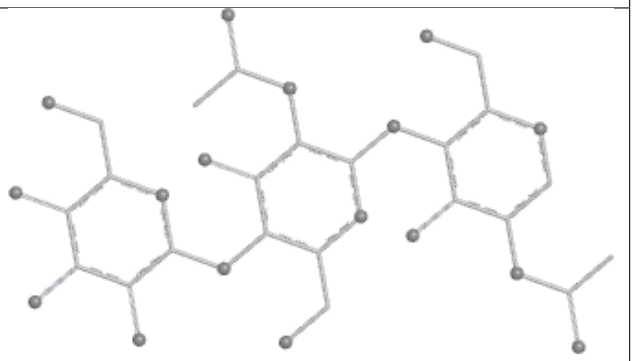


Rings

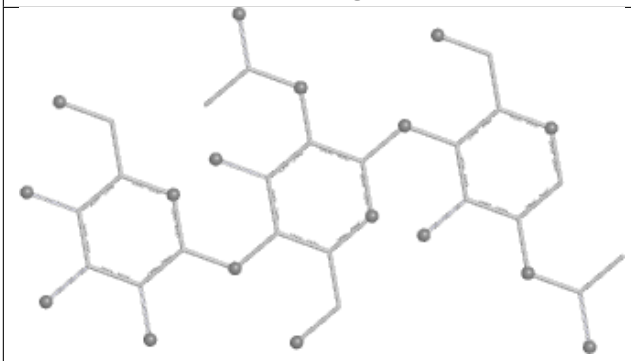
## Oligosaccharide Chain DA



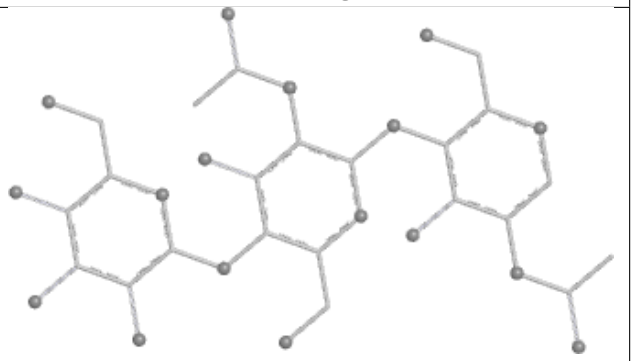
Bond lengths



Bond angles

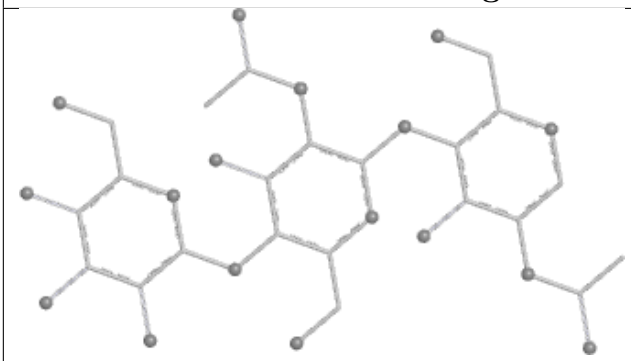


Torsions

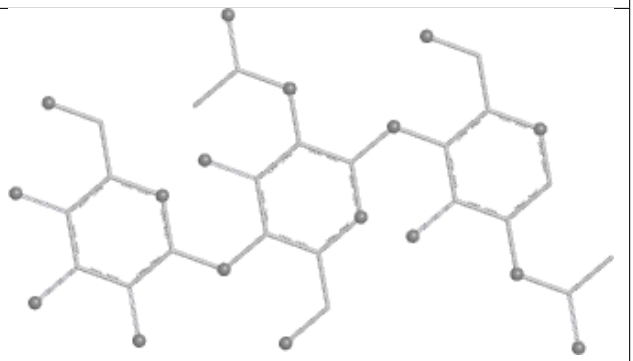


Rings

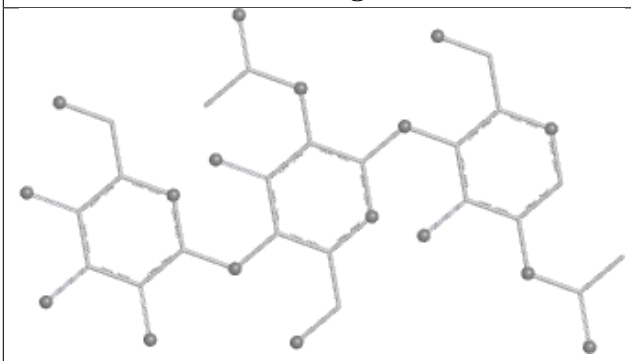
## Oligosaccharide Chain EA



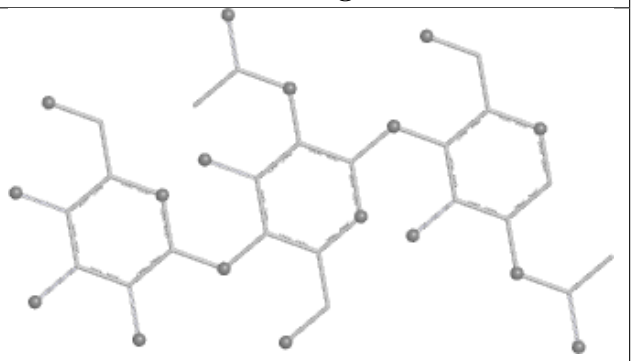
Bond lengths



Bond angles

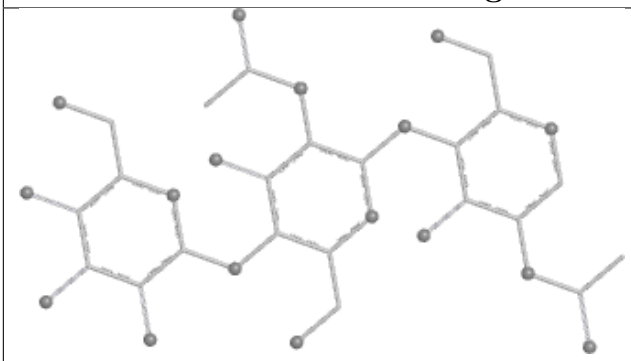


Torsions

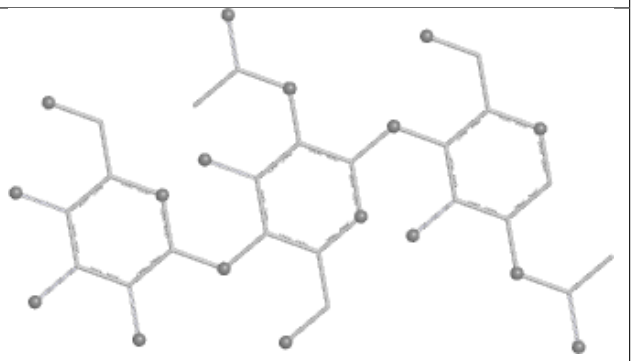


Rings

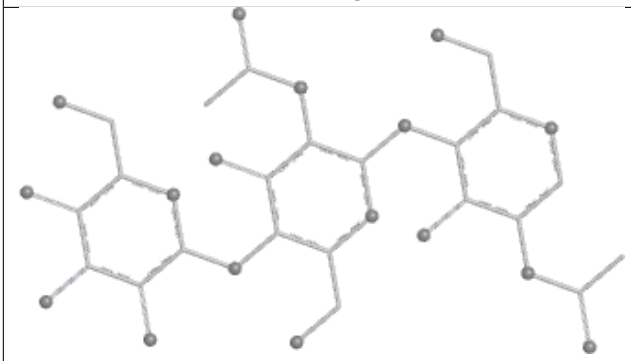
## Oligosaccharide Chain FA



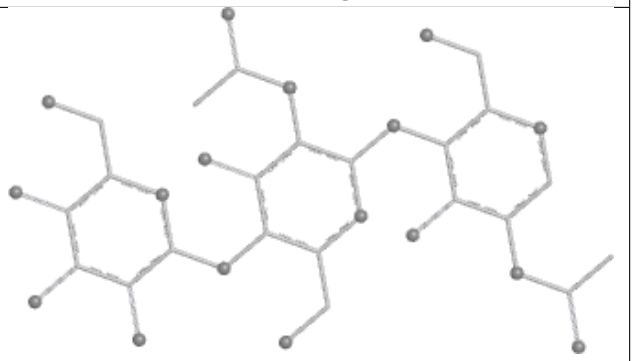
Bond lengths



Bond angles

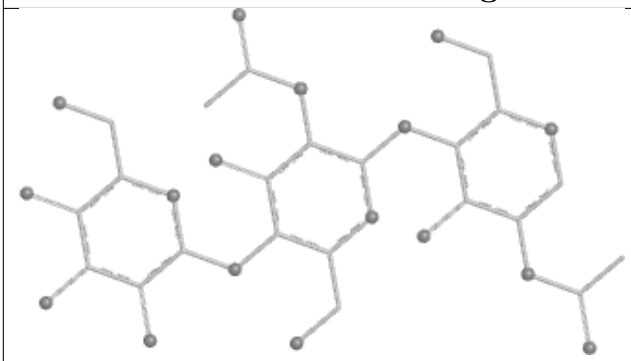


Torsions

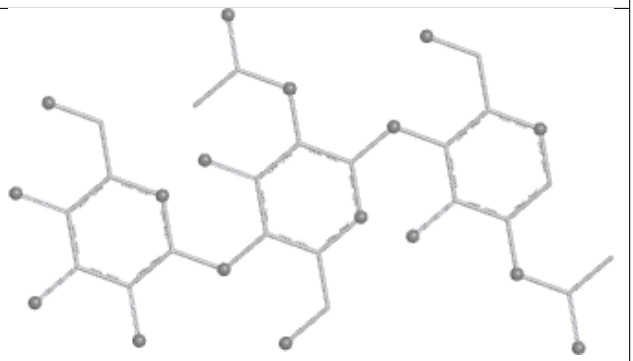


Rings

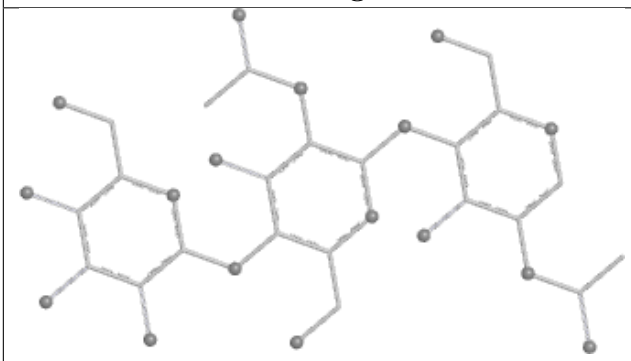
## Oligosaccharide Chain GA



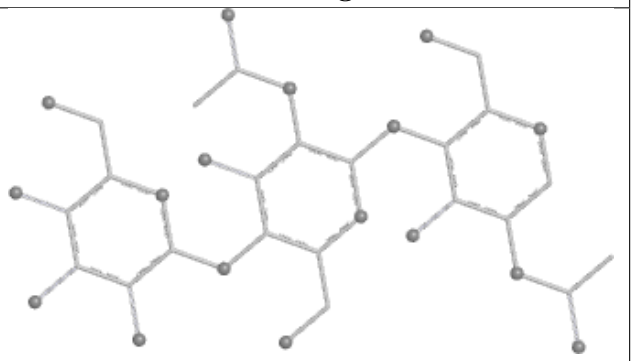
Bond lengths



Bond angles

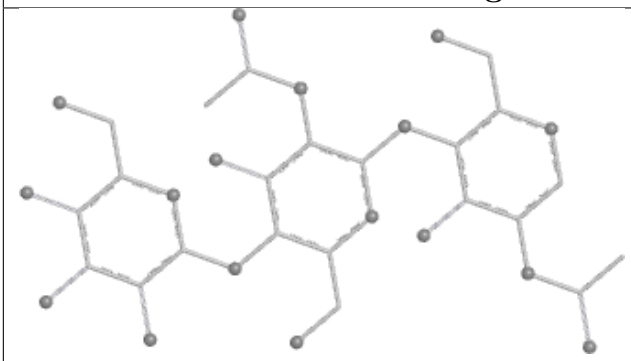


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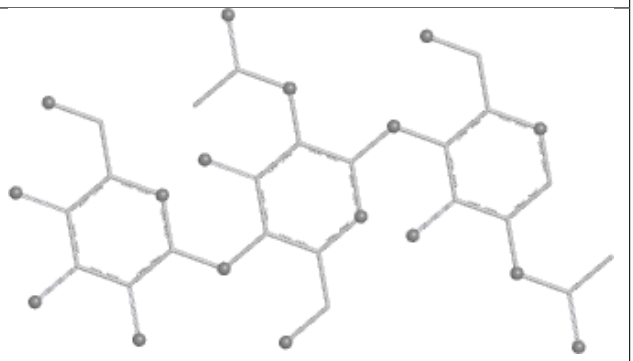


Rings

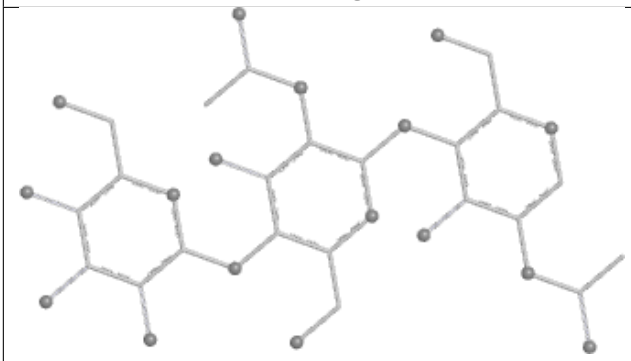
## Oligosaccharide Chain JA



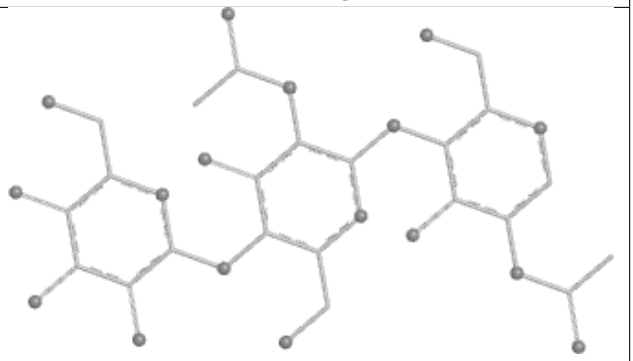
Bond lengths



Bond angles

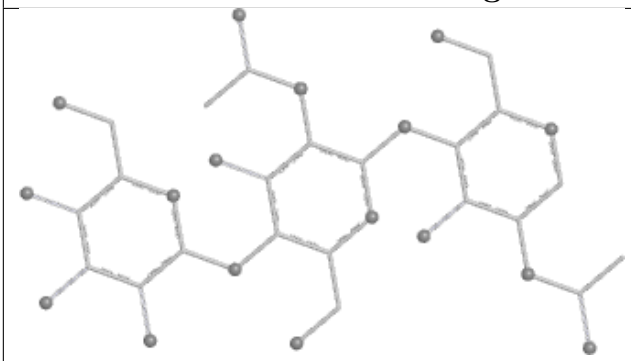


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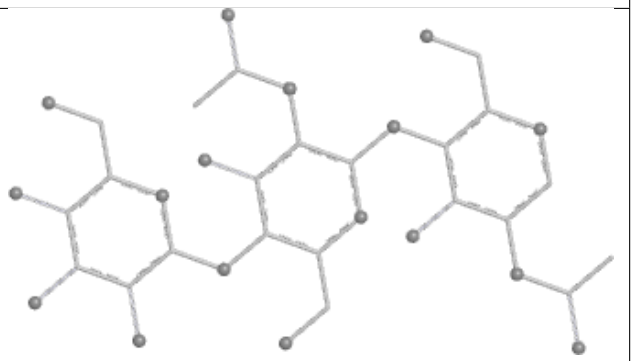


Rings

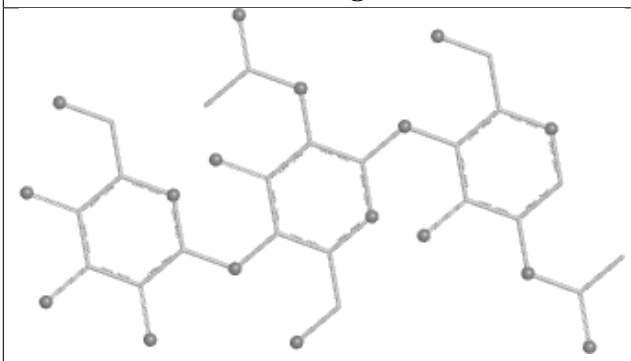
## Oligosaccharide Chain LA



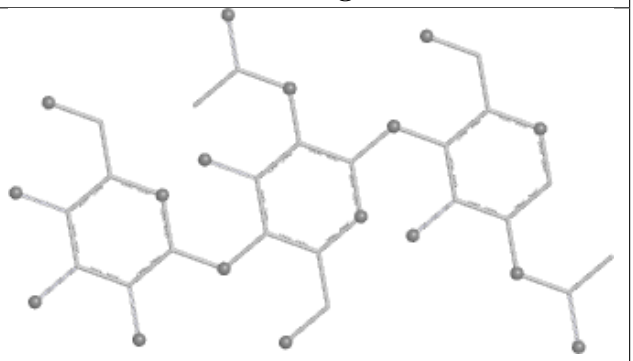
Bond lengths



Bond angles

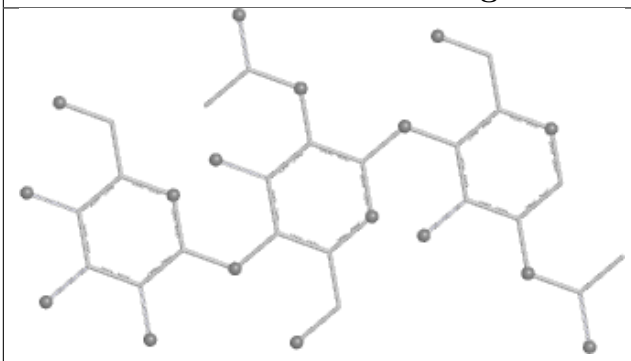


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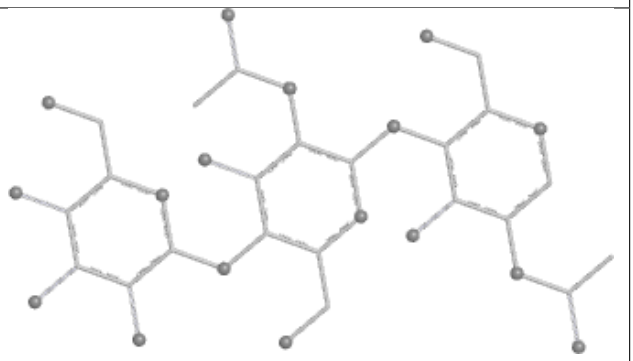


Rings

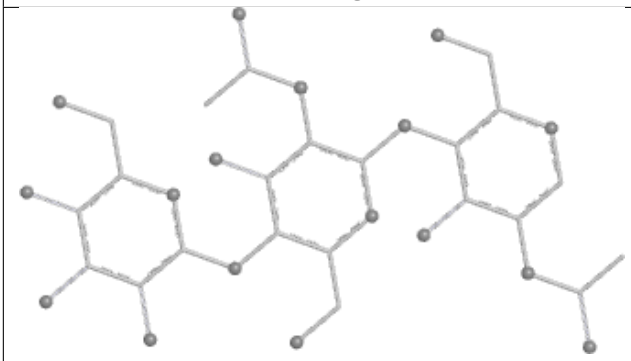
## Oligosaccharide Chain NA



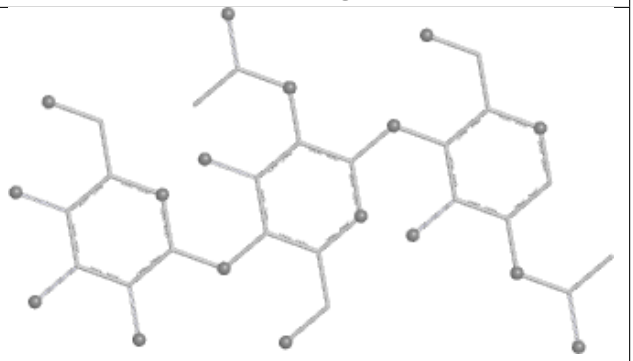
Bond lengths



Bond angles

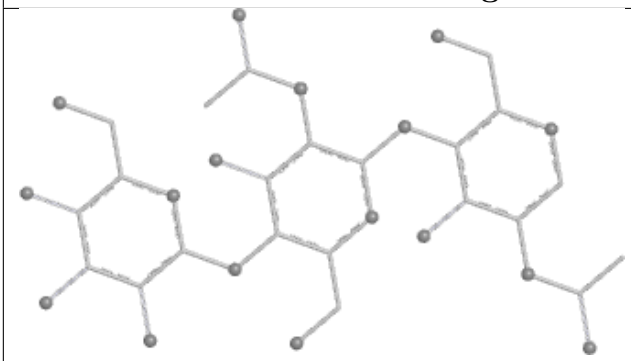


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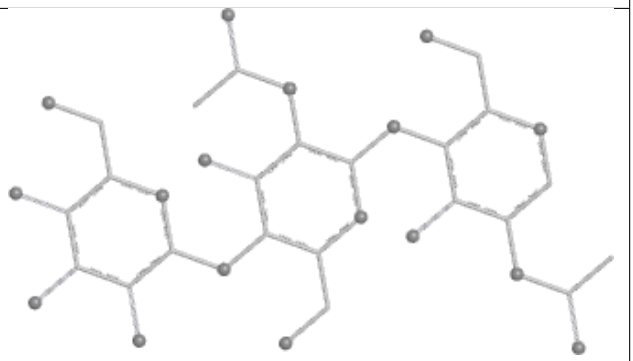


Rings

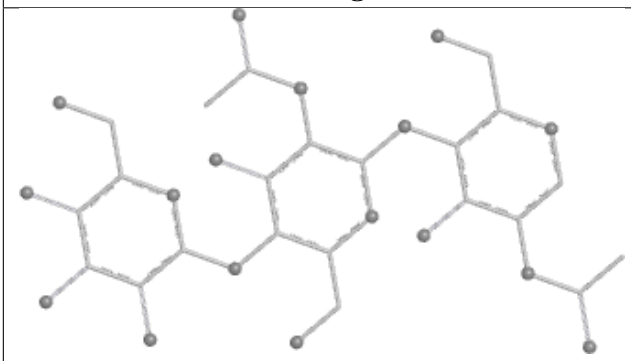
## Oligosaccharide Chain OA



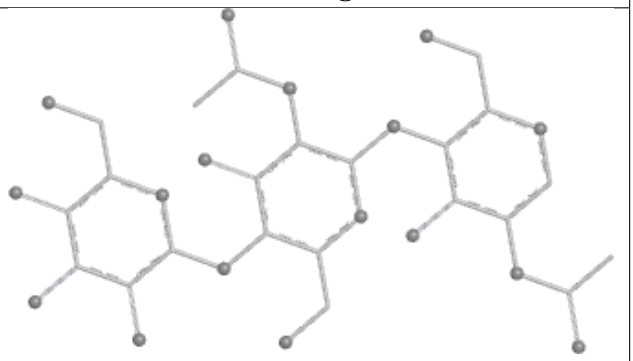
Bond lengths



Bond angles

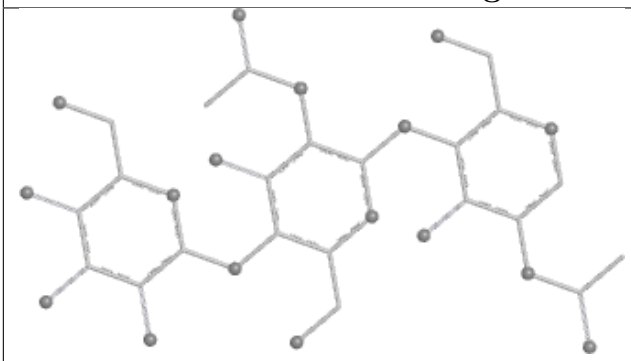


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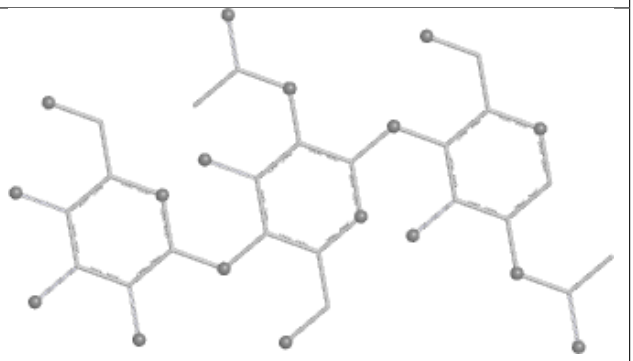


Rings

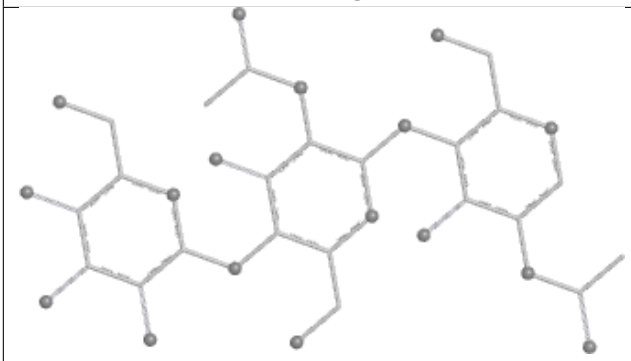
## Oligosaccharide Chain PA



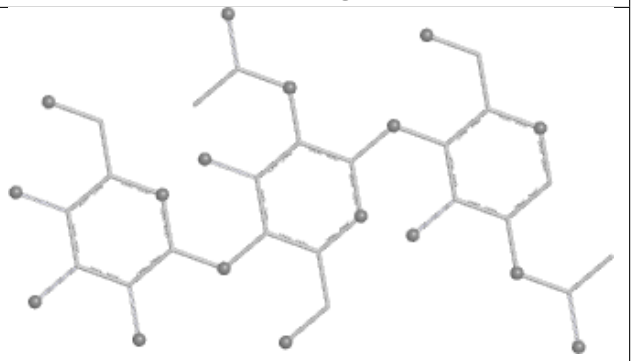
**Bond lengths**



**Bond angles**

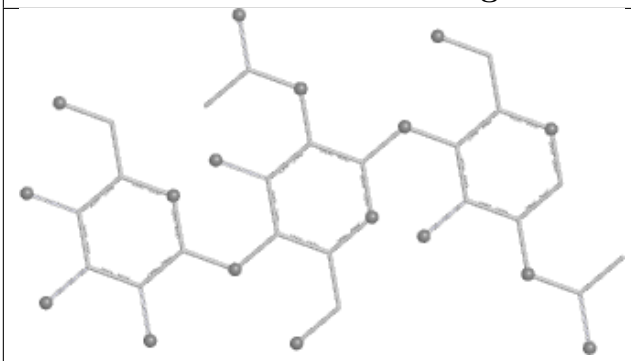


**Torsions**

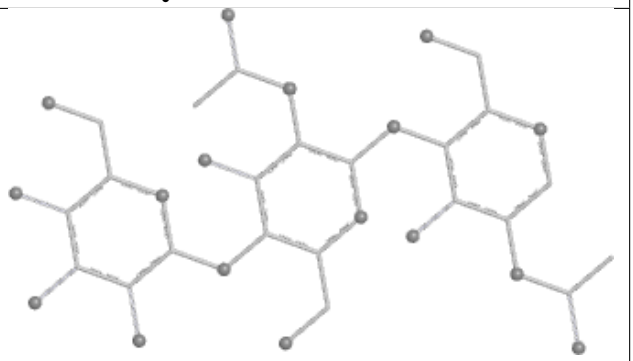


**Rings**

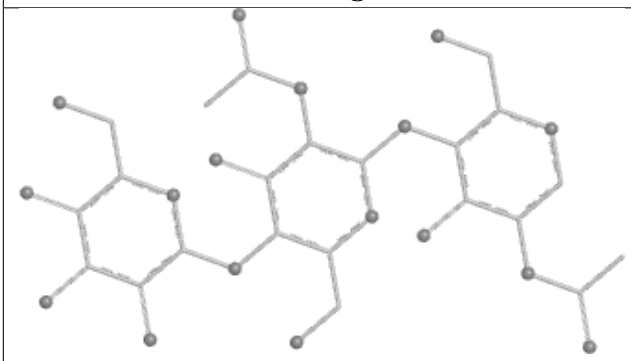
## Oligosaccharide Chain QA



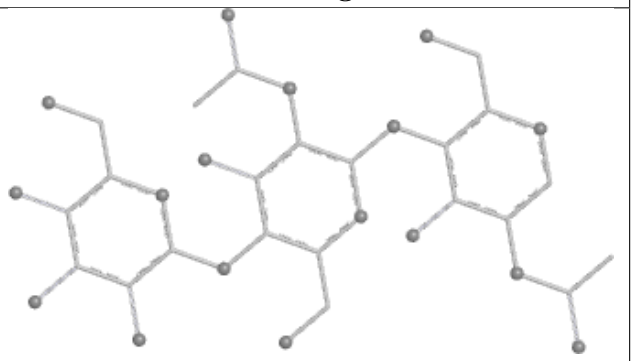
**Bond lengths**



**Bond angles**

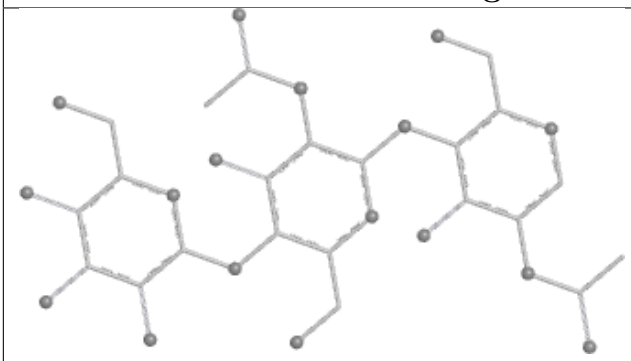


**Torsions**

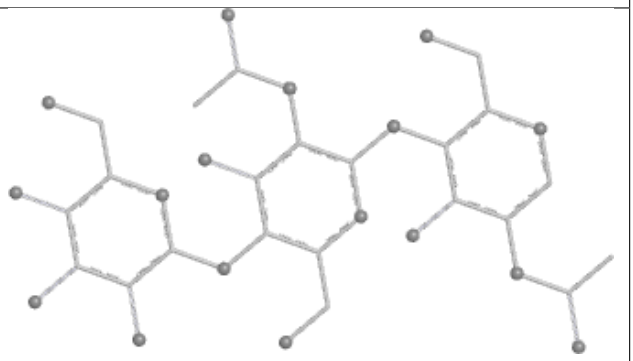


**Rings**

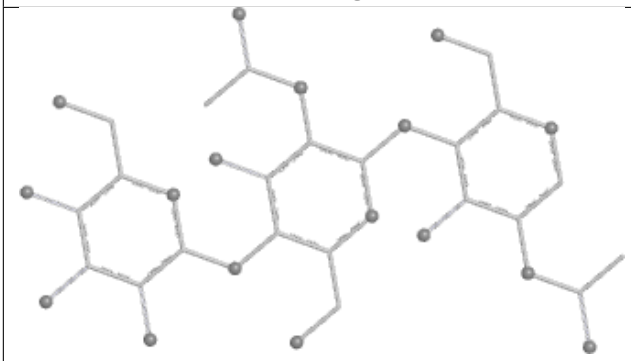
## Oligosaccharide Chain TA



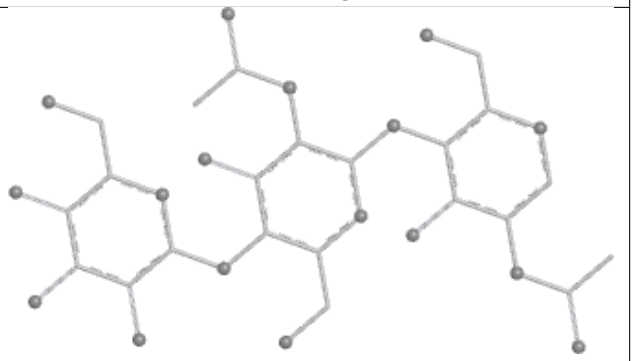
Bond lengths



Bond angles

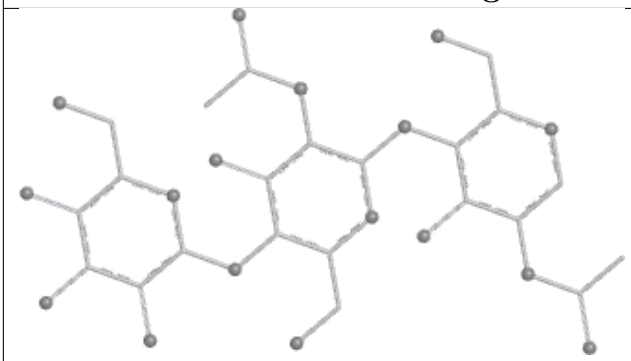


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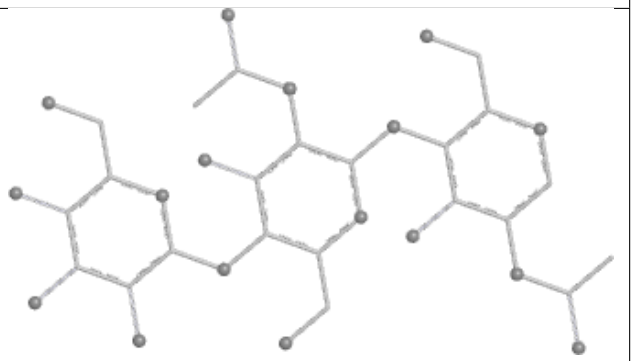


Rings

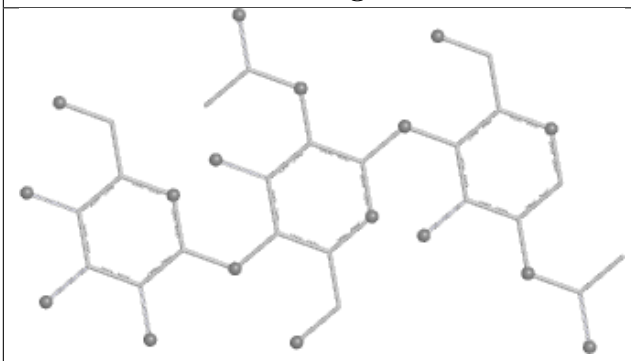
## Oligosaccharide Chain VA



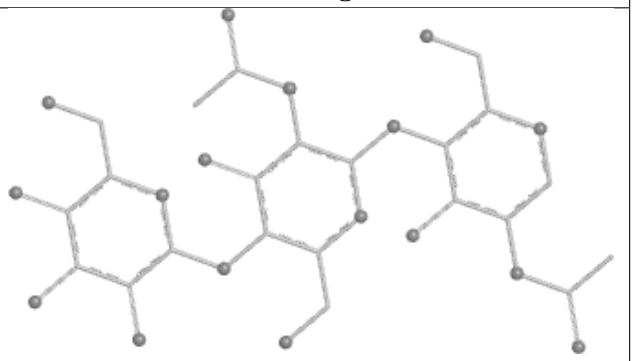
Bond lengths



Bond angles

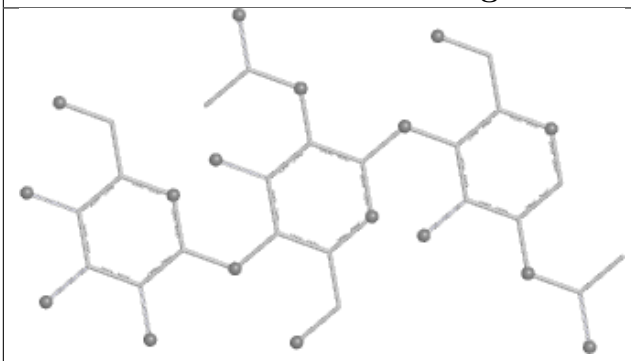


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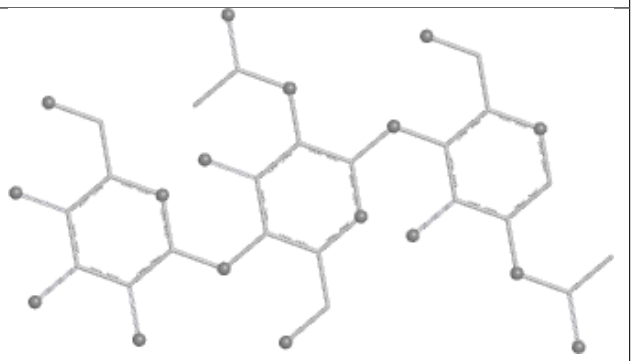


Rings

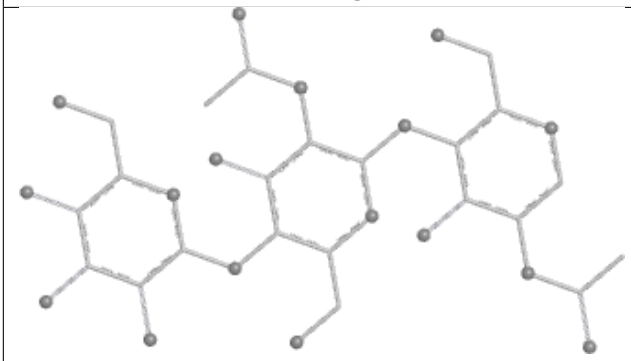
## Oligosaccharide Chain XA



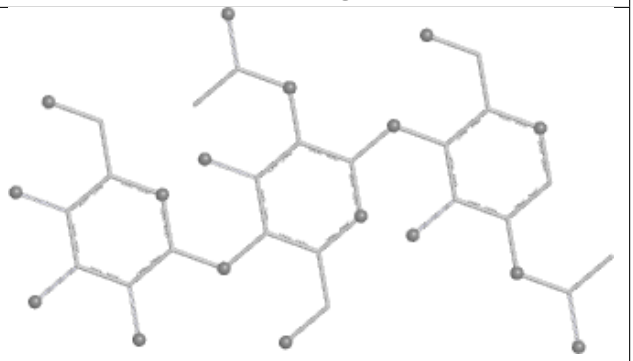
Bond lengths



Bond angles

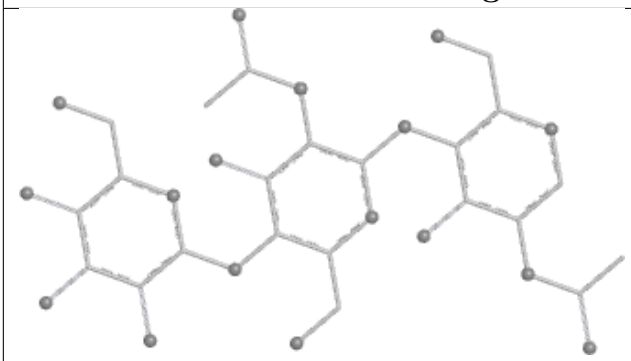


Torsions

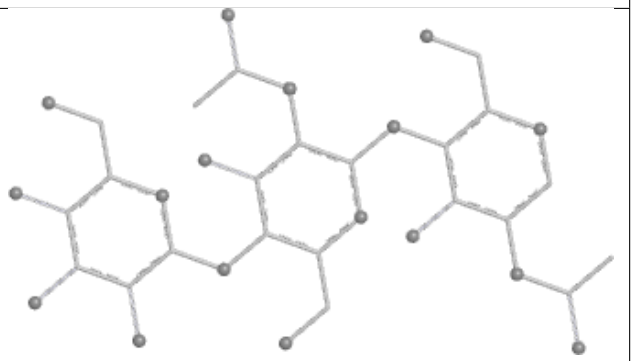


Rings

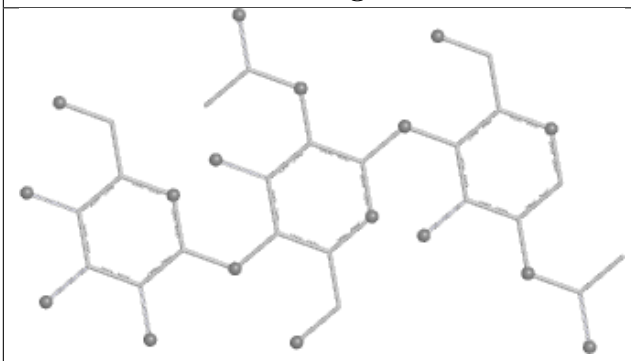
## Oligosaccharide Chain YA



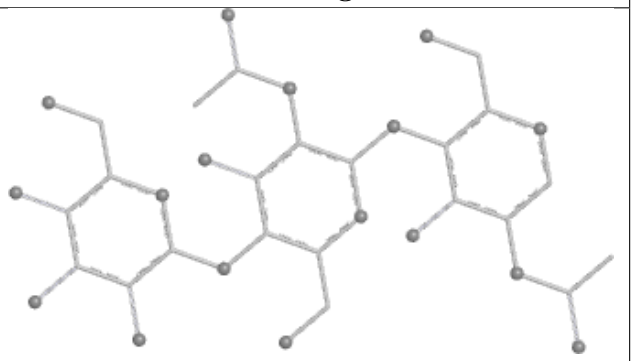
Bond lengths



Bond angles

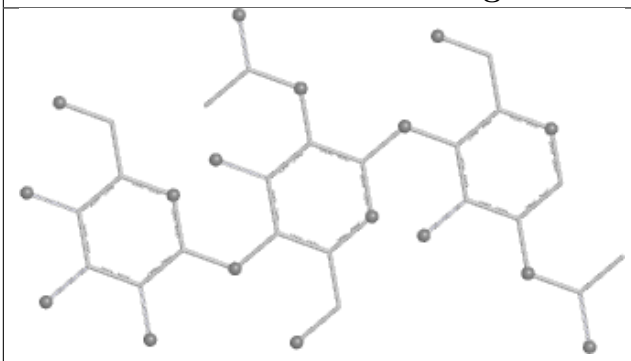


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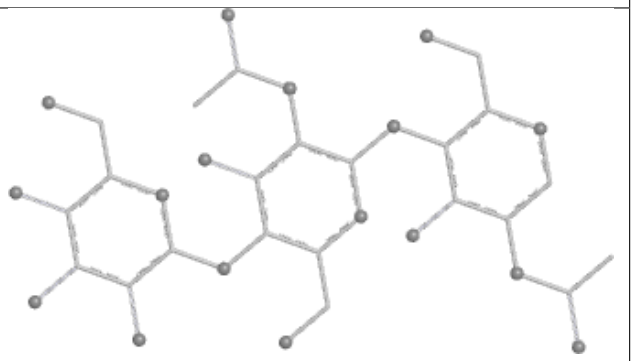


Rings

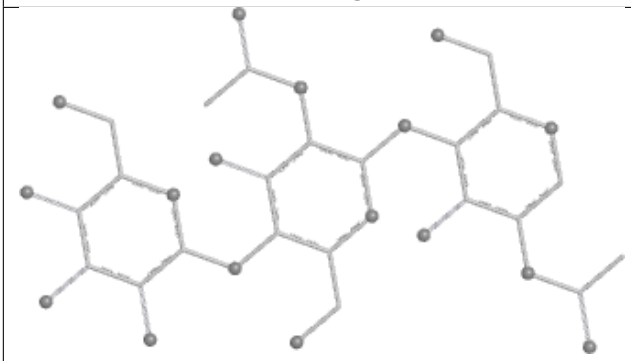
## Oligosaccharide Chain ZA



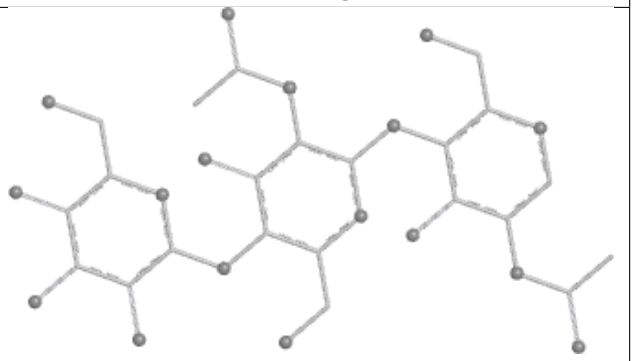
Bond lengths



Bond angles

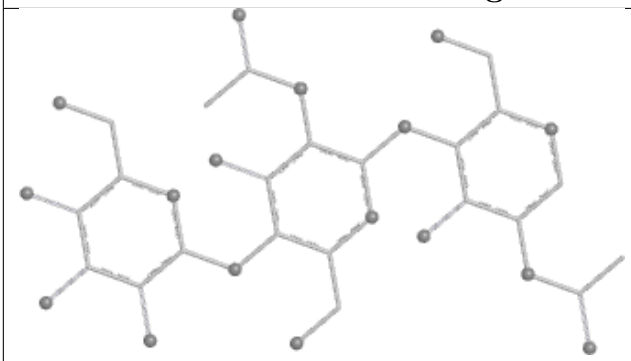


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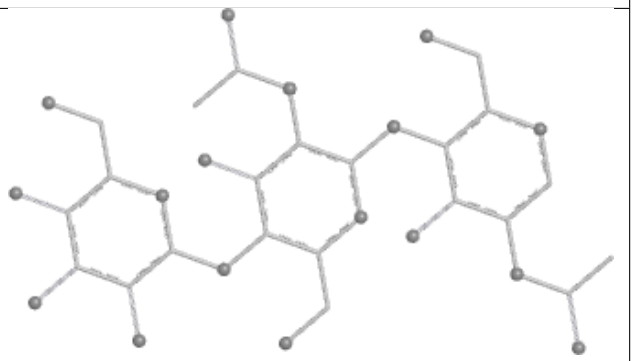


Rings

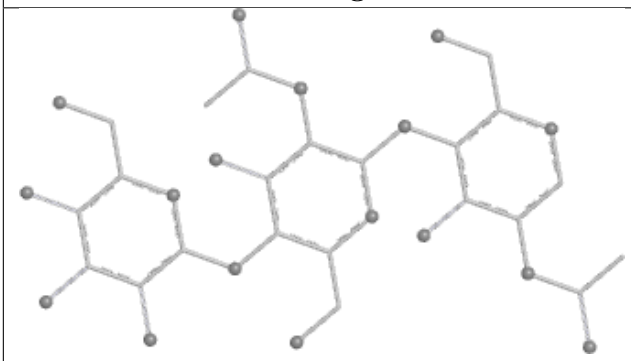
## Oligosaccharide Chain aA



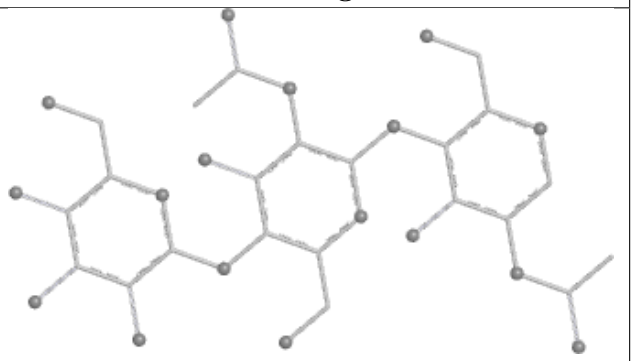
Bond lengths



Bond angles

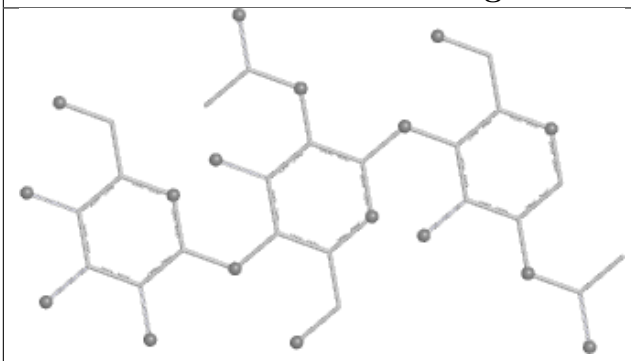


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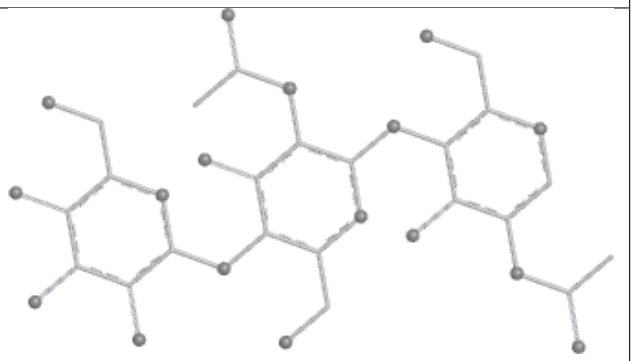


Rings

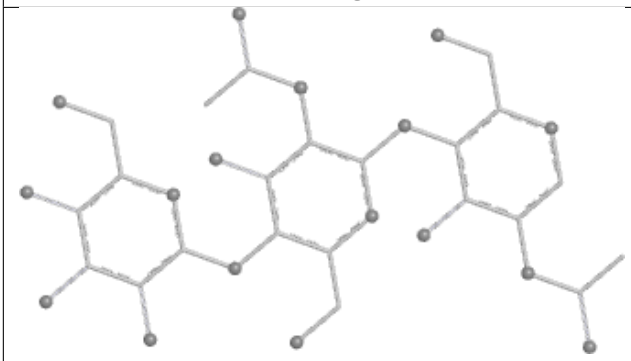
## Oligosaccharide Chain dA



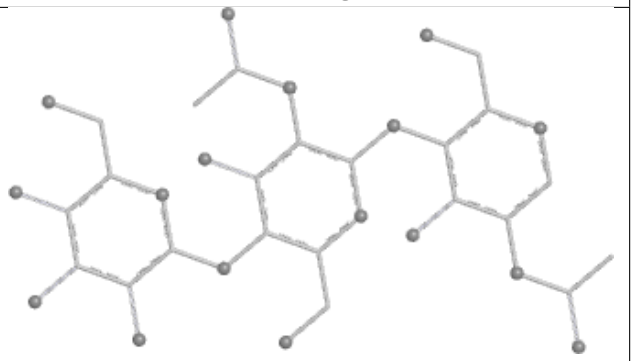
Bond lengths



Bond angles

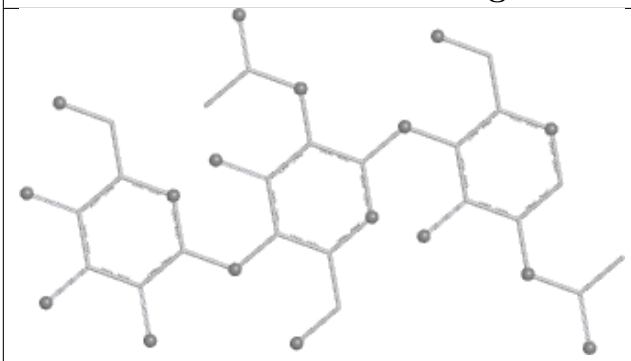


Torsions

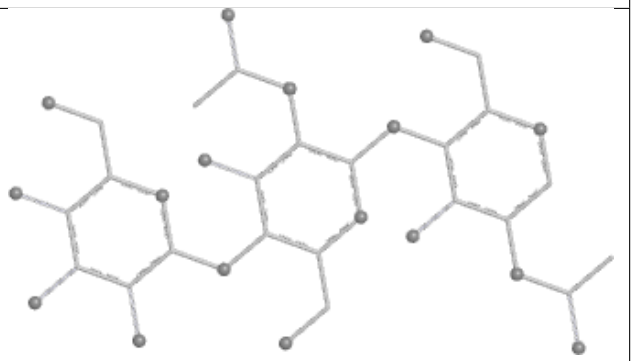


Rings

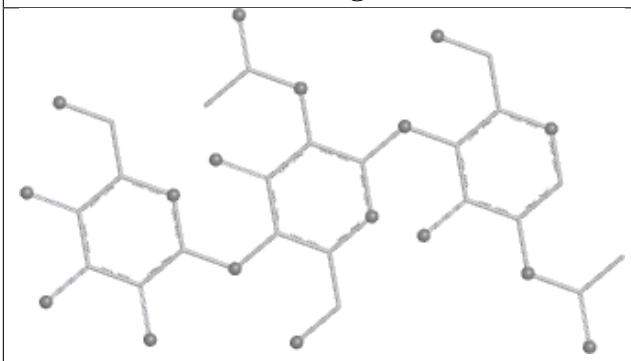
## Oligosaccharide Chain fA



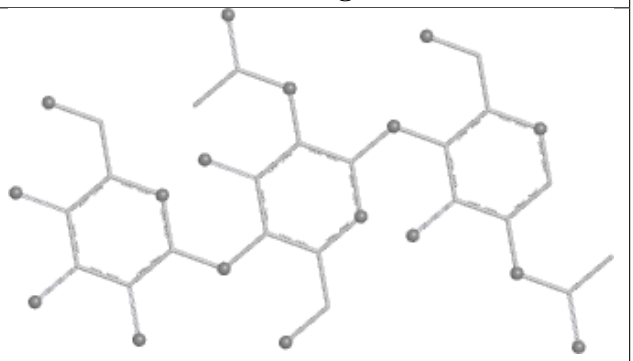
Bond lengths



Bond angles

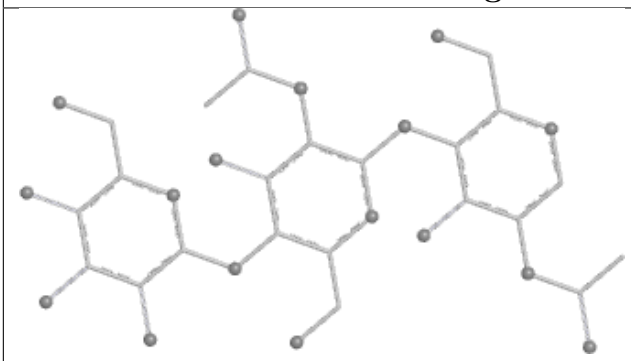


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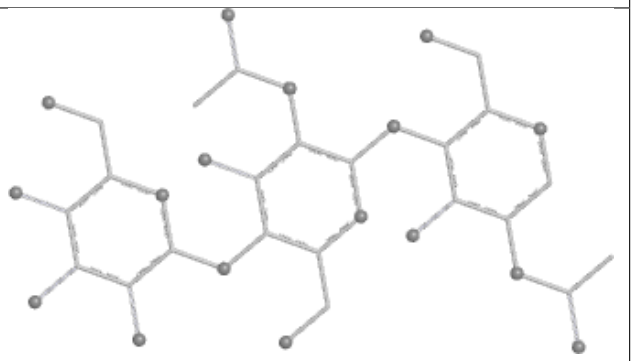


Rings

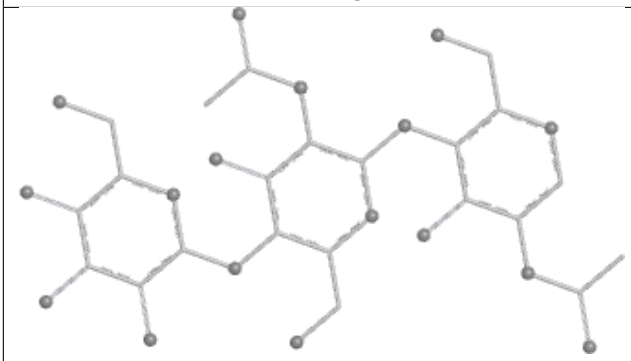
## Oligosaccharide Chain hA



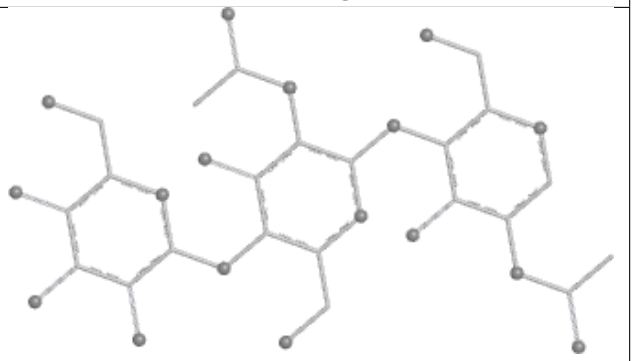
Bond lengths



Bond angles

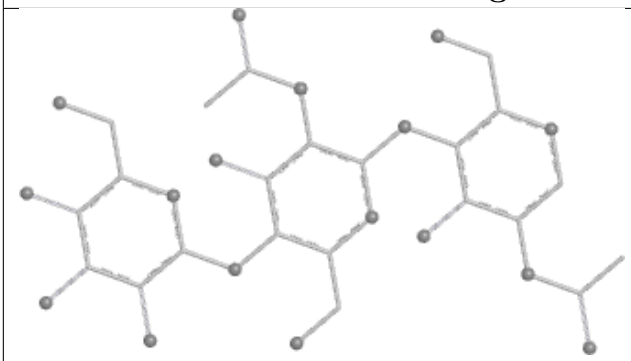


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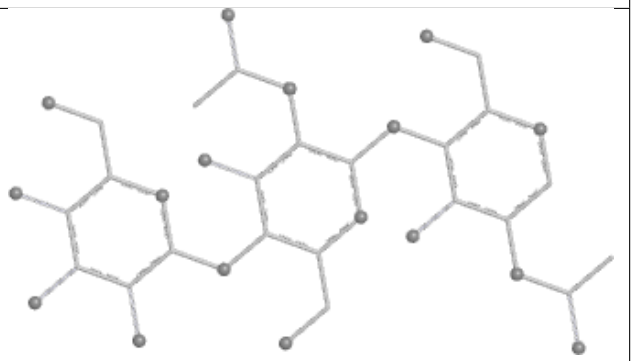


Rings

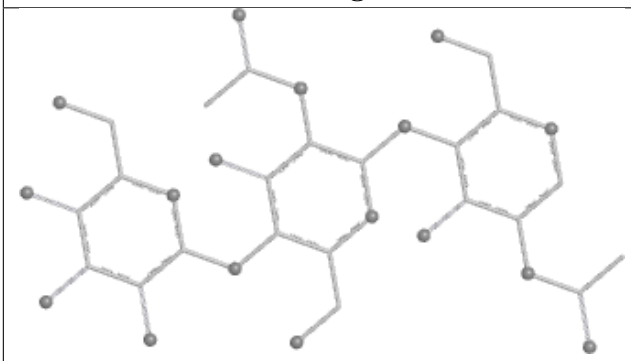
## Oligosaccharide Chain iA



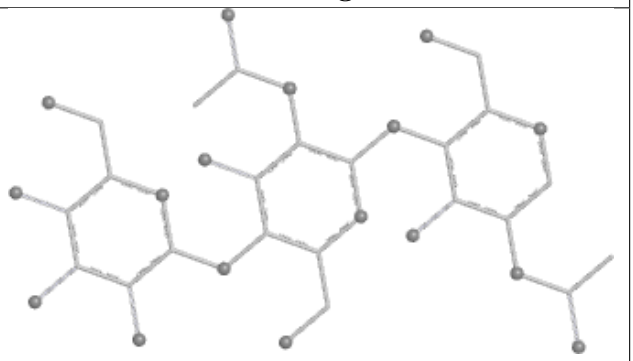
Bond lengths



Bond angles

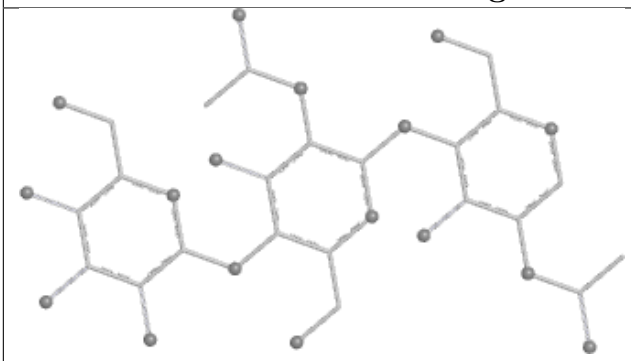


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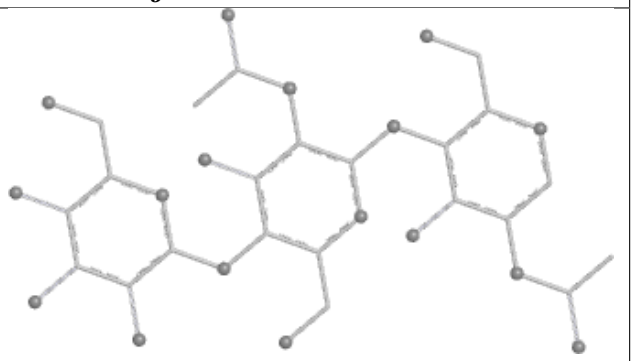


Rings

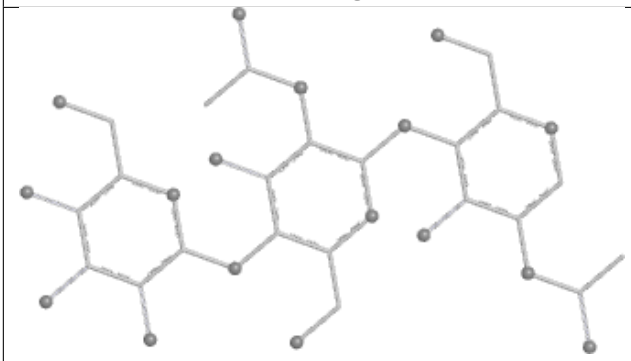
## Oligosaccharide Chain jA



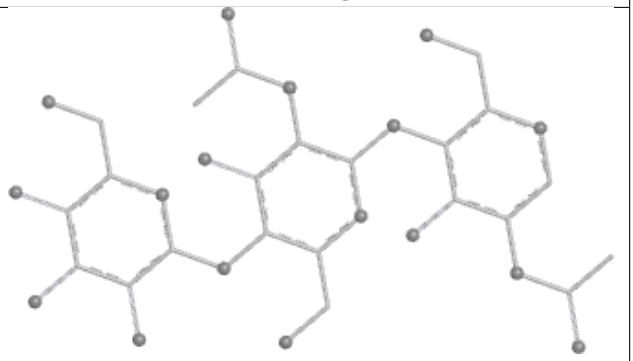
Bond lengths



Bond angles

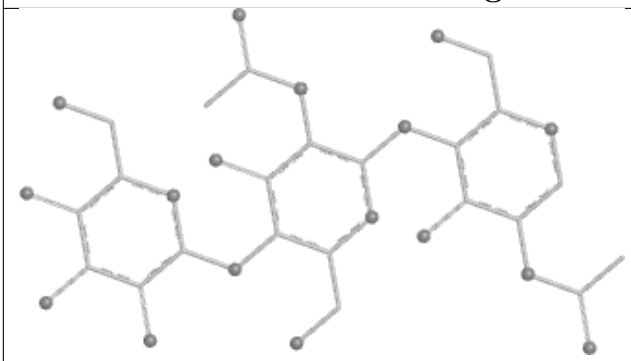


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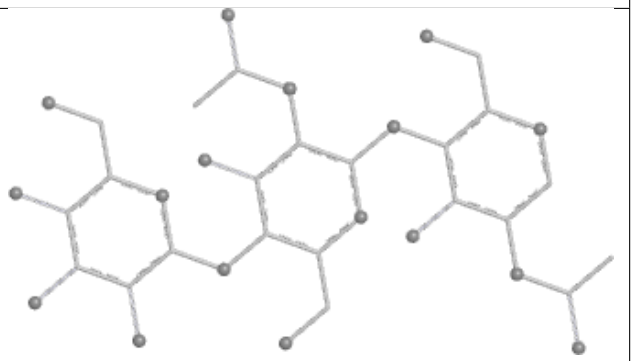


Rings

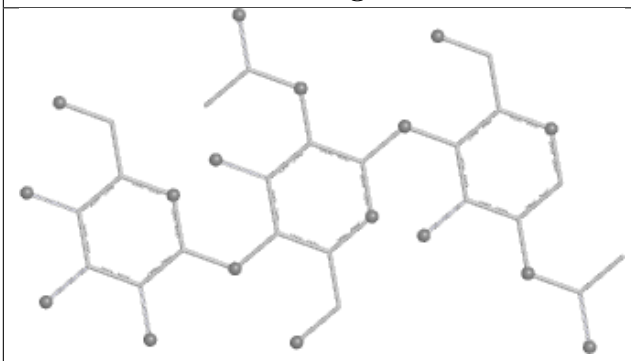
## Oligosaccharide Chain kA



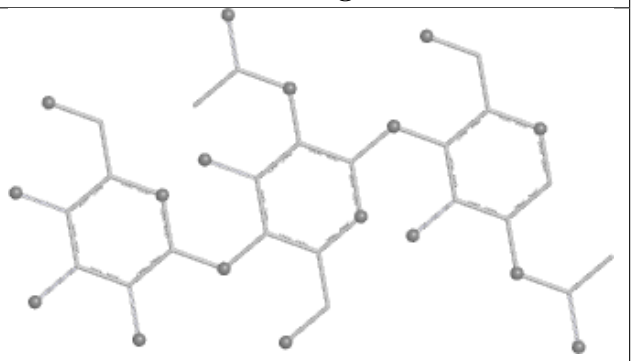
Bond lengths



Bond angles

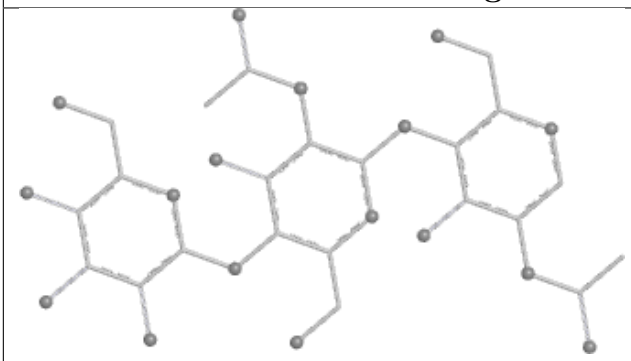


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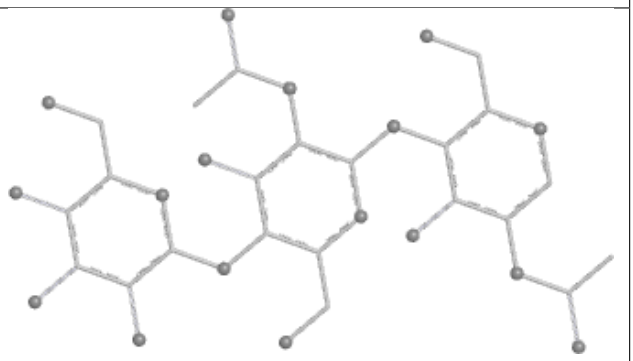


Rings

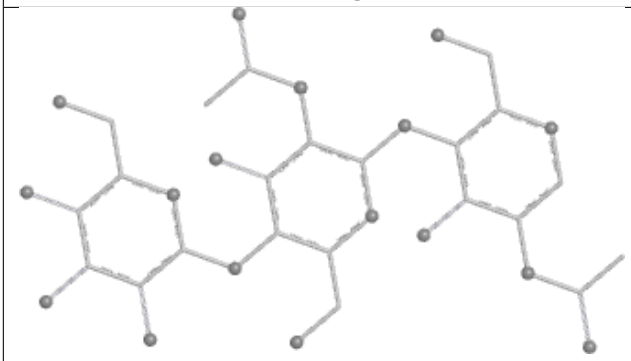
## Oligosaccharide Chain nA



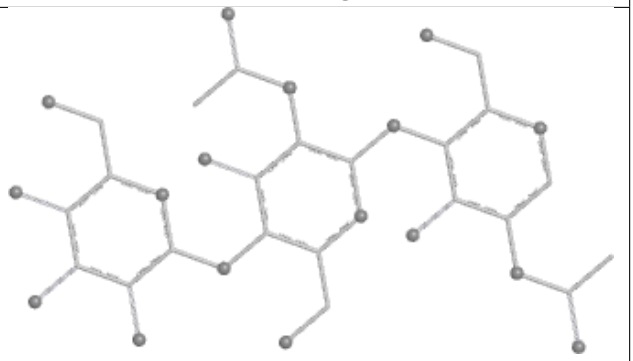
Bond lengths



Bond angles

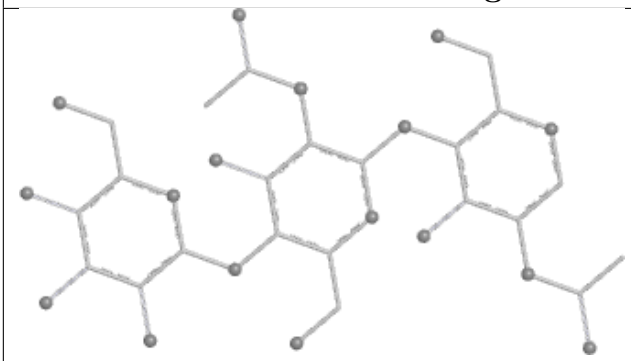


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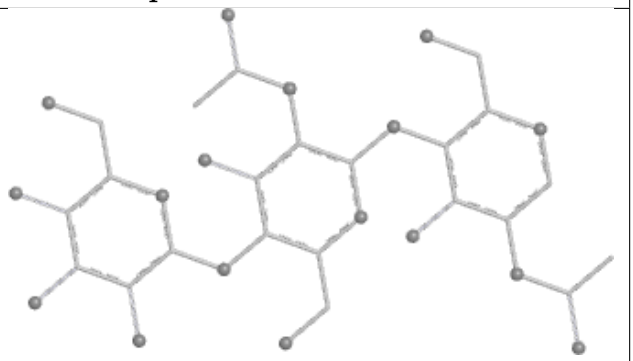


Rings

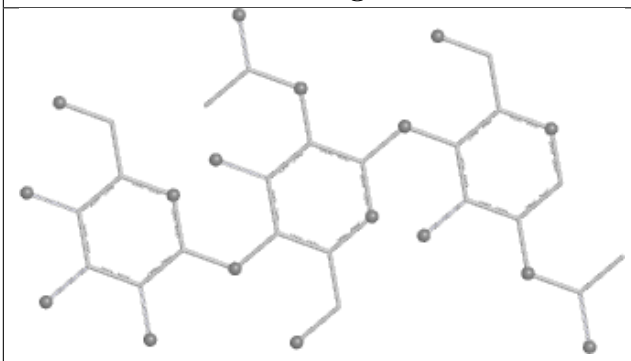
## Oligosaccharide Chain pA



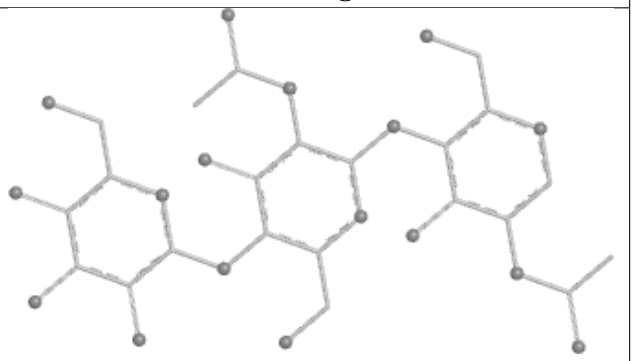
Bond lengths



Bond angles

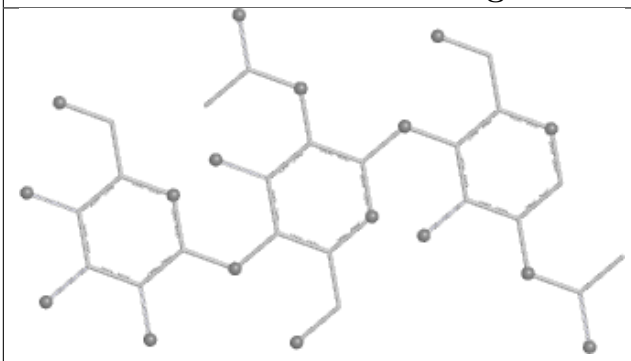


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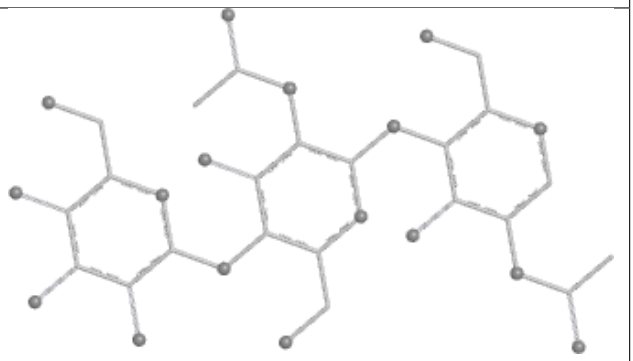


Rings

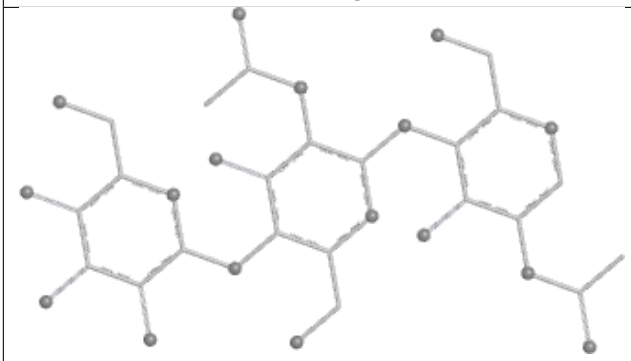
## Oligosaccharide Chain rA



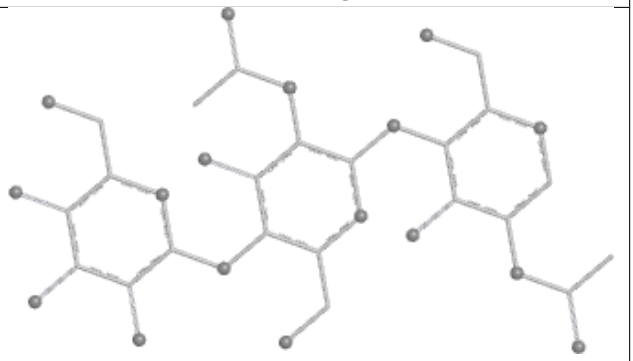
Bond lengths



Bond angles

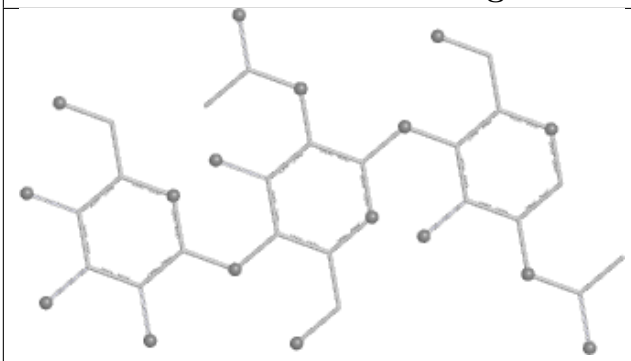


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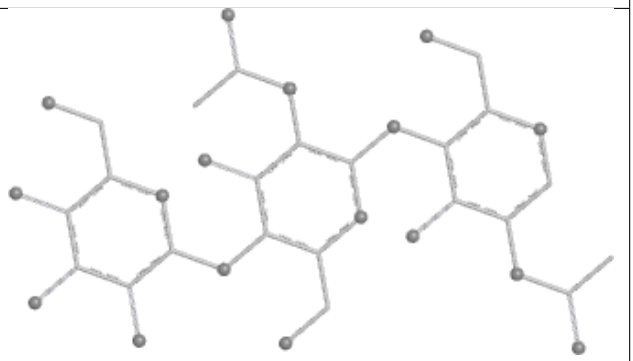


Rings

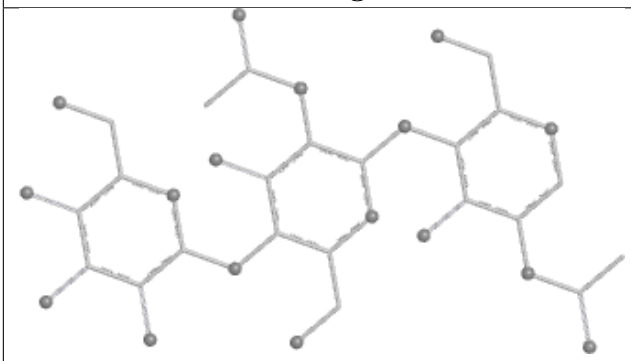
## Oligosaccharide Chain sA



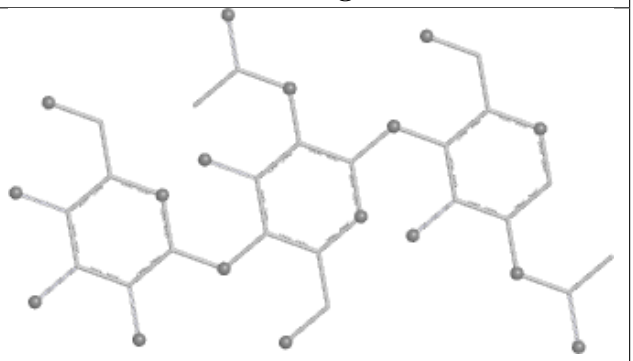
Bond lengths



Bond angles

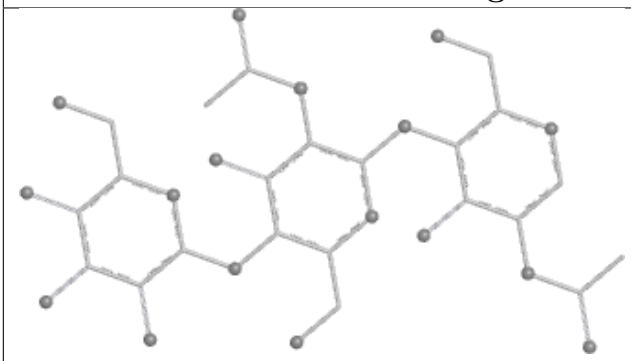


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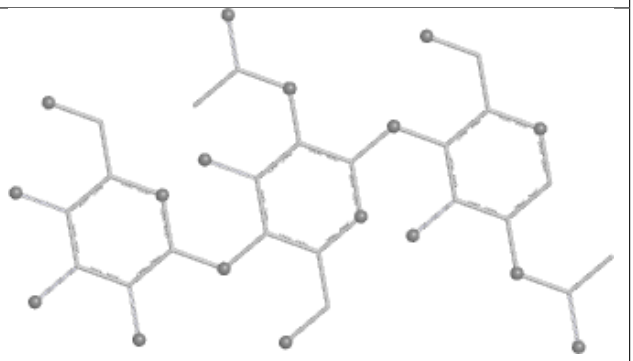


Rings

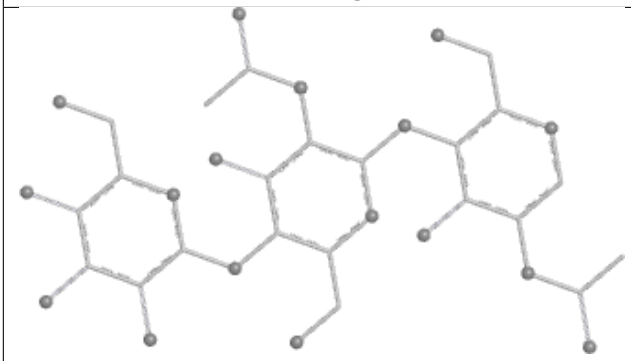
## Oligosaccharide Chain tA



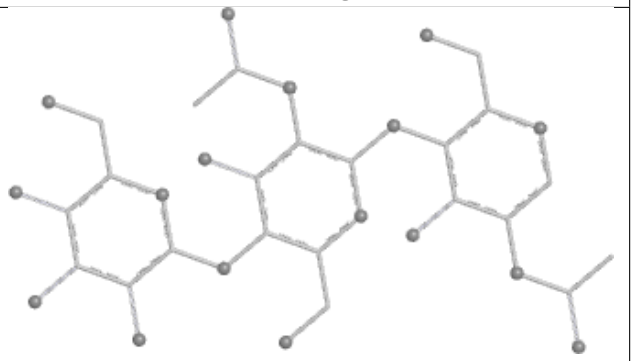
Bond lengths



Bond angles

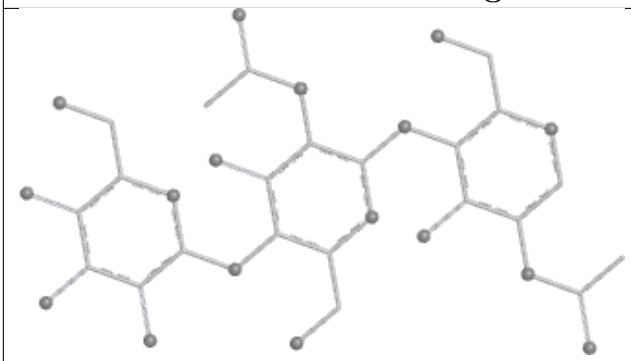


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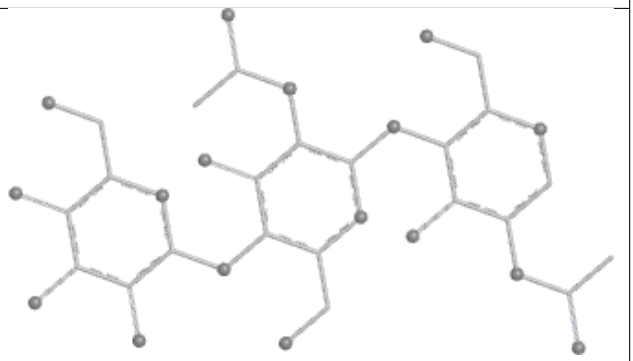


Rings

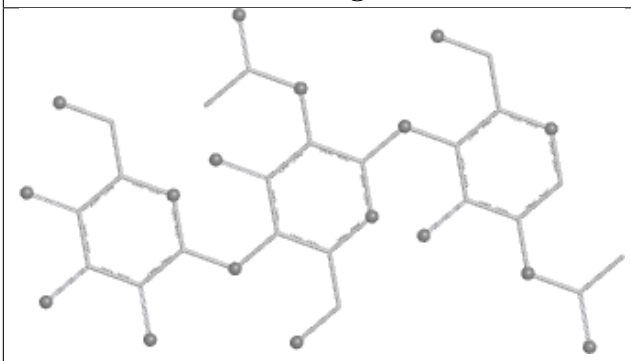
## Oligosaccharide Chain uA



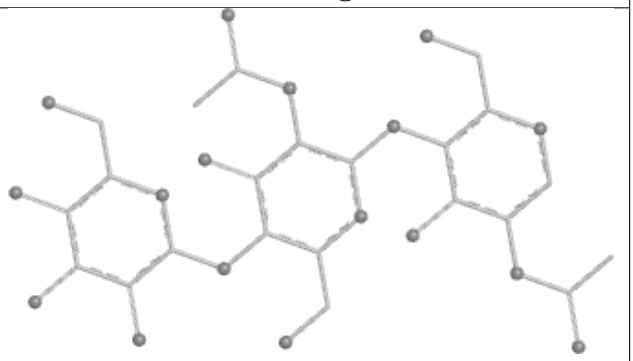
Bond lengths



Bond angles

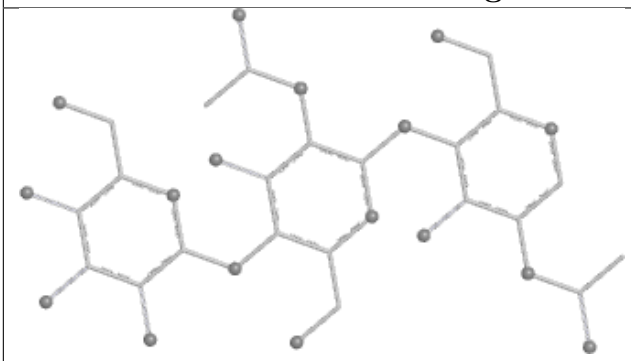


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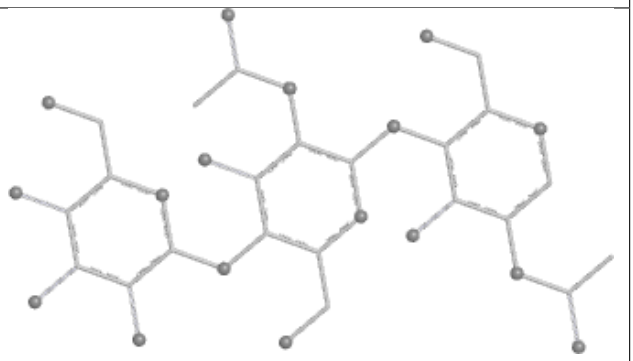


Rings

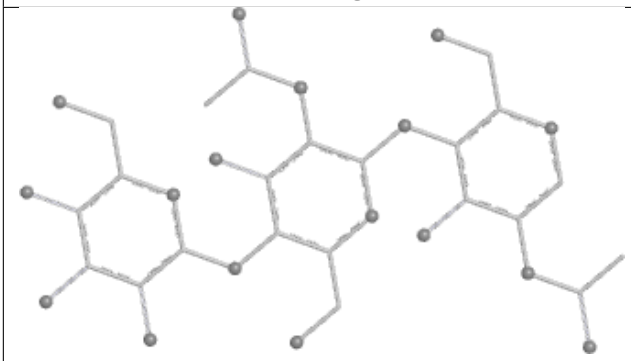
## Oligosaccharide Chain xA



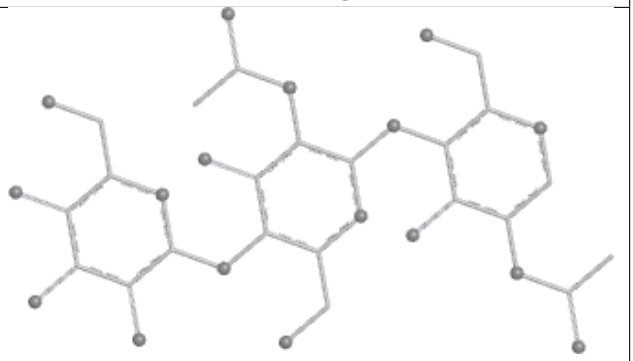
Bond lengths



Bond angles

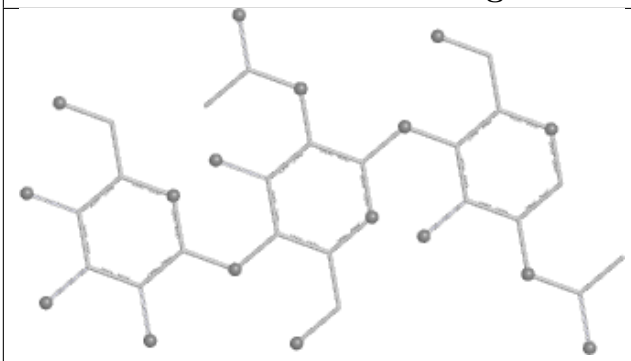


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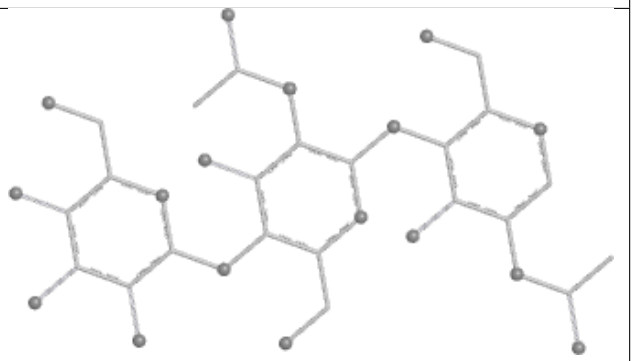


Rings

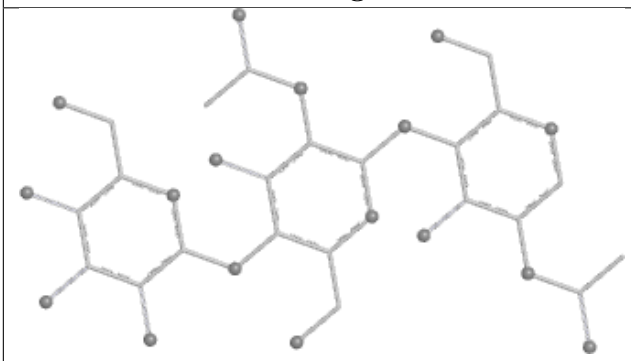
## Oligosaccharide Chain zA



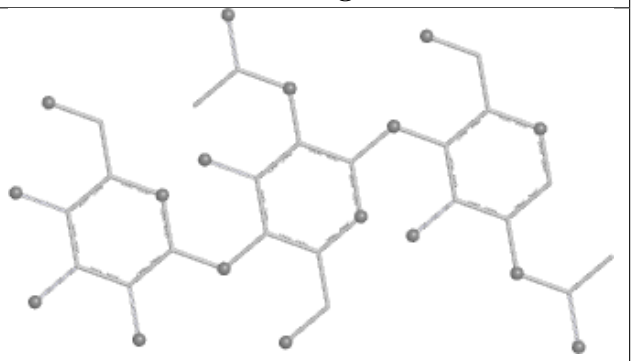
Bond lengths



Bond angles

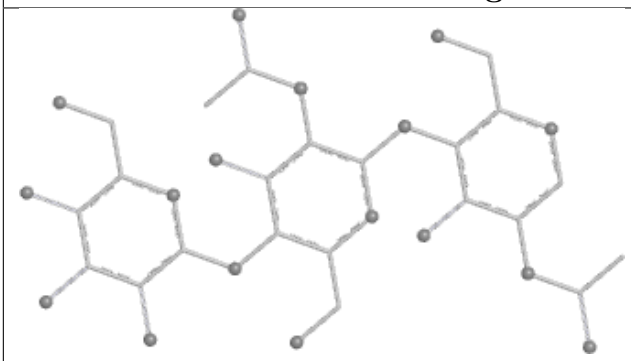


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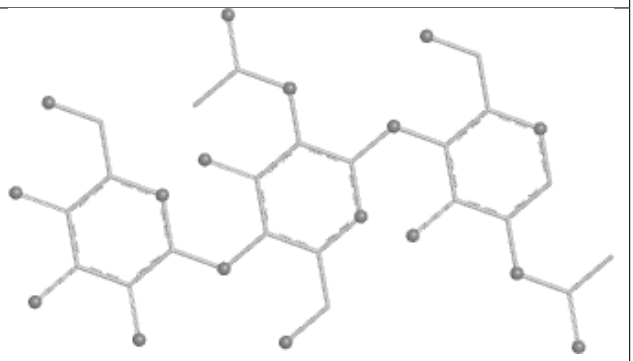


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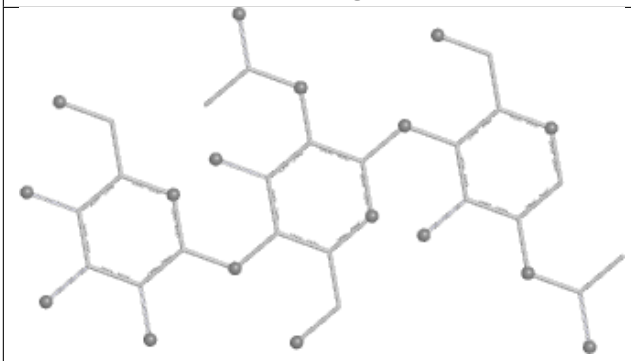
## Oligosaccharide Chain 1A



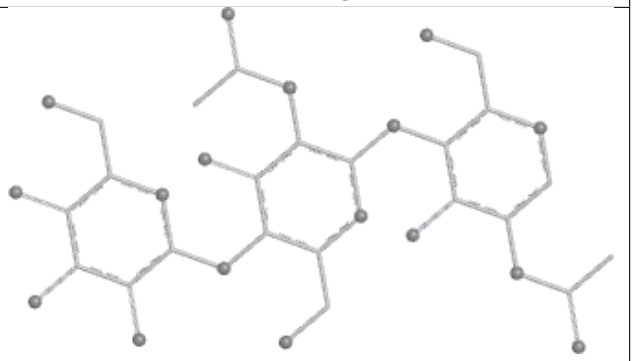
Bond lengths



Bond angles

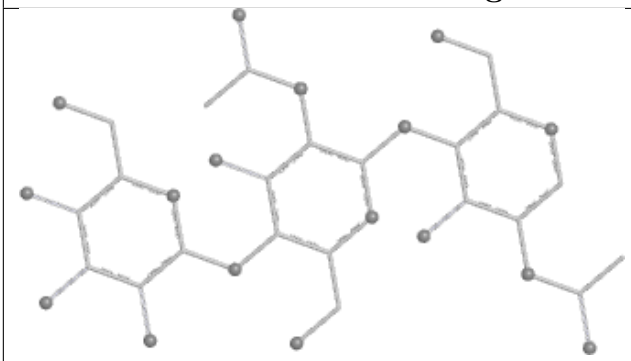


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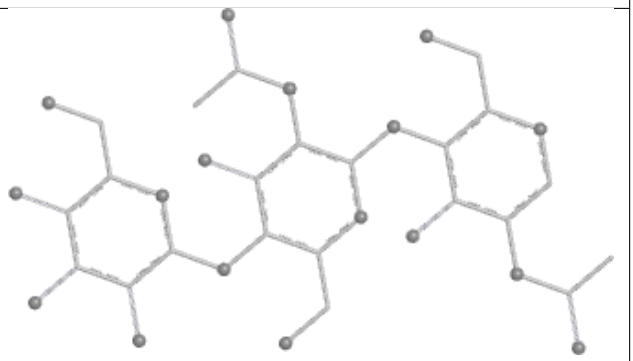


Rings

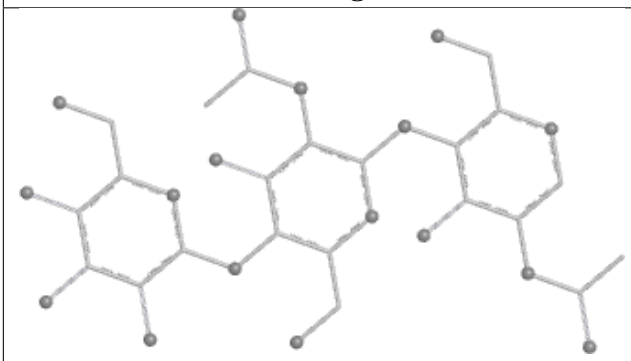
## Oligosaccharide Chain 2A



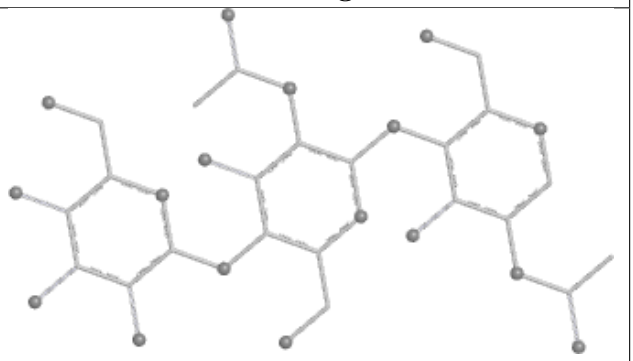
Bond lengths



Bond angles

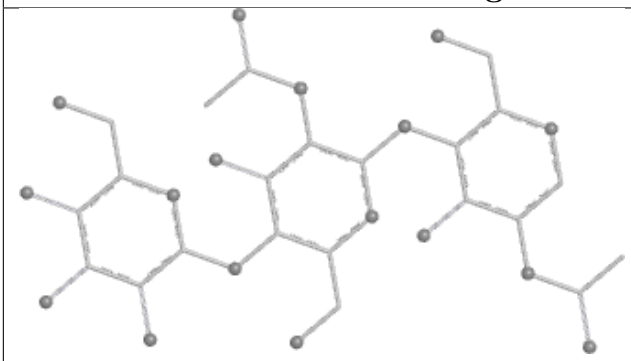


Torsions

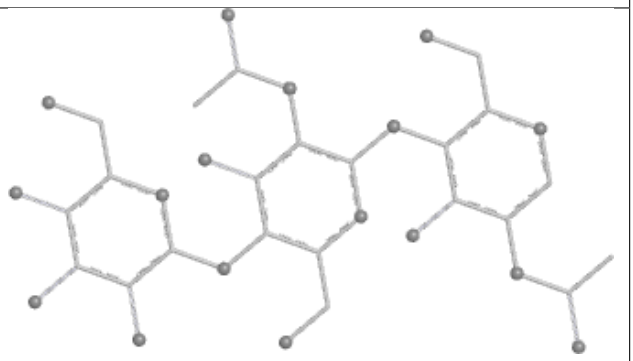


Rings

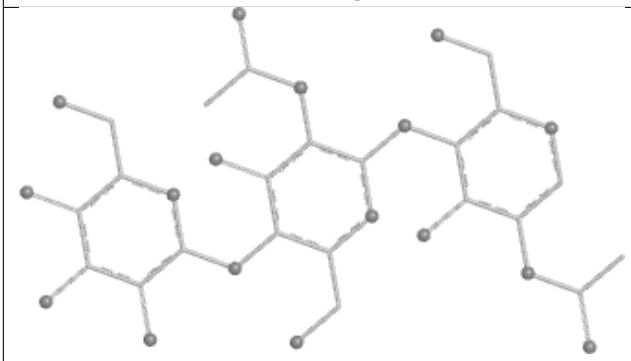
## Oligosaccharide Chain 3A



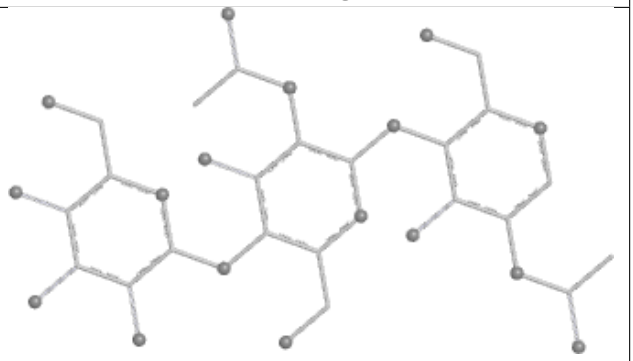
Bond lengths



Bond angles

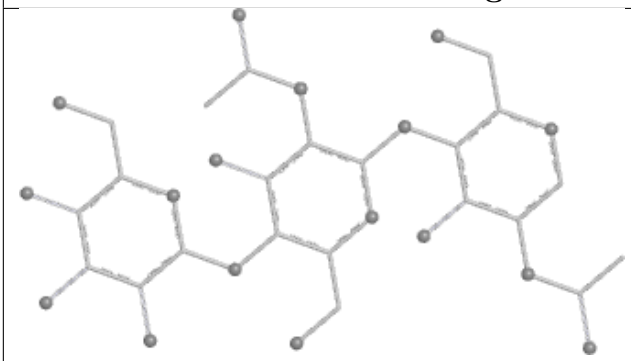


Torsions

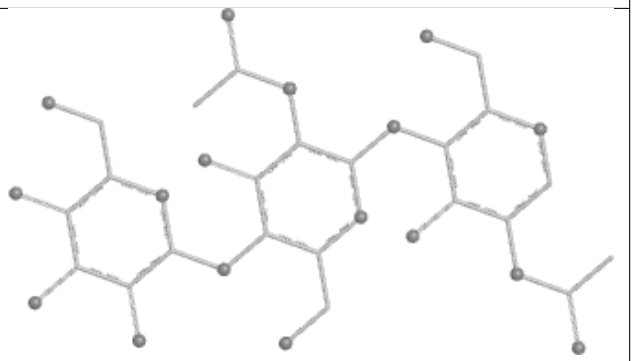


Rings

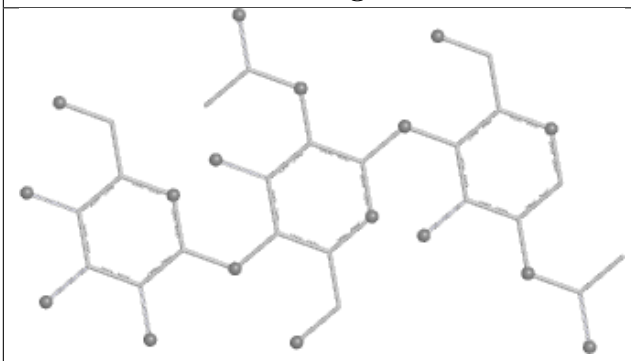
## Oligosaccharide Chain 4A



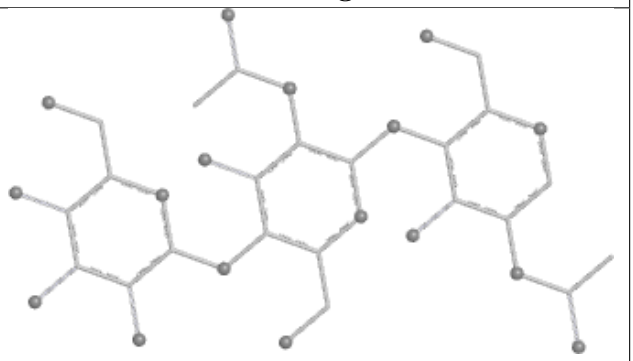
Bond lengths



Bond angles



Torsions



Rings

## 5.6 Ligand geometry (i)

20 ligands are modelled in this entry.

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

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\| > 2$ | Counts | RMSZ | $\#\|Z\| > 2$ |
| 4 | NAG | G | 3501 | 1 | 14,14,15 | 0.15 | 0 | 17,19,21 | 0.41 | 0 |
| 4 | NAG | C | 3501 | 1 | 14,14,15 | 0.18 | 0 | 17,19,21 | 0.48 | 0 |
| 4 | NAG | L | 3501 | 1 | 14,14,15 | 0.24 | 0 | 17,19,21 | 0.49 | 0 |
| 4 | NAG | D | 3501 | 1 | 14,14,15 | 0.24 | 0 | 17,19,21 | 0.39 | 0 |
| 4 | NAG | P | 3501 | 1 | 14,14,15 | 0.25 | 0 | 17,19,21 | 0.44 | 0 |
| 4 | NAG | Q | 3501 | 1 | 14,14,15 | 0.36 | 0 | 17,19,21 | 0.50 | 0 |
| 4 | NAG | N | 3501 | 1 | 14,14,15 | 0.21 | 0 | 17,19,21 | 0.36 | 0 |
| 4 | NAG | R | 3501 | 1 | 14,14,15 | 0.21 | 0 | 17,19,21 | 0.35 | 0 |
| 4 | NAG | T | 3501 | 1 | 14,14,15 | 0.24 | 0 | 17,19,21 | 0.65 | 0 |
| 4 | NAG | S | 3501 | 1 | 14,14,15 | 0.24 | 0 | 17,19,21 | 0.42 | 0 |
| 4 | NAG | E | 3501 | 1 | 14,14,15 | 0.16 | 0 | 17,19,21 | 0.44 | 0 |
| 4 | NAG | M | 3501 | 1 | 14,14,15 | 0.35 | 0 | 17,19,21 | 0.50 | 0 |
| 4 | NAG | K | 3501 | 1 | 14,14,15 | 0.15 | 0 | 17,19,21 | 0.42 | 0 |
| 4 | NAG | F | 3501 | 1 | 14,14,15 | 0.25 | 0 | 17,19,21 | 0.36 | 0 |
| 4 | NAG | O | 3501 | 1 | 14,14,15 | 0.35 | 0 | 17,19,21 | 0.46 | 0 |
| 4 | NAG | J | 3501 | 1 | 14,14,15 | 0.24 | 0 | 17,19,21 | 0.36 | 0 |
| 4 | NAG | B | 3501 | 1 | 14,14,15 | 0.30 | 0 | 17,19,21 | 0.41 | 0 |
| 4 | NAG | A | 3501 | 1 | 14,14,15 | 0.21 | 0 | 17,19,21 | 0.41 | 0 |
| 4 | NAG | H | 3501 | 1 | 14,14,15 | 0.28 | 0 | 17,19,21 | 0.46 | 0 |
| 4 | NAG | I | 3501 | 1 | 14,14,15 | 0.19 | 0 | 17,19,21 | 0.40 | 0 |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 4 | NAG | G | 3501 | 1 | - | 2/6/23/26 | 0/1/1/1 |
| 4 | NAG | C | 3501 | 1 | - | 2/6/23/26 | 0/1/1/1 |
| 4 | NAG | L | 3501 | 1 | - | 4/6/23/26 | 0/1/1/1 |
| 4 | NAG | D | 3501 | 1 | - | 4/6/23/26 | 0/1/1/1 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 4 | NAG | P | 3501 | 1 | - | 4/6/23/26 | 0/1/1/1 |
| 4 | NAG | Q | 3501 | 1 | - | 1/6/23/26 | 0/1/1/1 |
| 4 | NAG | N | 3501 | 1 | - | 3/6/23/26 | 0/1/1/1 |
| 4 | NAG | R | 3501 | 1 | - | 4/6/23/26 | 0/1/1/1 |
| 4 | NAG | T | 3501 | 1 | - | 4/6/23/26 | 0/1/1/1 |
| 4 | NAG | S | 3501 | 1 | - | 1/6/23/26 | 0/1/1/1 |
| 4 | NAG | E | 3501 | 1 | - | 2/6/23/26 | 0/1/1/1 |
| 4 | NAG | M | 3501 | 1 | - | 3/6/23/26 | 0/1/1/1 |
| 4 | NAG | K | 3501 | 1 | - | 2/6/23/26 | 0/1/1/1 |
| 4 | NAG | F | 3501 | 1 | - | 2/6/23/26 | 0/1/1/1 |
| 4 | NAG | O | 3501 | 1 | - | 1/6/23/26 | 0/1/1/1 |
| 4 | NAG | J | 3501 | 1 | - | 2/6/23/26 | 0/1/1/1 |
| 4 | NAG | B | 3501 | 1 | - | 4/6/23/26 | 0/1/1/1 |
| 4 | NAG | A | 3501 | 1 | - | 1/6/23/26 | 0/1/1/1 |
| 4 | NAG | H | 3501 | 1 | - | 4/6/23/26 | 0/1/1/1 |
| 4 | NAG | I | 3501 | 1 | - | 1/6/23/26 | 0/1/1/1 |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (51) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 4 | P | 3501 | NAG | O5-C5-C6-O6 |
| 4 | K | 3501 | NAG | C4-C5-C6-O6 |
| 4 | G | 3501 | NAG | C4-C5-C6-O6 |
| 4 | C | 3501 | NAG | C4-C5-C6-O6 |
| 4 | E | 3501 | NAG | C4-C5-C6-O6 |
| 4 | H | 3501 | NAG | O5-C5-C6-O6 |
| 4 | L | 3501 | NAG | C4-C5-C6-O6 |
| 4 | P | 3501 | NAG | C4-C5-C6-O6 |
| 4 | D | 3501 | NAG | O5-C5-C6-O6 |
| 4 | R | 3501 | NAG | O5-C5-C6-O6 |
| 4 | R | 3501 | NAG | C4-C5-C6-O6 |
| 4 | B | 3501 | NAG | O5-C5-C6-O6 |
| 4 | M | 3501 | NAG | O5-C5-C6-O6 |
| 4 | K | 3501 | NAG | O5-C5-C6-O6 |
| 4 | C | 3501 | NAG | O5-C5-C6-O6 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 4 | E | 3501 | NAG | O5-C5-C6-O6 |
| 4 | G | 3501 | NAG | O5-C5-C6-O6 |
| 4 | L | 3501 | NAG | O5-C5-C6-O6 |
| 4 | B | 3501 | NAG | C4-C5-C6-O6 |
| 4 | D | 3501 | NAG | C4-C5-C6-O6 |
| 4 | H | 3501 | NAG | C4-C5-C6-O6 |
| 4 | B | 3501 | NAG | C8-C7-N2-C2 |
| 4 | B | 3501 | NAG | O7-C7-N2-C2 |
| 4 | D | 3501 | NAG | C8-C7-N2-C2 |
| 4 | D | 3501 | NAG | O7-C7-N2-C2 |
| 4 | F | 3501 | NAG | C8-C7-N2-C2 |
| 4 | F | 3501 | NAG | O7-C7-N2-C2 |
| 4 | H | 3501 | NAG | C8-C7-N2-C2 |
| 4 | H | 3501 | NAG | O7-C7-N2-C2 |
| 4 | J | 3501 | NAG | C8-C7-N2-C2 |
| 4 | J | 3501 | NAG | O7-C7-N2-C2 |
| 4 | L | 3501 | NAG | C8-C7-N2-C2 |
| 4 | L | 3501 | NAG | O7-C7-N2-C2 |
| 4 | N | 3501 | NAG | C8-C7-N2-C2 |
| 4 | N | 3501 | NAG | O7-C7-N2-C2 |
| 4 | P | 3501 | NAG | C8-C7-N2-C2 |
| 4 | P | 3501 | NAG | O7-C7-N2-C2 |
| 4 | R | 3501 | NAG | C8-C7-N2-C2 |
| 4 | R | 3501 | NAG | O7-C7-N2-C2 |
| 4 | T | 3501 | NAG | C8-C7-N2-C2 |
| 4 | T | 3501 | NAG | O7-C7-N2-C2 |
| 4 | T | 3501 | NAG | O5-C5-C6-O6 |
| 4 | S | 3501 | NAG | O5-C5-C6-O6 |
| 4 | A | 3501 | NAG | O5-C5-C6-O6 |
| 4 | M | 3501 | NAG | C4-C5-C6-O6 |
| 4 | Q | 3501 | NAG | O5-C5-C6-O6 |
| 4 | I | 3501 | NAG | O5-C5-C6-O6 |
| 4 | O | 3501 | NAG | O5-C5-C6-O6 |
| 4 | T | 3501 | NAG | C4-C5-C6-O6 |
| 4 | N | 3501 | NAG | O5-C5-C6-O6 |
| 4 | M | 3501 | NAG | C1-C2-N2-C7 |

There are no ring outliers.

11 monomers are involved in 13 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 4 | G | 3501 | NAG | 1 | 0 |

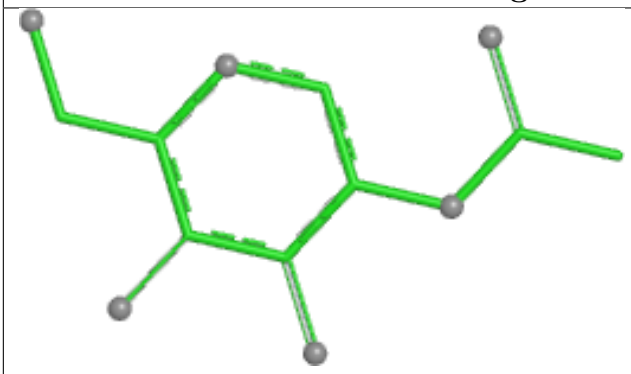
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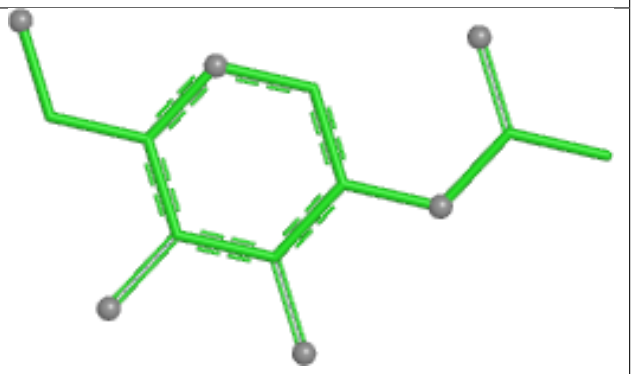
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 4 | C | 3501 | NAG | 1 | 0 |
| 4 | D | 3501 | NAG | 1 | 0 |
| 4 | N | 3501 | NAG | 1 | 0 |
| 4 | R | 3501 | NAG | 1 | 0 |
| 4 | T | 3501 | NAG | 3 | 0 |
| 4 | E | 3501 | NAG | 1 | 0 |
| 4 | K | 3501 | NAG | 1 | 0 |
| 4 | F | 3501 | NAG | 1 | 0 |
| 4 | H | 3501 | NAG | 1 | 0 |
| 4 | I | 3501 | NAG | 1 | 0 |

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

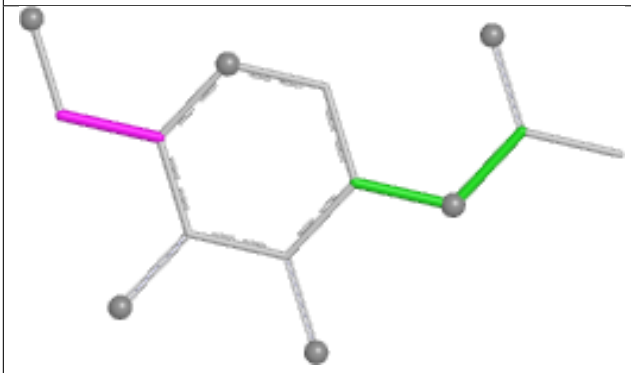
## Ligand NAG G 3501



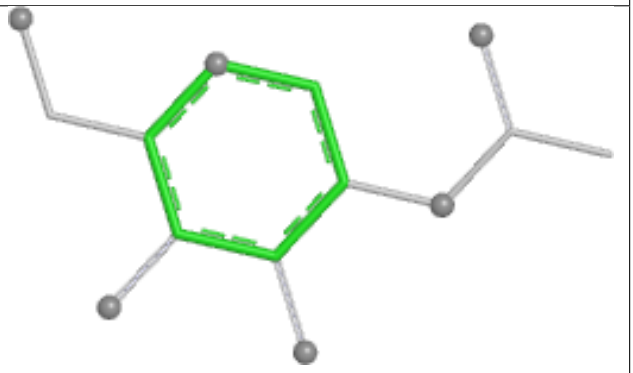
Bond lengths



Bond angles

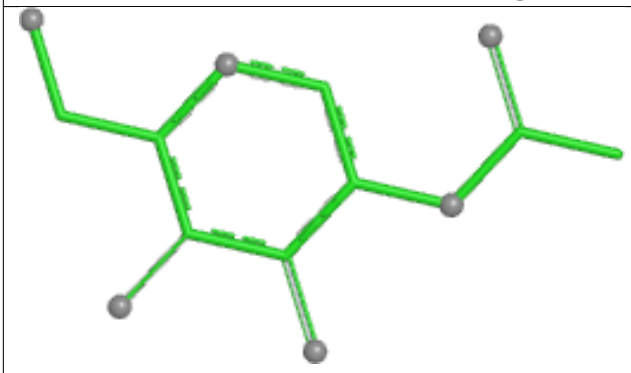


Torsions

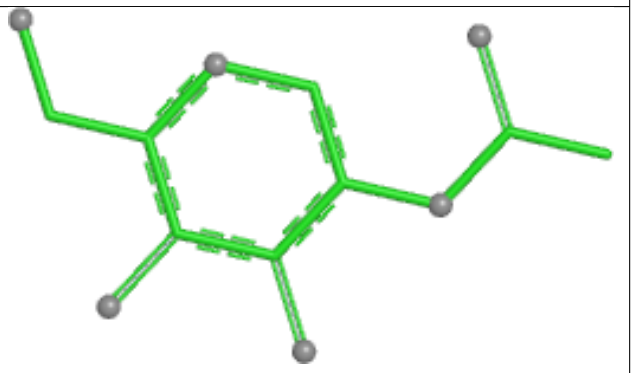


Rings

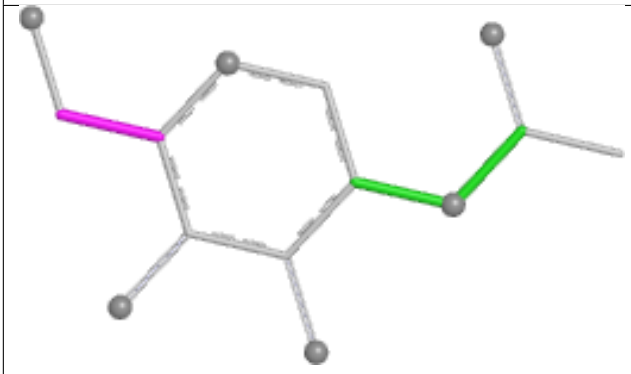
## Ligand NAG C 3501



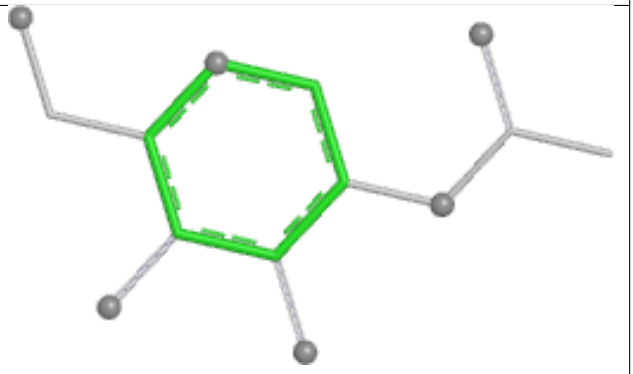
Bond lengths



Bond angles

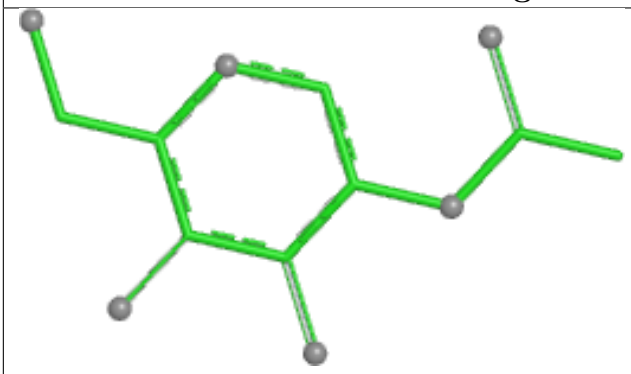


Torsions

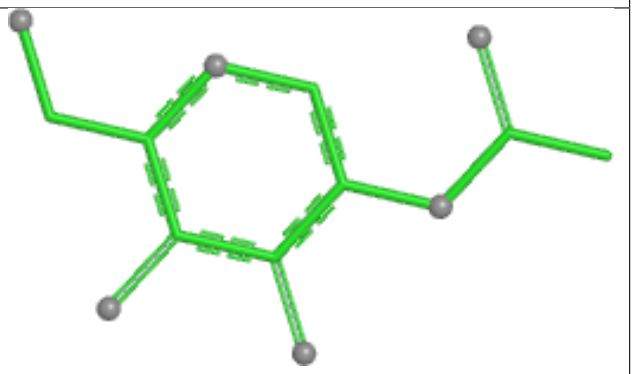


Rings

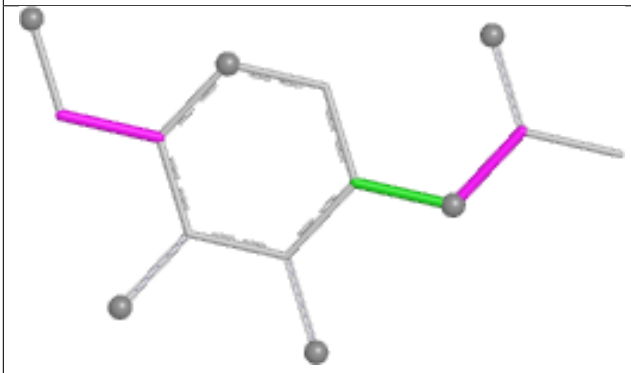
## Ligand NAG L 3501



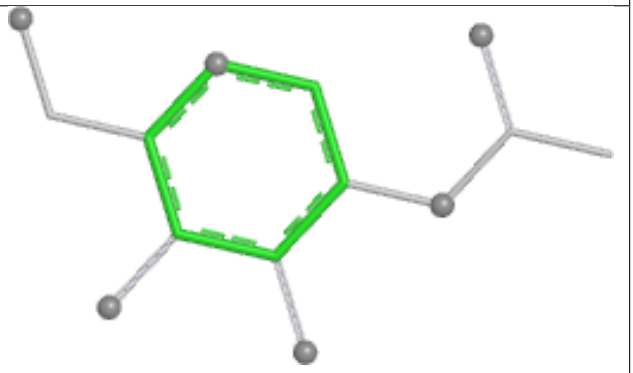
Bond lengths



Bond angles

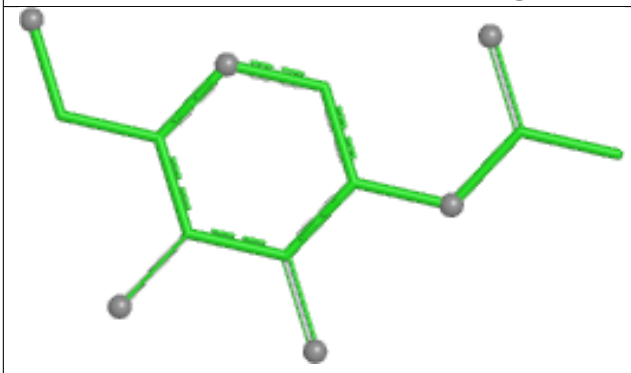


Torsions

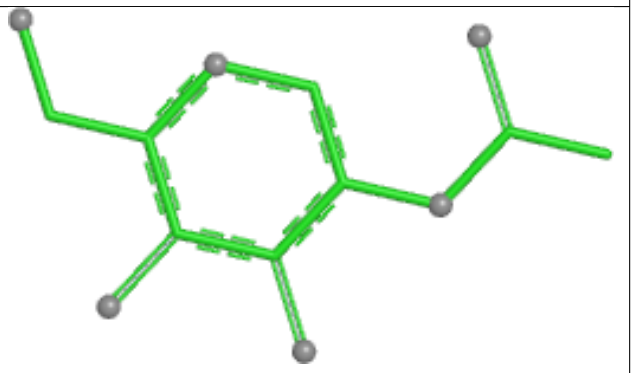


Rings

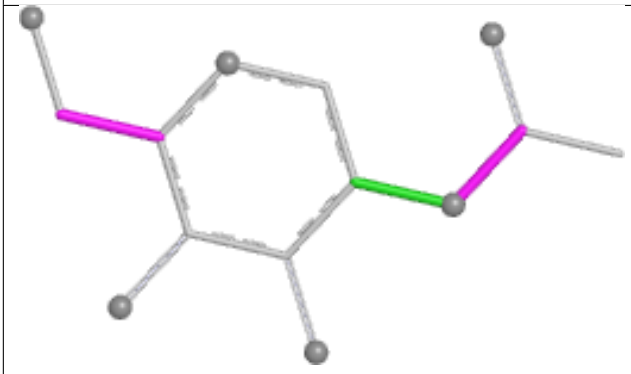
## Ligand NAG D 3501



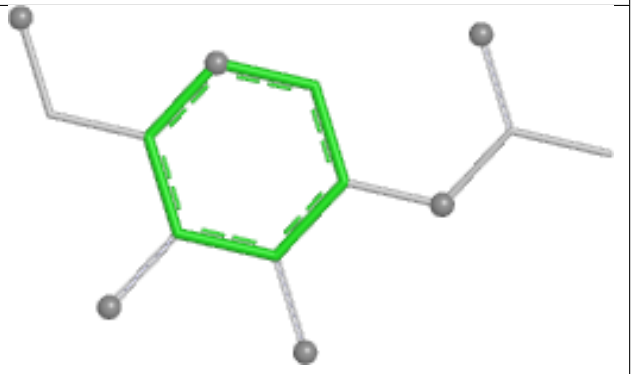
Bond lengths



Bond angles

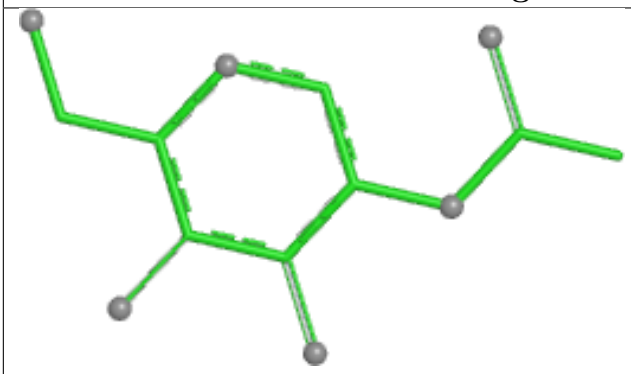


Torsions

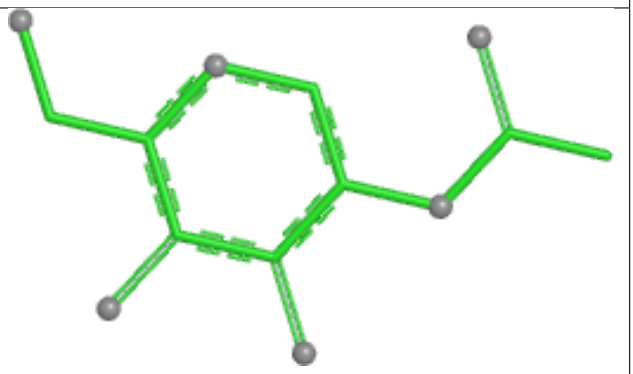


Rings

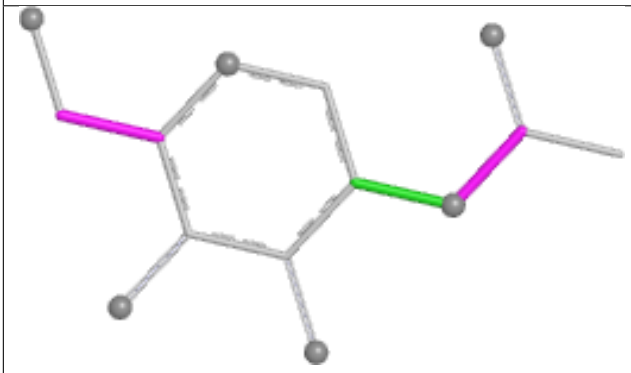
## Ligand NAG P 3501



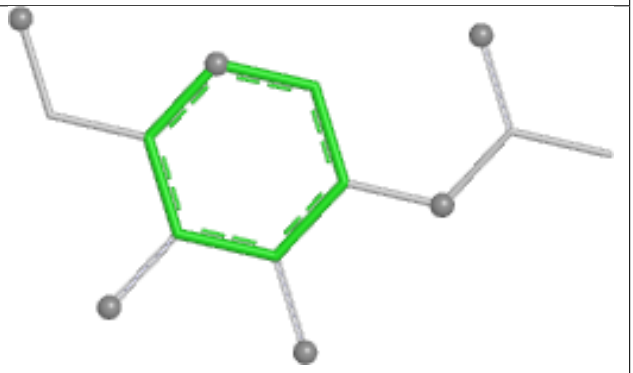
Bond lengths



Bond angles

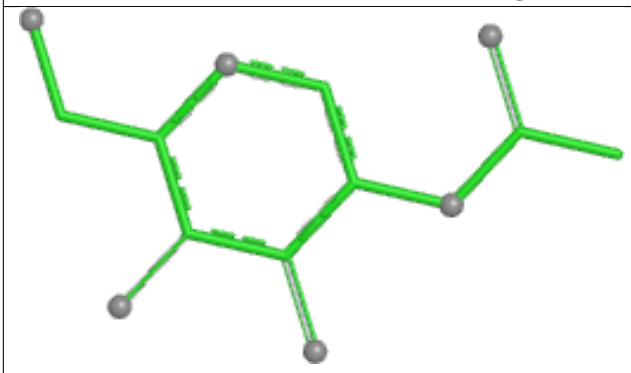


Torsions

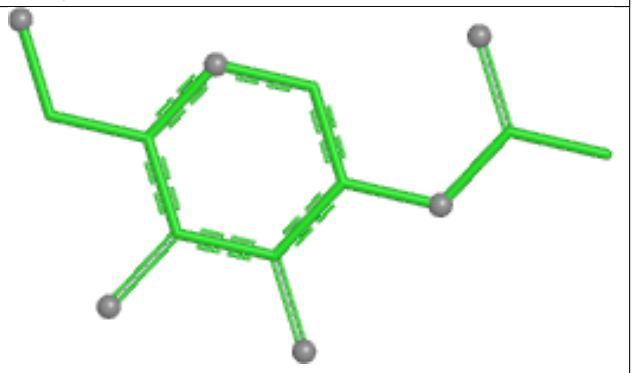


Rings

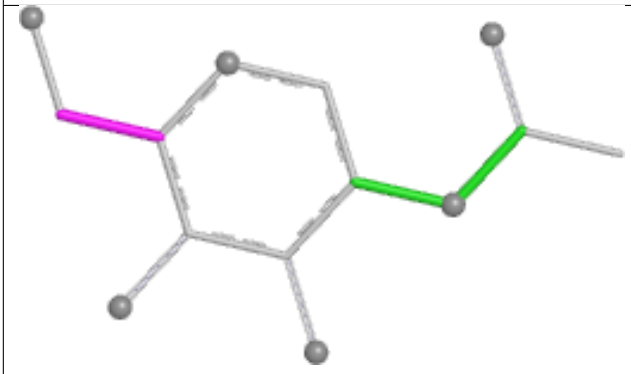
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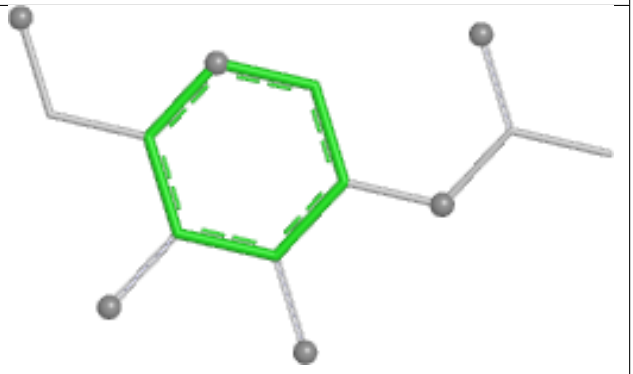
Bond lengths



Bond angles

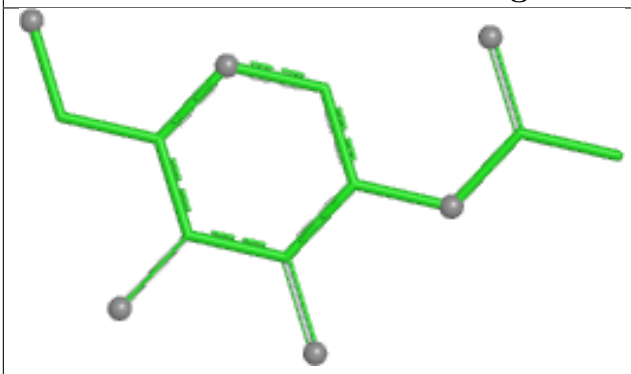


Torsions

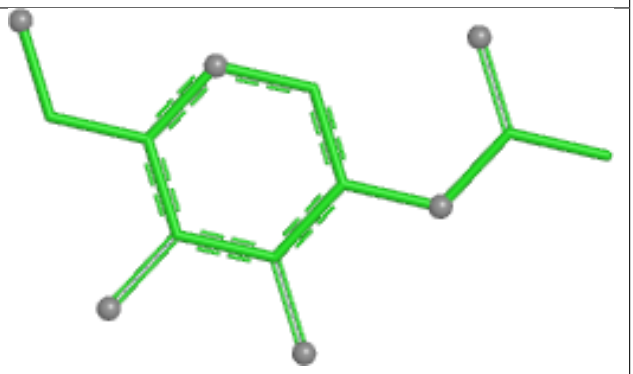


Rings

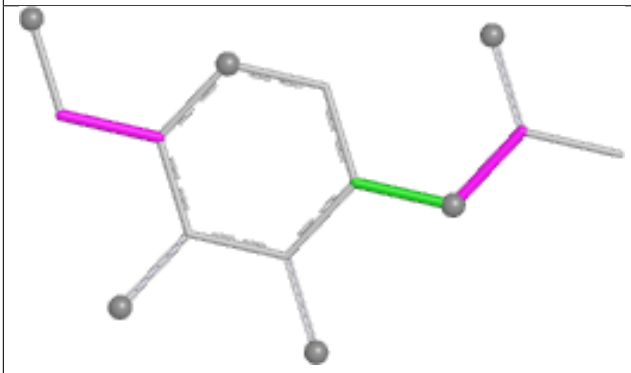
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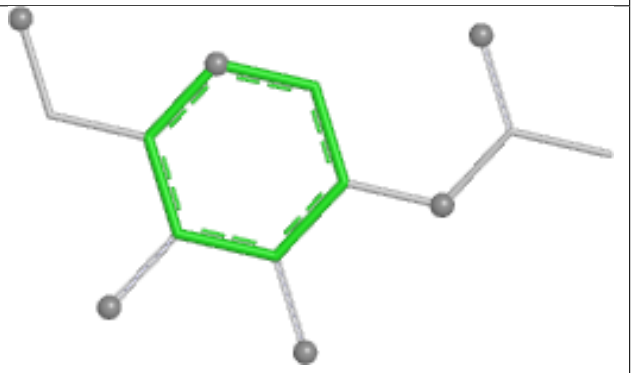
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Bond angles

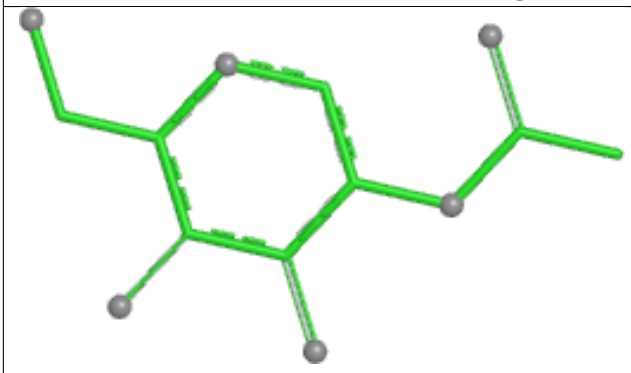


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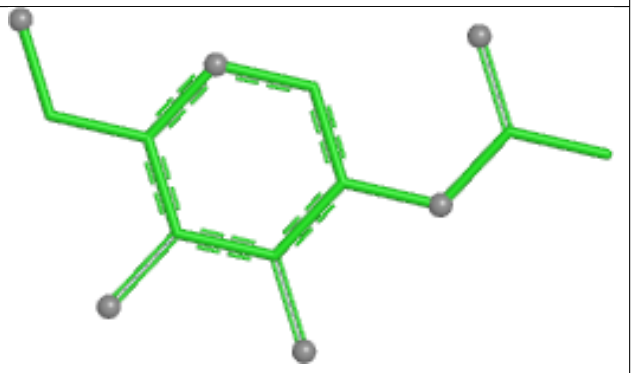


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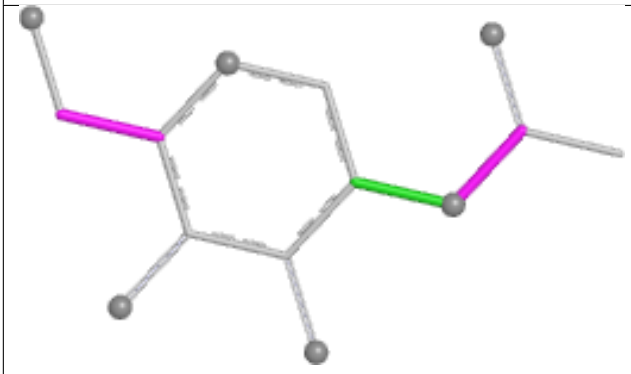
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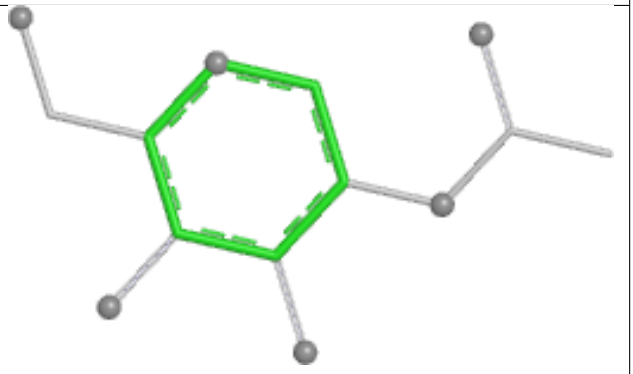
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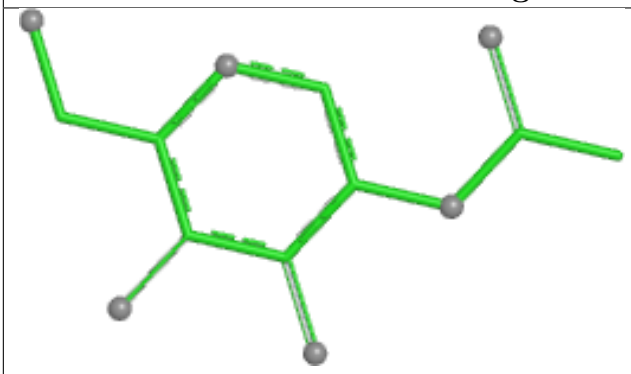


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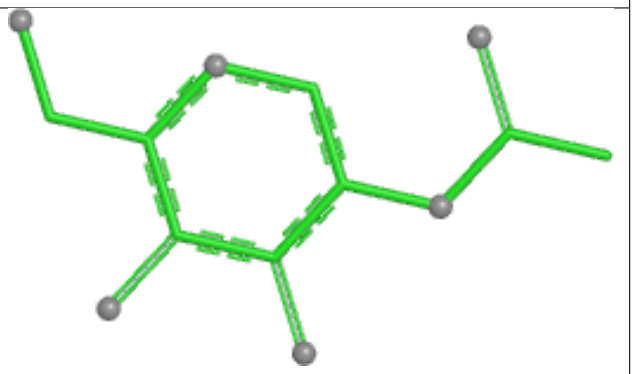


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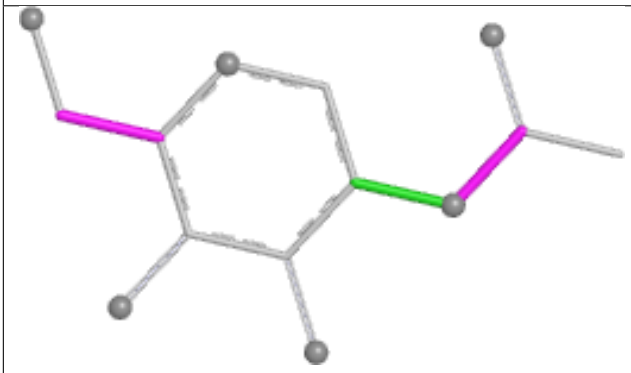
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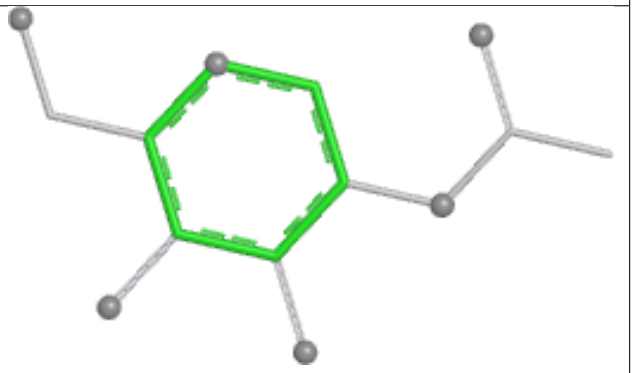
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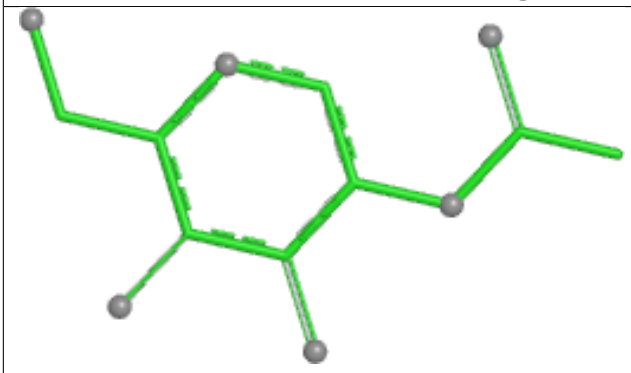


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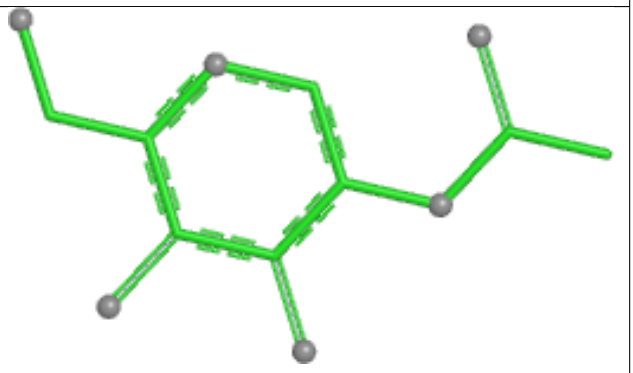


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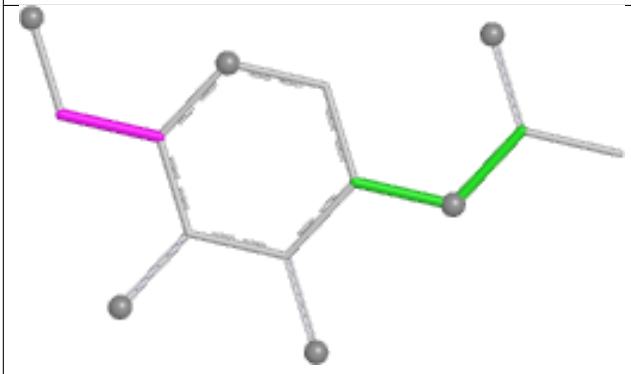
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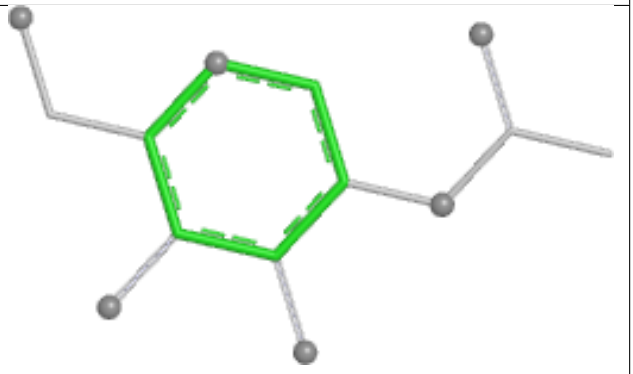
Bond lengths



Bond angles

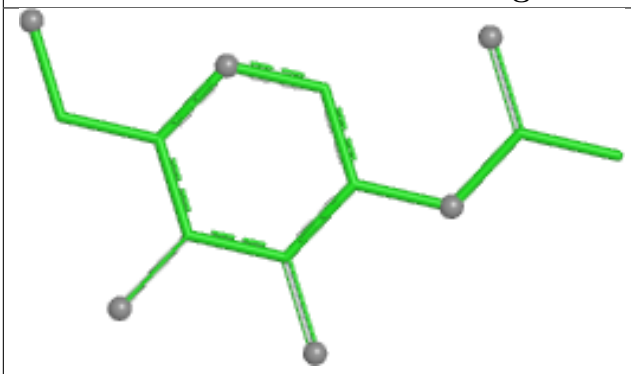


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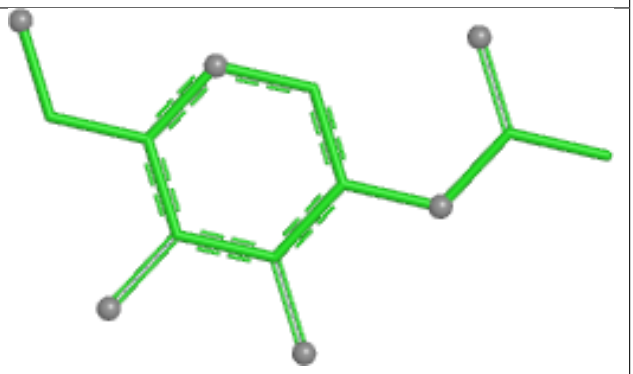


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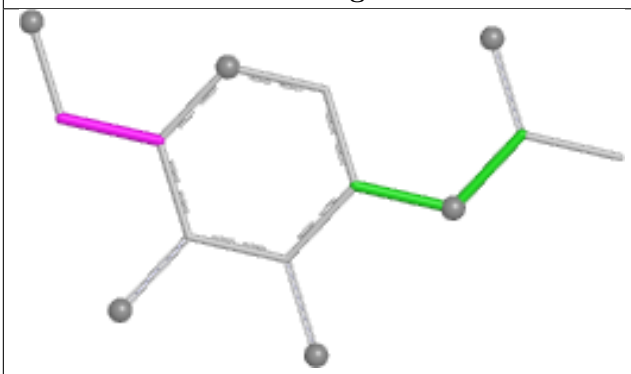
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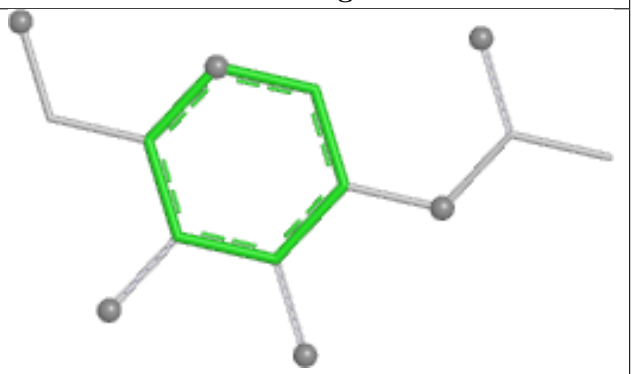
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Bond angles

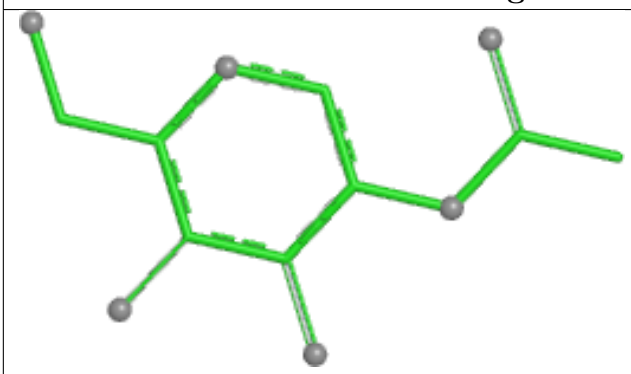


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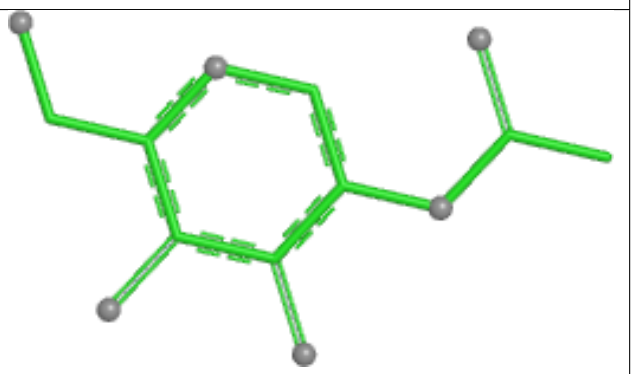


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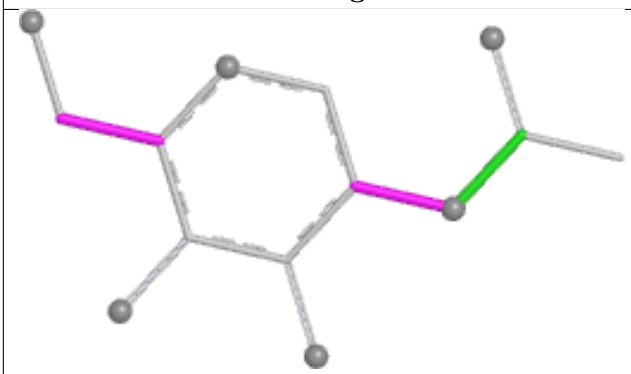
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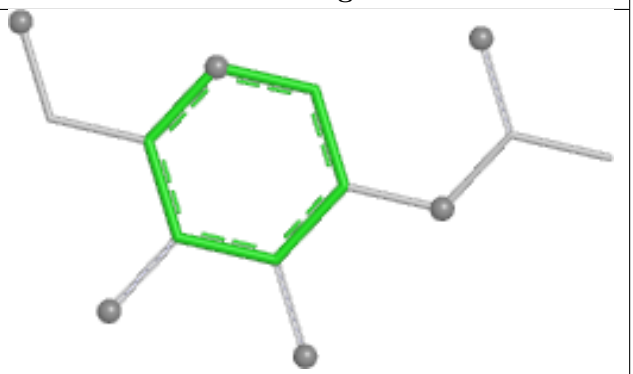
Bond lengths



Bond angles

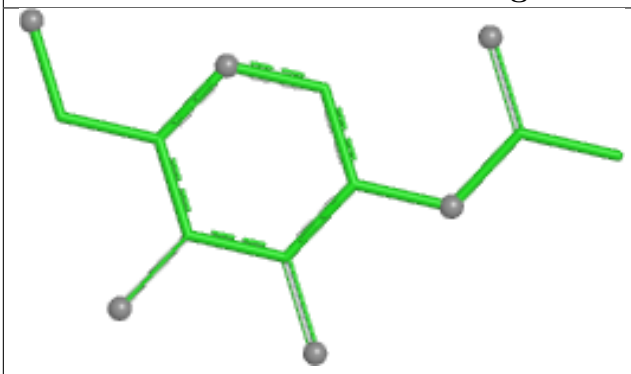


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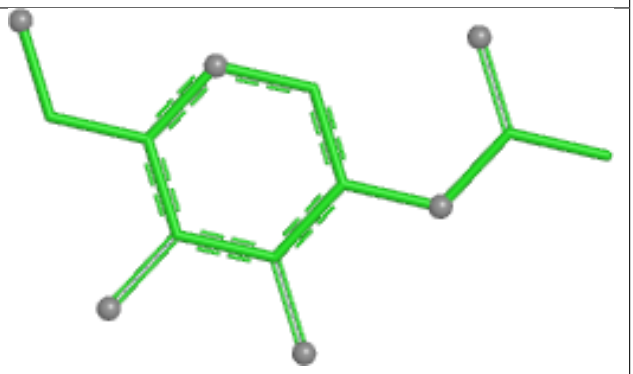


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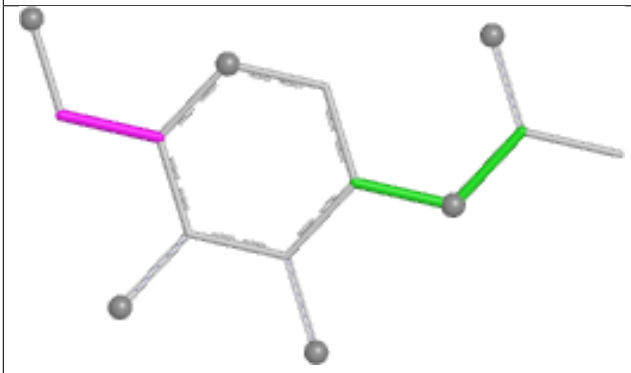
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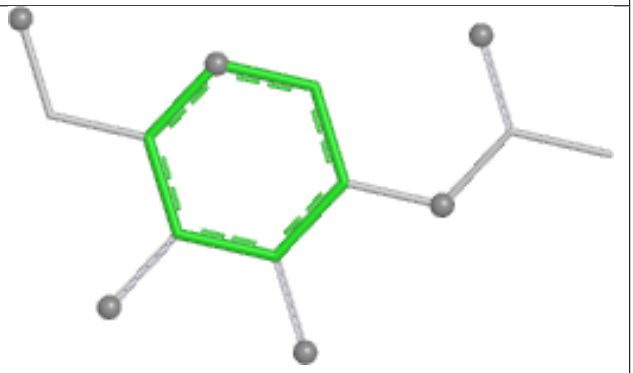
Bond lengths



Bond angles

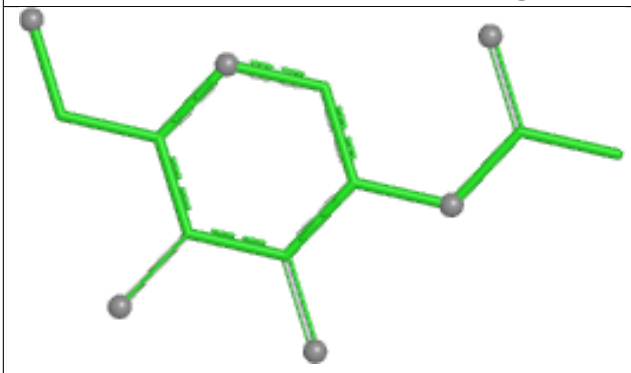


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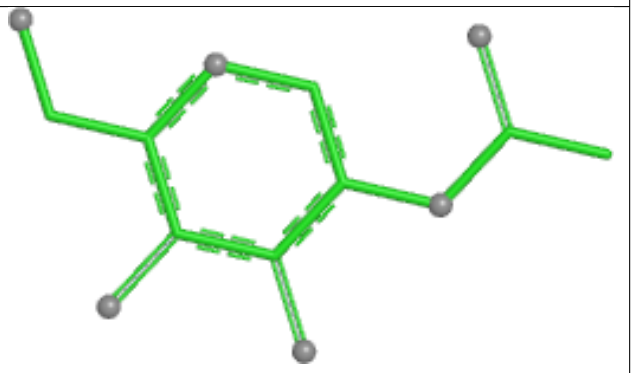


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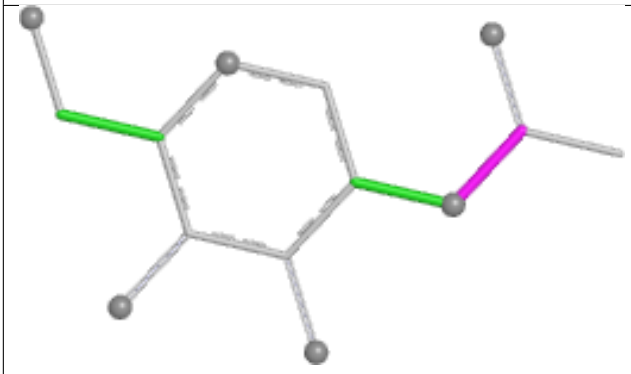
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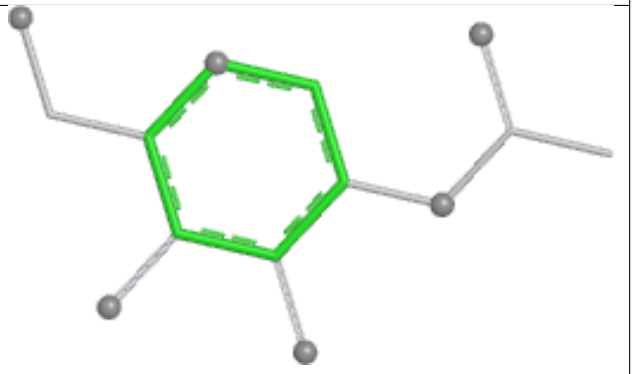
Bond lengths



Bond angles

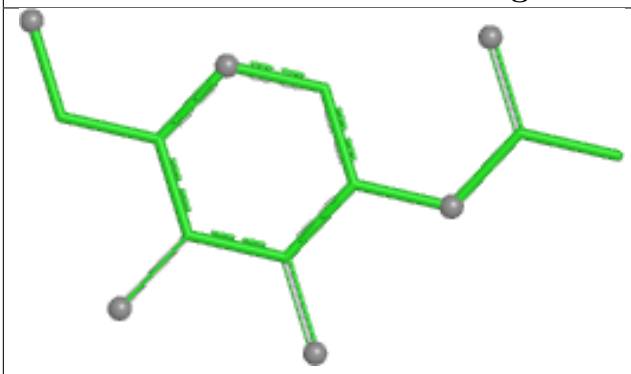


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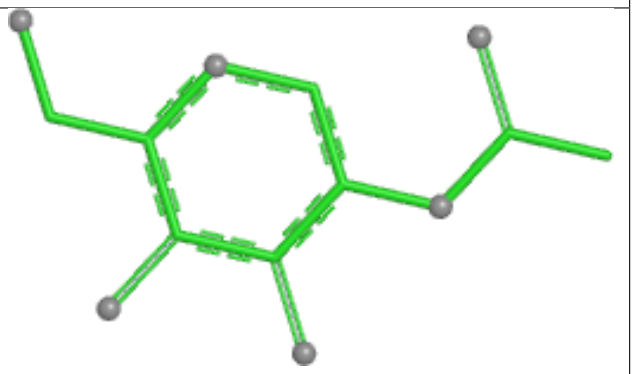


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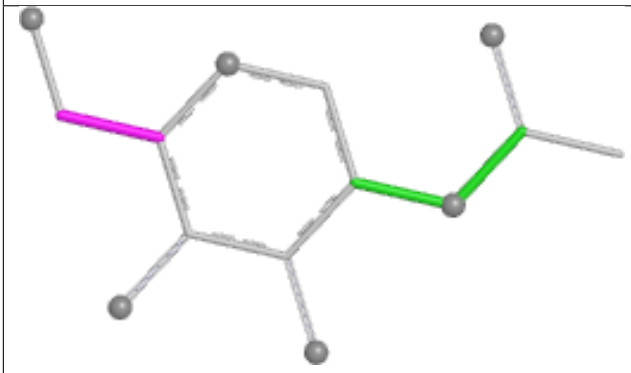
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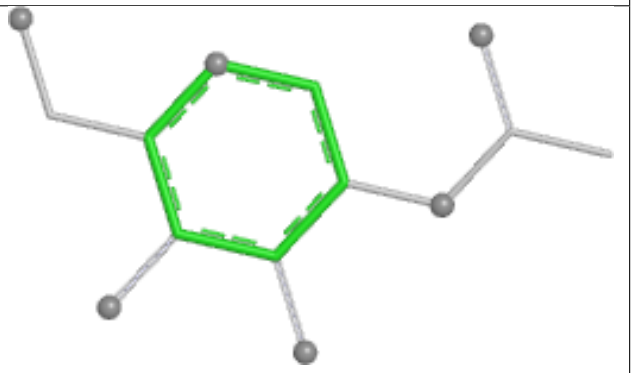
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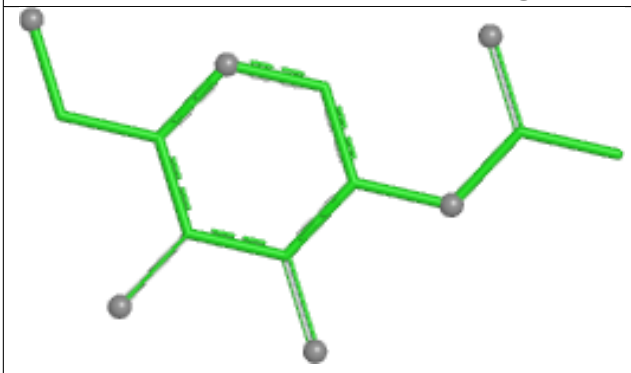


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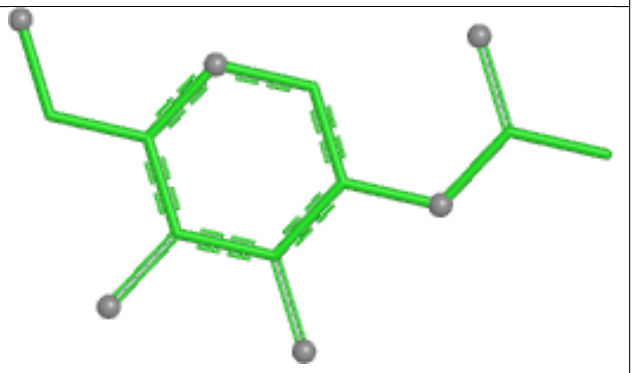


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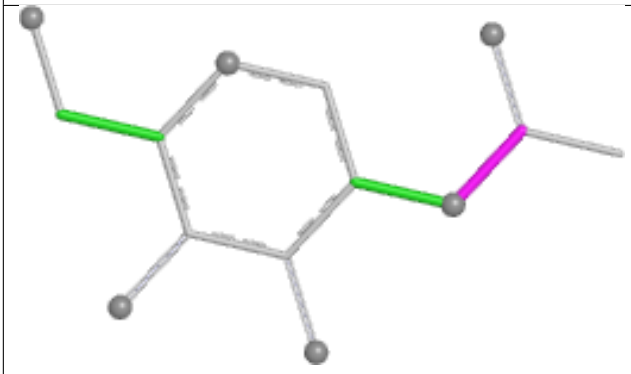
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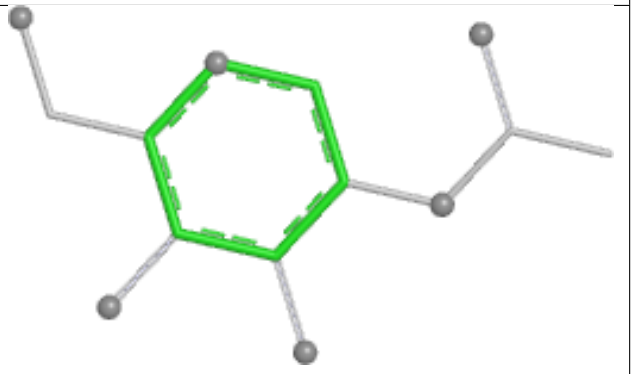
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Bond angles

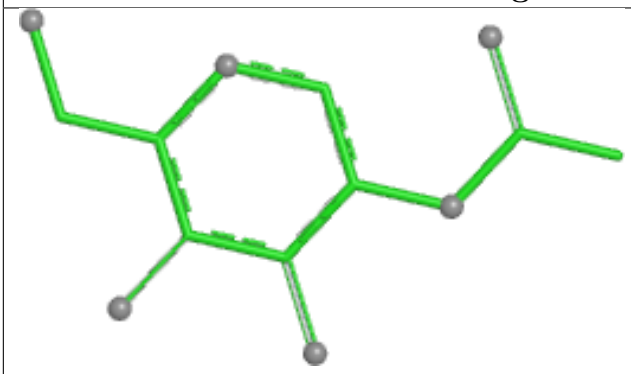


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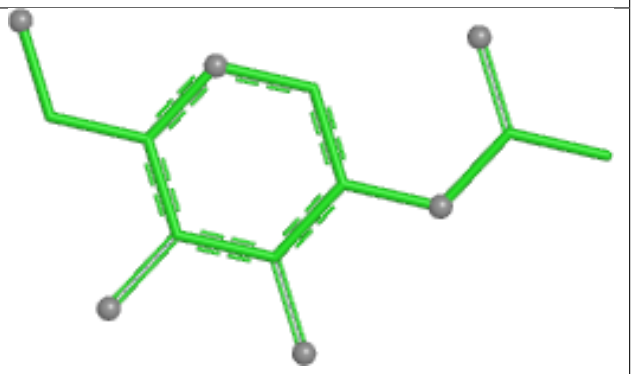


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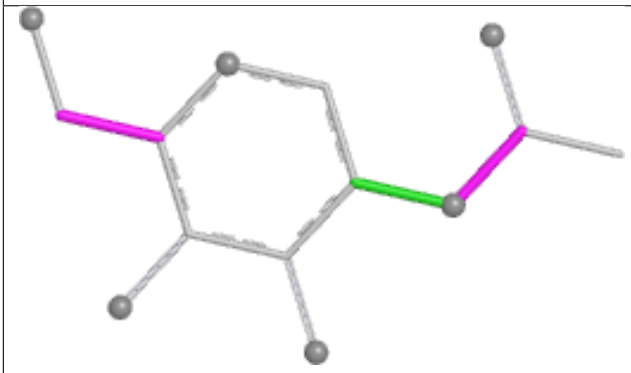
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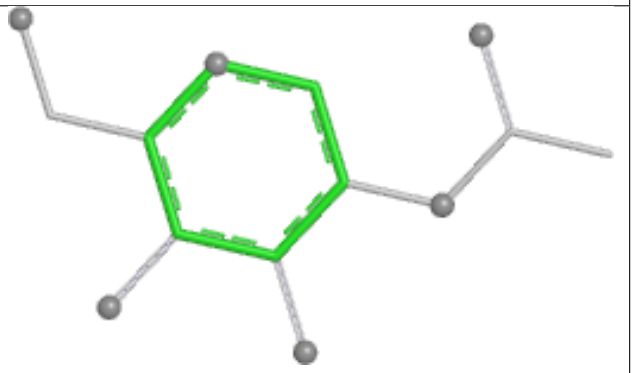
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Bond angles

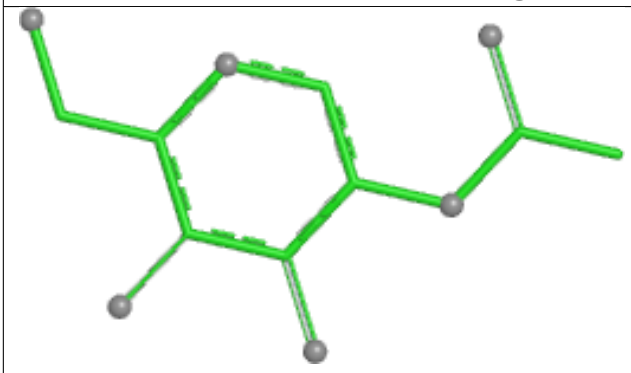


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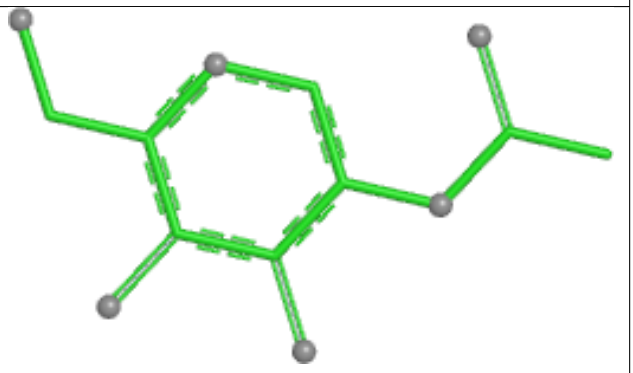


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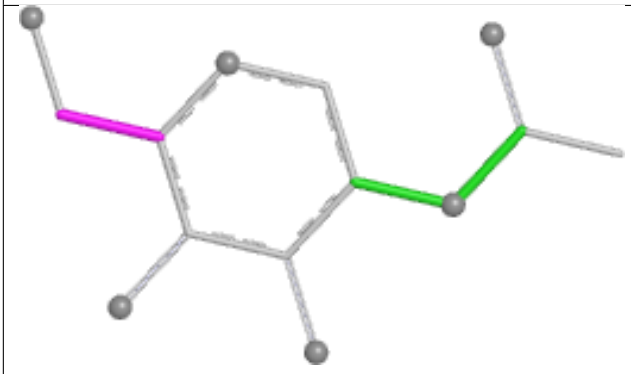
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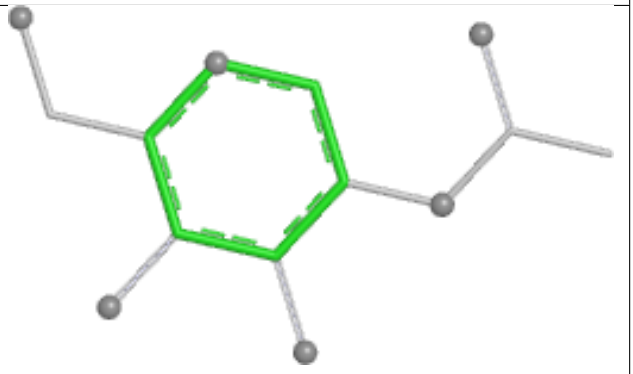
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Bond angles

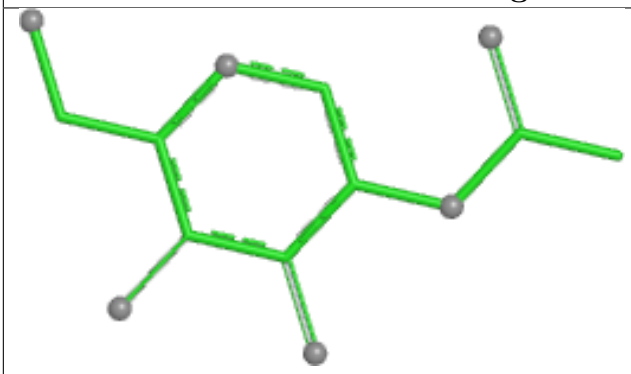


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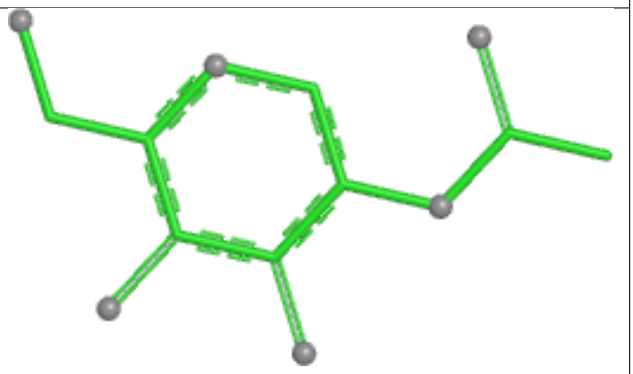


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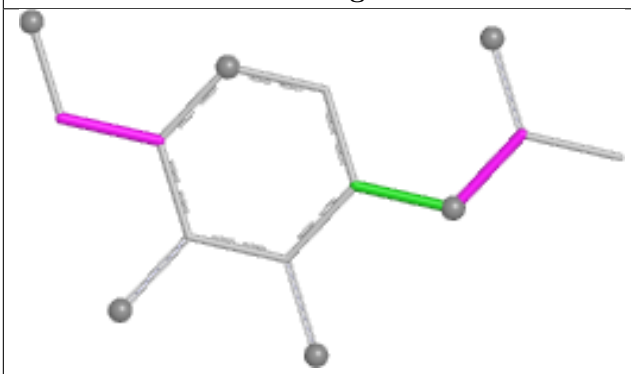
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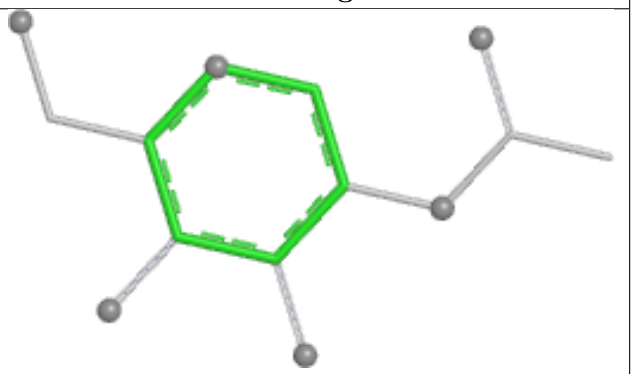
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Bond angles

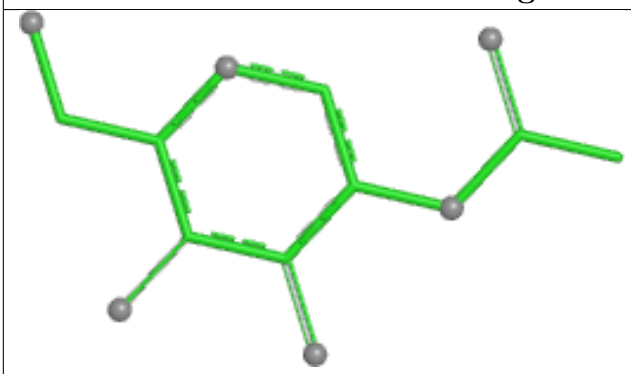


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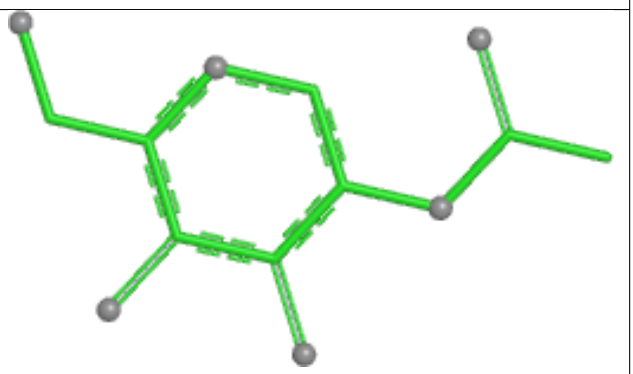


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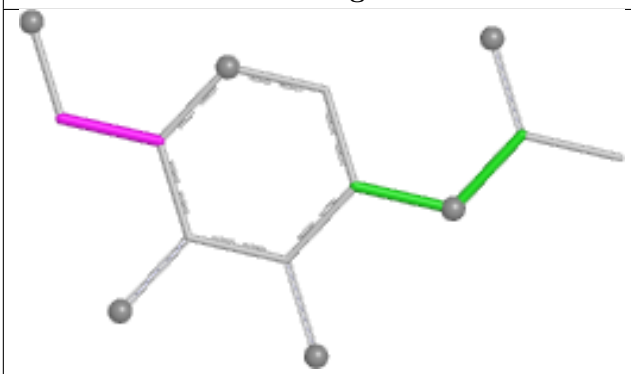
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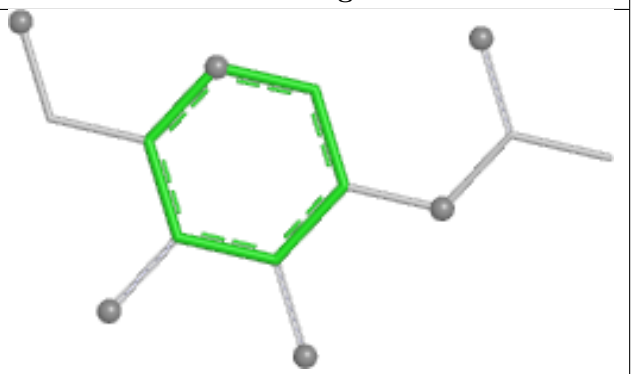
Bond lengths



Bond angles



Torsions



Rings

## 5.7 Other polymers (i)

There are no such residues in this entry.

## 5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

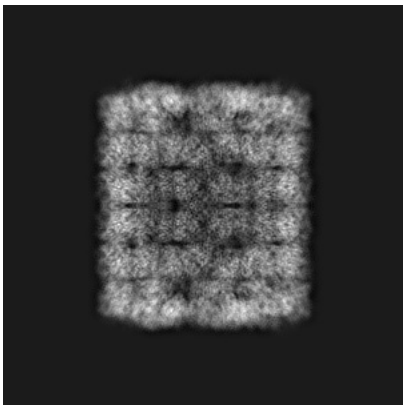
# 6 Map visualisation

This section contains visualisations of the EMDB entry EMD-41586. These allow visual inspection of the internal detail of the map and identification of artifacts.

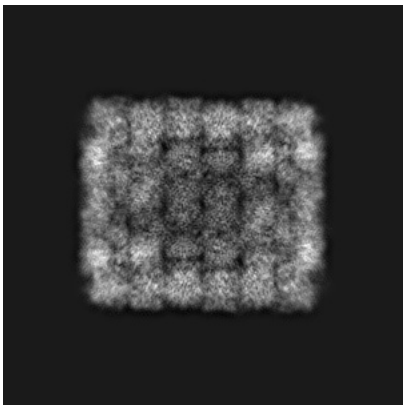
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

## 6.1 Orthogonal projections

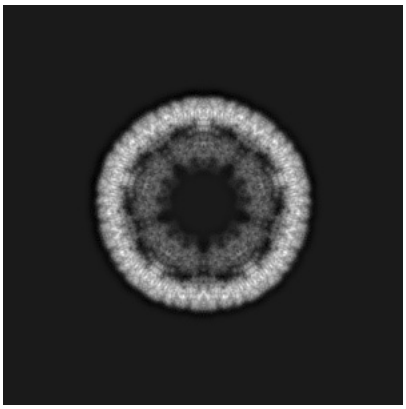
### 6.1.1 Primary map



X

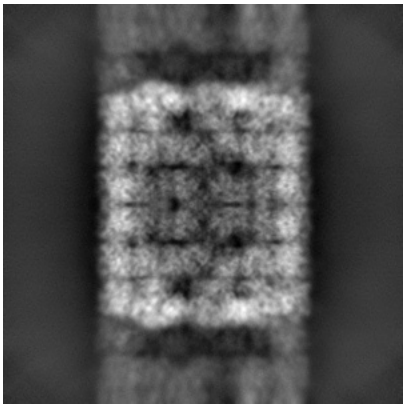


Y

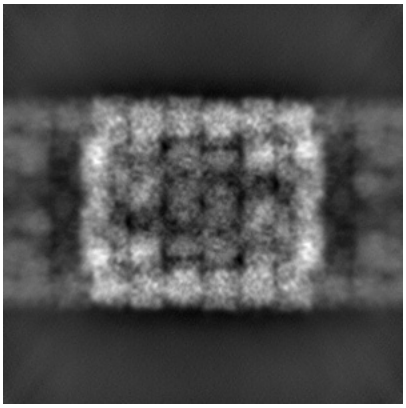


Z

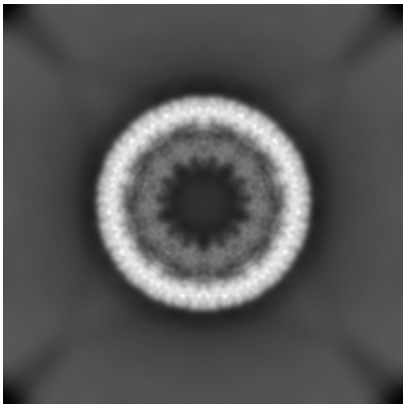
### 6.1.2 Raw map



X



Y

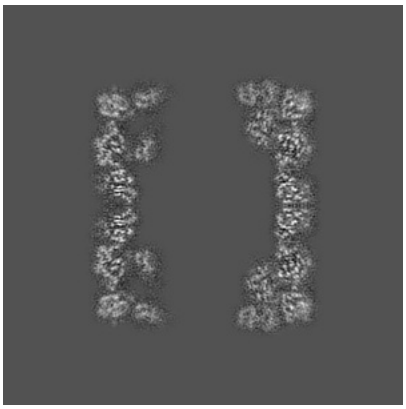


Z

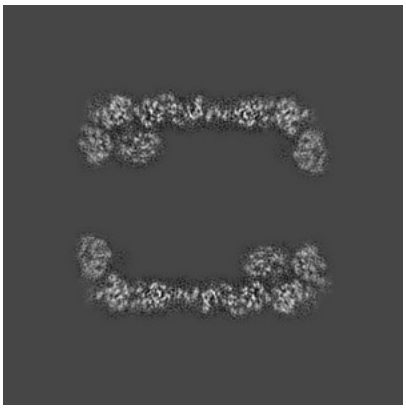
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices (i)

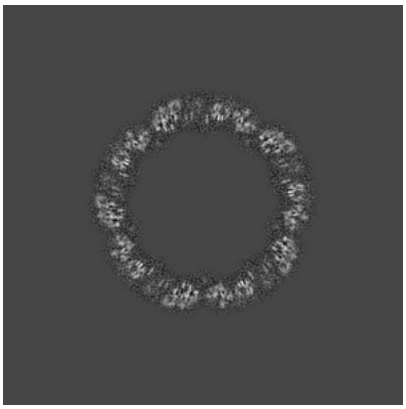
### 6.2.1 Primary map



X Index: 150

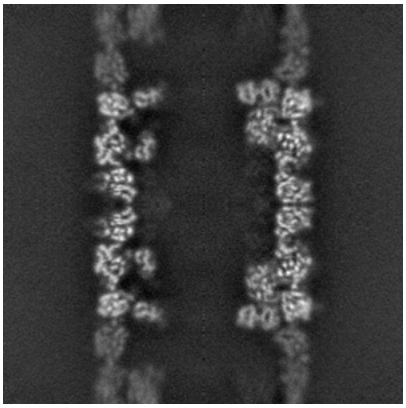


Y Index: 150

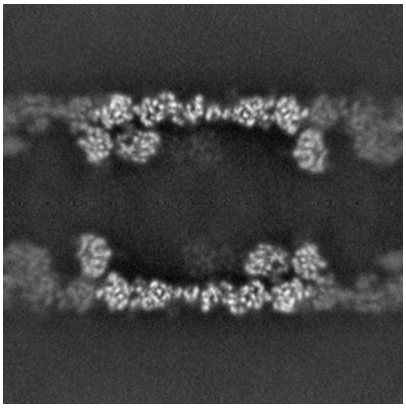


Z Index: 150

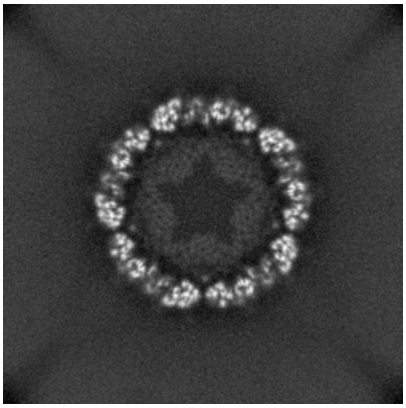
### 6.2.2 Raw map



X Index: 150



Y Index: 150

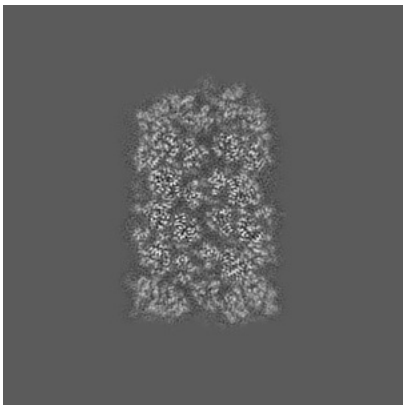


Z Index: 150

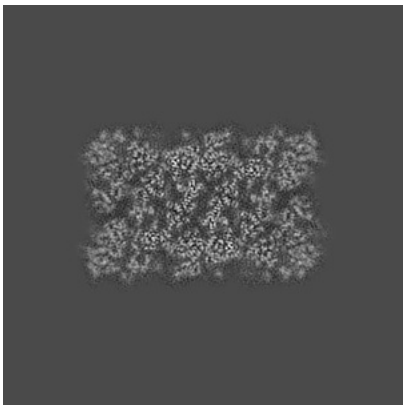
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices (i)

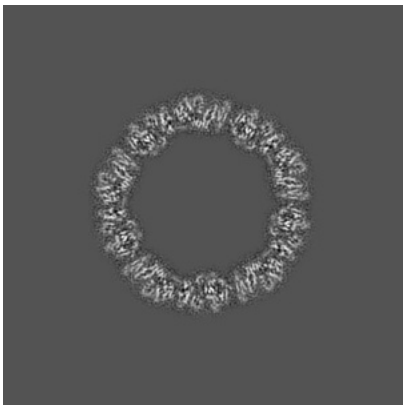
### 6.3.1 Primary map



X Index: 89

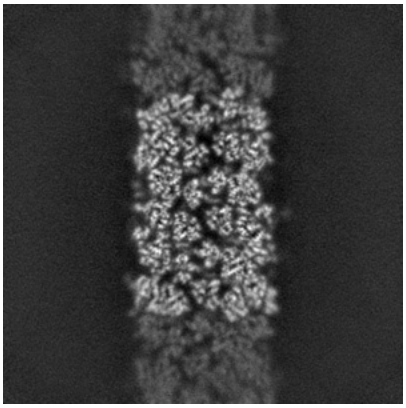


Y Index: 90

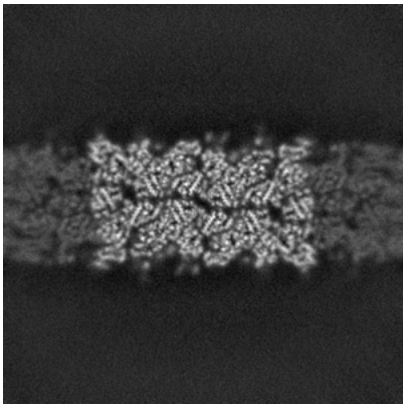


Z Index: 165

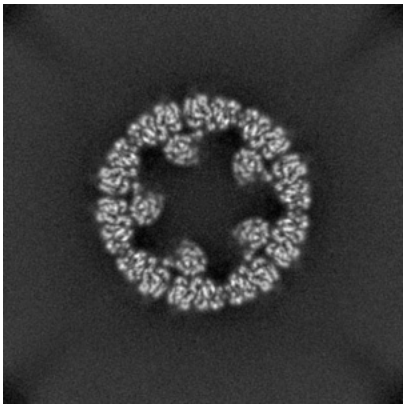
### 6.3.2 Raw map



X Index: 89



Y Index: 85

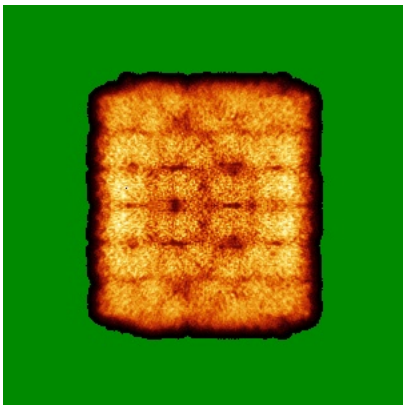


Z Index: 191

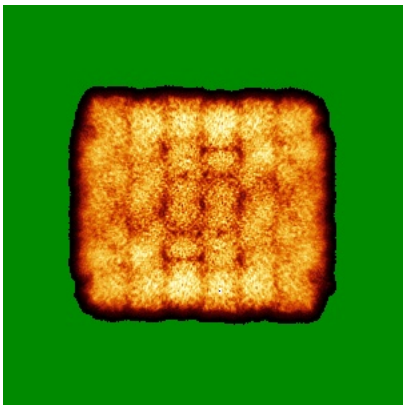
The images above show the largest variance slices of the map in three orthogonal directions.

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

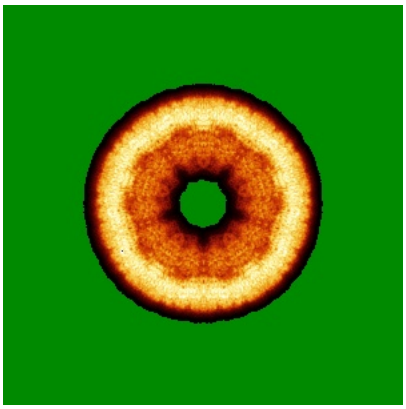
### 6.4.1 Primary map



X

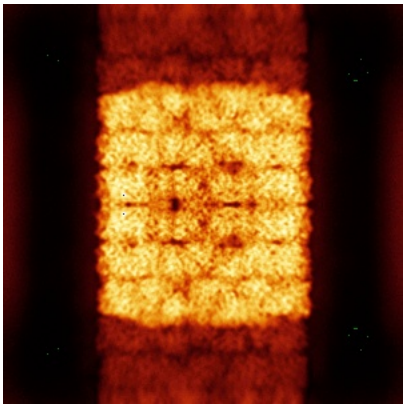


Y

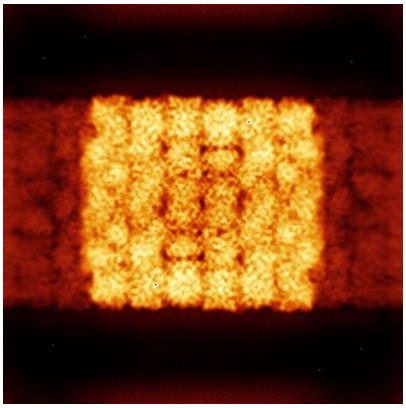


Z

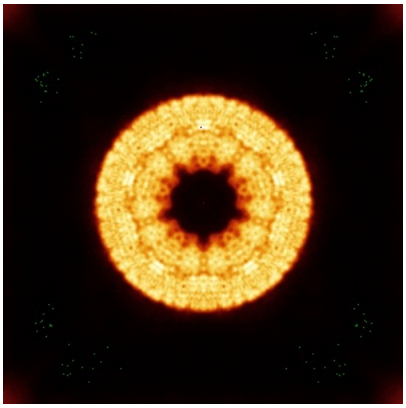
### 6.4.2 Raw map



X



Y



Z

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

## 6.5 Orthogonal surface views (i)

### 6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.637. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



X Y Z

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

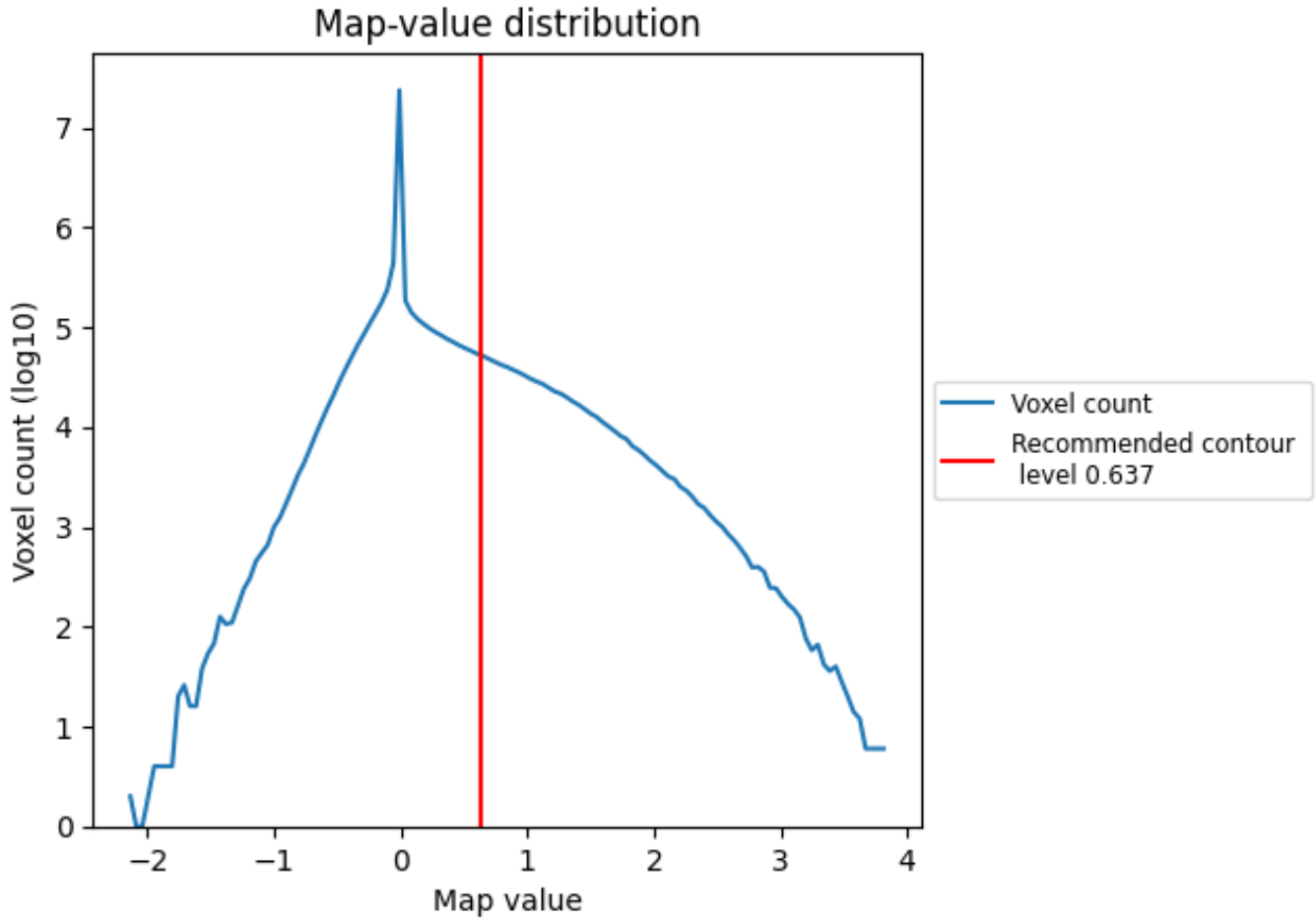
## 6.6 Mask visualisation (i)

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

# 7 Map analysis

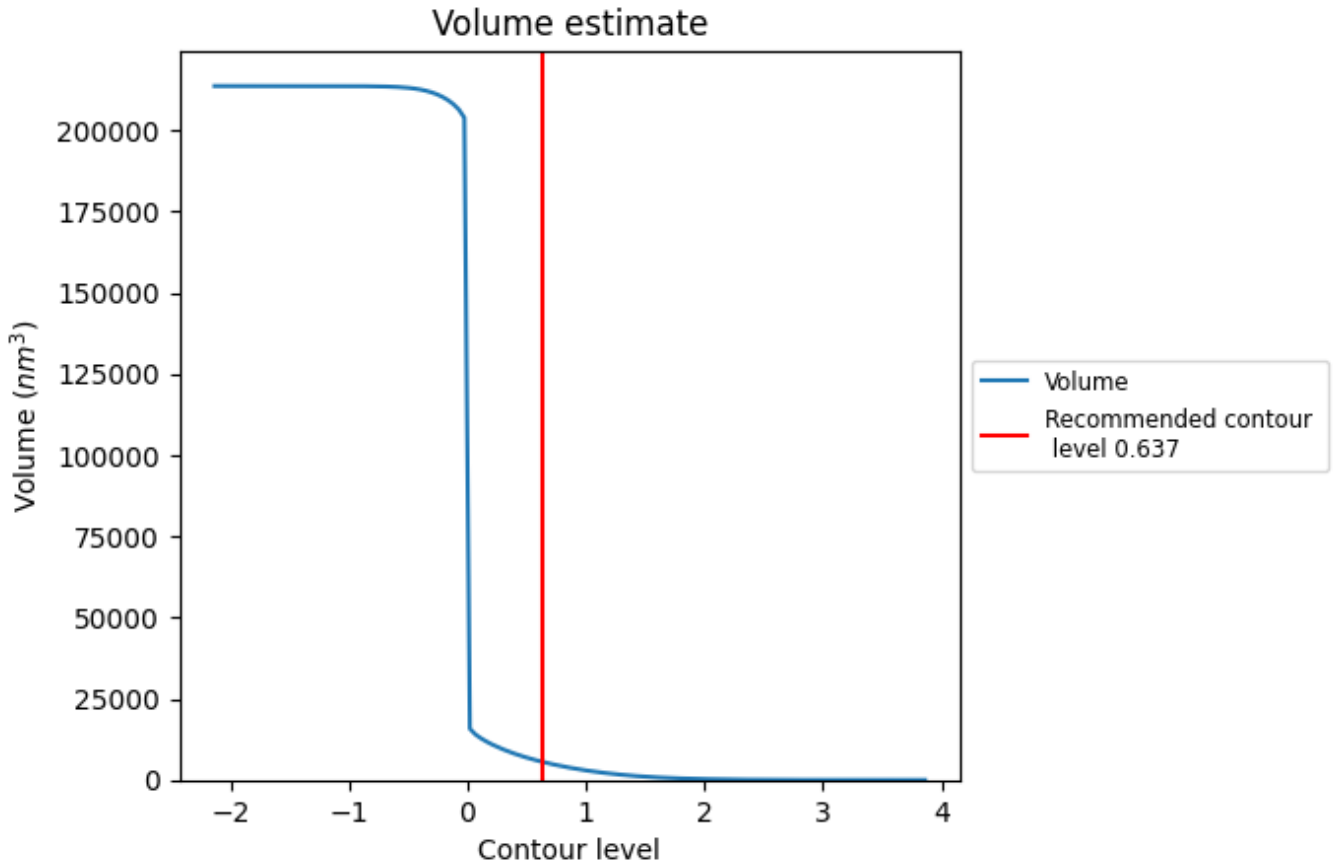
This section contains the results of statistical analysis of the map.

## 7.1 Map-value distribution




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

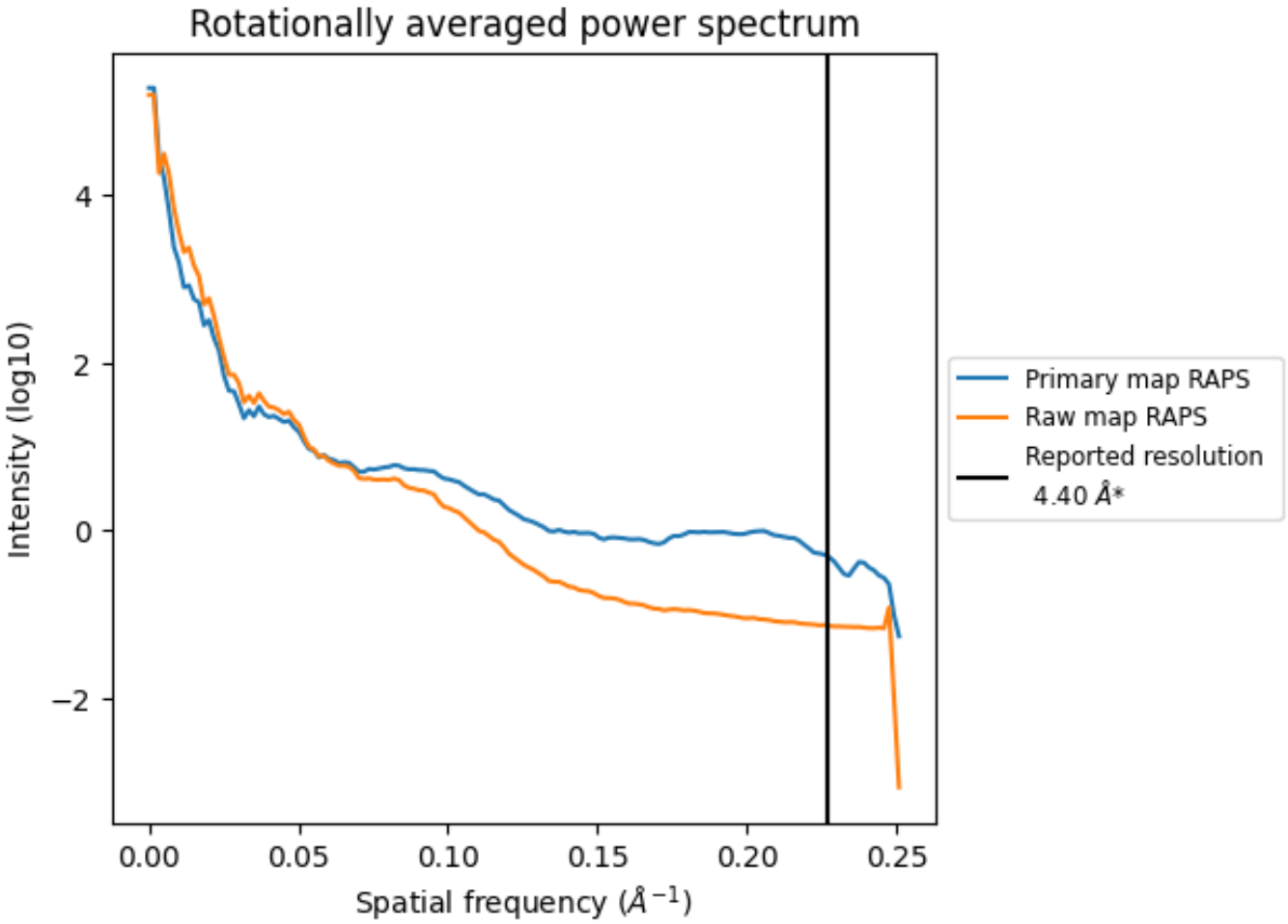
## 7.2 Volume estimate




The volume at the recommended contour level is 5531 $nm^3$; this corresponds to an approximate mass of 4996 kDa.

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

## 7.3 Rotationally averaged power spectrum (i)

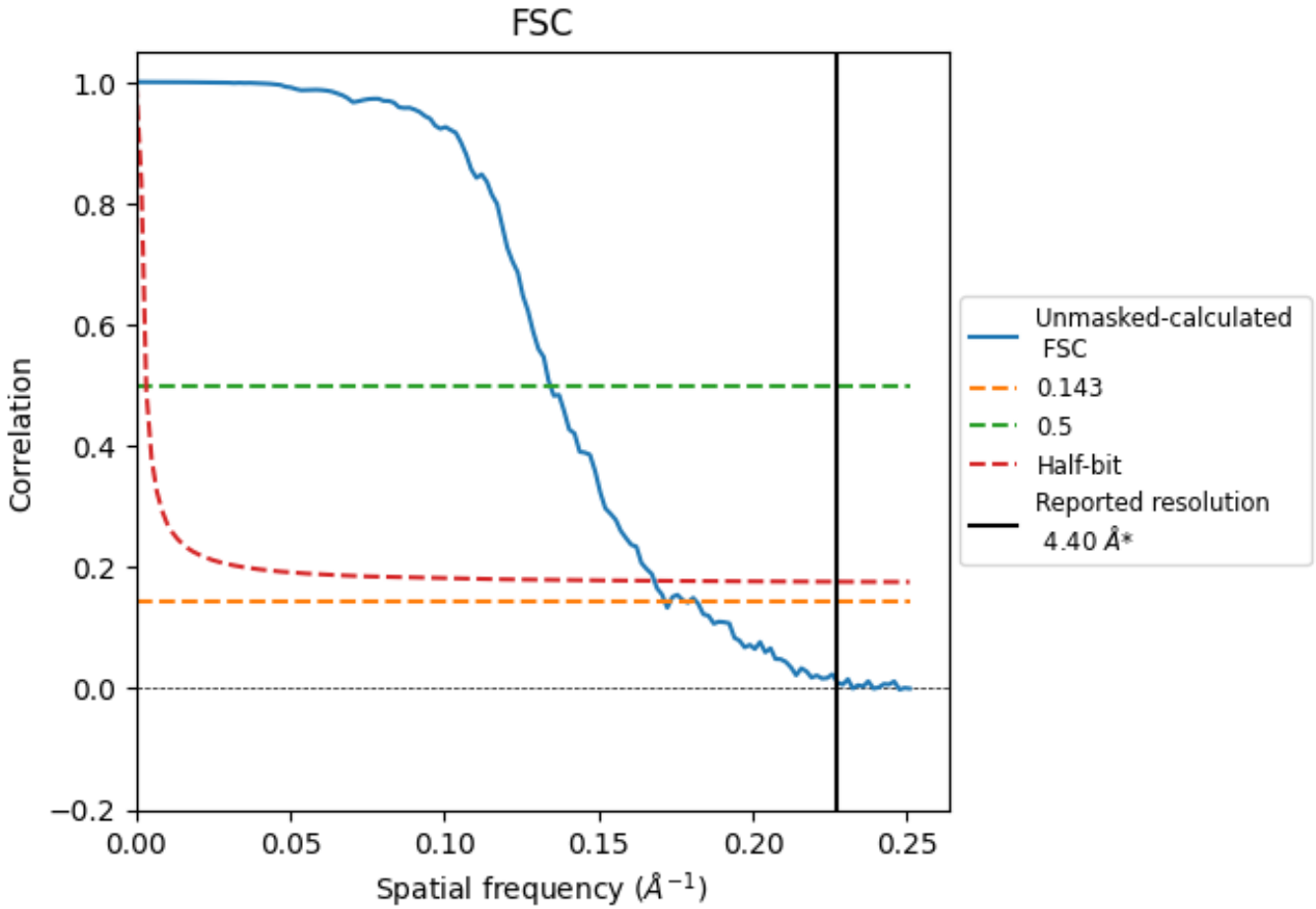



*Reported resolution corresponds to spatial frequency of 0.227 Å$^{-1}$

# 8 Fourier-Shell correlation

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

## 8.1 FSC




*Reported resolution corresponds to spatial frequency of 0.227 Å$^{-1}$

## 8.2 Resolution estimates (i)

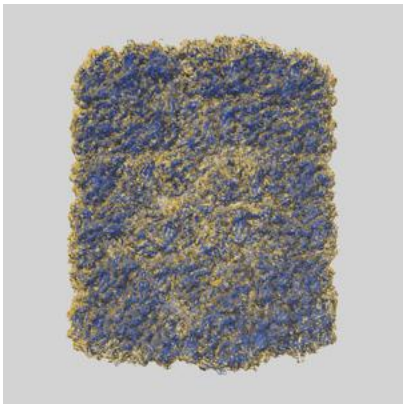
| Resolution estimate (Å) | Estimation criterion (FSC cut-off) | | |
|---|---|---|---|
| | 0.143 | 0.5 | Half-bit |
| Reported by author | 4.40 | - | - |
| Author-provided FSC curve | - | - | - |
| Unmasked-calculated* | 5.83 | 7.45 | 5.95 |

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 5.83 differs from the reported value 4.4 by more than 10 %

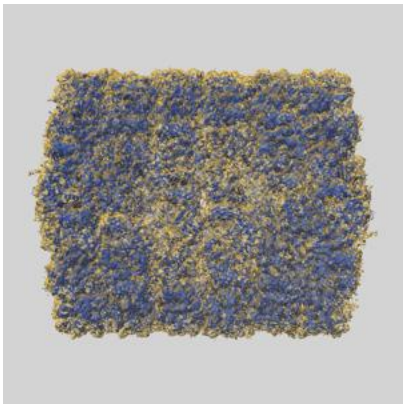
# 9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-41586 and PDB model 8TRZ. Per-residue inclusion information can be found in section 3 on page 16.

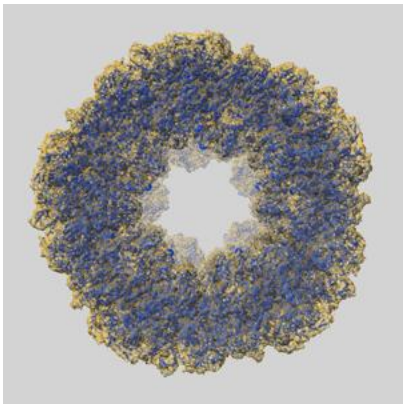
## 9.1 Map-model overlay



X



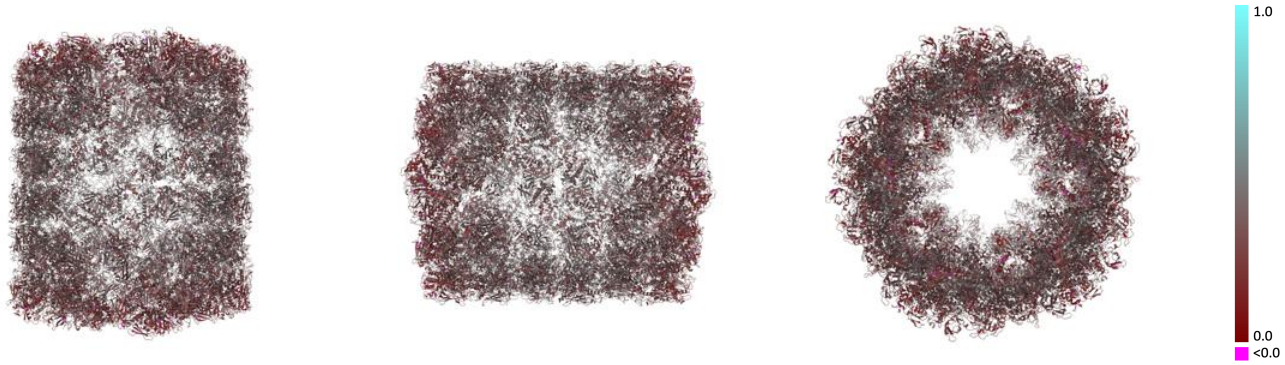
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.637 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

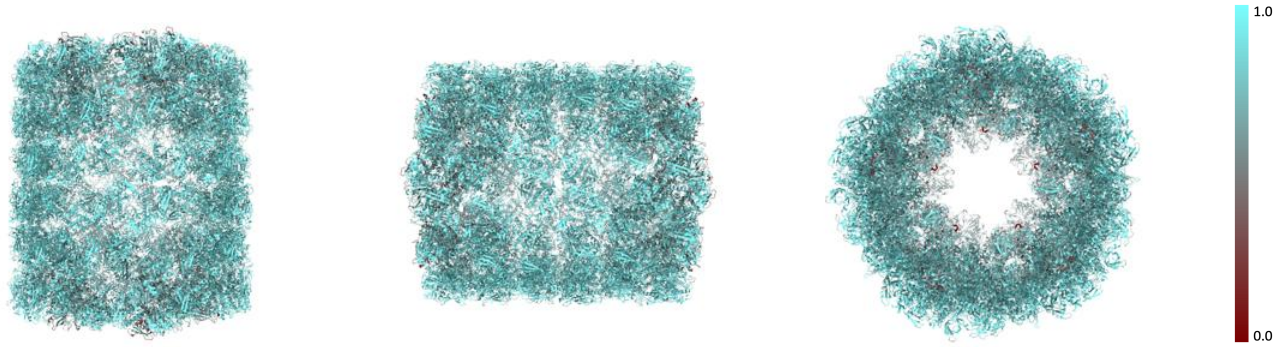
## 9.2 Q-score mapped to coordinate model




X Y Z

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

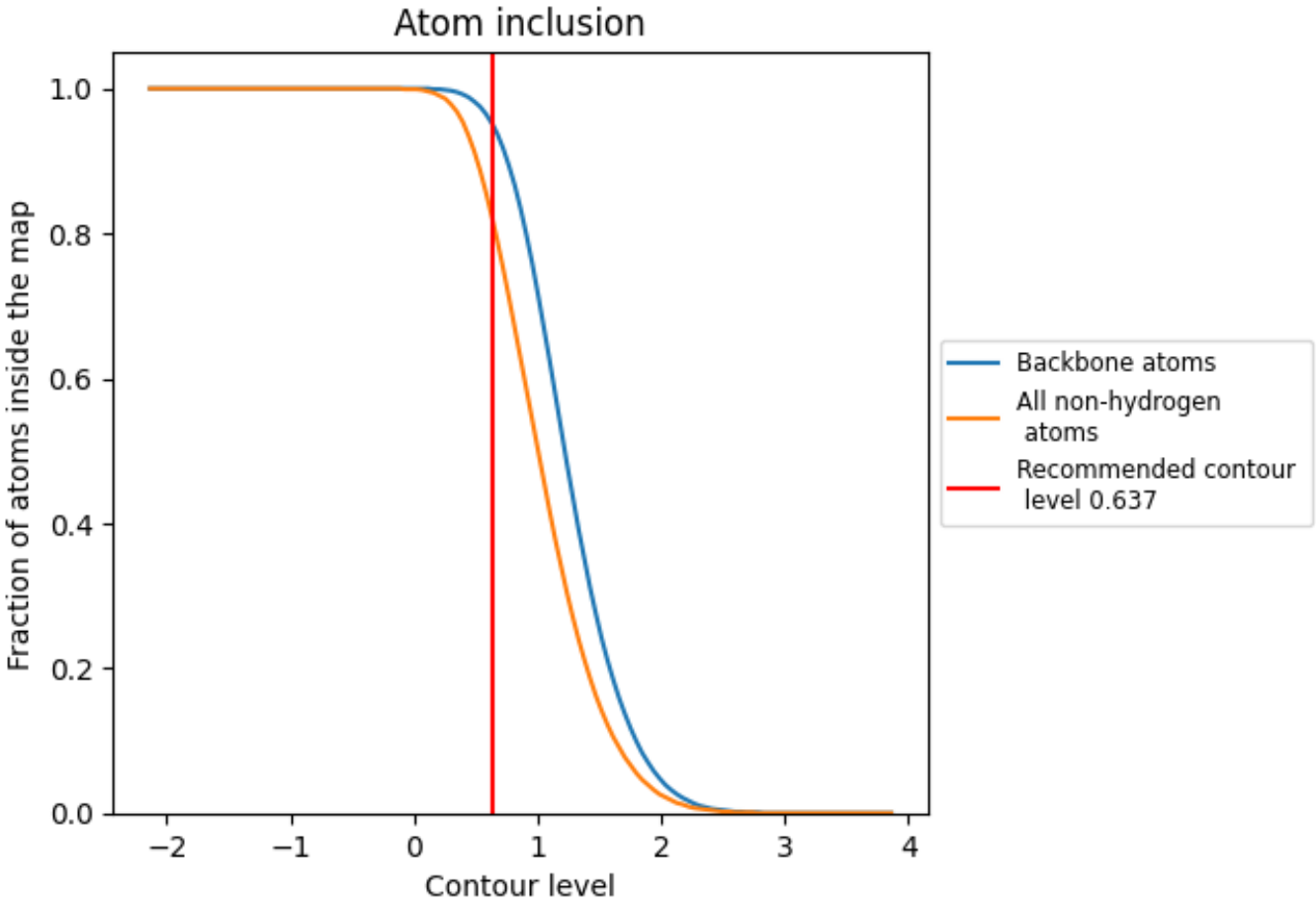
## 9.3 Atom inclusion mapped to coordinate model




X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.637).

## 9.4 Atom inclusion (i)




At the recommended contour level, 95% of all backbone atoms, 82% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.637) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion | Q-score |
|---|---|---|
| All | 0.8180 | 0.3460 |
| 0 | 0.8570 | 0.4210 |
| 0A | 0.6430 | 0.2730 |
| 1 | 0.8460 | 0.4420 |
| 1A | 0.9490 | 0.4190 |
| 2 | 0.7140 | 0.3260 |
| 2A | 0.7440 | 0.3960 |
| 3 | 0.9490 | 0.4180 |
| 3A | 0.8210 | 0.4200 |
| 4 | 0.7440 | 0.3860 |
| 4A | 0.8460 | 0.3690 |
| 5 | 0.8210 | 0.4350 |
| 5A | 0.7500 | 0.4130 |
| 6 | 0.8460 | 0.4270 |
| 7 | 0.7500 | 0.4250 |
| 8 | 0.9640 | 0.4330 |
| 9 | 0.9490 | 0.4620 |
| A | 0.8210 | 0.3590 |
| AA | 0.8570 | 0.4470 |
| B | 0.8180 | 0.3320 |
| BA | 0.8460 | 0.4330 |
| C | 0.8210 | 0.3580 |
| CA | 0.6070 | 0.2600 |
| D | 0.8160 | 0.3330 |
| DA | 0.9490 | 0.4330 |
| E | 0.8220 | 0.3590 |
| EA | 0.7950 | 0.4410 |
| F | 0.8140 | 0.3320 |
| FA | 0.8460 | 0.4350 |
| G | 0.8200 | 0.3580 |
| GA | 0.8210 | 0.4590 |
| H | 0.8150 | 0.3320 |
| HA | 0.7140 | 0.4060 |
| I | 0.8200 | 0.3580 |
| IA | 0.9290 | 0.4410 |




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| Chain | Atom inclusion | Q-score |
|---|---|---|
| J | 0.8190 | 0.3320 |
| JA | 0.9490 | 0.4600 |
| K | 0.8210 | 0.3570 |
| KA | 0.8570 | 0.3900 |
| L | 0.8140 | 0.3300 |
| LA | 0.8210 | 0.4390 |
| M | 0.8190 | 0.3580 |
| MA | 0.7500 | 0.3090 |
| N | 0.8160 | 0.3310 |
| NA | 0.9230 | 0.3900 |
| O | 0.8220 | 0.3600 |
| OA | 0.7440 | 0.3850 |
| P | 0.8180 | 0.3320 |
| PA | 0.8210 | 0.4320 |
| Q | 0.8210 | 0.3580 |
| QA | 0.8210 | 0.4470 |
| R | 0.8180 | 0.3330 |
| RA | 0.7500 | 0.4130 |
| S | 0.8210 | 0.3590 |
| SA | 0.8570 | 0.4200 |
| T | 0.8120 | 0.3320 |
| TA | 0.9490 | 0.4490 |
| U | 0.8930 | 0.4440 |
| UA | 0.8570 | 0.4460 |
| V | 0.9230 | 0.4860 |
| VA | 0.8460 | 0.4280 |
| W | 0.7860 | 0.4330 |
| WA | 0.7140 | 0.2600 |
| X | 0.8460 | 0.4110 |
| XA | 0.9490 | 0.4060 |
| Y | 0.6430 | 0.3080 |
| YA | 0.7950 | 0.4560 |
| Z | 0.9740 | 0.4590 |
| ZA | 0.8460 | 0.4390 |
| a | 0.7950 | 0.4010 |
| aA | 0.8460 | 0.4480 |
| b | 0.8460 | 0.4570 |
| bA | 0.7140 | 0.4030 |
| c | 0.7440 | 0.4650 |
| cA | 0.8930 | 0.4500 |
| d | 0.7500 | 0.4180 |
| dA | 0.9230 | 0.4750 |

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| Chain | Atom inclusion | Q-score |
|---|---|---|
| e | 0.8930 | 0.4480 |
| eA | 0.8570 | 0.4410 |
| f | 0.9490 | 0.4660 |
| fA | 0.8970 | 0.4330 |
| g | 0.7860 | 0.4400 |
| gA | 0.6430 | 0.2960 |
| h | 0.8720 | 0.4100 |
| hA | 0.9740 | 0.4690 |
| i | 0.6790 | 0.3330 |
| iA | 0.8210 | 0.4000 |
| j | 0.9230 | 0.4420 |
| jA | 0.8210 | 0.4460 |
| k | 0.7440 | 0.3850 |
| kA | 0.6920 | 0.4030 |
| l | 0.8210 | 0.4490 |
| lA | 0.6430 | 0.4200 |
| m | 0.7690 | 0.4140 |
| mA | 0.8930 | 0.4500 |
| n | 0.2860 | 0.3940 |
| nA | 0.9490 | 0.4720 |
| o | 0.8210 | 0.4050 |
| oA | 0.8570 | 0.4370 |
| p | 0.9230 | 0.4790 |
| pA | 0.7950 | 0.4200 |
| q | 0.8570 | 0.4090 |
| qA | 0.7860 | 0.3180 |
| r | 0.8720 | 0.4200 |
| rA | 0.8970 | 0.4090 |
| s | 0.6790 | 0.2760 |
| sA | 0.7440 | 0.3860 |
| t | 0.9230 | 0.4560 |
| tA | 0.8210 | 0.4520 |
| u | 0.7440 | 0.3950 |
| uA | 0.7690 | 0.4040 |
| v | 0.8210 | 0.4270 |
| vA | 0.7860 | 0.3800 |
| w | 0.7690 | 0.4100 |
| wA | 0.7860 | 0.4140 |
| x | 0.7140 | 0.4100 |
| xA | 0.9230 | 0.4420 |
| y | 0.8930 | 0.4310 |
| yA | 0.8570 | 0.4120 |

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| Chain | Atom inclusion | Q-score |
|---|---|---|
| z | 0.9490 | 0.4510 |
| zA | 0.7440 | 0.4040 |